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Supporting information for article:

Crystal and magnetic structures of $R_2Ni_{1.78}In$ compounds (R = Tb, Ho, Er and Tm)

Stanisław Baran, Aleksandra Deptuch, Andreas Hoser, Bogusław Penc, Yuriy Tyvanchuk and Andrzej Szytuła

Supporting Information

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The Supporting Information contains symmetry analysis of allowed magnetic structures in $R_2Ni_{1.78}In$ as generated by the BasIreps computer program as well as the .fst input files for FPStudio and parts of the .pcr input files for FullProf regarding the magnetic structures.

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1. Symmetry analysis for the *4h* Wyckoff site and $\boldsymbol{k_1} = \left[\frac{1}{4}, \frac{1}{4}, \frac{1}{2}\right]$

```
 +++++++++++++++++++++++++++++++++++++++++++++++++++++++
 +++ PROGRAM:BasIreps (Version 4.10, November 2012)+++
 +++              (JRC- ILL)               +++
 +++++++++++++++++++++++++++++++++++++++++++++++++++++++

 The calculation of the IRREPS of the little group is based in
 the procedure of ZAK provided within the program KAREP
 E. Hovestreydt, I. Aroyo et al, J.Appl.Cryst. 25, 544 (1992)
 Program based in CrysFML (Crystallographic Fortran-95 Modules Library)
 BasIreps -> (Version 4.10, November 2012), ILL-Juan Rodriguez-Carvajal

=> Title:Test of new BASIREPS
=> Symbol of the space group: P 4/m b m
=> The given space group P 4/m b m is standard, IT generators will be used
=> List of space group generators:  -x,-y,z; -y,x,z; -x+1/2,y+1/2,-z; -x,-y,-z
=> Propagation vector:   0.2500  0.2500  0.5000
=> BZ-point labelled as  G
=> The representations of Gk will be calculated



      Information on Space Group:
      ---------------------------

=>   Number of Space group: 127
=>  Hermann-Mauguin Symbol: P 4/m b m
=>           Hall Symbol: -P 4 2ab
=>          Setting Type: Generated from explicit IT generators
=>         Crystal System: Tetragonal
=>            Laue Class: 4/mmm
=>           Point Group: 4/mmm
=>        Bravais Lattice: P
=>         Lattice Symbol: tP
=>  Reduced Number of S.O.:   8
=>    General multiplicity:  16
=>         Centrosymmetry: Centric (-1 at origin)
=>  Generators (exc. -1&L):   3
=>        Asymmetric unit:  0.000 <= x <=  0.500
                            0.000 <= y <=  0.500
                            0.000 <= z <=  0.500
=> Centring vectors:  0


=> List of all Symmetry Operators and Symmetry Symbols

=> SYMM(  1): x,y,z                    Symbol: 1
=> SYMM(  2): -x,-y,z                  Symbol: 2 0,0,z
=> SYMM(  3): -y,x,z                   Symbol: 4+ 0,0,z
=> SYMM(  4): -x+1/2,y+1/2,-z          Symbol: 2 (0,1/2,0) 1/4,y,0
=> SYMM(  5): y,-x,z                   Symbol: 4- 0,0,z
=> SYMM(  6): x+1/2,-y+1/2,-z          Symbol: 2 (1/2,0,0) x,1/4,0
=> SYMM(  7): -y+1/2,-x+1/2,-z         Symbol: 2 x,-x+1/2,0
=> SYMM(  8): y+1/2,x+1/2,-z           Symbol: 2 (1/2,1/2,0) x,x,0
```

=> SYMM(9): -x,-y,-z Symbol: -1 0,0,0
=> SYMM(10): x,y,-z Symbol: m x,y,0
=> SYMM(11): y,-x,-z Symbol: -4+ 0,0,z; 0,0,0
=> SYMM(12): x+1/2,-y+1/2,z Symbol: a x,1/4,z
=> SYMM(13): -y,x,-z Symbol: -4- 0,0,z; 0,0,0
=> SYMM(14): -x+1/2,y+1/2,z Symbol: b 1/4,y,z
=> SYMM(15): y+1/2,x+1/2,z Symbol: n (1/2,1/2,0) x,x,z
=> SYMM(16): -y+1/2,-x+1/2,z Symbol: m x,-x+1/2,z

=> Special Wyckoff Positions for P 4/m b m

Multp	Site	Representative Coordinates (centring translations excluded)
8	k	x,x+1/2,z -x,-x+1/2,z -x+1/2,x,z -x+1/2,x,-z x+1/2,-x,z x+1/2,-x,-z -x,-x+1/2,-z x,x+1/2,-z
8	j	x,y,1/2 -x,-y,1/2 -y,x,1/2 -x+1/2,y+1/2,1/2 y,-x,1/2 x+1/2,-y+1/2,1/2 -y+1/2,-x+1/2,1/2 y+1/2,x+1/2,1/2
8	i	x,y,0 -x,-y,0 -y,x,0 -x+1/2,y+1/2,0 y,-x,0 x+1/2,-y+1/2,0 -y+1/2,-x+1/2,0 y+1/2,x+1/2,0
4	h	x,x+1/2,1/2 -x,-x+1/2,1/2 -x+1/2,x,1/2 x+1/2,-x,1/2
4	g	x,x+1/2,0 -x,-x+1/2,0 -x+1/2,x,0 x+1/2,-x,0
4	f	0,1/2,z 1/2,0,z 1/2,0,-z 0,1/2,-z
4	e	0,0,z 1/2,1/2,-z 0,0,-z 1/2,1/2,z
2	d	0,1/2,0 1/2,0,0
2	c	0,1/2,1/2 1/2,0,1/2
2	b	0,0,1/2 1/2,1/2,1/2
2	a	0,0,0 1/2,1/2,0

