



FOUNDATIONS  
ADVANCES

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**Supporting information for article:**

**Magnetic, electric and toroidal polarization modes describing the physical properties of crystals. NdFeO<sub>3</sub> case**

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In Table S1 one can find four magnetic modes with the corresponding parent magnetic point groups. These specific modes were chosen arbitrarily as an example to show the correspondence between magnetic and electric modes. To be specific, let us look at the electric modes in Table S2 which have the same labels as the magnetic modes from Table S1 i.e. **p-”FFF”**, **p-”AAA”**, **p-”FAF”** and **p-”AFA”**. These electric modes are obtained from the magnetic modes of Table S1 by replacing the magnetic moment components by irrational fractional coordinates, e.g.  $m_x \rightarrow x$ ,  $-m_x \rightarrow -x$ ,  $m_y \rightarrow y$ , etc... These simplified electric modes correspond to the set of atomic coordinates, i.e. the usual Wyckoff positions used in crystallography. This is because the contribution to the dipole moment  $q_j \mathbf{r}_j$  transform in the same way as the atomic position  $\mathbf{r}_j$ . The electric modes given in Table S2 can be described in magnetic point groups given in col. 3. In next sections we will explain how these equivalent groups can be obtained for such a transformation of a magnetic mode into an electric mode.

Table S1. Generalised magnetic modes (col. 1) with magnetic moment components (col. 2) of the representative ions (see text). These modes can be present in crystals with symmetry described by magnetic space groups obtained from the 'parent' magnetic point groups given in (col. 3). The crystal system is given in col. 4 (in the setting with unique monoclinic b-axis).

Mode	Magnetic moments	Parent magn. point gr.	system
<b>m – ”FFF”</b>	$(m_x \ m_y \ m_z)$	1 or $\bar{1}$	triclinic
<b>m – ”AAA”</b>	$(m_x \ m_y \ m_z) \ (\bar{m}_x \ \bar{m}_y \ \bar{m}_z)$	$\bar{1}'$ or $\bar{1}1'$ or $11'$	triclinic
<b>m – ”FAF”</b>	$(m_x \ m_y \ m_z) \ (m_x \ \bar{m}_y \ m_z)$	$2'$ or $m'$ or $2'/m'$	monoclinic
<b>m – ”AFA”</b>	$(m_x \ m_y \ m_z) \ (\bar{m}_x \ m_y \ \bar{m}_z)$	2 or $m$ or $2/m$	monoclinic

Table S2. Generalised electric modes (col. 1) with atomic coordinates (col. 2) of the representative ions (see text) equivalent to the generalised magnetic modes from Table S1. These modes can be present in crystals with symmetry described by magnetic space groups obtained from the 'parent' magnetic point groups given in (col. 3). The crystal system is given in col. 4 (in the setting with unique monoclinic b-axis).

Mode	Atomic coordinates	Parent magn. point gr.	system
<b>p – ”FFF”</b>	$(x \ y \ z)$	1 or $1'$	triclinic
<b>p – ”AAA”</b>	$(x \ y \ z) \ (\bar{x} \ \bar{y} \ \bar{z})$	$\bar{1}$ or $\bar{1}1'$	triclinic
<b>p – ”FAF”</b>	$(x \ y \ z) \ (x \ \bar{y} \ z)$	$m$ or $m'$ or $m1'$	monoclinic
<b>p – ”AFA”</b>	$(x \ y \ z) \ (\bar{x} \ y \ \bar{z})$	2 or $2'$ or $21'$	monoclinic

We need to consider the magnetic point groups  $2', m'$  and  $2'/m'$  for **m-”FAF”** and  $2, m$  and  $2/m$  for **m-”AFA”**. The transformation of the generalised inversions and of operations  $2, 2', m, m'$  by permutations  $A_3$  and  $A_5$  are given in Tables 9 and 10 (main paper).

The symmetry operations are given both in HM and RI notation. The transformation is easily visualised in RI notation, e.g. in permutation  $A_3$  the inversion  $\bar{1}$  changes to  $1'$ , so the mirror  $2\bar{1}=m$  changes to  $21'=2'$ . These changes of the symmetry operations by the permutations of generalised inversions  $A_3$  and  $A_5$  lead to changes of the magnetic point groups which are written down in Table S3.

Here in Table S4 the modes ”FAF” and ”AFA” are written without the preceding letter 'm' or 'p' indicating of the type i.e. magnetic or electric (polarisation). In fact the same symbol ”FAF” indicate the mode with a given set of directions of the components, given for the magnetic mode in Table S1, and for the electric mode in Table S2. There is also another important point, the magnetic **m-”FAF”** mode is invariant only with the three magnetic point groups  $2', m'$  and  $2'/m'$  as it was proven in our earlier study [2]. It means there are no other magnetic point groups that leave this mode invariant. The generalised inversions' permutations give a one-to-one correspondence between the magnetic point groups so only the three magnetic point groups  $m, m'$  and  $m1'$  leave the electric mode **p-”FAF”** invariant.

Table S3. Transformation of selected symmetry operations by the permutations of generalised inversions  $A_3$  and  $A_5$  which are explained in Tables 9 and 10 (main paper). For clarity the operations are given both in HM and RI notations (see text).

$A_0$		$A_3$		$A_5$	
<i>HM</i>	<i>RI</i>	<i>RI</i>	<i>HM</i>	<i>RI</i>	<i>HM</i>
1	= 11	11	= 1	11	= 1
$\bar{1}$	= $1\bar{1}$	$11'$	= $1'$	$11'$	= $1'$
$1'$	= $11'$	$1\bar{1}$	= $\bar{1}$	$1\bar{1}'$	= $\bar{1}'$
$\bar{1}'$	= $1\bar{1}'$	$1\bar{1}'$	= $\bar{1}'$	$1\bar{1}$	= $\bar{1}$
2	= 21	21	= 2	21	= 2
$2'$	= $21'$	$2\bar{1}$	= $m$	$2\bar{1}'$	= $m'$
$m$	= $2\bar{1}$	$21'$	= $2'$	$21'$	= $2'$
$m'$	= $2\bar{1}'$	$2\bar{1}'$	= $m'$	$2\bar{1}$	= $m$

Table S4. Changes of magnetic point groups by permutations of generalised inversions  $A_3$  and  $A_5$  as explained in Tables S1 and S2. The symbol  $m'$  means the group containing identity and the primed mirror while  $m1'$  means the grey group containing  $1, 1', m, m'$ . The first and second set of three lines refers to the mode "FAF" and "AFA", respectively.

$A_0$	$A_3$	$A_5$
Mode "FAF"		
$2'$	$m$	$m'$
$m'$	$m'$	$m$
$2'/m'$	$m1'$	$m1'$
Mode "AFA"		
2	2	2
$m$	$2'$	$2'$
$2/m$	$21'$	$21'$

Table S5. Double antisymmetry group types and Kopsky-categories. Third, forth and fifth columns show type behaviour in respect to  $\bar{1}$ ,  $1'$  and  $\bar{1}'$  generalised inversions, respectively. The column '# elements' shows the ratio of the number of elements for this groups vs. the number of elements of the corresponding full-white group. The column '# groups' shows number of magnetic point groups belonging to each type.

Category	Type	$\bar{1}$	$1'$	$\bar{1}'$	# elements	# groups
full-white	full-white	white	white	white	$\times 1$	11
full-gray	full-gray	gray	gray	gray	$\times 4$	11
full-B&W	full-B&W	B&W	B&W	B&W	$\times 1$	7
partially-gray	$\bar{1}$ -gray	gray	white	white	$\times 2$	11
	$1'$ -gray	white	gray	white	$\times 2$	11
	$\bar{1}'$ -gray	white	white	gray	$\times 2$	11
partially-B&W	$\bar{1}$ -B&W	B&W	white	white	$\times 1$	10
	$1'$ -B&W	white	B&W	white	$\times 1$	10
	$\bar{1}'$ -B&W	white	white	B&W	$\times 1$	10
B&W-partially-gray	B&W- $\bar{1}$ -gray	gray	B&W	B&W	$\times 2$	10
	B&W- $1'$ -gray	B&W	gray	B&W	$\times 2$	10
	B&W- $\bar{1}'$ -gray	B&W	B&W	gray	$\times 2$	10
					sum:	122

Table S6. Magnetic point group types explained in relation with the types proposed by Kopsky in [3].

Our type symbol	no.	structure according to Kopsky
full-white	0	$F_i = F_{e'} = F_{i'} = \phi \quad H = G \subset SO(3)$
full-gray	4	$F = F_i = F_{e'} = F_{i'} = G \quad H = G \times E_0 \subset O'(3)$
full-B&W	11	All $F, F_i, F_{e'}, F_{i'}$ disjoint, not empty $H = F + iF_1 + e'F_2 + i'F_3 \subset O'(3)$ ; $F_1, F_2, F_3$ mean all possible combinations of $F_i, F_{e'}, F_{i'}$
$\bar{1}$ -gray	1	$F = F_i = G, \quad F_{e'} = F_{i'} = \phi \quad H = G \times I \subset O(3)$
$1'$ -gray	3	$F = F_{e'} = G, \quad F_i = F_{i'} = \phi \quad H = G \times E' \subset SO'(3)$
$\bar{1}'$ -gray	2	$F = F_{i'} = G, \quad F_{i'} = F_i = \phi \quad H = G \times I' \subset \bar{SO}(3)$
$\bar{1}$ -B&W	5	$F + F_i = G, \quad F_{e'} = F_{i'} = \phi \quad H = F + i(G - F) \subset O(3)$
$1'$ -B&W	7	$F + F_{e'} = G, \quad F_{i'} = F_i = \phi \quad H = F + e'(G - F) \subset SO'(3)$
$\bar{1}'$ -B&W	6	$F + F_{i'} = G, \quad F_i = F_{e'} = \phi \quad H = F + i'(G - F) \subset \bar{SO}(3)$
B&W- $\bar{1}$ -gray	8	$F = F_i, \quad F_{e'} = F_{i'} = G - F \quad H = F(e + i) + (G - F)(e' + i') \subset O'(3)$
B&W- $1'$ -gray	10	$F = F_{e'}, \quad F_{i'} = F_i = G - F \quad H = F(e + e') + (G - F)(i' + i) \subset O'(3)$
B&W- $\bar{1}'$ -gray	9	$F = F_{i'}, \quad F_i = F_{e'} = G - F \quad H = F(e + i') + (G - F)(i + i') \subset O'(3)$

Table S7. Magnetic point group types explained in relation with the Double Antisymmetry Space Groups (DASG) proposed by Van Leeuwen et al. [4].

Our type symbol	no.	DASG category symbol	Category structure
full-white	1	$Q$	$Q$
full-gray	5	$Q1'\bar{1}$	$Q + Q1' + Q\bar{1} + Q\bar{1}'$
full-B&W	12	$Q(H)\{K\}$	$H \cap K + (H - K)\bar{1} + (K - H)1' + (Q - (H + K))\bar{1}'$
$\bar{1}$ -gray	4	$Q\bar{1}$	$Q + Q\bar{1}$
$1'$ -gray	2	$Q1'$	$Q + Q1'$
$\bar{1}'$ -gray	8	$Q\bar{1}'$	$Q + Q\bar{1}'$
$\bar{1}$ -B&W	7	$Q\{H\}$	$H + (Q - H)\bar{1}$
$1'$ -B&W	3	$Q(H)$	$H + (Q - H)1'$
$\bar{1}'$ -B&W	11	$Q(H)\{H\}$	$H + (Q - H)\bar{1}'$
B&W- $\bar{1}$ -gray	6	$Q(H)\bar{1}$	$H + H\bar{1} + (Q - H)1' + (Q - H)\bar{1}'$
B&W- $1'$ -gray	9	$Q\{H\}1'$	$H + H1' + (Q - H)\bar{1} + (Q - H)\bar{1}'$
B&W- $\bar{1}'$ -gray	10	$Q(H)\bar{1}'$	$H + H\bar{1}' + (Q - H)1' + (Q - H)\bar{1}$

Table S8a. List of the 122 magnetic point groups given in the order proposed in ITD [1]. The Hermann-Mauguin i.e. international notation (both short and full symbols), rotation-inversion (RI), Shubnikov and Schoenflies notation are given. For each group the assigned type, e.g. 'full-white', 'full-gray' etc. is also given.