=> Number of generators of space group: 4

GEN(1): -x,-y,z
GEN(2): -y,x,z
GEN(3): -x+1/2,y+1/2,-z
GEN(4): -x,-y,-z

TRANSLATIONAL COSET REPRESENTATIVES OF SPACE GROUP: P 4/m b m

Num	Symmetry-Element	Eqv. Positions
(1)	1	x,y,z

```
(  2)   2 0,0,z                      -x,-y,z
(  3)   4+ 0,0,z                      -y,x,z
(  4)   2 (0,1/2,0) 1/4,y,0              y,-x,z
(  5)   4- 0,0,z                      -x+1/2,y+1/2,-z
(  6)   2 (1/2,0,0) x,1/4,0              x+1/2,-y+1/2,-z
(  7)   2 x,-x+1/2,0                   y+1/2,x+1/2,-z
(  8)   2 (1/2,1/2,0) x,x,0              -y+1/2,-x+1/2,-z
(  9)   -1 0,0,0                      -x,-y,-z
( 10)   m x,y,0                        x,y,-z
( 11)   -4+ 0,0,z; 0,0,0                 y,-x,-z
( 12)   a x,1/4,z                      -y,x,-z
( 13)   -4- 0,0,z; 0,0,0                 x-1/2,-y-1/2,z
( 14)   b 1/4,y,z                      -x-1/2,y-1/2,z
( 15)   n (1/2,1/2,0) x,x,z              -y-1/2,-x-1/2,z
( 16)   m x,-x+1/2,z                   y-1/2,x-1/2,z


=> The lattice symbol is tP


 The conventional k-vector is
   0.25000     0.25000     0.50000

THE GENERATORS OF THE LITTLE GROUP OF BRILLOUIN ZONE POINT  G

The little group can be generated from the following 2 elements:-

 => GENk(1): y+1/2,x+1/2,-z
 => GENk(2): x,y,-z

REPRESENTATIVE ELEMENTS OF THE LITTLE GROUP OF BRILLOUIN ZONE POINT  G

 Operator of Gk Number( 1): x,y,z
 Operator of Gk Number( 2): y+1/2,x+1/2,-z
 Operator of Gk Number( 3): x,y,-z
 Operator of Gk Number( 4): y+1/2,x+1/2,z

------------------------------------------------------------
=> Number of elements of G_k:   4
=> Number of irreducible representations of G_k:   4
=> Dimensions:  1 1 1 1

=> Symmetry elements of G_k and irreps:
   Symmetry elements reduced to the standard form (positive translations < 1)
   The matrices of IRreps have been multiplied by the appropriate phase factor

-> SYMM_K( 1):  x,y,z                :  1          ->  h1          Int. symbol: 1
   Phase factor for correcting input data:  0.0000
   Matrix of IRrep( 1):
                1
   Matrix of IRrep( 2):
                1
   Matrix of IRrep( 3):
                1
   Matrix of IRrep( 4):
                1
-> SYMM_K( 2):  y+1/2,x+1/2,-z          :  2 ( x, x, 0) -> h16          Int. symbol: 2 (1/2,1/2,0) x,x,0
```

Phase factor for correcting input data: 0.0000
Matrix of IRrep(1):
i
Matrix of IRrep(2):
i
Matrix of IRrep(3):
-i
Matrix of IRrep(4):
-i
-> SYMM_K(3): x,y,-z : m (x, y, 0) -> h28 Int. symbol: m x,y,0
Phase factor for correcting input data: 0.0000
Matrix of IRrep(1):
1
Matrix of IRrep(2):
-1
Matrix of IRrep(3):
1
Matrix of IRrep(4):
-1
-> SYMM_K(4): y+1/2,x+1/2,z : m (x, x, z) -> h37 Int. symbol: n (1/2,1/2,0) x,x,z
Phase factor for correcting input data: 0.0000
Matrix of IRrep(1):
i
Matrix of IRrep(2):
-i
Matrix of IRrep(3):
-i
Matrix of IRrep(4):
i

==========
Writing of Irreps matrices in symbolic form: Module:Phase (fractions of 2pi)
Numeric values of symbols a,b,c,d, ... are given at the end of the table
==========

In this section the translations associated to Seitz symbols are simplified as
1/2 1/3 2/3 1/4 3/4 1/6 5/6 1/8 3/8 5/8 7/8
p q r s t u v w x y z

The rotational part of Seitz symbols contains information about the orientation as defined in Kovalev. The international symbols may be truncated (for format reasons) in the table below. The complete international symbols can be found in the previous list.

Ireps Symmetry operators ->
v 1 2 (1/2,1/2,0) m x,y,0 n (1/2,1/2,0)
v {1|000} {2_xx0|pp0} {m_xy0|000} {m_xxz|pp0}
v Symm(1) Symm(2) Symm(3) Symm(4)

IRrep(1): 1 i 1 i

IRrep(2): 1 i -1 -i

IRrep(3): 1 -i 1 -i

IRrep(4): 1 -i -1 i

List of constants and phase factors defined in the above table
---

The propagation vector is k=(0.25000, 0.25000, 0.50000)
Phase factor: i = exp{2.pi.i. 0.25000} = (0.00000, 1.00000) Exponent(fraction 2pi) = 1/4
Phase factor: -i = exp{2.pi.i. 0.75000} = (-0.00000,-1.00000) Exponent(fraction 2pi) = 3/4

=> Alternative evaluation of the propagation vector group.
The ordering of the symmetry operators may be different
than the sequence numbering given above

PROPAGATION VECTOR GROUP INFORMATION
==========

=> The input propagation vector is: K=(0.2500 0.2500 0.5000)
=> K .. IS NOT .. equivalent to -K
=> The operators following the k-vectors constitute the co-set decomposition G[Gk]
The list of equivalent k-vectors are also given on the right of operators.
=> The star of K is formed by the following 4 vectors:

k_1 = (0.2500 0.2500 0.5000) Op: (1) x,y,z
Op: (8) y+1/2,x+1/2,-z -> (0.2500 0.2500 -0.5000)
Op: (10) x,y,-z -> (0.2500 0.2500 -0.5000)
Op: (15) y+1/2,x+1/2,z -> (0.2500 0.2500 0.5000)

Eqv. -K: k_2 = (-0.2500 -0.2500 0.5000) Op: (2) -x,-y,z
Op: (7) -y+1/2,-x+1/2,-z -> (-0.2500 -0.2500 -0.5000)
Op: (9) -x,-y,-z -> (-0.2500 -0.2500 -0.5000)
Op: (16) -y+1/2,-x+1/2,z -> (-0.2500 -0.2500 0.5000)

k_3 = (0.2500 -0.2500 0.5000) Op: (3) -y,x,z
Op: (6) x+1/2,-y+1/2,-z -> (0.2500 -0.2500 -0.5000)
Op: (12) x+1/2,-y+1/2,z -> (0.2500 -0.2500 0.5000)
Op: (13) -y,x,-z -> (0.2500 -0.2500 -0.5000)

k_4 = (-0.2500 0.2500 -0.5000) Op: (4) -x+1/2,y+1/2,-z
Op: (5) y,-x,z -> (-0.2500 0.2500 0.5000)
Op: (11) y,-x,-z -> (-0.2500 0.2500 -0.5000)
Op: (14) -x+1/2,y+1/2,z -> (-0.2500 0.2500 0.5000)

=> G_k has the following symmetry operators:

1 SYMM(1) = x,y,z
2 SYMM(8) = y+1/2,x+1/2,-z
3 SYMM(10) = x,y,-z
4 SYMM(15) = y+1/2,x+1/2,z

```
   DATA ABOUT ATOMS
   ================

 -> The atom site: Tm1   is split in  3 orbits
 -> The total number of sites has been increased consequently

=> No. of sites:    3

=> Calculation for axial vectors

=> List of atoms within a primitive unit cell:
           X      Y      Z         for site:  1
-> Tm11_1 :  0.1741  0.6741  0.5000  : (x,y,z)
           X      Y      Z         for site:  2
-> Tm12_1 :  0.8259  0.3259  0.5000  : (x,y,z)
           X      Y      Z         for site:  3
-> Tm13_1 :  0.3259  0.1741  0.5000  : (x,y,z)
-> Tm13_2 :  0.6741  0.8259  0.5000  : (y+1/2,x+1/2,-z) + (0,0,1)


   CALCULATIONS FOR SITE : 1

================================================================================
    Sym.Op.     Atoms Numbers, phases and returning Vectors
   Vector Rep.    Character(V)    Character(Perm)(r,i)  ChM
================================================================================
SYMM_K( 1): x,y,z                   :  1          ->  h1
    Atoms:         1
    Phase:       0.0000
   Vector:     0.0 0.0 0.0
   Vector Representation: ( Mx, My, Mz)
   Ch(V):  3.000 Chr(P):  1.000 Chi(P):  0.000 Chr(T):  3.000 Chi(T):  0.000
--------------------------------------------------------------------------------
SYMM_K( 2): y+1/2,x+1/2,-z              :  2 ( x, x, 0) -> h16
    Atoms:         1
    Phase:       0.2500
   Vector:    -1.0 0.0 1.0
   Vector Representation: ( My, Mx,-Mz)
   Ch(V): -1.000 Chr(P):  0.000 Chi(P): -1.000 Chr(T): -0.000 Chi(T):  1.000
--------------------------------------------------------------------------------
SYMM_K( 3): x,y,-z                  :  m ( x, y, 0) -> h28
    Atoms:         1
    Phase:       0.5000
   Vector:     0.0 0.0 1.0
   Vector Representation: (-Mx,-My, Mz)
   Ch(V): -1.000 Chr(P): -1.000 Chi(P): -0.000 Chr(T):  1.000 Chi(T):  0.000
--------------------------------------------------------------------------------
SYMM_K( 4): y+1/2,x+1/2,z               :  m ( x, x, z) -> h37
    Atoms:         1
    Phase:      -0.2500
   Vector:    -1.0 0.0 0.0
   Vector Representation: (-My,-Mx,-Mz)
   Ch(V): -1.000 Chr(P):  0.000 Chi(P):  1.000 Chr(T): -0.000 Chi(T): -1.000
--------------------------------------------------------------------------------

 => Decomposition of the Magnetic/Mechanic representation:
```

-> Characters of GAMMA and IRreps:

GAMMA G(1) G(2) G(3) G(4)
3.0 0.0 -0.0 1.0 1.0 0.0 -0.0-1.0

Irep_k(1) G(1) G(2) G(3) G(4)
1.0 0.0 0.0 1.0 1.0 0.0 0.0 1.0

Irep_k(2) G(1) G(2) G(3) G(4)
1.0 0.0 0.0 1.0 -1.0 0.0 -0.0-1.0

Irep_k(3) G(1) G(2) G(3) G(4)
1.0 0.0 -0.0-1.0 1.0 0.0 -0.0-1.0

Irep_k(4) G(1) G(2) G(3) G(4)
1.0 0.0 -0.0-1.0 -1.0 0.0 0.0 1.0

-> GAMMA(Magnetic): 1 Irep_k(1) + 1 Irep_k(2) + 1 Irep_k(3)

=> Decomposition of the Permutational Representation:

-> GAMMA(Permutation): 1 Irep_k(4)

=> Exchange multiplets:

Representation Irep_k(4) x Axial: 1 Irep_k(1) + 1 Irep_k(2) + 1 Irep_k(3)

General information relating the calculated basis functions with the magnetic structure

---

The fundamental hypothesis of the representational analysis is that the vectorial Fourier coefficients are LINEAR COMBINATIONS of Basis Functions, in a simplified form: Sk(j) = Sum{n}{C(n).BsV(n,j)}
The index 'j' labels the sublatices (j=1,2,...na) of the current site: Tm11_1
The simplified notation for C(n) used below, is given by the symbols: u,v,w,p,q ....(may be complex!)
The Fourier coefficients are written as: Sk(j) = u BsV(1,j)+ v BsV(2,j)+ w BsV(3,j)+ p BsV(4,j)+ q BsV(5,j)+ ...
The atomic components of the basis functions BsV(n,j) are 3D constant vectors (may be complex) written as row matrices
BsV(n,j) represents the basis vector 'n' attached to the atom 'j'
BsV(n,1:na) represents the basis vectors 'n' of the atoms 1 up to na (row of na 3D-vectors)
The magnetic moments should be calculated from the Fourier coefficients using the general formula:

$$m(L,j) = \mathrm{Sum}\{k\}\{ Sk(j) \exp[-2\pi i.k.R(L)] \}$$

or for a single pair (k,-k)

$$m(L,j) = Sk(j) \exp\{-2\pi i.k.R(L)\} + Sk^*(j) \exp\{2\pi i.k.R(L)\}$$

Where R(L) is the LATTICE translation giving the vector position of the cell labelled 'L': R(L) = L1 a + L2 b + L3 c

If the lattice is CENTRED the expression of R(L) contains also fractional indices (L1,L2,L3)

The components of m(L,j), Sk(j) and BsV(n,j) are given with respect to a frame with unit vectors along a,b,c

We consider only the propagation vector pair (k,-k) with k = (0.25000, 0.25000, 0.50000)

=> Atomic components of the BASIS FUNCTIONS using PROJECTION OPERATORS:
Calculation for SITE number: 1
(Only non-null functions are written)

++
=> Basis functions of Representation IRrep(1) of dimension 1 contained 1 times in GAMMA
++

SYMM x,y,z
Atoms: Tm11_1
BsV(1, 1: 1):Re (1 -1 0)

----- The Fourier coefficients are LINEAR COMBINATIONS of Basis Functions: coefficients u,v,w,p,q ....(may be complex!)

The general expressions of the Fourier coefficients Sk(j) of the atoms non-related
by lattice translations are the following:

SYMM x,y,z Atom: Tm11_1 0.1741 0.6741 0.5000
Sk(1): (u,-u,0)

++
=> Basis functions of Representation IRrep(2) of dimension 1 contained 1 times in GAMMA
++

SYMM x,y,z
Atoms: Tm11_1
BsV(1, 1: 1):Re (0 0 1)

----- The Fourier coefficients are LINEAR COMBINATIONS of Basis Functions: coefficients u,v,w,p,q ....(may be complex!)

The general expressions of the Fourier coefficients Sk(j) of the atoms non-related
by lattice translations are the following:

SYMM x,y,z Atom: Tm11_1 0.1741 0.6741 0.5000
Sk(1): (0,0,u)

++
=> Basis functions of Representation IRrep(3) of dimension 1 contained 1 times in GAMMA
++

SYMM x,y,z
Atoms: Tm11_1
BsV(1, 1: 1):Re (1 1 0)

----- The Fourier coefficients are LINEAR COMBINATIONS of Basis Functions: coefficients u,v,w,p,q ....(may be complex!)

The general expressions of the Fourier coefficients Sk(j) of the atoms non-related by lattice translations are the following:

SYMM x,y,z Atom: Tm11_1 0.1741 0.6741 0.5000
Sk(1): (u,u,0)

CALCULATIONS FOR SITE : 2

==========

Sym.Op. Atoms Numbers, phases and returning Vectors
Vector Rep. Character(V) Character(Perm)(r,i) ChM

==========

SYMM_K(1): x,y,z : 1 -> h1
Atoms: 1
Phase: 0.0000
Vector: 0.0 0.0 0.0
Vector Representation: (Mx, My, Mz)
Ch(V): 3.000 Chr(P): 1.000 Chi(P): 0.000 Chr(T): 3.000 Chi(T): 0.000

SYMM_K(2): y+1/2,x+1/2,-z : 2 (x, x, 0) -> h16
Atoms: 1
Phase: 0.2500
Vector: 0.0-1.0 1.0
Vector Representation: (My, Mx,-Mz)
Ch(V): -1.000 Chr(P): 0.000 Chi(P): -1.000 Chr(T): -0.000 Chi(T): 1.000

SYMM_K(3): x,y,-z : m (x, y, 0) -> h28
Atoms: 1
Phase: 0.5000
Vector: 0.0 0.0 1.0
Vector Representation: (-Mx,-My, Mz)
Ch(V): -1.000 Chr(P): -1.000 Chi(P): -0.000 Chr(T): 1.000 Chi(T): 0.000