No.	Hermann-Mauguin		RI	Shubnikov	Schoenflies	type
	Short	Full				
1.1.1	1	1	1	1	$C_1$	full-white
1.2.2	11'	11'	11'	$1 \times \underline{1}$	$C'_1$	1'-gray
2.1.3	$\bar{1}$	$\bar{1}$	1 $\bar{1}$	$\bar{2}$	$C_i$	$\bar{1}$ -gray
2.2.4	$\bar{1}1'$	$\bar{1}1'$	1 $\bar{1}1'\bar{1}'$	$\bar{2} \times \underline{1}$	$C'_i$	full-gray
2.3.5	$\bar{1}'$	$\bar{1}'$	1 $\bar{1}'$	$\underline{2}$	$C_i(C_1)$	$\bar{1}'$ -gray
3.1.6	2	121	2	2	$C_2$	full-white
3.2.7	21'	1211'	21'	$2 \times \underline{1}$	$C'_2$	1'-gray
3.3.8	2'	12'1	2'	$\underline{2}$	$C_2(C_1)$	1'-B&W
4.1.9	$m$	1m1	$\bar{2}$	$m$	$C_s$	$\bar{1}$ -B&W
4.2.10	$m1'$	1m11'	$\frac{\bar{2}}{2'}1'$	$m \times \underline{1}$	$C'_s$	B&W-1'-gray
4.3.11	$m'$	1m'1	$\bar{2}'$	$\underline{m}$	$C_s(C_1)$	$\bar{1}'$ -B&W
5.1.12	2/m	1 $\frac{2}{m}$ 1	2 $\bar{1}$	2 : $m$	$C_{2h}$	$\bar{1}$ -gray
5.2.13	2/m1'	1 $\frac{2}{m}$ 11'	2 $\bar{1}1'\bar{1}'$	2 : $m \times \underline{1}$	$C'_{2h}$	full-gray
5.3.14	2'/m	1 $\frac{2'}{m}$ 1	$\frac{\bar{2}}{2'}\bar{1}'$	$\underline{2} : m$	$C_{2h}(C_s)$	B&W- $\bar{1}'$ -gray
5.4.15	2/m'	1 $\frac{2}{m'}$ 1	2 $\bar{1}'$	2 : $\underline{m}$	$C_{2h}(C_2)$	$\bar{1}'$ -gray
5.5.16	2'/m'	1 $\frac{2'}{m'}$ 1	$\frac{2'}{2'}\bar{1}$	$\underline{2} : \underline{m}$	$C_{2h}(C_i)$	B&W- $\bar{1}$ -gray
6.1.17	222	222	222	2 : 2	$D_2$	full-white
6.2.18	2221'	2221'	2221'	2 : 2 $\times \underline{1}$	$D'_2$	1'-gray
6.3.19	22'2'	22'2'	22'2'	2 : $\underline{2}$	$D_2(C_2)$	1'-B&W
7.1.20	2mm	2mm	2 $\bar{2}\bar{2}$	2 · $m$	$C_{2v}$	$\bar{1}$ -B&W
7.2.21	2mm1'	2mm1'	2 $\frac{\bar{2}}{2'}\frac{\bar{2}}{2'}1'$	2 · $m \times \underline{1}$	$C'_{2v}$	B&W-1'-gray
7.3.22	$m2'm'$	$m2'm'$	2 $\bar{2}'\bar{2}'$	$\underline{2} \cdot m$	$C_{2v}(C_s)$	full-B&W
7.4.23	2m'm'	2m'm'	2 $\bar{2}'\bar{2}'$	2 · $\underline{m}$	$C_{2v}(C_2)$	$\bar{1}'$ -B&W
8.1.24	mmm	$\frac{2}{m}\frac{2}{m}\frac{2}{m}$	222 $\bar{1}$	$m \cdot 2 : m$	$D_{2h}$	$\bar{1}$ -gray
8.2.25	mmm1'	$\frac{2}{m}\frac{2}{m}\frac{2}{m}1'$	222 $\bar{1}1'\bar{1}'$	$m \cdot 2 : m \times \underline{1}$	$D'_{2h}$	full-gray
8.3.26	$m'mm$	$\frac{2}{m'}\frac{2'}{m'}\frac{2'}{m'}$	2 $\frac{\bar{2}}{2'}\frac{\bar{2}}{2'}\bar{1}'$	$m \cdot 2 : \underline{m}$	$D_{2h}(C_{2v})$	B&W- $\bar{1}'$ -gray
8.4.27	$mm'm'$	$\frac{2}{m}\frac{2'}{m'}\frac{2'}{m'}$	2 $\frac{2'}{2'}\frac{2'}{2'}\bar{1}$	$\underline{m} \cdot 2 : m$	$D_{2h}(C_{2h})$	B&W- $\bar{1}$ -gray
8.5.28	$m'm'm'$	$\frac{2}{m'}\frac{2}{m'}\frac{2}{m'}$	222 $\bar{1}'$	$\underline{m} \cdot 2 : \underline{m}$	$D_{2h}(D_2)$	$\bar{1}'$ -gray
9.1.29	4	4	4	4	$C_4$	full-white
9.2.30	41'	41'	41'	$4 \times \underline{1}$	$C'_4$	1'-gray
9.3.31	4'	4'	4'	$\underline{4}$	$C_4(C_2)$	1'-B&W
10.1.32	$\bar{4}$	$\bar{4}$	$\bar{4}$	$\bar{4}$	$S_4$	$\bar{1}$ -B&W
10.2.33	$\bar{4}1'$	$\bar{4}1'$	$\frac{\bar{4}}{4'}1'$	$\bar{4} \times \underline{1}$	$S'_4$	B&W-1'-gray
10.3.34	$\bar{4}'$	$\bar{4}'$	$\bar{4}'$	$\bar{\underline{4}}$	$S_4(C_2)$	$\bar{1}'$ -B&W
11.1.35	4/m	$\frac{4}{m}$	4 $\bar{1}$	4 : $m$	$C_{4h}$	$\bar{1}$ -gray
11.2.36	4/m1'	$\frac{4}{m}1'$	4 $\bar{1}1'\bar{1}'$	4 : $m \times \underline{1}$	$C'_{4h}$	full-gray
11.3.37	4'/m	$\frac{4'}{m}$	$\frac{4'}{4'}\bar{1}$	$\underline{4} : m$	$C_{4h}(C_{2h})$	B&W- $\bar{1}$ -gray
11.4.38	4/m'	$\frac{4}{m'}$	4 $\bar{1}'$	4 : $\underline{m}$	$C_{4h}(C_4)$	$\bar{1}'$ -gray
11.5.39	4'/m'	$\frac{4'}{m'}$	$\frac{\bar{4}}{4'}\bar{1}'$	$\underline{4} : \underline{m}$	$C_{4h}(S_4)$	B&W- $\bar{1}'$ -gray

Table S8a. Standard order (continuation)

No.	Hermann-Mauguin		RI	Shubnikov	Schoenflies	type
	Short	Full				
12.1.40	422	422	422	4 : 2	$D_4$	full-white
12.2.41	4221'	4221'	4221'	4 : 2 × $\underline{1}$	$D'_4$	1'-gray
12.3.42	4'22'	4'22'	4'22'	$\underline{4}$ : 2	$D_4(D_2)$	1'-B&W
12.4.43	42'2'	42'2'	42'2'	4 : $\underline{2}$	$D_4(C_2)$	1'-B&W
13.1.44	4mm	4mm	4 $\bar{2}\bar{2}$	4 · m	$C_{4v}$	$\bar{1}$ -B&W
13.2.45	4mm1'	4mm1'	4 $\frac{\bar{2}}{2'}\frac{\bar{2}}{2'}1'$	4 · m × $\underline{1}$	$C'_{4v}$	B&W-1'-gray
13.3.46	4'mm'	4'mm'	4'2 $\bar{2}$ '	$\underline{4}$ · m	$C_{4v}(C_{2v})$	full-B&W
13.4.47	4m'm'	4m'm'	4 $\bar{2}'\bar{2}'$	4 · $\underline{m}$	$C_{4v}(C_4)$	$\bar{1}'$ -B&W
14.1.48	$\bar{4}2m$	$\bar{4}2m$	4 $\bar{2}\bar{2}$	$\bar{4}$ · m	$D_{2d}$	$\bar{1}$ -B&W
14.2.49	$\bar{4}2m1'$	$\bar{4}2m1'$	$\bar{4}\frac{2\bar{2}}{4'}1'$	$\bar{4}$ · m × $\underline{1}$	$D'_{2d}$	B&W-1'-gray
14.3.50	$\bar{4}'m2'$	$\bar{4}'m2'$	4'2 $\bar{2}'$	$\bar{4}$ · m	$D_{2d}(C_{2v})$	full-B&W
14.4.51	$\bar{4}'2m'$	$\bar{4}'2m'$	4'2 $\bar{2}'$	$\bar{4}$ · $\underline{m}$	$D_{2d}(D_2)$	$\bar{1}'$ -B&W
14.5.52	$\bar{4}2'm'$	$\bar{4}2'm'$	4 $\bar{2}'\bar{2}'$	$\bar{4}$ · $\underline{m}$	$D_{2d}(S_4)$	full-B&W
15.1.53	4/mmm	$\frac{4}{m}\frac{2}{m}\frac{2}{m}$	422 $\bar{1}$	m · 4 : m	$D_{4h}$	$\bar{1}$ -gray
15.2.54	4/mmm1'	$\frac{4}{m}\frac{2}{m}\frac{2}{m}1'$	422 $\bar{1}1'\bar{1}'$	m · 4 : m × $\underline{1}$	$D'_{4h}$	full-gray
15.3.55	4/m'mm	$\frac{4}{m'}\frac{2'}{m}\frac{2'}{m}$	4 $\frac{2}{2'}\frac{2}{2'}\bar{1}'$	m · 4 : $\underline{m}$	$D_{4h}(C_{4v})$	B&W- $\bar{1}'$ -gray
15.4.56	4'/mmm'	$\frac{4'}{m}\frac{2}{m}\frac{2'}{m'}$	4' $\frac{2}{4'}\frac{2'}{2'}\bar{1}$	m · $\underline{4}$ : m	$D_{4h}(D_{2h})$	B&W- $\bar{1}$ -gray
15.5.57	4'/m'm'm	$\frac{4'}{m'}\frac{2}{m'}\frac{2'}{m}$	4' $\frac{2}{4'}\frac{2'}{2'}\bar{1}'$	m · $\underline{4}$ : $\underline{m}$	$D_{4h}(D_{2d})$	B&W- $\bar{1}'$ -gray
15.6.58	4/mm'm'	$\frac{4}{m}\frac{2'}{m'}\frac{2'}{m'}$	4 $\frac{2'}{2'}\frac{2'}{2'}\bar{1}$	$\underline{m}$ · 4 : m	$D_{4h}(C_{4h})$	B&W- $\bar{1}$ -gray
15.7.59	4/m'm'm'	$\frac{4}{m'}\frac{2}{m'}\frac{2'}{m'}$	422 $\bar{1}'$	$\underline{m}$ · 4 : $\underline{m}$	$D_{4h}(D_4)$	$\bar{1}'$ -gray

Table S8a. Standard order (continuation)

No.	Hermann-Mauguin		RI	Shubnikov	Schoenflies	type
	Short	Full				
16.1.60	3	3	3	3	$C_3$	full-white
16.2.61	31'	31'	31'	$3 \times \underline{1}$	$C'_3$	1'-gray
17.1.62	$\bar{3}$	$\bar{3}$	3 $\bar{1}$	$\bar{6}$	$S_6$	$\bar{1}$ -gray
17.2.63	$\bar{3}1'$	$\bar{3}1'$	3 $\bar{1}1'\bar{1}'$	$\bar{6} \times \underline{1}$	$S'_6$	full-gray
17.3.64	$\bar{3}'$	$\bar{3}'$	3 $\bar{1}'$	$\bar{6}$	$S_6(C_3)$	$\bar{1}'$ -gray
18.1.65	32	321	32	3 : 2	$D_3$	full-white
18.2.66	321'	3211'	321'	3 : 2 $\times \underline{1}$	$D'_3$	1'-gray
18.3.67	32'	32'1	32'	3 : $\underline{2}$	$D_3(C_3)$	1'-B&W
19.1.68	3m	3m1	3 $\bar{2}$	3 · m	$C_{3v}$	$\bar{1}$ -B&W
19.2.69	3m1'	3m11'	3 $\bar{2}'1'$	3 · m $\times \underline{1}$	$C'_{3v}$	B&W-1'-gray
19.3.70	3m'	3m'1	3 $\bar{2}'$	3 · $\underline{m}$	$C_{3v}(C_3)$	$\bar{1}'$ -B&W
20.1.71	$\bar{3}m$	$\bar{3}\frac{2}{m}1$	32 $\bar{1}$	$\bar{6} \cdot m$	$D_{3d}$	$\bar{1}$ -gray
20.2.72	$\bar{3}m1'$	$\bar{3}\frac{2}{m}11'$	32 $\bar{1}1'\bar{1}'$	$\bar{6} \cdot m \times \underline{1}$	$D'_{3d}$	full-gray
20.3.73	$\bar{3}'m$	$\bar{3}'\frac{2}{m}1$	3 $\bar{2}'\bar{1}'$	$\bar{6} \cdot m$	$D_{3d}(C_{3v})$	B&W- $\bar{1}'$ -gray
20.4.74	$\bar{3}'m'$	$\bar{3}'\frac{2}{m'}1$	32 $\bar{1}'$	$\bar{6} \cdot \underline{m}$	$D_{3d}(D_3)$	$\bar{1}'$ -gray
20.5.75	$\bar{3}m'$	$\bar{3}\frac{2}{m'}1$	3 $\bar{2}'\bar{1}$	$\bar{6} \cdot \underline{m}$	$D_{3d}(S_6)$	B&W- $\bar{1}$ -gray
21.1.76	6	6	6	6	$C_6$	full-white
21.2.77	61'	61'	61'	$6 \times \underline{1}$	$C'_6$	1'-gray
21.3.78	6'	6'	6'	$\underline{6}$	$C_6(C_3)$	1'-B&W
22.1.79	$\bar{6}$	$\bar{6}$	$\bar{6}$	3 : m	$C_{3h}$	$\bar{1}$ -B&W
22.2.80	$\bar{6}1'$	$\bar{6}1'$	$\bar{6}\bar{6}'1'$	3 : m $\times \underline{1}$	$C'_{3h}$	B&W-1'-gray
22.3.81	$\bar{6}'$	$\bar{6}'$	$\bar{6}'$	3 : $\underline{m}$	$C_{3h}(C_3)$	$\bar{1}'$ -B&W
23.1.82	6/m	$\frac{6}{m}$	6 $\bar{1}$	6 : m	$C_{6h}$	$\bar{1}$ -gray
23.2.83	6/m1'	$\frac{6}{m}1'$	6 $\bar{1}1'\bar{1}'$	6 : m $\times \underline{1}$	$C'_{6h}$	full-gray
23.3.84	6'/m	$\frac{6'}{m}$	$\bar{6}\bar{6}'\bar{1}'$	$\underline{6} : m$	$C_{6h}(C_{3h})$	B&W- $\bar{1}'$ -gray
23.4.85	6/m'	$\frac{6}{m'}$	6 $\bar{1}'$	6 : $\underline{m}$	$C_{6h}(C_6)$	$\bar{1}'$ -gray
23.5.86	6'/m'	$\frac{6'}{m'}$	$\bar{6}'\bar{1}$	$\underline{6} : \underline{m}$	$C_{6h}(S_6)$	B&W- $\bar{1}$ -gray



Table S8a. Standard order (continuation)

No.	Hermann-Mauguin		RI	Shubnikov	Schoenflies	type
	Short	Full				
24.1.87	622	622	622	6 : 2	$D_6$	full-white
24.2.88	6221'	6221'	6221'	6 : 2 × $\underline{1}$	$D'_6$	1'-gray
24.3.89	6'22'	6'22'	6'22'	6 : 2	$D_6(D_3)$	1'-B&W
24.4.90	62'2'	62'2'	62'2'	6 : $\underline{2}$	$D_6(C_6)$	1'-B&W
25.1.91	6mm	6mm	6 $\bar{2}\bar{2}$	6 · m	$C_{6v}$	1-B&W
25.2.92	6mm1'	6mm1'	6 $\frac{\bar{2}}{2'}\frac{\bar{2}}{2'}1'$	6 · m × $\underline{1}$	$C'_{6v}$	B&W-1'-gray
25.3.93	6'mm'	6'mm'	6' $\bar{2}\bar{2}'$	6 · m	$C_{6v}(C_{3v})$	full-B&W
25.4.94	6m'm'	6m'm'	6 $\bar{2}'\bar{2}'$	6 · $\underline{m}$	$C_{6v}(C_6)$	1'-B&W
26.1.95	$\bar{6}2m$	$\bar{6}2m$	$\bar{6}2\bar{2}$	m · 3 : m	$D_{3h}$	1-B&W
26.2.96	$\bar{6}2m1'$	$\bar{6}2m1'$	$\bar{6}\frac{2}{6'}\frac{\bar{2}}{2'}1'$	m · 3 : m × $\underline{1}$	$D'_{3h}$	B&W-1'-gray
26.3.97	$\bar{6}'2m'$	$\bar{6}'2m'$	$\bar{6}'2\bar{2}'$	$\underline{m}$ · 3 : $\underline{m}$	$D_{3h}(D_3)$	1'-B&W
26.4.98	$\bar{6}'m2'$	$\bar{6}'m2'$	$\bar{6}'\bar{2}\bar{2}'$	m · 3 : $\underline{m}$	$D_{3h}(C_{3v})$	full-B&W
26.5.99	$\bar{6}2'm'$	$\bar{6}2'm'$	$\bar{6}2'\bar{2}'$	$\underline{m}$ · 3 : m	$D_{3h}(C_{3h})$	full-B&W
27.1.100	6/mmm	$\frac{6}{m}\frac{2}{m}\frac{2}{m}$	622 $\bar{1}$	m · 6 : m	$D_{6h}$	1-gray
27.2.101	6/mmm1'	$\frac{6}{m}\frac{2}{m}\frac{2}{m}1'$	622 $\bar{1}1'\bar{1}'$	m · 6 : m × $\underline{1}$	$D'_{6h}$	full-gray
27.3.102	6/m'mm	$\frac{6}{m'}\frac{2'}{m}\frac{2'}{m}$	6 $\frac{\bar{2}}{2'}\frac{\bar{2}}{2'}\bar{1}'$	m · 6 : $\underline{m}$	$D_{6h}(C_{6v})$	B&W-1'-gray
27.4.103	6'/mm'm	$\frac{6'}{m'}\frac{2'}{m'}\frac{2'}{m}$	6' $\frac{\bar{2}}{2'}\frac{\bar{2}}{2'}\bar{1}'$	m · $\underline{6}$ : m	$D_{6h}(D_{3h})$	B&W-1'-gray
27.5.104	6'/m'mm'	$\frac{6'}{m'}\frac{2'}{m}\frac{2'}{m'}$	6' $\frac{\bar{2}}{2'}\frac{\bar{2}}{2'}\bar{1}$	m · $\underline{6}$ : $\underline{m}$	$D_{6h}(D_{3d})$	B&W-1-gray
27.6.105	6/mm'm'	$\frac{6}{m}\frac{2'}{m'}\frac{2'}{m'}$	6 $\frac{\bar{2}'}{2'}\frac{\bar{2}'}{2'}\bar{1}$	$\underline{m}$ · 6 : m	$D_{6h}(C_{6h})$	B&W-1-gray
27.7.106	6/m'm'm'	$\frac{6}{m'}\frac{2}{m'}\frac{2}{m'}$	622 $\bar{1}'$	$\underline{m}$ · 6 : $\underline{m}$	$D_{6h}(D_6)$	1'-gray
28.1.107	23	23	23	3/2	$T$	full-white
28.2.108	231'	231'	231'	3/2 × $\underline{1}$	$T'$	1'-gray
29.1.109	$m\bar{3}$	$\frac{2}{m}\bar{3}$	23 $\bar{1}$	$\bar{6}/2$	$T_h$	1-gray
29.2.110	$m\bar{3}1'$	$\frac{2}{m}\bar{3}1'$	23 $\bar{1}1'\bar{1}'$	$\bar{6}/2$ × $\underline{1}$	$T'_h$	full-gray
29.3.111	$m'\bar{3}'$	$\frac{2}{m'}\bar{3}'$	23 $\bar{1}'$	$\underline{\bar{6}}/2$	$T(T_h)$	1'-gray
30.1.112	432	432	432	3/4	$O$	full-white
30.2.113	4321'	4321'	4321'	3/4 × $\underline{1}$	$O'$	1'-gray
30.3.114	4'32'	4'32'	4'32'	3/ $\underline{4}$	$O(T)$	1'-B&W
31.1.115	$\bar{4}3m$	$\bar{4}3m$	$\bar{4}3\bar{2}$	3/ $\bar{4}$	$T_d$	1-B&W
31.2.116	$\bar{4}3m1'$	$\bar{4}3m1'$	$\bar{4}\frac{3}{4'}\frac{\bar{2}}{2'}1'$	3/ $\bar{4}$ × $\underline{1}$	$T'_d$	B&W-1'-gray
31.3.117	$\bar{4}'3m'$	$\bar{4}'3m'$	$\bar{4}'3\bar{2}'$	3/ $\underline{\bar{4}}$	$T_d(T)$	1'-B&W
32.1.118	$m\bar{3}m$	$\frac{4}{m}\frac{\bar{3}}{m}\frac{2}{m}$	432 $\bar{1}$	$\bar{6}/4$	$O_h$	1-gray
32.2.119	$m\bar{3}m1'$	$\frac{4}{m}\frac{\bar{3}}{m}\frac{2}{m}1'$	432 $\bar{1}1'\bar{1}'$	$\bar{6}/4$ × $\underline{1}$	$O'_h$	full-gray
32.3.120	$m'\bar{3}'m$	$\frac{4'}{m'}\frac{\bar{3}'}{m'}\frac{2'}{m}$	$\bar{4}\frac{3}{4'}\frac{\bar{2}}{2'}\bar{1}'$	$\underline{\bar{6}}/4$	$O_h(T_d)$	B&W-1'-gray
32.4.121	$m\bar{3}m'$	$\frac{4}{m}\frac{\bar{3}}{m'}\frac{2'}{m'}$	$\bar{4}'\frac{3}{4'}\frac{\bar{2}}{2'}\bar{1}$	$\bar{6}/\underline{4}$	$O_h(T_h)$	B&W-1-gray
32.5.122	$m'\bar{3}'m'$	$\frac{4}{m'}\frac{\bar{3}'}{m'}\frac{2}{m'}$	432 $\bar{1}'$	$\underline{\bar{6}}/4$	$O_h(O)$	1'-gray

Table S8b. List of the 122 magnetic point groups given in blocks related to the 11 chiral groups listed in the following order: 1, 3, 23, 2, 4, 32, 6, 432, 222, 422, 622. Hermann-Mauguin i.e. international notation (both short and full symbols), rotation-inversion (RI), Shubnikov and Schoenflies notation are given. For each group the assigned type, e.g. 'full-white', 'full-gray' etc. is also given.

No.	Hermann-Mauguin		RI	Shubnikov	Schoenflies	type
	Short	Full				
1.1.1	1	1	1	1	$C_1$	full-white
2.2.4	$\bar{1}1'$	$\bar{1}1'$	$1\bar{1}'\bar{1}'$	$\bar{2} \times \underline{1}$	$C'_i$	full-gray
2.1.3	$\bar{1}$	$\bar{1}$	$1\bar{1}$	$\bar{2}$	$C_i$	$\bar{1}$ -gray
1.2.2	$11'$	$11'$	$11'$	$1 \times \underline{1}$	$C'_1$	$1'$ -gray
2.3.5	$\bar{1}'$	$\bar{1}'$	$1\bar{1}'$	$\bar{2}$	$C_i(C_1)$	$\bar{1}'$ -gray
16.1.60	3	3	3	3	$C_3$	full-white
17.2.63	$\bar{3}1'$	$\bar{3}1'$	$3\bar{1}'\bar{1}'$	$\bar{6} \times \underline{1}$	$S'_6$	full-gray
17.1.62	$\bar{3}$	$\bar{3}$	$3\bar{1}$	$\bar{6}$	$S_6$	$\bar{1}$ -gray
16.2.61	$31'$	$31'$	$31'$	$3 \times \underline{1}$	$C'_3$	$1'$ -gray
17.3.64	$\bar{3}'$	$\bar{3}'$	$3\bar{1}'$	$\bar{6}$	$S_6(C_3)$	$\bar{1}'$ -gray
28.1.107	23	23	23	3/2	$T$	full-white
29.2.110	$m\bar{3}1'$	$\frac{2}{m}\bar{3}1'$	$23\bar{1}'\bar{1}'$	$\bar{6}/2 \times \underline{1}$	$T'_h$	full-gray
29.1.109	$m\bar{3}$	$\frac{2}{m}\bar{3}$	$23\bar{1}$	$\bar{6}/2$	$T_h$	$\bar{1}$ -gray
28.2.108	$231'$	$231'$	$231'$	$3/2 \times \underline{1}$	$T'$	$1'$ -gray
29.3.111	$m'\bar{3}'$	$\frac{2}{m'}\bar{3}'$	$23\bar{1}'$	$\bar{6}/2$	$T(T_h)$	$\bar{1}'$ -gray

Table S8b. Chiral order (continuation)

No.	Hermann-Mauguin		RI	Shubnikov	Schoenflies	type
	Short	Full				
3.1.6	2	121	2	2	$C_2$	full-white
5.2.13	$2/m1'$	$1\frac{2}{m}11'$	$2\bar{1}1'\bar{1}'$	$2 : m \times \underline{1}$	$C'_{2h}$	full-gray
5.1.12	$2/m$	$1\frac{2}{m}1$	$2\bar{1}$	$2 : m$	$C_{2h}$	$\bar{1}$ -gray
3.2.7	$21'$	$1211'$	$21'$	$2 \times \underline{1}$	$C'_2$	$1'$ -gray
5.4.15	$2/m'$	$1\frac{2}{m'}1$	$2\bar{1}'$	$2 : \underline{m}$	$C_{2h}(C_2)$	$\bar{1}'$ -gray
4.1.9	$m$	$1m1$	$\bar{2}$	$m$	$C_s$	$\bar{1}$ -B&W
3.3.8	$2'$	$12'1$	$2'$	$\underline{2}$	$C_2(C_1)$	$1'$ -B&W
4.3.11	$m'$	$1m'1$	$\bar{2}'$	$\underline{m}$	$C_s(C_1)$	$\bar{1}'$ -B&W
5.5.16	$2'/m'$	$1\frac{2'}{m'}1$	$2'\bar{1}$	$\underline{2} : \underline{m}$	$C_{2h}(C_i)$	B&W- $\bar{1}$ -gray
4.2.10	$m1'$	$1m11'$	$\bar{2}'1'$	$m \times \underline{1}$	$C'_s$	B&W- $1'$ -gray
5.3.14	$2'/m$	$1\frac{2'}{m}1$	$\bar{2}'\bar{1}'$	$\underline{2} : m$	$C_{2h}(C_s)$	B&W- $\bar{1}'$ -gray
9.1.29	4	4	4	4	$C_4$	full-white
11.2.36	$4/m1'$	$\frac{4}{m}1'$	$4\bar{1}1'\bar{1}'$	$4 : m \times \underline{1}$	$C'_{4h}$	full-gray
11.1.35	$4/m$	$\frac{4}{m}$	$4\bar{1}$	$4 : m$	$C_{4h}$	$\bar{1}$ -gray
9.2.30	$41'$	$41'$	$41'$	$4 \times \underline{1}$	$C'_4$	$1'$ -gray
11.4.38	$4/m'$	$\frac{4}{m'}$	$4\bar{1}'$	$4 : \underline{m}$	$C_{4h}(C_4)$	$\bar{1}'$ -gray
10.1.32	$\bar{4}$	$\bar{4}$	$\bar{4}$	$\bar{4}$	$S_4$	$\bar{1}$ -B&W
9.3.31	$4'$	$4'$	$4'$	$\underline{4}$	$C_4(C_2)$	$1'$ -B&W
10.3.34	$\bar{4}'$	$\bar{4}'$	$\bar{4}'$	$\underline{\bar{4}}$	$S_4(C_2)$	$\bar{1}'$ -B&W
11.3.37	$4'/m$	$\frac{4'}{m}$	$\bar{4}'\bar{1}$	$\underline{4} : m$	$C_{4h}(C_{2h})$	B&W- $\bar{1}$ -gray
10.2.33	$\bar{4}1'$	$\bar{4}1'$	$\bar{4}'1'$	$\underline{\bar{4}} \times \underline{1}$	$S'_4$	B&W- $1'$ -gray
11.5.39	$4'/m'$	$\frac{4'}{m'}$	$\bar{4}'\bar{1}'$	$\underline{\bar{4}} : \underline{m}$	$C_{4h}(S_4)$	B&W- $\bar{1}'$ -gray
18.1.65	32	321	32	$3 : 2$	$D_3$	full-white
20.2.72	$\bar{3}m1'$	$\bar{3}\frac{2}{m}11'$	$32\bar{1}1'\bar{1}'$	$\bar{6} \cdot m \times \underline{1}$	$D'_{3d}$	full-gray
20.1.71	$\bar{3}m$	$\bar{3}\frac{2}{m}1$	$32\bar{1}$	$\bar{6} \cdot m$	$D_{3d}$	$\bar{1}$ -gray
18.2.66	$321'$	$3211'$	$321'$	$3 : 2 \times \underline{1}$	$D'_3$	$1'$ -gray
20.4.74	$\bar{3}'m'$	$\bar{3}'\frac{2}{m'}1$	$32\bar{1}'$	$\bar{6} \cdot \underline{m}$	$D_{3d}(D_3)$	$\bar{1}'$ -gray
19.1.68	$3m$	$3m1$	$3\bar{2}$	$3 \cdot m$	$C_{3v}$	$\bar{1}$ -B&W
18.3.67	$32'$	$32'1$	$32'$	$3 : \underline{2}$	$D_3(C_3)$	$1'$ -B&W
19.3.70	$3m'$	$3m'1$	$3\bar{2}'$	$3 \cdot \underline{m}$	$C_{3v}(C_3)$	$\bar{1}'$ -B&W
20.5.75	$\bar{3}m'$	$\bar{3}\frac{2'}{m'}1$	$3\bar{2}'\bar{1}$	$\bar{6} \cdot \underline{m}$	$D_{3d}(S_6)$	B&W- $\bar{1}$ -gray
19.2.69	$3m1'$	$3m11'$	$3\bar{2}'1'$	$3 \cdot m \times \underline{1}$	$C'_{3v}$	B&W- $1'$ -gray
20.3.73	$\bar{3}'m$	$\bar{3}'\frac{2'}{m}1$	$3\bar{2}'\bar{1}'$	$\bar{6} \cdot m$	$D_{3d}(C_{3v})$	B&W- $\bar{1}'$ -gray