SYMM_K(4): y+1/2,x+1/2,z : m (x, x, z) -> h37
Atoms: 1
Phase: -0.2500
Vector: 0.0-1.0 0.0
Vector Representation: (-My,-Mx,-Mz)
Ch(V): -1.000 Chr(P): 0.000 Chi(P): 1.000 Chr(T): -0.000 Chi(T): -1.000

=> Decomposition of the Magnetic/Mechanic representation:

-> Characters of GAMMA and IRreps:

GAMMA G(1) G(2) G(3) G(4)
3.0 0.0 -0.0 1.0 1.0 0.0 -0.0-1.0

Irep_k(1) G(1) G(2) G(3) G(4)
1.0 0.0 0.0 1.0 1.0 0.0 0.0 1.0

Irep_k(2) G(1) G(2) G(3) G(4)

1.0 0.0 0.0 1.0 -1.0 0.0 -0.0-1.0

Irep_k(3) G(1) G(2) G(3) G(4)
1.0 0.0 -0.0-1.0 1.0 0.0 -0.0-1.0

Irep_k(4) G(1) G(2) G(3) G(4)
1.0 0.0 -0.0-1.0 -1.0 0.0 0.0 1.0

-> GAMMA(Magnetic): 1 Irep_k(1) + 1 Irep_k(2) + 1 Irep_k(3)

=> Decomposition of the Permutational Representation:

-> GAMMA(Permutation): 1 Irep_k(4)

=> Exchange multiplets:

Representation Irep_k(4) x Axial: 1 Irep_k(1) + 1 Irep_k(2) + 1 Irep_k(3)

General information relating the calculated basis functions with the magnetic structure
---

The fundamental hypothesis of the representational analysis is that the vectorial Fourier coefficients are LINEAR COMBINATIONS of Basis Functions, in a simplified form: Sk(j) = Sum{n}{C(n).BsV(n,j)}
The index 'j' labels the sublatices (j=1,2,...na) of the current site: Tm12_1
The simplified notation for C(n) used below, is given by the symbols: u,v,w,p,q ....(may be complex!)
The Fourier coefficients are written as: Sk(j) = u BsV(1,j)+ v BsV(2,j)+ w BsV(3,j)+ p BsV(4,j)+ q BsV(5,j)+ ...
The atomic components of the basis functions BsV(n,j) are 3D constant vectors (may be complex) written as row matrices
BsV(n,j) represents the basis vector 'n' attached to the atom 'j'
BsV(n,1:na) represents the basis vectors 'n' of the atoms 1 up to na (row of na 3D-vectors)
The magnetic moments should be calculated from the Fourier coefficients using the general formula:

m(L,j) = Sum{k}{ Sk(j) exp[-2pi.i.k.R(L)] }

or for a single pair (k,-k)

m(L,j) = Sk(j) exp{-2pi.i.k.R(L)} + Sk*(j) exp{2pi.i.k.R(L)}

Where R(L) is the LATTICE translation giving the vector position of the cell labelled 'L': R(L) = L1 a + L2 b + L3 c

If the lattice is CENTRED the expression of R(L) contains also fractional indices (L1,L2,L3)
The components of m(L,j), Sk(j) and BsV(n,j) are given with respect to a frame with unit vectors along a,b,c

We consider only the propagation vector pair (k,-k) with k = (0.25000, 0.25000, 0.50000)

=> Atomic components of the BASIS FUNCTIONS using PROJECTION OPERATORS:
Calculation for SITE number: 2
(Only non-null functions are written)

++
=> Basis functions of Representation IRrep(1) of dimension 1 contained 1 times in GAMMA
++

SYMM x,y,z
Atoms: Tm12_1
BsV(1, 1: 1):Re (1 -1 0)

----- The Fourier coefficients are LINEAR COMBINATIONS of Basis Functions: coefficients u,v,w,p,q ....(may be complex!)

The general expressions of the Fourier coefficients Sk(j) of the atoms non-related
by lattice translations are the following:

SYMM x,y,z Atom: Tm12_1 0.8259 0.3259 0.5000
Sk(1): (u,-u,0)

++
=> Basis functions of Representation IRrep(2) of dimension 1 contained 1 times in GAMMA
++

SYMM x,y,z
Atoms: Tm12_1
BsV(1, 1: 1):Re (0 0 1)

----- The Fourier coefficients are LINEAR COMBINATIONS of Basis Functions: coefficients u,v,w,p,q ....(may be complex!)

The general expressions of the Fourier coefficients Sk(j) of the atoms non-related
by lattice translations are the following:

SYMM x,y,z Atom: Tm12_1 0.8259 0.3259 0.5000
Sk(1): (0,0,u)

++
=> Basis functions of Representation IRrep(3) of dimension 1 contained 1 times in GAMMA
++

SYMM x,y,z
Atoms: Tm12_1
BsV(1, 1: 1):Re (1 1 0)

----- The Fourier coefficients are LINEAR COMBINATIONS of Basis Functions: coefficients u,v,w,p,q ....(may be complex!)

The general expressions of the Fourier coefficients Sk(j) of the atoms non-related
by lattice translations are the following:

SYMM x,y,z Atom: Tm12_1 0.8259 0.3259 0.5000
Sk(1): (u,u,0)

CALCULATIONS FOR SITE : 3

```
================================================================================
     Sym.Op.     Atoms Numbers, phases and returning Vectors
    Vector Rep.    Character(V)    Character(Perm)(r,i)  ChM
================================================================================
 SYMM_K( 1): x,y,z                  :  1          ->  h1
     Atoms:        1            2
     Phase:      0.0000       0.0000
    Vector:    0.0 0.0 0.0    0.0 0.0 0.0
    Vector Representation: ( Mx, My, Mz)
    Ch(V):  3.000 Chr(P):  2.000 Chi(P):  0.000 Chr(T):  6.000 Chi(T):  0.000
--------------------------------------------------------------------------------
 SYMM_K( 2): y+1/2,x+1/2,-z            :  2 ( x, x, 0) -> h16
     Atoms:        2            1
     Phase:      0.5000       0.0000
    Vector:    0.0 0.0 1.0   -1.0-1.0 1.0
    Vector Representation: ( My, Mx,-Mz)
    Ch(V): -1.000 Chr(P):  0.000 Chi(P):  0.000 Chr(T):  0.000 Chi(T):  0.000
--------------------------------------------------------------------------------
 SYMM_K( 3): x,y,-z                 :  m ( x, y, 0) -> h28
     Atoms:        1            2
     Phase:      0.5000       0.5000
    Vector:    0.0 0.0 1.0    0.0 0.0 1.0
    Vector Representation: (-Mx,-My, Mz)
    Ch(V): -1.000 Chr(P): -2.000 Chi(P): -0.000 Chr(T):  2.000 Chi(T):  0.000
--------------------------------------------------------------------------------
 SYMM_K( 4): y+1/2,x+1/2,z              :  m ( x, x, z) -> h37
     Atoms:        2            1
     Phase:      0.0000      -0.5000
    Vector:    0.0 0.0 0.0   -1.0-1.0 0.0
    Vector Representation: (-My,-Mx,-Mz)
    Ch(V): -1.000 Chr(P):  0.000 Chi(P):  0.000 Chr(T):  0.000 Chi(T):  0.000
--------------------------------------------------------------------------------

 => Decomposition of the Magnetic/Mechanic representation:

 -> Characters of GAMMA and IRreps:

  GAMMA      G( 1)   G( 2)   G( 3)   G( 4)
         6.0 0.0  0.0 0.0  2.0 0.0  0.0 0.0

Irep_k( 1)   G( 1)   G( 2)   G( 3)   G( 4)
         1.0 0.0  0.0 1.0  1.0 0.0  0.0 1.0

Irep_k( 2)   G( 1)   G( 2)   G( 3)   G( 4)
         1.0 0.0  0.0 1.0 -1.0 0.0 -0.0-1.0

Irep_k( 3)   G( 1)   G( 2)   G( 3)   G( 4)
         1.0 0.0 -0.0-1.0  1.0 0.0 -0.0-1.0

Irep_k( 4)   G( 1)   G( 2)   G( 3)   G( 4)
         1.0 0.0 -0.0-1.0 -1.0 0.0  0.0 1.0

 -> GAMMA(Magnetic):   2 Irep_k( 1) + 1 Irep_k( 2) + 2 Irep_k( 3) + 1 Irep_k( 4)

--------------------------------------------------------------------------------
```

=> Decomposition of the Permutational Representation:

-> GAMMA(Permutation): 1 Irep_k(2) + 1 Irep_k(4)

=> Exchange multiplets:

Representation Irep_k(2) x Axial: 1 Irep_k(1) + 1 Irep_k(3) + 1 Irep_k(4)

Representation Irep_k(4) x Axial: 1 Irep_k(1) + 1 Irep_k(2) + 1 Irep_k(3)

General information relating the calculated basis functions with the magnetic structure

----

The fundamental hypothesis of the representational analysis is that the vectorial Fourier coefficients are LINEAR COMBINATIONS of Basis Functions, in a simplified form: Sk(j) = Sum{n}{C(n).BsV(n,j)}
The index 'j' labels the sublatices (j=1,2,...na) of the current site: Tm13_1 Tm13_2
The simplified notation for C(n) used below, is given by the symbols: u,v,w,p,q ....(may be complex!)
The Fourier coefficients are written as: Sk(j) = u BsV(1,j)+ v BsV(2,j)+ w BsV(3,j)+ p BsV(4,j)+ q BsV(5,j)+ ...
The atomic components of the basis functions BsV(n,j) are 3D constant vectors (may be complex) written as row matrices
BsV(n,j) represents the basis vector 'n' attached to the atom 'j'
BsV(n,1:na) represents the basis vectors 'n' of the atoms 1 up to na (row of na 3D-vectors)
The magnetic moments should be calculated from the Fourier coefficients using the general formula:

m(L,j) = Sum{k}{ Sk(j) exp[-2pi.i.k.R(L)] }

or for a single pair (k,-k)

m(L,j) = Sk(j) exp{-2pi.i.k.R(L)} + Sk*(j) exp{2pi.i.k.R(L)}

Where R(L) is the LATTICE translation giving the vector position of the cell labelled 'L': R(L) = L1 a + L2 b + L3 c

If the lattice is CENTRED the expression of R(L) contains also fractional indices (L1,L2,L3)
The components of m(L,j), Sk(j) and BsV(n,j) are given with respect to a frame with unit vectors along a,b,c

We consider only the propagation vector pair (k,-k) with k = (0.25000, 0.25000, 0.50000)

=> Atomic components of the BASIS FUNCTIONS using PROJECTION OPERATORS:
Calculation for SITE number: 3
(Only non-null functions are written)

++
=> Basis functions of Representation IRrep(1) of dimension 1 contained 2 times in GAMMA
++

```
        SYMM  x,y,z   y+1/2,x+1/2,-z+1
        Atoms:     Tm13_1         Tm13_2
BsV( 1, 1: 2):Re (   1   0   0) (   0   0   0)
              Im (   0   0   0) (   0   1   0)
```

BsV(2, 1: 2):Re (0 1 0) (0 0 0)
Im (0 0 0) (1 0 0)

----- The Fourier coefficients are LINEAR COMBINATIONS of Basis Functions: coefficients u,v,w,p,q ....(may be complex!)

The general expressions of the Fourier coefficients Sk(j) of the atoms non-related by lattice translations are the following:

SYMM x,y,z Atom: Tm13_1 0.3259 0.1741 0.5000
Sk(1): (u,v,0)

SYMM y+1/2,x+1/2,-z+1 Atom: Tm13_2 0.6741 0.8259 0.5000
Sk(2): i.(v,u,0)

++
=> Basis functions of Representation IRrep(2) of dimension 1 contained 1 times in GAMMA
++

SYMM x,y,z y+1/2,x+1/2,-z+1
Atoms: Tm13_1 Tm13_2
BsV(1, 1: 2):Re (0 0 1) (0 0 0)
Im (0 0 0) (0 0 -1)

----- The Fourier coefficients are LINEAR COMBINATIONS of Basis Functions: coefficients u,v,w,p,q ....(may be complex!)

The general expressions of the Fourier coefficients Sk(j) of the atoms non-related by lattice translations are the following:

SYMM x,y,z Atom: Tm13_1 0.3259 0.1741 0.5000
Sk(1): (0,0,u)

SYMM y+1/2,x+1/2,-z+1 Atom: Tm13_2 0.6741 0.8259 0.5000
Sk(2): i.(0,0,-u)

++
=> Basis functions of Representation IRrep(3) of dimension 1 contained 2 times in GAMMA
++

SYMM x,y,z y+1/2,x+1/2,-z+1
Atoms: Tm13_1 Tm13_2
BsV(1, 1: 2):Re (1 0 0) (0 0 0)
Im (0 0 0) (0 -1 0)
BsV(2, 1: 2):Re (0 1 0) (0 0 0)
Im (0 0 0) (-1 0 0)

----- The Fourier coefficients are LINEAR COMBINATIONS of Basis Functions: coefficients u,v,w,p,q ....(may be complex!)

The general expressions of the Fourier coefficients Sk(j) of the atoms non-related by lattice translations are the following:

SYMM x,y,z Atom: Tm13_1 0.3259 0.1741 0.5000

Sk(1): (u,v,0)

SYMM y+1/2,x+1/2,-z+1 Atom: Tm13_2 0.6741 0.8259 0.5000
Sk(2): i.(-v,-u,0)

++
=> Basis functions of Representation IRrep(4) of dimension 1 contained 1 times in GAMMA
++

SYMM x,y,z y+1/2,x+1/2,-z+1
Atoms: Tm13_1 Tm13_2
BsV(1, 1: 2):Re (0 0 1) (0 0 0)
Im (0 0 0) (0 0 1)

----- The Fourier coefficients are LINEAR COMBINATIONS of Basis Functions: coefficients u,v,w,p,q ....(may be complex!)