Table S8b. Chiral order (continuation)

No.	Hermann-Mauguin		RI	Shubnikov	Schoenflies	type
	Short	Full				
21.1.76	6	6	6	6	$C_6$	full-white
23.2.83	$6/m1'$	$\frac{6}{m}1'$	$6\bar{1}'\bar{1}'$	$6 : m \times \underline{1}$	$C'_{6h}$	full-gray
23.1.82	$6/m$	$\frac{6}{m}$	$6\bar{1}$	$6 : m$	$C_{6h}$	$\bar{1}$ -gray
21.2.77	$61'$	$61'$	$61'$	$6 \times \underline{1}$	$C'_6$	$1'$ -gray
23.4.85	$6/m'$	$\frac{6}{m'}$	$6\bar{1}'$	$6 : \underline{m}$	$C_{6h}(C_6)$	$\bar{1}'$ -gray
22.1.79	$\bar{6}$	$\bar{6}$	$\bar{6}$	$3 : m$	$C_{3h}$	$\bar{1}$ -B&W
21.3.78	$6'$	$6'$	$6'$	$\underline{6}$	$C_6(C_3)$	$1'$ -B&W
22.3.81	$\bar{6}'$	$\bar{6}'$	$\bar{6}'$	$3 : \underline{m}$	$C_{3h}(C_3)$	$\bar{1}'$ -B&W
23.5.86	$6'/m'$	$\frac{6'}{m'}$	$\frac{6'}{6'}\bar{1}$	$\underline{6} : \underline{m}$	$C_{6h}(S_6)$	B&W- $\bar{1}$ -gray
22.2.80	$\bar{6}1'$	$\bar{6}1'$	$\frac{6}{6'}1'$	$3 : m \times \underline{1}$	$C'_{3h}$	B&W- $1'$ -gray
23.3.84	$6'/m$	$\frac{6'}{m}$	$\frac{6}{6'}\bar{1}'$	$\underline{6} : m$	$C_{6h}(C_{3h})$	B&W- $\bar{1}'$ -gray
30.1.112	432	432	432	3/4	$O$	full-white
32.2.119	$m\bar{3}m1'$	$\frac{4}{m}\bar{3}\frac{2}{m}1'$	$432\bar{1}'\bar{1}'$	$\bar{6}/4 \times \underline{1}$	$O'_h$	full-gray
32.1.118	$m\bar{3}m$	$\frac{4}{m}\bar{3}\frac{2}{m}$	$432\bar{1}$	$\bar{6}/4$	$O_h$	$\bar{1}$ -gray
30.2.113	$4321'$	$4321'$	$4321'$	$3/4 \times \underline{1}$	$O'$	$1'$ -gray
32.5.122	$m'\bar{3}'m'$	$\frac{4}{m'}\bar{3}'\frac{2}{m'}$	$432\bar{1}'$	$\bar{6}/4$	$O_h(O)$	$\bar{1}'$ -gray
31.1.115	$\bar{4}3m$	$\bar{4}3m$	$\bar{4}3\bar{2}$	3/4	$T_d$	$\bar{1}$ -B&W
30.3.114	$4'32'$	$4'32'$	$4'32'$	$3/\underline{4}$	$O(T)$	$1'$ -B&W
31.3.117	$\bar{4}'3m'$	$\bar{4}'3m'$	$\bar{4}'3\bar{2}'$	$3/\underline{4}$	$T_d(T)$	$\bar{1}'$ -B&W
32.4.121	$m\bar{3}m'$	$\frac{4'}{m}\bar{3}'\frac{2'}{m'}$	$\frac{4'}{4'}3\frac{2'}{2'}\bar{1}$	$\bar{6}/\underline{4}$	$O_h(T_h)$	B&W- $\bar{1}$ -gray
31.2.116	$\bar{4}3m1'$	$\bar{4}3m1'$	$\frac{4'}{4'}3\frac{2'}{2'}1'$	$3/\bar{4} \times \underline{1}$	$T'_d$	B&W- $1'$ -gray
32.3.120	$m'\bar{3}'m$	$\frac{4'}{m'}\bar{3}'\frac{2'}{m}$	$\frac{4'}{4'}3\frac{2'}{2'}\bar{1}'$	$\bar{6}/\underline{4}$	$O_h(T_d)$	B&W- $\bar{1}'$ -gray

Table S8b. Chiral order (continuation)

No.	Hermann-Mauguin		RI	Shubnikov	Schoenflies	type
	Short	Full				
6.1.17	222	222	222	$2 : 2$	$D_2$	full-white
8.2.25	$mmm1'$	$\frac{2}{m} \frac{2}{m} \frac{2}{m} 1'$	$222\bar{1}'\bar{1}'$	$m \cdot 2 : m \times \underline{1}$	$D'_{2h}$	full-gray
7.3.22	$m2'm'$	$m2'm'$	$\bar{2}'\bar{2}'$	$\underline{2} \cdot m$	$C_{2v}(C_s)$	full-B&W
8.1.24	$mmm$	$\frac{2}{m} \frac{2}{m} \frac{2}{m}$	$222\bar{1}$	$m \cdot 2 : m$	$D_{2h}$	$\bar{1}$ -gray
6.2.18	2221'	2221'	2221'	$2 : 2 \times \underline{1}$	$D'_2$	1'-gray
8.5.28	$m'm'm'$	$\frac{2}{m'} \frac{2}{m'} \frac{2}{m'}$	$222\bar{1}'$	$\underline{m} \cdot 2 : \underline{m}$	$D_{2h}(D_2)$	$\bar{1}'$ -gray
7.1.20	2mm	2mm	$\bar{2}\bar{2}$	$2 \cdot m$	$C_{2v}$	$\bar{1}$ -B&W
6.3.19	$22'2'$	$22'2'$	$22'2'$	$2 : \underline{2}$	$D_2(C_2)$	1'-B&W
7.4.23	$2m'm'$	$2m'm'$	$\bar{2}'\bar{2}'$	$2 \cdot \underline{m}$	$C_{2v}(C_2)$	$\bar{1}'$ -B&W
8.4.27	$mm'm'$	$\frac{2}{m} \frac{2'}{m'} \frac{2'}{m'}$	$2 \frac{2'}{2'} \frac{2'}{2'} \bar{1}$	$\underline{m} \cdot 2 : m$	$D_{2h}(C_{2h})$	B&W- $\bar{1}$ -gray
7.2.21	$2mm1'$	$2mm1'$	$2 \frac{2'}{2'} \frac{2'}{2'} 1'$	$2 \cdot m \times \underline{1}$	$C'_{2v}$	B&W-1'-gray
8.3.26	$m'mm$	$\frac{2}{m'} \frac{2'}{m'} \frac{2'}{m'}$	$2 \frac{2'}{2'} \frac{2'}{2'} \bar{1}'$	$m \cdot 2 : \underline{m}$	$D_{2h}(C_{2v})$	B&W- $\bar{1}'$ -gray
12.1.40	422	422	422	$4 : 2$	$D_4$	full-white
15.2.54	$4/mmm1'$	$\frac{4}{m} \frac{2}{m} \frac{2}{m} 1'$	$422\bar{1}'\bar{1}'$	$m \cdot 4 : m \times \underline{1}$	$D'_{4h}$	full-gray
14.5.52	$\bar{4}2'm'$	$\bar{4}2'm'$	$\bar{4}2'\bar{2}'$	$\bar{4} \cdot \underline{m}$	$D_{2d}(S_4)$	full-B&W
13.3.46	$4'mm'$	$4'mm'$	$4'\bar{2}'\bar{2}'$	$\underline{4} \cdot m$	$C_{4v}(C_{2v})$	full-B&W
14.3.50	$\bar{4}'m2'$	$\bar{4}'m2'$	$\bar{4}'\bar{2}'\bar{2}'$	$\bar{4} \cdot m$	$D_{2d}(C_{2v})$	full-B&W
15.1.53	$4/mmm$	$\frac{4}{m} \frac{2}{m} \frac{2}{m}$	$422\bar{1}$	$m \cdot 4 : m$	$D_{4h}$	$\bar{1}$ -gray
12.2.41	4221'	4221'	4221'	$4 : 2 \times \underline{1}$	$D'_4$	1'-gray
15.7.59	$4/m'm'm'$	$\frac{4}{m'} \frac{2}{m'} \frac{2}{m'}$	$422\bar{1}'$	$\underline{m} \cdot 4 : \underline{m}$	$D_{4h}(D_4)$	$\bar{1}'$ -gray
13.1.44	4mm	4mm	$\bar{4}\bar{2}\bar{2}$	$4 \cdot m$	$C_{4v}$	$\bar{1}$ -B&W
14.1.48	$\bar{4}2m$	$\bar{4}2m$	$\bar{4}\bar{2}\bar{2}$	$\bar{4} \cdot m$	$D_{2d}$	$\bar{1}$ -B&W
12.4.43	$42'2'$	$42'2'$	$42'2'$	$4 : \underline{2}$	$D_4(C_2)$	1'-B&W
12.3.42	$4'22'$	$4'22'$	$4'22'$	$\underline{4} : 2$	$D_4(D_2)$	1'-B&W
13.4.47	$4m'm'$	$4m'm'$	$4\bar{2}'\bar{2}'$	$4 \cdot \underline{m}$	$C_{4v}(C_4)$	$\bar{1}'$ -B&W
14.4.51	$\bar{4}'2m'$	$\bar{4}'2m'$	$\bar{4}'\bar{2}'\bar{2}'$	$\bar{4} \cdot \underline{m}$	$D_{2d}(D_2)$	$\bar{1}'$ -B&W
15.6.58	$4/mm'm'$	$\frac{4}{m} \frac{2'}{m'} \frac{2'}{m'}$	$4 \frac{2'}{2'} \frac{2'}{2'} \bar{1}$	$\underline{m} \cdot 4 : m$	$D_{4h}(C_{4h})$	B&W- $\bar{1}$ -gray
15.4.56	$4'/mmm'$	$\frac{4'}{m} \frac{2}{m} \frac{2'}{m'}$	$4' \frac{2}{2'} \frac{2'}{2'} \bar{1}$	$m \cdot \underline{4} : m$	$D_{4h}(D_{2h})$	B&W- $\bar{1}$ -gray
13.2.45	$4mm1'$	$4mm1'$	$4 \frac{2}{2'} \frac{2}{2'} 1'$	$4 \cdot m \times \underline{1}$	$C'_{4v}$	B&W-1'-gray
14.2.49	$\bar{4}2m1'$	$\bar{4}2m1'$	$\bar{4} \frac{2}{2'} \frac{2}{2'} 1'$	$\bar{4} \cdot m \times \underline{1}$	$D'_{2d}$	B&W-1'-gray
15.3.55	$4/m'mm$	$\frac{4}{m'} \frac{2'}{m'} \frac{2'}{m'}$	$4 \frac{2'}{2'} \frac{2'}{2'} \bar{1}'$	$m \cdot 4 : \underline{m}$	$D_{4h}(C_{4v})$	B&W- $\bar{1}'$ -gray
15.5.57	$4'/m'm'm'$	$\frac{4'}{m'} \frac{2}{m'} \frac{2'}{m'}$	$4' \frac{2}{2'} \frac{2'}{2'} \bar{1}'$	$m \cdot \underline{4} : \underline{m}$	$D_{4h}(D_{2d})$	B&W- $\bar{1}'$ -gray

Table S8b. Chiral order (continuation)

No.	Hermann-Mauguin		RI	Shubnikov	Schoenflies	type
	Short	Full				
24.1.87	622	622	622	6 : 2	$D_6$	full-white
27.2.101	$6/mmm1'$	$\frac{6}{m} \frac{2}{m} \frac{2}{m} 1'$	$622\bar{1}1'\bar{1}'$	$m \cdot 6 : m \times \underline{1}$	$D'_{6h}$	full-gray
26.5.99	$\bar{6}2'm'$	$\bar{6}2'm'$	$\bar{6}2'2'$	$\underline{m} \cdot 3 : m$	$D_{3h}(C_{3h})$	full-B&W
25.3.93	$6'mm'$	$6'mm'$	$6'2'2'$	$\underline{6} \cdot m$	$C_{6v}(C_{3v})$	full-B&W
26.4.98	$\bar{6}'m2'$	$\bar{6}'m2'$	$\bar{6}'2'2'$	$m \cdot 3 : \underline{m}$	$D_{3h}(C_{3v})$	full-B&W
27.1.100	$6/mmm$	$\frac{6}{m} \frac{2}{m} \frac{2}{m}$	622 $\bar{1}$	$m \cdot 6 : m$	$D_{6h}$	$\bar{1}$ -gray
24.2.88	6221'	6221'	6221'	6 : 2 $\times \underline{1}$	$D'_6$	1'-gray
27.7.106	$6/m'm'm'$	$\frac{6}{m'} \frac{2}{m'} \frac{2}{m'}$	622 $\bar{1}'$	$\underline{m} \cdot 6 : \underline{m}$	$D_{6h}(D_6)$	$\bar{1}'$ -gray
25.1.91	6mm	6mm	6 $\bar{2}\bar{2}$	6 $\cdot$ m	$C_{6v}$	$\bar{1}$ -B&W
26.1.95	$\bar{6}2m$	$\bar{6}2m$	$\bar{6}2\bar{2}$	$m \cdot 3 : m$	$D_{3h}$	$\bar{1}$ -B&W
24.4.90	62'2'	62'2'	62'2'	6 : $\underline{2}$	$D_6(C_6)$	1'-B&W
24.3.89	6'22'	6'22'	6'22'	$\underline{6} : 2$	$D_6(D_3)$	1'-B&W
25.4.94	6m'm'	6m'm'	6 $\bar{2}'\bar{2}'$	6 $\cdot$ $\underline{m}$	$C_{6v}(C_6)$	$\bar{1}'$ -B&W
26.3.97	$\bar{6}'2m'$	$\bar{6}'2m'$	$\bar{6}'2\bar{2}'$	$\underline{m} \cdot 3 : \underline{m}$	$D_{3h}(D_3)$	$\bar{1}'$ -B&W
27.6.105	$6/mm'm'$	$\frac{6}{m} \frac{2'}{m'} \frac{2'}{m'}$	6 $\frac{2'}{2'} \frac{2'}{2'} \bar{1}$	$\underline{m} \cdot 6 : m$	$D_{6h}(C_{6h})$	B&W- $\bar{1}$ -gray
27.5.104	$6'/m'mm'$	$\frac{6'}{m'} \frac{2}{m} \frac{2'}{m'}$	6' $\frac{2}{2} \frac{2'}{2'} \bar{1}$	$m \cdot \underline{6} : \underline{m}$	$D_{6h}(D_{3d})$	B&W- $\bar{1}$ -gray
25.2.92	6mm1'	6mm1'	6 $\frac{2}{2'} \frac{2}{2'} 1'$	6 $\cdot$ m $\times \underline{1}$	$C'_{6v}$	B&W-1'-gray
26.2.96	$\bar{6}2m1'$	$\bar{6}2m1'$	6 $\frac{2}{6'} \frac{2}{2'} 1'$	$m \cdot 3 : m \times \underline{1}$	$D'_{3h}$	B&W-1'-gray
27.3.102	$6/m'mm$	$\frac{6}{m'} \frac{2'}{m} \frac{2'}{m}$	6 $\frac{2}{2'} \frac{2}{2'} \bar{1}'$	$m \cdot 6 : \underline{m}$	$D_{6h}(C_{6v})$	B&W- $\bar{1}'$ -gray
27.4.103	$6'/mm'm$	$\frac{6'}{m} \frac{2}{m'} \frac{2'}{m}$	6' $\frac{2}{6'} \frac{2}{2'} \bar{1}'$	$m \cdot \underline{6} : m$	$D_{6h}(D_{3h})$	B&W- $\bar{1}'$ -gray

Table S8c. List of the 122 magnetic point groups given in the order of magnetic point groups types, i.e.: 'Full-white', 'Full-gray', 'Full-black-and-white', 'Partially-gray', 'Partially-black-and-white' and 'Black-and-white-Partially-gray'. The Hermann-Mauguin i.e. international notation (both short and full symbols), rotation-inversion (RI), Shubnikov and Schoenflies notation are given. For each group the assigned type is also given.