The general expressions of the Fourier coefficients Sk(j) of the atoms non-related
by lattice translations are the following:

SYMM x,y,z Atom: Tm13_1 0.3259 0.1741 0.5000
Sk(1): (0,0,u)

SYMM y+1/2,x+1/2,-z+1 Atom: Tm13_2 0.6741 0.8259 0.5000
Sk(2): i.(0,0,u)

---

2. Symmetry analysis for the *4h* Wyckoff site and $\boldsymbol{k}_1''' = \left[-\frac{1}{4}, \frac{1}{4}, -\frac{1}{2}\right]$

```
 ++++++++++++++++++++++++++++++++++++++++++++++++++++++
 +++ PROGRAM:BasIreps (Version 4.10, November 2012)+++
 +++              (JRC- ILL)              +++
 ++++++++++++++++++++++++++++++++++++++++++++++++++++++

 The calculation of the IRREPS of the little group is based in
 the procedure of ZAK provided within the program KAREP
 E. Hovestreydt, I. Aroyo et al, J.Appl.Cryst. 25, 544 (1992)
 Program based in CrysFML (Crystallographic Fortran-95 Modules Library)
 BasIreps -> (Version 4.10, November 2012), ILL-Juan Rodriguez-Carvajal

=> Title:Test of new BASIREPS
=> Symbol of the space group: P 4/m b m
=> The given space group P 4/m b m is standard, IT generators will be used
=> List of space group generators:  -x,-y,z; -y,x,z; -x+1/2,y+1/2,-z; -x,-y,-z
=> Propagation vector:  -0.2500  0.2500 -0.5000
=> BZ-point labelled as  G
=> The representations of Gk will be calculated



      Information on Space Group:
      ---------------------------

=>   Number of Space group: 127
=>  Hermann-Mauguin Symbol: P 4/m b m
=>           Hall Symbol: -P 4 2ab
=>          Setting Type: Generated from explicit IT generators
=>         Crystal System: Tetragonal
=>            Laue Class: 4/mmm
=>           Point Group: 4/mmm
=>        Bravais Lattice: P
=>         Lattice Symbol: tP
=>  Reduced Number of S.O.:   8
=>    General multiplicity:  16
=>         Centrosymmetry: Centric (-1 at origin)
=>  Generators (exc. -1&L):   3
=>        Asymmetric unit:  0.000 <= x <=  0.500
                            0.000 <= y <=  0.500
                            0.000 <= z <=  0.500
=> Centring vectors:  0


=> List of all Symmetry Operators and Symmetry Symbols

=> SYMM(  1): x,y,z                    Symbol: 1
=> SYMM(  2): -x,-y,z                  Symbol: 2 0,0,z
=> SYMM(  3): -y,x,z                   Symbol: 4+ 0,0,z
=> SYMM(  4): -x+1/2,y+1/2,-z          Symbol: 2 (0,1/2,0) 1/4,y,0
=> SYMM(  5): y,-x,z                   Symbol: 4- 0,0,z
=> SYMM(  6): x+1/2,-y+1/2,-z          Symbol: 2 (1/2,0,0) x,1/4,0
=> SYMM(  7): -y+1/2,-x+1/2,-z         Symbol: 2 x,-x+1/2,0
=> SYMM(  8): y+1/2,x+1/2,-z           Symbol: 2 (1/2,1/2,0) x,x,0
```

=> SYMM(9): -x,-y,-z Symbol: -1 0,0,0
=> SYMM(10): x,y,-z Symbol: m x,y,0
=> SYMM(11): y,-x,-z Symbol: -4+ 0,0,z; 0,0,0
=> SYMM(12): x+1/2,-y+1/2,z Symbol: a x,1/4,z
=> SYMM(13): -y,x,-z Symbol: -4- 0,0,z; 0,0,0
=> SYMM(14): -x+1/2,y+1/2,z Symbol: b 1/4,y,z
=> SYMM(15): y+1/2,x+1/2,z Symbol: n (1/2,1/2,0) x,x,z
=> SYMM(16): -y+1/2,-x+1/2,z Symbol: m x,-x+1/2,z

=> Special Wyckoff Positions for P 4/m b m

Multp	Site	Representative Coordinates (centring translations excluded)
8	k	x,x+1/2,z -x,-x+1/2,z -x+1/2,x,z -x+1/2,x,-z x+1/2,-x,z x+1/2,-x,-z -x,-x+1/2,-z x,x+1/2,-z
8	j	x,y,1/2 -x,-y,1/2 -y,x,1/2 -x+1/2,y+1/2,1/2 y,-x,1/2 x+1/2,-y+1/2,1/2 -y+1/2,-x+1/2,1/2 y+1/2,x+1/2,1/2
8	i	x,y,0 -x,-y,0 -y,x,0 -x+1/2,y+1/2,0 y,-x,0 x+1/2,-y+1/2,0 -y+1/2,-x+1/2,0 y+1/2,x+1/2,0
4	h	x,x+1/2,1/2 -x,-x+1/2,1/2 -x+1/2,x,1/2 x+1/2,-x,1/2
4	g	x,x+1/2,0 -x,-x+1/2,0 -x+1/2,x,0 x+1/2,-x,0
4	f	0,1/2,z 1/2,0,z 1/2,0,-z 0,1/2,-z
4	e	0,0,z 1/2,1/2,-z 0,0,-z 1/2,1/2,z
2	d	0,1/2,0 1/2,0,0
2	c	0,1/2,1/2 1/2,0,1/2
2	b	0,0,1/2 1/2,1/2,1/2
2	a	0,0,0 1/2,1/2,0

=> Number of generators of space group: 4

GEN(1): -x,-y,z
GEN(2): -y,x,z
GEN(3): -x+1/2,y+1/2,-z
GEN(4): -x,-y,-z

TRANSLATIONAL COSET REPRESENTATIVES OF SPACE GROUP: P 4/m b m

Num	Symmetry-Element	Eqv. Positions
(1)	1	x,y,z

```
(  2)   2 0,0,z                      -x,-y,z
(  3)   4+ 0,0,z                      -y,x,z
(  4)   2 (0,1/2,0) 1/4,y,0              y,-x,z
(  5)   4- 0,0,z                      -x+1/2,y+1/2,-z
(  6)   2 (1/2,0,0) x,1/4,0              x+1/2,-y+1/2,-z
(  7)   2 x,-x+1/2,0                   y+1/2,x+1/2,-z
(  8)   2 (1/2,1/2,0) x,x,0              -y+1/2,-x+1/2,-z
(  9)   -1 0,0,0                      -x,-y,-z
( 10)   m x,y,0                        x,y,-z
( 11)   -4+ 0,0,z; 0,0,0                 y,-x,-z
( 12)   a x,1/4,z                      -y,x,-z
( 13)   -4- 0,0,z; 0,0,0                 x-1/2,-y-1/2,z
( 14)   b 1/4,y,z                      -x-1/2,y-1/2,z
( 15)   n (1/2,1/2,0) x,x,z              -y-1/2,-x-1/2,z
( 16)   m x,-x+1/2,z                   y-1/2,x-1/2,z


=> The lattice symbol is tP


 The conventional k-vector is
  -0.25000     0.25000    -0.50000

THE GENERATORS OF THE LITTLE GROUP OF BRILLOUIN ZONE POINT  G

The little group can be generated from the following 2 elements:-

 => GENk(1): -y+1/2,-x+1/2,-z
 => GENk(2): x,y,-z

REPRESENTATIVE ELEMENTS OF THE LITTLE GROUP OF BRILLOUIN ZONE POINT  G

 Operator of Gk Number( 1): x,y,z
 Operator of Gk Number( 2): -y+1/2,-x+1/2,-z
 Operator of Gk Number( 3): x,y,-z
 Operator of Gk Number( 4): -y+1/2,-x+1/2,z

------------------------------------------------------------
=> Number of elements of G_k:   4
=> Number of irreducible representations of G_k:   4
=> Dimensions:  1 1 1 1

=> Symmetry elements of G_k and irreps:
   Symmetry elements reduced to the standard form (positive translations < 1)
   The matrices of IRreps have been multiplied by the appropriate phase factor

-> SYMM_K( 1):  x,y,z                :  1          ->  h1         Int. symbol: 1
   Phase factor for correcting input data:  0.0000
   Matrix of IRrep( 1):
                1
   Matrix of IRrep( 2):
                1
   Matrix of IRrep( 3):
                1
   Matrix of IRrep( 4):
                1
-> SYMM_K( 2):  -y+1/2,-x+1/2,-z        :  2 ( x,-x, 0) -> h13         Int. symbol: 2 x,-x+1/2,0
```