No.	Hermann-Mauguin		RI	Shubnikov	Schoenflies	type
	Short	Full				
1.1.1	1	1	1	1	$C_1$	full-white
3.1.6	2	121	2	2	$C_2$	full-white
16.1.60	3	3	3	3	$C_3$	full-white
9.1.29	4	4	4	4	$C_4$	full-white
21.1.76	6	6	6	6	$C_6$	full-white
6.1.17	222	222	222	2 : 2	$D_2$	full-white
18.1.65	32	321	32	3 : 2	$D_3$	full-white
12.1.40	422	422	422	4 : 2	$D_4$	full-white
24.1.87	622	622	622	6 : 2	$D_6$	full-white
28.1.107	23	23	23	3/2	$T$	full-white
30.1.112	432	432	432	3/4	$O$	full-white
2.2.4	$\bar{1}1'$	$\bar{1}1'$	$1\bar{1}1'\bar{1}'$	$\bar{2} \times \underline{1}$	$C'_i$	full-gray
5.2.13	$2/m1'$	$1\frac{2}{m}11'$	$2\bar{1}1'\bar{1}'$	$2 : m \times \underline{1}$	$C'_{2h}$	full-gray
17.2.63	$\bar{3}1'$	$\bar{3}1'$	$3\bar{1}1'\bar{1}'$	$\bar{6} \times \underline{1}$	$S'_6$	full-gray
11.2.36	$4/m1'$	$\frac{4}{m}1'$	$4\bar{1}1'\bar{1}'$	$4 : m \times \underline{1}$	$C'_{4h}$	full-gray
23.2.83	$6/m1'$	$\frac{6}{m}1'$	$6\bar{1}1'\bar{1}'$	$6 : m \times \underline{1}$	$C'_{6h}$	full-gray
8.2.25	$mmm1'$	$\frac{2}{m}\frac{2}{m}\frac{2}{m}1'$	$222\bar{1}1'\bar{1}'$	$m \cdot 2 : m \times \underline{1}$	$D'_{2h}$	full-gray
20.2.72	$\bar{3}m1'$	$\bar{3}\frac{2}{m}11'$	$32\bar{1}1'\bar{1}'$	$\bar{6} \cdot m \times \underline{1}$	$D'_{3d}$	full-gray
15.2.54	$4/mmm1'$	$\frac{4}{m}\frac{2}{m}\frac{2}{m}1'$	$422\bar{1}1'\bar{1}'$	$m \cdot 4 : m \times \underline{1}$	$D'_{4h}$	full-gray
27.2.101	$6/mmm1'$	$\frac{6}{m}\frac{2}{m}\frac{2}{m}1'$	$622\bar{1}1'\bar{1}'$	$m \cdot 6 : m \times \underline{1}$	$D'_{6h}$	full-gray
29.2.110	$m\bar{3}1'$	$\frac{2}{m}\bar{3}1'$	$23\bar{1}1'\bar{1}'$	$\bar{6}/2 \times \underline{1}$	$T'_h$	full-gray
32.2.119	$m\bar{3}m1'$	$\frac{4}{m}\bar{3}\frac{2}{m}1'$	$432\bar{1}1'\bar{1}'$	$\bar{6}/4 \times \underline{1}$	$O'_h$	full-gray
7.3.22	$m2'm'$	$m2'm'$	$\bar{2}2'\bar{2}'$	$\underline{2} \cdot m$	$C_{2v}(C_s)$	full-B&W
14.5.52	$\bar{4}2'm'$	$\bar{4}2'm'$	$\bar{4}2'\bar{2}'$	$\bar{4} \cdot \underline{m}$	$D_{2d}(S_4)$	full-B&W
13.3.46	$4'mm'$	$4'mm'$	$4'\bar{2}\bar{2}'$	$\underline{4} \cdot m$	$C_{4v}(C_{2v})$	full-B&W
14.3.50	$\bar{4}'m2'$	$\bar{4}'m2'$	$\bar{4}'\bar{2}\bar{2}'$	$\bar{4} \cdot m$	$D_{2d}(C_{2v})$	full-B&W
26.5.99	$\bar{6}2'm'$	$\bar{6}2'm'$	$\bar{6}2'\bar{2}'$	$\underline{m} \cdot 3 : m$	$D_{3h}(C_{3h})$	full-B&W
25.3.93	$6'mm'$	$6'mm'$	$6'\bar{2}\bar{2}'$	$\underline{6} \cdot m$	$C_{6v}(C_{3v})$	full-B&W
26.4.98	$\bar{6}'m2'$	$\bar{6}'m2'$	$\bar{6}'\bar{2}\bar{2}'$	$m \cdot 3 : \underline{m}$	$D_{3h}(C_{3v})$	full-B&W

Table S8c. Types order (continuation)

No.	Hermann-Mauguin		RI	Shubnikov	Schoenflies	type
	Short	Full				
2.1.3	$\bar{1}$	$\bar{1}$	$1\bar{1}$	$\bar{2}$	$C_i$	$\bar{1}$ -gray
5.1.12	$2/m$	$1\frac{2}{m}1$	$2\bar{1}$	$2 : m$	$C_{2h}$	$\bar{1}$ -gray
17.1.62	$\bar{3}$	$\bar{3}$	$3\bar{1}$	$\bar{6}$	$S_6$	$\bar{1}$ -gray
11.1.35	$4/m$	$\frac{4}{m}$	$4\bar{1}$	$4 : m$	$C_{4h}$	$\bar{1}$ -gray
23.1.82	$6/m$	$\frac{6}{m}$	$6\bar{1}$	$6 : m$	$C_{6h}$	$\bar{1}$ -gray
8.1.24	$mmm$	$\frac{2}{m}\frac{2}{m}\frac{2}{m}$	$222\bar{1}$	$m \cdot 2 : m$	$D_{2h}$	$\bar{1}$ -gray
20.1.71	$\bar{3}m$	$\bar{3}\frac{2}{m}1$	$32\bar{1}$	$\bar{6} \cdot m$	$D_{3d}$	$\bar{1}$ -gray
15.1.53	$4/mmm$	$\frac{4}{m}\frac{2}{m}\frac{2}{m}$	$422\bar{1}$	$m \cdot 4 : m$	$D_{4h}$	$\bar{1}$ -gray
27.1.100	$6/mmm$	$\frac{6}{m}\frac{2}{m}\frac{2}{m}$	$622\bar{1}$	$m \cdot 6 : m$	$D_{6h}$	$\bar{1}$ -gray
29.1.109	$m\bar{3}$	$\frac{2}{m}\bar{3}$	$23\bar{1}$	$\bar{6}/2$	$T_h$	$\bar{1}$ -gray
32.1.118	$m\bar{3}m$	$\frac{4}{m}\bar{3}\frac{2}{m}$	$432\bar{1}$	$\bar{6}/4$	$O_h$	$\bar{1}$ -gray
1.2.2	$11'$	$11'$	$11'$	$1 \times \underline{1}$	$C'_1$	$1'$ -gray
3.2.7	$21'$	$1211'$	$21'$	$2 \times \underline{1}$	$C'_2$	$1'$ -gray
16.2.61	$31'$	$31'$	$31'$	$3 \times \underline{1}$	$C'_3$	$1'$ -gray
9.2.30	$41'$	$41'$	$41'$	$4 \times \underline{1}$	$C'_4$	$1'$ -gray
21.2.77	$61'$	$61'$	$61'$	$6 \times \underline{1}$	$C'_6$	$1'$ -gray
6.2.18	$2221'$	$2221'$	$2221'$	$2 : 2 \times \underline{1}$	$D'_2$	$1'$ -gray
18.2.66	$321'$	$3211'$	$321'$	$3 : 2 \times \underline{1}$	$D'_3$	$1'$ -gray
12.2.41	$4221'$	$4221'$	$4221'$	$4 : 2 \times \underline{1}$	$D'_4$	$1'$ -gray
24.2.88	$6221'$	$6221'$	$6221'$	$6 : 2 \times \underline{1}$	$D'_6$	$1'$ -gray
28.2.108	$231'$	$231'$	$231'$	$3/2 \times \underline{1}$	$T'$	$1'$ -gray
30.2.113	$4321'$	$4321'$	$4321'$	$3/4 \times \underline{1}$	$O'$	$1'$ -gray
2.3.5	$\bar{1}'$	$\bar{1}'$	$1\bar{1}'$	$\bar{2}$	$C_i(C_1)$	$\bar{1}'$ -gray
5.4.15	$2/m'$	$1\frac{2}{m'}1$	$2\bar{1}'$	$2 : \underline{m}$	$C_{2h}(C_2)$	$\bar{1}'$ -gray
17.3.64	$\bar{3}'$	$\bar{3}'$	$3\bar{1}'$	$\bar{6}$	$S_6(C_3)$	$\bar{1}'$ -gray
11.4.38	$4/m'$	$\frac{4}{m'}$	$4\bar{1}'$	$4 : \underline{m}$	$C_{4h}(C_4)$	$\bar{1}'$ -gray
23.4.85	$6/m'$	$\frac{6}{m'}$	$6\bar{1}'$	$6 : \underline{m}$	$C_{6h}(C_6)$	$\bar{1}'$ -gray
8.5.28	$m'm'm'$	$\frac{2}{m'}\frac{2}{m'}\frac{2}{m'}$	$222\bar{1}'$	$\underline{m} \cdot 2 : \underline{m}$	$D_{2h}(D_2)$	$\bar{1}'$ -gray
20.4.74	$\bar{3}'m'$	$\bar{3}'\frac{2}{m'}1$	$32\bar{1}'$	$\bar{6} \cdot \underline{m}$	$D_{3d}(D_3)$	$\bar{1}'$ -gray
15.7.59	$4/m'm'm'$	$\frac{4}{m'}\frac{2}{m'}\frac{2}{m'}$	$422\bar{1}'$	$\underline{m} \cdot 4 : \underline{m}$	$D_{4h}(D_4)$	$\bar{1}'$ -gray
27.7.106	$6/m'm'm'$	$\frac{6}{m'}\frac{2}{m'}\frac{2}{m'}$	$622\bar{1}'$	$\underline{m} \cdot 6 : \underline{m}$	$D_{6h}(D_6)$	$\bar{1}'$ -gray
29.3.111	$m'\bar{3}'$	$\frac{2}{m'}\bar{3}'$	$23\bar{1}'$	$\bar{6}/2$	$T(T_h)$	$\bar{1}'$ -gray
32.5.122	$m'\bar{3}'m'$	$\frac{4}{m'}\bar{3}'\frac{2}{m'}$	$432\bar{1}'$	$\bar{6}/4$	$O_h(O)$	$\bar{1}'$ -gray



Table S8c. Types order (continuation)

No.	Hermann-Mauguin		RI	Shubnikov	Schoenflies	type
	Short	Full				
4.1.9	$m$	$1m1$	$\bar{2}$	$m$	$C_s$	$\bar{1}$ -B&W
10.1.32	$\bar{4}$	$\bar{4}$	$\bar{4}$	$\bar{4}$	$S_4$	$\bar{1}$ -B&W
22.1.79	$\bar{6}$	$\bar{6}$	$\bar{6}$	$3 : m$	$C_{3h}$	$\bar{1}$ -B&W
7.1.20	$2mm$	$2mm$	$2\bar{2}\bar{2}$	$2 \cdot m$	$C_{2v}$	$\bar{1}$ -B&W
19.1.68	$3m$	$3m1$	$3\bar{2}$	$3 \cdot m$	$C_{3v}$	$\bar{1}$ -B&W
13.1.44	$4mm$	$4mm$	$4\bar{2}\bar{2}$	$4 \cdot m$	$C_{4v}$	$\bar{1}$ -B&W
14.1.48	$\bar{4}2m$	$\bar{4}2m$	$\bar{4}2\bar{2}$	$\bar{4} \cdot m$	$D_{2d}$	$\bar{1}$ -B&W
25.1.91	$6mm$	$6mm$	$6\bar{2}\bar{2}$	$6 \cdot m$	$C_{6v}$	$\bar{1}$ -B&W
26.1.95	$\bar{6}2m$	$\bar{6}2m$	$\bar{6}2\bar{2}$	$m \cdot 3 : m$	$D_{3h}$	$\bar{1}$ -B&W
31.1.115	$\bar{4}3m$	$\bar{4}3m$	$\bar{4}3\bar{2}$	$3/\bar{4}$	$T_d$	$\bar{1}$ -B&W
3.3.8	$2'$	$12'1$	$2'$	$\underline{2}$	$C_2(C_1)$	$1'$ -B&W
9.3.31	$4'$	$4'$	$4'$	$\underline{4}$	$C_4(C_2)$	$1'$ -B&W
21.3.78	$6'$	$6'$	$6'$	$\underline{6}$	$C_6(C_3)$	$1'$ -B&W
6.3.19	$22'2'$	$22'2'$	$22'2'$	$2 : \underline{2}$	$D_2(C_2)$	$1'$ -B&W
18.3.67	$32'$	$32'1$	$32'$	$3 : \underline{2}$	$D_3(C_3)$	$1'$ -B&W
12.4.43	$42'2'$	$42'2'$	$42'2'$	$4 : \underline{2}$	$D_4(C_2)$	$1'$ -B&W
12.3.42	$4'22'$	$4'22'$	$4'22'$	$\underline{4} : 2$	$D_4(D_2)$	$1'$ -B&W
24.4.90	$62'2'$	$62'2'$	$62'2'$	$6 : \underline{2}$	$D_6(C_6)$	$1'$ -B&W
24.3.89	$6'22'$	$6'22'$	$6'22'$	$\underline{6} : 2$	$D_6(D_3)$	$1'$ -B&W
30.3.114	$4'32'$	$4'32'$	$4'32'$	$3/\underline{4}$	$O(T)$	$1'$ -B&W
4.3.11	$m'$	$1m'1$	$\bar{2}'$	$\underline{m}$	$C_s(C_1)$	$\bar{1}'$ -B&W
10.3.34	$\bar{4}'$	$\bar{4}'$	$\bar{4}'$	$\underline{\bar{4}}$	$S_4(C_2)$	$\bar{1}'$ -B&W
22.3.81	$\bar{6}'$	$\bar{6}'$	$\bar{6}'$	$3 : \underline{m}$	$C_{3h}(C_3)$	$\bar{1}'$ -B&W
7.4.23	$2m'm'$	$2m'm'$	$2\bar{2}'\bar{2}'$	$2 \cdot \underline{m}$	$C_{2v}(C_2)$	$\bar{1}'$ -B&W
19.3.70	$3m'$	$3m'1$	$3\bar{2}'$	$3 \cdot \underline{m}$	$C_{3v}(C_3)$	$\bar{1}'$ -B&W
13.4.47	$4m'm'$	$4m'm'$	$4\bar{2}'\bar{2}'$	$4 \cdot \underline{m}$	$C_{4v}(C_4)$	$\bar{1}'$ -B&W
14.4.51	$\bar{4}'2m'$	$\bar{4}'2m'$	$\bar{4}'2\bar{2}'$	$\underline{\bar{4}} \cdot \underline{m}$	$D_{2d}(D_2)$	$\bar{1}'$ -B&W
25.4.94	$6m'm'$	$6m'm'$	$6\bar{2}'\bar{2}'$	$6 \cdot \underline{m}$	$C_{6v}(C_6)$	$\bar{1}'$ -B&W
26.3.97	$\bar{6}'2m'$	$\bar{6}'2m'$	$\bar{6}'2\bar{2}'$	$\underline{m} \cdot 3 : \underline{m}$	$D_{3h}(D_3)$	$\bar{1}'$ -B&W
31.3.117	$\bar{4}'3m'$	$\bar{4}'3m'$	$\bar{4}'3\bar{2}'$	$3/\underline{\bar{4}}$	$T_d(T)$	$\bar{1}'$ -B&W

Table S8c. Types order (continuation)

No.	Hermann-Mauguin		RI	Shubnikov	Schoenflies	type
	Short	Full				
5.5.16	$2'/m'$	$1\frac{2'}{m'}1$	$\frac{2'}{2'}\bar{1}$	$\underline{2} : \underline{m}$	$C_{2h}(C_i)$	B&W- $\bar{1}$ -gray
11.3.37	$4'/m$	$\frac{4'}{m}$	$\frac{4'}{4'}\bar{1}$	$\underline{4} : \underline{m}$	$C_{4h}(C_{2h})$	B&W- $\bar{1}$ -gray
23.5.86	$6'/m'$	$\frac{6'}{m'}$	$\frac{6'}{6'}\bar{1}$	$\underline{6} : \underline{m}$	$C_{6h}(S_6)$	B&W- $\bar{1}$ -gray
8.4.27	$mm'm'$	$\frac{2}{m} \frac{2'}{m'} \frac{2'}{m'}$	$2\frac{2'}{2'}\frac{2'}{2'}\bar{1}$	$\underline{m} \cdot \underline{2} : \underline{m}$	$D_{2h}(C_{2h})$	B&W- $\bar{1}$ -gray
20.5.75	$\bar{3}m'$	$\frac{3}{m'}\frac{2'}{m'}$	$3\frac{2'}{2'}\bar{1}$	$\bar{6} \cdot \underline{m}$	$D_{3d}(S_6)$	B&W- $\bar{1}$ -gray
15.6.58	$4/mm'm'$	$\frac{4}{m} \frac{2'}{m'} \frac{2'}{m'}$	$4\frac{2'}{2'}\frac{2'}{2'}\bar{1}$	$\underline{m} \cdot \underline{4} : \underline{m}$	$D_{4h}(C_{4h})$	B&W- $\bar{1}$ -gray
15.4.56	$4'/mmm'$	$\frac{4'}{m} \frac{2}{m} \frac{2'}{m'}$	$\frac{4'}{4'} 2\frac{2'}{2'}\bar{1}$	$m \cdot \underline{4} : \underline{m}$	$D_{4h}(D_{2h})$	B&W- $\bar{1}$ -gray
27.6.105	$6/mm'm'$	$\frac{6}{m} \frac{2'}{m'} \frac{2'}{m'}$	$6\frac{2'}{2'}\frac{2'}{2'}\bar{1}$	$\underline{m} \cdot \underline{6} : \underline{m}$	$D_{6h}(C_{6h})$	B&W- $\bar{1}$ -gray
27.5.104	$6'/m'mm'$	$\frac{6'}{m'} \frac{2}{m} \frac{2'}{m'}$	$\frac{6'}{6'} 2\frac{2'}{2'}\bar{1}$	$m \cdot \underline{6} : \underline{m}$	$D_{6h}(D_{3d})$	B&W- $\bar{1}$ -gray
32.4.121	$m\bar{3}m'$	$\frac{4'}{m} \frac{3}{m'} \frac{2'}{m'}$	$\frac{4'}{4'} 3\frac{2'}{2'}\bar{1}$	$\bar{6}/\underline{4}$	$O_h(T_h)$	B&W- $\bar{1}$ -gray
4.2.10	$m1'$	$1m11'$	$\frac{2}{2'}1'$	$m \times \underline{1}$	$C'_s$	B&W- $1'$ -gray
10.2.33	$\bar{4}1'$	$\bar{4}1'$	$\frac{4}{4'}1'$	$\bar{4} \times \underline{1}$	$S'_4$	B&W- $1'$ -gray
22.2.80	$\bar{6}1'$	$\bar{6}1'$	$\frac{6}{6'}1'$	$3 : m \times \underline{1}$	$C'_{3h}$	B&W- $1'$ -gray
7.2.21	$2mm1'$	$2mm1'$	$2\frac{2}{2'}\frac{2}{2'}1'$	$2 \cdot m \times \underline{1}$	$C'_{2v}$	B&W- $1'$ -gray
19.2.69	$3m1'$	$3m11'$	$3\frac{2}{2'}\frac{2}{2'}1'$	$3 \cdot m \times \underline{1}$	$C'_{3v}$	B&W- $1'$ -gray
13.2.45	$4mm1'$	$4mm1'$	$4\frac{2}{2'}\frac{2}{2'}\frac{2}{2'}1'$	$4 \cdot m \times \underline{1}$	$C'_{4v}$	B&W- $1'$ -gray
14.2.49	$\bar{4}2m1'$	$\bar{4}2m1'$	$\frac{4}{4'} 2\frac{2}{2'}\frac{2}{2'}1'$	$\bar{4} \cdot m \times \underline{1}$	$D'_{2d}$	B&W- $1'$ -gray
25.2.92	$6mm1'$	$6mm1'$	$6\frac{2}{2'}\frac{2}{2'}\frac{2}{2'}1'$	$6 \cdot m \times \underline{1}$	$C'_{6v}$	B&W- $1'$ -gray
26.2.96	$\bar{6}2m1'$	$\bar{6}2m1'$	$\frac{6}{6'} 2\frac{2}{2'}\frac{2}{2'}1'$	$m \cdot 3 : m \times \underline{1}$	$D'_{3h}$	B&W- $1'$ -gray
31.2.116	$\bar{4}3m1'$	$\bar{4}3m1'$	$\frac{4}{4'} 3\frac{2}{2'}\frac{2}{2'}1'$	$3/\bar{4} \times \underline{1}$	$T'_d$	B&W- $1'$ -gray
5.3.14	$2'/m$	$1\frac{2'}{m}1$	$\frac{2}{2'}\bar{1}'$	$\underline{2} : \underline{m}$	$C_{2h}(C_s)$	B&W- $\bar{1}'$ -gray
11.5.39	$4'/m'$	$\frac{4'}{m'}$	$\frac{4'}{4'}\bar{1}'$	$\underline{4} : \underline{m}$	$C_{4h}(S_4)$	B&W- $\bar{1}'$ -gray
23.3.84	$6'/m$	$\frac{6'}{m}$	$\frac{6'}{6'}\bar{1}'$	$\underline{6} : \underline{m}$	$C_{6h}(C_{3h})$	B&W- $\bar{1}'$ -gray
8.3.26	$m'mm$	$\frac{2}{m'} \frac{2'}{m} \frac{2'}{m}$	$2\frac{2'}{2'}\frac{2}{2'}\bar{1}'$	$\underline{m} \cdot \underline{2} : \underline{m}$	$D_{2h}(C_{2v})$	B&W- $\bar{1}'$ -gray
20.3.73	$\bar{3}'m$	$\frac{3}{m'}\frac{2'}{m}$	$3\frac{2'}{2'}\bar{1}'$	$\bar{6} \cdot \underline{m}$	$D_{3d}(C_{3v})$	B&W- $\bar{1}'$ -gray
15.3.55	$4/m'mm$	$\frac{4}{m'} \frac{2'}{m} \frac{2'}{m}$	$4\frac{2'}{2'}\frac{2}{2'}\bar{1}'$	$\underline{m} \cdot \underline{4} : \underline{m}$	$D_{4h}(C_{4v})$	B&W- $\bar{1}'$ -gray
15.5.57	$4'/m'm'm$	$\frac{4'}{m'} \frac{2}{m'} \frac{2'}{m}$	$\frac{4'}{4'} 2\frac{2'}{2'}\bar{1}'$	$m \cdot \underline{4} : \underline{m}$	$D_{4h}(D_{2d})$	B&W- $\bar{1}'$ -gray
27.3.102	$6/m'mm$	$\frac{6}{m'} \frac{2'}{m} \frac{2'}{m}$	$6\frac{2}{2'}\frac{2}{2'}\bar{1}'$	$\underline{m} \cdot \underline{6} : \underline{m}$	$D_{6h}(C_{6v})$	B&W- $\bar{1}'$ -gray
27.4.103	$6'/mm'm$	$\frac{6'}{m'} \frac{2}{m'} \frac{2'}{m}$	$\frac{6'}{6'} 2\frac{2}{2'}\bar{1}'$	$m \cdot \underline{6} : \underline{m}$	$D_{6h}(D_{3h})$	B&W- $\bar{1}'$ -gray
32.3.120	$m'\bar{3}'m$	$\frac{4'}{m'} \frac{3}{m'} \frac{2'}{m}$	$\frac{4'}{4'} 3\frac{2}{2'}\bar{1}'$	$\bar{6}/\underline{4}$	$O_h(T_d)$	B&W- $\bar{1}'$ -gray

Table S9a. List of the 122 magnetic point groups, using the sequence used in ITD [1], with allowed components of the order parameters **M**, **P** and **T**. Cols. 1 and 2 show the group number and group name in the Hermann-Mauguin (international notation). Col. 3 gives the group name in rotation-inversion 'RI' notation. Cols. 4-6 show which components of **M**, **P** and **T** can be non-zero, e.g.  $xy$  means that both  $x$  and  $y$  components can be non-zero.

No.	HM	RI	<i>M</i>	<i>P</i>	<i>T</i>
1.1.1	1	1	$xyz$	$xyz$	$xyz$
1.2.2	11'	11'		$xyz$	
2.1.3	$\bar{1}$	1 $\bar{1}$	$xyz$		
2.2.4	$\bar{1}1'$	1 $\bar{1}1'\bar{1}'$			
2.3.5	$\bar{1}'$	1 $\bar{1}'$			$xyz$
3.1.6	2	2	$z$	$z$	$z$
3.2.7	21'	21'		$z$	
3.3.8	2'	2'	$xy$	$z$	$xy$
4.1.9	$m$	$\bar{2}$	$z$	$xy$	$xy$
4.2.10	$m1'$	$\frac{\bar{2}}{2'}1'$		$xy$	
4.3.11	$m'$	$\bar{2}'$	$xy$	$xy$	$z$
5.1.12	2/ $m$	2 $\bar{1}$	$z$		
5.2.13	2/ $m1'$	2 $\bar{1}1'\bar{1}'$			
5.3.14	2'/ $m$	$\frac{\bar{2}}{2'}\bar{1}'$			$xy$
5.4.15	2/ $m'$	2 $\bar{1}'$			$z$
5.5.16	2'/ $m'$	$\frac{2'}{2'}\bar{1}$	$xy$		
6.1.17	222	222			
6.2.18	2221'	2221'			
6.3.19	2'2'2	2'2'2	$z$		$z$
7.1.20	$mm2$	$\bar{2}\bar{2}2$		$z$	$z$
7.2.21	$mm21'$	$\frac{\bar{2}}{2'}\frac{\bar{2}}{2'}21'$		$z$	
7.3.22	$m'm2'$	$\bar{2}'\bar{2}'2'$	$y$	$z$	$x$
7.4.23	$m'm'2$	$\bar{2}'\bar{2}'2$	$z$	$z$	
8.1.24	$mmm$	222 $\bar{1}$			
8.2.25	$mmm1'$	222 $\bar{1}1'\bar{1}'$			
8.3.26	$mmm'$	$\frac{\bar{2}}{2'}\frac{\bar{2}}{2'}2\bar{1}'$			$z$
8.4.27	$m'm'm$	$\frac{2'}{2'}\frac{2'}{2'}2\bar{1}$	$z$		
8.5.28	$m'm'm'$	222 $\bar{1}'$			
9.1.29	4	4	$z$	$z$	$z$
9.2.30	41'	41'		$z$	
9.3.31	4'	4'		$z$	
10.1.32	$\bar{4}$	$\bar{4}$	$z$		
10.2.33	$\bar{4}1'$	$\frac{\bar{4}}{4'}1'$			
10.3.34	$\bar{4}'$	$\bar{4}'$			$z$
11.1.35	4/ $m$	4 $\bar{1}$	$z$		
11.2.36	4/ $m1'$	4 $\bar{1}1'\bar{1}'$			
11.3.37	4'/ $m$	$\frac{4'}{4'}\bar{1}$			
11.4.38	4/ $m'$	4 $\bar{1}'$			$z$
11.5.39	4'/ $m'$	$\frac{4'}{4'}\bar{1}'$			

Table S9a. Standard order (continuation)

No.	HM	RI	$M$	$P$	$T$
12.1.40	422	422			
12.2.41	4221'	4221'			
12.3.42	4'22'	4'22'			
12.4.43	42'2'	42'2'	$z$		$z$
13.1.44	4mm	422		$z$	$z$
13.2.45	4mm1'	4 $\frac{2}{2'}\frac{2}{2'}1'$		$z$	
13.3.46	4'mm'	4'22'		$z$	
13.4.47	4m'm'	42'2'	$z$	$z$	
14.1.48	42m	422			
14.2.49	42m1'	4 $\frac{2}{4'}2\frac{2}{2'}1'$			
14.3.50	4'm2'	4'22'			$z$
14.4.51	4'2m'	4'22'			
14.5.52	42'm'	42'2'	$z$		
15.1.53	4/mmm	422			
15.2.54	4/mmm1'	4221'1'1'			
15.3.55	4/m'mm	4 $\frac{2}{2'}\frac{2}{2'}\bar{1}'$			$z$
15.4.56	4'/mmm'	4' $\frac{2}{4'}2\frac{2}{2'}\bar{1}$			
15.5.57	4'/m'm'm	4 $\frac{2}{4'}2\frac{2}{2'}\bar{1}'$			
15.6.58	4/mm'm'	4 $\frac{2'}{2'}\frac{2'}{2'}\bar{1}$	$z$		
15.7.59	4/m'm'm'	4221'			
16.1.60	3	3	$z$	$z$	$z$
16.2.61	31'	31'		$z$	
17.1.62	3	3	$z$		
17.2.63	31'	31'1'1'			
17.3.64	3'	31'			$z$
18.1.65	32	32			
18.2.66	321'	321'			
18.3.67	32'	32'	$z$		$z$
19.1.68	3m	32		$z$	$z$
19.2.69	3m1'	3 $\frac{2}{2'}1'$		$z$	
19.3.70	3m'	32'	$z$	$z$	
20.1.71	3m	32			
20.2.72	3m1'	321'1'1'			
20.3.73	3'm	3 $\frac{2}{2'}\bar{1}'$			$z$
20.4.74	3'm'	321'			
20.5.75	3m'	3 $\frac{2'}{2'}\bar{1}$	$z$		
21.1.76	6	6	$z$	$z$	$z$
21.2.77	61'	61'		$z$	
21.3.78	6'	6'		$z$	
22.1.79	6	6	$z$		
22.2.80	61'	6 $\frac{6}{6'}1'$			
22.3.81	6'	6'			$z$
23.1.82	6/m	6	$z$		
23.2.83	6/m1'	61'1'1'			
23.3.84	6'/m	6 $\frac{6}{6'}\bar{1}'$			
23.4.85	6/m'	61'			$z$
23.5.86	6'/m'	6 $\frac{6'}{6'}\bar{1}$			

Table S9a. Standard order (continuation)

No.	HM	RI	<i>M</i>	<i>P</i>	<i>T</i>
24.1.87	622	622			
24.2.88	6221'	6221'			
24.3.89	6'22'	6'22'			
24.4.90	62'2'	62'2'	z		z
25.1.91	6mm	6 $\bar{2}\bar{2}$		z	z
25.2.92	6mm1'	6 $\frac{2}{2'}\frac{2}{2'}1'$		z	
25.3.93	6'mm'	6' $\bar{2}\bar{2}'$		z	
25.4.94	6m'm'	6 $\bar{2}'\bar{2}'$	z	z	
26.1.95	$\bar{6}2m$	$\bar{6}2\bar{2}$			
26.2.96	$\bar{6}2m1'$	$\bar{6}\frac{2}{6'}2\frac{2}{2'}1'$			
26.3.97	$\bar{6}'2m'$	$\bar{6}'2\bar{2}'$			
26.4.98	$\bar{6}'m2'$	$\bar{6}'\bar{2}\bar{2}'$			z
26.5.99	$\bar{6}2'm'$	$\bar{6}2'\bar{2}'$	z		
27.1.100	6/mmm	622 $\bar{1}$			
27.2.101	6/mmm1'	622 $\bar{1}1'\bar{1}'$			
27.3.102	6/m'mm	6 $\frac{2}{2'}\frac{2}{2'}\bar{1}'$			z
27.4.103	6'/mm'm	$\bar{6}\frac{2}{6'}2\frac{2}{2'}\bar{1}'$			
27.5.104	6'/m'mm'	$\bar{6}'2\frac{2}{6'}\bar{1}$			
27.6.105	6/mm'm'	6 $\frac{2'}{2'}\frac{2'}{2'}\bar{1}$	z		
27.7.106	6/m'm'm'	622 $\bar{1}'$			
28.1.107	23	23			
28.2.108	231'	231'			
29.1.109	$m\bar{3}$	23 $\bar{1}$			
29.2.110	$m\bar{3}1'$	23 $\bar{1}1'\bar{1}'$			
29.3.111	$m'\bar{3}'$	23 $\bar{1}'$			
30.1.112	432	432			
30.2.113	4321'	4321'			
30.3.114	4'32'	4'32'			
31.1.115	$\bar{4}3m$	$\bar{4}3\bar{2}$			
31.2.116	$\bar{4}3m1'$	$\bar{4}\frac{3}{4'}3\frac{2}{2'}1'$			
31.3.117	$\bar{4}'3m'$	$\bar{4}'3\bar{2}'$			
32.1.118	$m\bar{3}m$	432 $\bar{1}$			
32.2.119	$m\bar{3}m1'$	432 $\bar{1}1'\bar{1}'$			
32.3.120	$m'\bar{3}'m$	$\bar{4}\frac{3}{4'}3\frac{2}{2'}\bar{1}'$			
32.4.121	$m\bar{3}m'$	$\bar{4}'3\frac{2'}{2'}\bar{1}$			
32.5.122	$m'\bar{3}'m'$	432 $\bar{1}'$			

Table S9b. List of the 122 magnetic point groups shown in blocks of those allowing for 3, 2, 1 and zero order parameters. The components of the allowed order parameters  $M$ ,  $P$  and  $T$  are given explicitly. Cols. 1 and 2 show the group number and group name in the Hermann-Mauguin (international notation). Col. 3 gives the group name in rotation-inversion 'RI' notation. Cols. 4-6 show which components of  $M$ ,  $P$  and  $T$  can be non-zero, e.g.  $xy$  means that both  $x$  and  $y$  components can be non-zero.

No.	HM	RI	$M$	$P$	$T$
1.1.1	1	1	$xyz$	$xyz$	$xyz$
3.1.6	2	2	$z$	$z$	$z$
16.1.60	3	3	$z$	$z$	$z$
9.1.29	4	4	$z$	$z$	$z$
21.1.76	6	6	$z$	$z$	$z$
7.3.22	$m'm2'$	$\bar{2}'\bar{2}'$	$y$	$z$	$x$
4.1.9	$m$	$\bar{2}$	$z$	$xy$	$xy$
3.3.8	$2'$	$2'$	$xy$	$z$	$xy$
4.3.11	$m'$	$\bar{2}'$	$xy$	$xy$	$z$
7.1.20	$mm2$	$\bar{2}\bar{2}$		$z$	$z$
19.1.68	$3m$	$3\bar{2}$		$z$	$z$
13.1.44	$4mm$	$4\bar{2}\bar{2}$		$z$	$z$
25.1.91	$6mm$	$6\bar{2}\bar{2}$		$z$	$z$
6.3.19	$2'2'2$	$2'2'2$	$z$		$z$
18.3.67	$32'$	$32'$	$z$		$z$
12.4.43	$42'2'$	$42'2'$	$z$		$z$
24.4.90	$62'2'$	$62'2'$	$z$		$z$
7.4.23	$m'm'2$	$\bar{2}'\bar{2}'2$	$z$	$z$	
19.3.70	$3m'$	$3\bar{2}'$	$z$	$z$	
13.4.47	$4m'm'$	$4\bar{2}'\bar{2}'$	$z$	$z$	
25.4.94	$6m'm'$	$6\bar{2}'\bar{2}'$	$z$	$z$	

Table S9b. Number of order parameters (continuation)

No.	HM	RI	$M$	$P$	$T$
2.1.3	$\bar{1}$	$1\bar{1}$	$xyz$		
5.5.16	$2'/m'$	$\frac{2'}{2'}\bar{1}$	$xy$		
5.1.12	$2/m$	$2\bar{1}$	$z$		
17.1.62	$\bar{3}$	$3\bar{1}$	$z$		
11.1.35	$4/m$	$4\bar{1}$	$z$		
23.1.82	$6/m$	$6\bar{1}$	$z$		
10.1.32	$\bar{4}$	$\bar{4}$	$z$		
22.1.79	$\bar{6}$	$\bar{6}$	$z$		
8.4.27	$m'm'm$	$\frac{2'}{2'}\frac{2'}{2'}2\bar{1}$	$z$		
20.5.75	$\bar{3}m'$	$3\frac{2'}{2'}\bar{1}$	$z$		
15.6.58	$4/mm'm'$	$4\frac{2'}{2'}\frac{2'}{2'}\bar{1}$	$z$		
27.6.105	$6/mm'm'$	$6\frac{2'}{2'}\frac{2'}{2'}\bar{1}$	$z$		
14.5.52	$\bar{4}2'm'$	$\bar{4}2'\bar{2}'$	$z$		
26.5.99	$\bar{6}2'm'$	$\bar{6}2'\bar{2}'$	$z$		
1.2.2	$11'$	$11'$		$xyz$	
4.2.10	$m1'$	$\frac{2}{2'}1'$		$xy$	
3.2.7	$21'$	$21'$		$z$	
16.2.61	$31'$	$31'$		$z$	
9.2.30	$41'$	$41'$		$z$	
21.2.77	$61'$	$61'$		$z$	
9.3.31	$4'$	$4'$		$z$	
21.3.78	$6'$	$6'$		$z$	
7.2.21	$mm21'$	$\frac{2}{2'}\frac{2}{2'}21'$		$z$	
19.2.69	$3m1'$	$3\frac{2}{2'}1'$		$z$	
13.2.45	$4mm1'$	$4\frac{2}{2'}\frac{2}{2'}1'$		$z$	
25.2.92	$6mm1'$	$6\frac{2}{2'}\frac{2}{2'}1'$		$z$	
13.3.46	$4'mm'$	$4'\bar{2}\bar{2}'$		$z$	
25.3.93	$6'mm'$	$6'\bar{2}\bar{2}'$		$z$	
2.3.5	$\bar{1}'$	$1\bar{1}'$			$xyz$
5.3.14	$2'/m$	$\frac{2}{2'}\bar{1}'$			$xy$
5.4.15	$2/m'$	$2\bar{1}'$			$z$
17.3.64	$\bar{3}'$	$3\bar{1}'$			$z$
11.4.38	$4/m'$	$4\bar{1}'$			$z$
10.3.34	$\bar{4}'$	$\bar{4}'$			$z$
22.3.81	$\bar{6}'$	$\bar{6}'$			$z$
23.4.85	$6/m'$	$6\bar{1}'$			$z$
8.3.26	$mmm'$	$\frac{2}{2'}\frac{2}{2'}2\bar{1}'$			$z$
20.3.73	$\bar{3}'m$	$3\frac{2}{2'}\bar{1}'$			$z$
15.3.55	$4/m'mm$	$4\frac{2}{2'}\frac{2}{2'}\bar{1}'$			$z$
27.3.102	$6/m'mm$	$6\frac{2}{2'}\frac{2}{2'}\bar{1}'$			$z$
26.4.98	$\bar{6}'m2'$	$\bar{6}'\bar{2}2'$			$z$
14.3.50	$\bar{4}'m2'$	$\bar{4}'\bar{2}2'$			$z$

Table S9b. Number of order parameters (continuation)

No.	HM	RI	<i>M</i>	<i>P</i>	<i>T</i>
2.2.4	$\bar{1}1'$	$1\bar{1}'\bar{1}'$			
5.2.13	$2/m1'$	$2\bar{1}'\bar{1}'$			
6.1.17	222	222			
8.1.24	<i>mmm</i>	$222\bar{1}$			
6.2.18	2221'	$2221'$			
8.5.28	$m'm'm'$	$222\bar{1}'$			
8.2.25	$mmm1'$	$222\bar{1}'\bar{1}'$			
12.1.40	422	422			
18.1.65	32	32			
24.1.87	622	622			
20.1.71	$\bar{3}m$	$32\bar{1}$			
15.1.53	$4/mmm$	$422\bar{1}$			
27.1.100	$6/mmm$	$622\bar{1}$			
14.1.48	$\bar{4}2m$	$\bar{4}2\bar{2}$			
26.1.95	$\bar{6}2m$	$\bar{6}2\bar{2}$			
18.2.66	321'	$321'$			
12.2.41	4221'	$4221'$			
24.2.88	6221'	$6221'$			
12.3.42	$4'22'$	$4'22'$			
24.3.89	$6'22'$	$6'22'$			
20.4.74	$\bar{3}'m'$	$32\bar{1}'$			
15.7.59	$4/m'm'm'$	$422\bar{1}'$			
27.7.106	$6/m'm'm'$	$622\bar{1}'$			
14.4.51	$\bar{4}'2m'$	$\bar{4}'2\bar{2}'$			
26.3.97	$\bar{6}'2m'$	$\bar{6}'2\bar{2}'$			
11.2.36	$4/m1'$	$4\bar{1}'\bar{1}'$			
17.2.63	$\bar{3}1'$	$3\bar{1}'\bar{1}'$			
23.2.83	$6/m1'$	$6\bar{1}'\bar{1}'$			
11.3.37	$4'/m$	$\frac{4'}{4'}\bar{1}$			
23.5.86	$6'/m'$	$\frac{6'}{6'}\bar{1}$			
10.2.33	$\bar{4}1'$	$\frac{4}{4'}1'$			
22.2.80	$\bar{6}1'$	$\frac{6}{6'}1'$			
11.5.39	$4'/m'$	$\frac{4}{4'}\bar{1}'$			
23.3.84	$6'/m$	$\frac{6}{6'}\bar{1}'$			
20.2.72	$\bar{3}m1'$	$32\bar{1}'\bar{1}'$			
15.2.54	$4/mmm1'$	$422\bar{1}'\bar{1}'$			
27.2.101	$6/mmm1'$	$622\bar{1}'\bar{1}'$			
15.4.56	$4'/mmm'$	$\frac{4'}{4'}2\frac{2'}{2'}\bar{1}$			
27.5.104	$6'/m'mm'$	$\frac{6'}{6'}2\frac{2'}{2'}\bar{1}$			
14.2.49	$\bar{4}2m1'$	$\frac{4}{4'}2\frac{2}{2'}1'$			
26.2.96	$\bar{6}2m1'$	$\frac{6}{6'}2\frac{2}{2'}1'$			
15.5.57	$4'/m'm'm$	$\frac{4}{4'}2\frac{2}{2'}\bar{1}'$			
27.4.103	$6'/mm'm$	$\frac{6}{6'}2\frac{2}{2'}\bar{1}'$			



Table S9b. Number of order parameters (continuation)

No.	HM	RI	$M$	$P$	$T$
28.1.107	23	23			
30.1.112	432	432			
29.2.110	$m\bar{3}1'$	$23\bar{1}'\bar{1}'$			
32.2.119	$m\bar{3}m1'$	$432\bar{1}'\bar{1}'$			
29.1.109	$m\bar{3}$	$23\bar{1}$			
32.1.118	$m\bar{3}m$	$432\bar{1}$			
28.2.108	$231'$	$231'$			
30.2.113	$4321'$	$4321'$			
29.3.111	$m'\bar{3}'$	$23\bar{1}'$			
32.5.122	$m'\bar{3}'m'$	$432\bar{1}'$			
32.4.121	$m\bar{3}m'$	$\frac{4'}{4'}3\frac{2'}{2'}\bar{1}$			
31.2.116	$\bar{4}3m1'$	$\frac{4}{4}3\frac{2}{2'}1'$			
32.3.120	$m'\bar{3}'m$	$\frac{4}{4}3\frac{2}{2'}\bar{1}'$			
31.1.115	$\bar{4}3m$	$\bar{4}3\bar{2}$			
30.3.114	$4'32'$	$4'32'$			
31.3.117	$\bar{4}'3m'$	$\bar{4}'3\bar{2}'$			

Table S10. Complete list of parent magnetic point groups (classes) that allow continuous ferromagnetic, ferroelectric and ferrotoroidic moment reorientation. Please note that ferro-continuous reorientation is possible for ions located in each Wyckoff position.

mode	crystal system	ferromagnetic	ferroelectric	ferrotoroidic
"FFF"	triclinic	$1\bar{1}$ ( $\bar{1}$ ) 1 (1)	$11'$ ( $11'$ ) 1 (1)	$1\bar{1}'$ ( $\bar{1}'$ ) 1 (1)
"FAF" and "FOF"	monoclinic	$\frac{2'}{2'}\bar{1}$ ( $2'/m'$ ) $2'$ ( $2'$ ) $\bar{2}'$ ( $m'$ )	$\frac{2}{2'}1'$ ( $m1'$ ) $\bar{2}$ ( $m$ ) $\bar{2}'$ ( $m'$ )	$\frac{2}{2'}\bar{1}'$ ( $2'/m$ ) $\bar{2}$ ( $m$ ) $2'$ ( $2'$ )

Table S11. Complete list of parent magnetic point groups (classes) that allow continuous antiferromagnetic, antiferroelectric and antiferrotoroidic moment reorientation. Please note that antiferro-continuous reorientation is possible only for ions in Wyckoff positions with magnetic site-symmetry point groups given in rows denoted "(3 components)" and "(2 components)" in Tables 1, 4 and 5 in the main text.

mode	crystal system	antiferromagnetic	antiferroelectric	antiferrotoroidic
"AAA"	triclinic	$1\bar{1}'\bar{1}'$ ( $\bar{1}1'$ ) $11'$ ( $11'$ ) $1\bar{1}'$ ( $\bar{1}'$ )	$1\bar{1}'\bar{1}'$ ( $\bar{1}1'$ ) $1\bar{1}$ ( $\bar{1}$ ) $1\bar{1}'$ ( $\bar{1}'$ )	$1\bar{1}'\bar{1}'$ ( $\bar{1}1'$ ) $1\bar{1}$ ( $\bar{1}$ ) $11'$ ( $11'$ )
"AFA"	monoclinic	$2\bar{1}$ ( $2/m$ ) 2 (2) $\bar{2}$ ( $m$ )	$21'$ ( $21'$ ) 2 (2) $2'$ ( $2'$ )	$2\bar{1}'$ ( $2/m'$ ) 2 (2) $\bar{2}'$ ( $m'$ )
"ABA" and "A0A"	monoclinic	$2\bar{1}'\bar{1}'$ ( $2/m1'$ ) $21'$ ( $21'$ ) $2\bar{1}'$ ( $2/m'$ ) $\frac{2}{2'}1'$ ( $m1'$ ) $\frac{2}{2'}\bar{1}'$ ( $2'/m$ )	$2\bar{1}'\bar{1}'$ ( $2/m1'$ ) $2\bar{1}$ ( $2/m$ ) $2\bar{1}'$ ( $2/m'$ ) $\frac{2'}{2'}\bar{1}$ ( $2'/m'$ ) $\frac{2}{2'}\bar{1}'$ ( $2'/m$ )	$2\bar{1}'\bar{1}'$ ( $2/m1'$ ) $2\bar{1}$ ( $2/m$ ) $21'$ ( $21'$ ) $\frac{2'}{2'}\bar{1}$ ( $2'/m'$ ) $\frac{2}{2'}1'$ ( $m1'$ )

Table S12. Complete list of parent magnetic point groups (classes) that allow nearly collinear antiferromagnetism with (weak) ferromagnetism, nearly collinear antiferroelectricity with (weak) ferroelectricity and nearly collinear antiferrotoroidicity with (weak) ferrotoroidicity. Please note that nearly collinear antiferro- with ferro- ordering is possible only for ions in Wyckoff positions with magnetic site-symmetry point groups specified in Tables 1, 4 and 5 in the main text.

mode	crystal system	magnetic	electric	toroidic
"AFA"	monoclinic	$2\bar{1}$ ( $2/m$ ) 2 (2) $\bar{2}$ ( $m$ )	$21'$ ( $21'$ ) 2 (2) $2'$ ( $2'$ )	$2\bar{1}'$ ( $2/m'$ ) 2 (2) $\bar{2}'$ ( $m'$ )
"FAF"	monoclinic	$\frac{2'}{2'}\bar{1}$ ( $2'/m'$ ) $2'$ ( $2'$ ) $\bar{2}'$ ( $m'$ )	$\frac{2}{2'}1'$ ( $m1'$ ) $\bar{2}$ ( $m$ ) $\bar{2}'$ ( $m'$ )	$\frac{2}{2'}\bar{1}'$ ( $2'/m$ ) $\bar{2}$ ( $m$ ) $2'$ ( $2'$ )
"AFB" and "AF0"	orthorhombic	$2\frac{2'}{2'}\frac{2'}{2'}\bar{1}$ ( $mm'm'$ ) $22'2'$ ( $22'2'$ ) $2\bar{2}'\bar{2}'$ ( $2m'm'$ ) $\bar{2}2'\bar{2}'$ ( $m2'm'$ )	$2\frac{2}{2'}\frac{2}{2'}1'$ ( $2mm1'$ ) $2\bar{2}\bar{2}$ ( $2mm$ ) $2\bar{2}'\bar{2}'$ ( $2m'm'$ ) $2'\bar{2}\bar{2}'$ ( $2'mm'$ )	$2\frac{2}{2'}\frac{2}{2'}\bar{1}'$ ( $m'mm$ ) $2\bar{2}\bar{2}$ ( $2mm$ ) $22'2'$ ( $22'2'$ ) $\bar{2}'\bar{2}2'$ ( $m'm2'$ )

Table S13. All 122 parent magnetic point groups (classes) divided into Kopsky-categories and types. Eight last columns denote which of ferromagnetic, **M**, ferroelectric, **P**, and ferrotoroidic, **T**, moment is allowed, e.g. "•" symbol in "MP" column means that both **M** and **P** can be non-zero.

Groups	Category	Type	none	M	P	T	PT	MT	MP	MPT
222, 32, 422, 622, 23, 432 1, 2, 3, 4, 6	full-white	full-white	•							•
1 $\bar{1}\bar{1}'\bar{1}'$ , 2 $\bar{1}\bar{1}'\bar{1}'$ , 3 $\bar{1}\bar{1}'\bar{1}'$ , 4 $\bar{1}\bar{1}'\bar{1}'$ , 6 $\bar{1}\bar{1}'\bar{1}'$ , 222 $\bar{1}\bar{1}'\bar{1}'$ , 32 $\bar{1}\bar{1}'\bar{1}'$ , 422 $\bar{1}\bar{1}'\bar{1}'$ , 622 $\bar{1}\bar{1}'\bar{1}'$ 23 $\bar{1}\bar{1}'\bar{1}'$ , 432 $\bar{1}\bar{1}'\bar{1}'$	full-gray	full-gray	• • •							
4 $\bar{2}'\bar{2}'$ , 6 $\bar{2}'\bar{2}'$ 4' $\bar{2}\bar{2}'$ , 6' $\bar{2}\bar{2}'$ 4' $\bar{2}\bar{2}'$ , 6' $\bar{2}\bar{2}'$ 2 $\bar{2}'\bar{2}'$	full-B&W	full-B&W		•		•				•
222 $\bar{1}$ , 32 $\bar{1}$ , 422 $\bar{1}$ , 622 $\bar{1}$ , 23 $\bar{1}$ , 432 $\bar{1}$ 2221', 321', 4221', 6221', 231', 4321' 222 $\bar{1}'$ , 32 $\bar{1}'$ , 422 $\bar{1}'$ , 622 $\bar{1}'$ , 23 $\bar{1}'$ , 432 $\bar{1}'$ 1 $\bar{1}$ , 2 $\bar{1}$ , 3 $\bar{1}$ , 4 $\bar{1}$ , 6 $\bar{1}$ 11', 21', 31', 41', 61' 1 $\bar{1}'$ , 2 $\bar{1}'$ , 3 $\bar{1}'$ , 4 $\bar{1}'$ , 6 $\bar{1}'$	partially-gray	$\bar{1}$ -gray 1'-gray $\bar{1}'$ -gray $\bar{1}$ -gray 1'-gray $\bar{1}'$ -gray	• • •			•		•		
4 $\bar{3}\bar{2}$ and 4 $\bar{2}\bar{2}$ , 6 $\bar{2}\bar{2}$ 4'32' and 4'22', 6'22' 4' $\bar{3}\bar{2}'$ and 4' $\bar{2}\bar{2}'$ , 6' $\bar{2}\bar{2}'$ 4, 6 4', 6' 4, 6' 3 $\bar{2}$ , 2 $\bar{2}\bar{2}$ , 4 $\bar{2}\bar{2}$ , 6 $\bar{2}\bar{2}$ 32', 22'2', 42'2', 62'2' 3 $\bar{2}'$ , 2 $\bar{2}'\bar{2}'$ , 4 $\bar{2}'\bar{2}'$ , 6 $\bar{2}'\bar{2}'$ 2 2' 2'	partially-B&W	$\bar{1}$ -B&W 1'-B&W $\bar{1}'$ -B&W $\bar{1}$ -B&W 1'-B&W $\bar{1}'$ -B&W $\bar{1}$ -B&W 1'-B&W $\bar{1}'$ -B&W $\bar{1}$ -B&W 1'-B&W $\bar{1}'$ -B&W	• • •		•		•		•	• • •
4' $\bar{4}$ , 6' $\bar{4}$ , 4' $\bar{3}\bar{2}'\bar{1}$ and 4' $\bar{2}\bar{2}'\bar{1}$ , 6' $\bar{2}\bar{2}'\bar{1}$ 4' $\bar{4}'$ , 6' $\bar{4}'$ , 4' $\bar{3}\bar{2}'\bar{1}'$ and 4' $\bar{2}\bar{2}'\bar{1}'$ , 6' $\bar{2}\bar{2}'\bar{1}'$ 4' $\bar{4}'$ , 6' $\bar{4}'$ , 4' $\bar{3}\bar{2}'\bar{1}'$ and 4' $\bar{2}\bar{2}'\bar{1}'$ , 6' $\bar{2}\bar{2}'\bar{1}'$ 2' $\bar{4}$ , 3' $\bar{2}'\bar{1}$ , 2' $\bar{2}'\bar{2}'\bar{1}$ , 4' $\bar{2}'\bar{2}'\bar{1}$ , 6' $\bar{2}'\bar{2}'\bar{1}$ 2' $\bar{4}'$ , 3' $\bar{2}'\bar{1}'$ , 2' $\bar{2}'\bar{2}'\bar{1}'$ , 4' $\bar{2}'\bar{2}'\bar{1}'$ , 6' $\bar{2}'\bar{2}'\bar{1}'$ 2' $\bar{4}'$ , 3' $\bar{2}'\bar{1}'$ , 2' $\bar{2}'\bar{2}'\bar{1}'$ , 4' $\bar{2}'\bar{2}'\bar{1}'$ , 6' $\bar{2}'\bar{2}'\bar{1}'$	B&W-partially-gray	B&W- $\bar{1}$ -gray B&W-1'-gray B&W- $\bar{1}'$ -gray B&W- $\bar{1}$ -gray B&W-1'-gray B&W- $\bar{1}'$ -gray	• • •			•		•		

## References

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