Phase factor for correcting input data: 0.0000
Matrix of IRrep(1):
1
Matrix of IRrep(2):
1
Matrix of IRrep(3):
-1
Matrix of IRrep(4):
-1
-> SYMM_K(3): x,y,-z : m (x, y, 0) -> h28 Int. symbol: m x,y,0
Phase factor for correcting input data: 0.0000
Matrix of IRrep(1):
1
Matrix of IRrep(2):
-1
Matrix of IRrep(3):
1
Matrix of IRrep(4):
-1
-> SYMM_K(4): -y+1/2,-x+1/2,z : m (x,-x, z) -> h40 Int. symbol: m x,-x+1/2,z
Phase factor for correcting input data: 0.0000
Matrix of IRrep(1):
1
Matrix of IRrep(2):
-1
Matrix of IRrep(3):
-1
Matrix of IRrep(4):
1

==========
Writing of Irreps matrices in symbolic form: Module:Phase (fractions of 2pi)
Numeric values of symbols a,b,c,d, ... are given at the end of the table
==========

In this section the translations associated to Seitz symbols are simplified as
1/2 1/3 2/3 1/4 3/4 1/6 5/6 1/8 3/8 5/8 7/8
p q r s t u v w x y z

The rotational part of Seitz symbols contains information about the orientation as defined in Kovalev. The international symbols may be truncated (for format reasons) in the table below. The complete international symbols can be found in the previous list.

Ireps Symmetry operators ->
v 1 2 x,-x+1/2,0 m x,y,0 m x,-x+1/2,z
v {1|000} {2_x-x0|pp0} {m_xy0|000} {m_x-xz|pp0}
v Symm(1) Symm(2) Symm(3) Symm(4)

IRrep(1): 1 1 1 1

IRrep(2): 1 1 -1 -1

IRrep(3): 1 -1 1 -1

IRrep(4): 1 -1 -1 1

List of constants and phase factors defined in the above table

---

The propagation vector is k=(-0.25000, 0.25000,-0.50000)

=> Alternative evaluation of the propagation vector group.
The ordering of the symmetry operators may be different
than the sequence numbering given above

PROPAGATION VECTOR GROUP INFORMATION

==========

=> The input propagation vector is: K=(-0.2500 0.2500 -0.5000)
=> K .. IS NOT .. equivalent to -K
=> The operators following the k-vectors constitute the co-set decomposition G[Gk]
The list of equivalent k-vectors are also given on the right of operators.
=> The star of K is formed by the following 4 vectors:

k_1 = (-0.2500 0.2500 -0.5000) Op: (1) x,y,z
Op: (7) -y+1/2,-x+1/2,-z -> (-0.2500 0.2500 0.5000)
Op: (10) x,y,-z -> (-0.2500 0.2500 0.5000)
Op: (16) -y+1/2,-x+1/2,z -> (-0.2500 0.2500 -0.5000)

Eqv. -K: k_2 = (0.2500 -0.2500 -0.5000) Op: (2) -x,-y,z
Op: (8) y+1/2,x+1/2,-z -> (0.2500 -0.2500 0.5000)
Op: (9) -x,-y,-z -> (0.2500 -0.2500 0.5000)
Op: (15) y+1/2,x+1/2,z -> (0.2500 -0.2500 -0.5000)

k_3 = (0.2500 0.2500 -0.5000) Op: (3) -y,x,z
Op: (4) -x+1/2,y+1/2,-z -> (0.2500 0.2500 0.5000)
Op: (13) -y,x,-z -> (0.2500 0.2500 0.5000)
Op: (14) -x+1/2,y+1/2,z -> (0.2500 0.2500 -0.5000)

k_4 = (-0.2500 -0.2500 -0.5000) Op: (5) y,-x,z
Op: (6) x+1/2,-y+1/2,-z -> (-0.2500 -0.2500 0.5000)
Op: (11) y,-x,-z -> (-0.2500 -0.2500 0.5000)
Op: (12) x+1/2,-y+1/2,z -> (-0.2500 -0.2500 -0.5000)

=> G_k has the following symmetry operators:

1 SYMM(1) = x,y,z
2 SYMM(7) = -y+1/2,-x+1/2,-z
3 SYMM(10) = x,y,-z
4 SYMM(16) = -y+1/2,-x+1/2,z

DATA ABOUT ATOMS

```
    ================

  -> The atom site: Tm1   is split in  3 orbits
  -> The total number of sites has been increased consequently

 => No. of sites:    3

 => Calculation for axial vectors

 => List of atoms within a primitive unit cell:
            X      Y      Z         for site:  1
 -> Tm11_1 :   0.1741  0.6741  0.5000  : (x,y,z)
 -> Tm11_2 :   0.8259  0.3259  0.5000  : (-y+1/2,-x+1/2,-z) + (1,0,1)
            X      Y      Z         for site:  2
 -> Tm12_1 :   0.3259  0.1741  0.5000  : (x,y,z)
            X      Y      Z         for site:  3
 -> Tm13_1 :   0.6741  0.8259  0.5000  : (x,y,z)


    CALCULATIONS FOR SITE : 1

 ================================================================================
      Sym.Op.     Atoms Numbers, phases and returning Vectors
     Vector Rep.    Character(V)    Character(Perm)(r,i)  ChM
 ================================================================================
  SYMM_K( 1): x,y,z                    :   1          ->  h1
      Atoms:         1             2
      Phase:       0.0000         0.0000
     Vector:     0.0 0.0 0.0     0.0 0.0 0.0
     Vector Representation: ( Mx, My, Mz)
     Ch(V):  3.000 Chr(P):  2.000 Chi(P):  0.000 Chr(T):  6.000 Chi(T):  0.000
 --------------------------------------------------------------------------------
  SYMM_K( 2): -y+1/2,-x+1/2,-z             :   2 ( x,-x, 0) -> h13
      Atoms:         2             1
      Phase:      -0.7500        -0.2500
     Vector:     1.0 0.0 1.0     0.0 1.0 1.0
     Vector Representation: (-My,-Mx,-Mz)
     Ch(V): -1.000 Chr(P):  0.000 Chi(P):  0.000 Chr(T):  0.000 Chi(T):  0.000
 --------------------------------------------------------------------------------
  SYMM_K( 3): x,y,-z                   :   m ( x, y, 0) -> h28
      Atoms:         1             2
      Phase:      -0.5000        -0.5000
     Vector:     0.0 0.0 1.0     0.0 0.0 1.0
     Vector Representation: (-Mx,-My, Mz)
     Ch(V): -1.000 Chr(P): -2.000 Chi(P):  0.000 Chr(T):  2.000 Chi(T): -0.000
 --------------------------------------------------------------------------------
  SYMM_K( 4): -y+1/2,-x+1/2,z              :   m ( x,-x, z) -> h40
      Atoms:         2             1
      Phase:      -0.2500         0.2500
     Vector:     1.0 0.0 0.0     0.0 1.0 0.0
     Vector Representation: ( My, Mx,-Mz)
     Ch(V): -1.000 Chr(P):  0.000 Chi(P):  0.000 Chr(T):  0.000 Chi(T):  0.000
 --------------------------------------------------------------------------------

 => Decomposition of the Magnetic/Mechanic representation:

 -> Characters of GAMMA and IRreps:
```

```
 GAMMA      G( 1)    G( 2)    G( 3)    G( 4)
        6.0 0.0  0.0 0.0  2.0-0.0  0.0 0.0

Irep_k( 1)    G( 1)    G( 2)    G( 3)    G( 4)
        1.0 0.0  1.0 0.0  1.0 0.0  1.0 0.0

Irep_k( 2)    G( 1)    G( 2)    G( 3)    G( 4)
        1.0 0.0  1.0 0.0 -1.0 0.0 -1.0 0.0

Irep_k( 3)    G( 1)    G( 2)    G( 3)    G( 4)
        1.0 0.0 -1.0 0.0  1.0 0.0 -1.0 0.0

Irep_k( 4)    G( 1)    G( 2)    G( 3)    G( 4)
        1.0 0.0 -1.0 0.0 -1.0 0.0  1.0 0.0

 -> GAMMA(Magnetic):   2 Irep_k( 1) + 1 Irep_k( 2) + 2 Irep_k( 3) + 1 Irep_k( 4)

-------------------------------------------------------------------------------

 => Decomposition of the Permutational Representation:

 -> GAMMA(Permutation):   1 Irep_k( 2) + 1 Irep_k( 4)

 => Exchange multiplets:

   Representation Irep_k( 2) x Axial:   1 Irep_k( 1) + 1 Irep_k( 3) + 1 Irep_k( 4)

   Representation Irep_k( 4) x Axial:   1 Irep_k( 1) + 1 Irep_k( 2) + 1 Irep_k( 3)

-------------------------------------------------------------------------------

 ------------------------------------------------------------------------------------------------------------------------
              General information relating the calculated basis functions with the magnetic structure
 ------------------------------------------------------------------------------------------------------------------------

     The fundamental hypothesis of the representational analysis is that the vectorial Fourier coefficients are
     LINEAR COMBINATIONS of Basis Functions, in a simplified form: Sk(j) = Sum{n}{C(n).BsV(n,j)}
     The index 'j' labels the sublatices (j=1,2,...na) of the current site: Tm11_1 Tm11_2
     The simplified notation for C(n) used below, is given by the symbols: u,v,w,p,q ....(may be complex!)
     The Fourier coefficients are written as: Sk(j) = u BsV(1,j)+ v BsV(2,j)+ w BsV(3,j)+ p BsV(4,j)+ q BsV(5,j)+ ...
     The atomic components of the basis functions BsV(n,j) are 3D constant vectors (may be complex) written as
row matrices
     BsV(n,j) represents the basis vector 'n' attached to the atom 'j'
     BsV(n,1:na) represents the basis vectors 'n' of the atoms 1 up to na (row of na 3D-vectors)
     The magnetic moments should be calculated from the Fourier coefficients using the general formula:

                          m(L,j) = Sum{k}{ Sk(j) exp[-2pi.i.k.R(L)] }

     or for a single pair (k,-k)

                          m(L,j) = Sk(j) exp{-2pi.i.k.R(L)} +  Sk*(j) exp{2pi.i.k.R(L)}

     Where R(L) is the LATTICE translation giving the vector position of the cell labelled 'L':  R(L) = L1 a + L2 b + L3
c

     If the lattice is CENTRED the expression of R(L) contains also fractional indices (L1,L2,L3)
```

The components of m(L,j), Sk(j) and BsV(n,j) are given with respect to a frame with unit vectors along a,b,c

We consider only the propagation vector pair (k,-k) with k = (-0.25000, 0.25000,-0.50000)

=> Atomic components of the BASIS FUNCTIONS using PROJECTION OPERATORS:
Calculation for SITE number: 1
(Only non-null functions are written)

++
=> Basis functions of Representation IRrep(1) of dimension 1 contained 2 times in GAMMA
++

SYMM x,y,z -y+3/2,-x+1/2,-z+1
Atoms: Tm11_1 Tm11_2
BsV(1, 1: 2):Re (1 0 0) (0 0 0)
Im (0 0 0) (0 1 0)
BsV(2, 1: 2):Re (0 1 0) (0 0 0)
Im (0 0 0) (1 0 0)

----- The Fourier coefficients are LINEAR COMBINATIONS of Basis Functions: coefficients u,v,w,p,q ....(may be complex!)

The general expressions of the Fourier coefficients Sk(j) of the atoms non-related
by lattice translations are the following:

SYMM x,y,z Atom: Tm11_1 0.1741 0.6741 0.5000
Sk(1): (u,v,0)

SYMM -y+3/2,-x+1/2,-z+1 Atom: Tm11_2 0.8259 0.3259 0.5000
Sk(2): i.(v,u,0)

++
=> Basis functions of Representation IRrep(2) of dimension 1 contained 1 times in GAMMA
++

SYMM x,y,z -y+3/2,-x+1/2,-z+1
Atoms: Tm11_1 Tm11_2
BsV(1, 1: 2):Re (0 0 1) (0 0 0)
Im (0 0 0) (0 0 1)

----- The Fourier coefficients are LINEAR COMBINATIONS of Basis Functions: coefficients u,v,w,p,q ....(may be complex!)

The general expressions of the Fourier coefficients Sk(j) of the atoms non-related
by lattice translations are the following:

SYMM x,y,z Atom: Tm11_1 0.1741 0.6741 0.5000
Sk(1): (0,0,u)

SYMM -y+3/2,-x+1/2,-z+1 Atom: Tm11_2 0.8259 0.3259 0.5000
Sk(2): i.(0,0,u)

```
 ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
=> Basis functions of Representation IRrep( 3) of dimension  1 contained 2 times in GAMMA
 ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

        SYMM  x,y,z   -y+3/2,-x+1/2,-z+1
        Atoms:     Tm11_1          Tm11_2
BsV( 1, 1: 2):Re (    1    0    0) (    0    0    0)
         Im (    0    0    0) (    0   -1    0)
BsV( 2, 1: 2):Re (    0    1    0) (    0    0    0)
         Im (    0    0    0) (   -1    0    0)
```

----- The Fourier coefficients are LINEAR COMBINATIONS of Basis Functions: coefficients u,v,w,p,q ....(may be complex!)

The general expressions of the Fourier coefficients Sk(j) of the atoms non-related by lattice translations are the following:

SYMM x,y,z Atom: Tm11_1 0.1741 0.6741 0.5000
Sk(1): (u,v,0)

SYMM -y+3/2,-x+1/2,-z+1 Atom: Tm11_2 0.8259 0.3259 0.5000
Sk(2): i.(-v,-u,0)

```
 ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
=> Basis functions of Representation IRrep( 4) of dimension  1 contained 1 times in GAMMA
 ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

        SYMM  x,y,z   -y+3/2,-x+1/2,-z+1
        Atoms:     Tm11_1          Tm11_2
BsV( 1, 1: 2):Re (    0    0    1) (    0    0    0)
         Im (    0    0    0) (    0    0   -1)
```

----- The Fourier coefficients are LINEAR COMBINATIONS of Basis Functions: coefficients u,v,w,p,q ....(may be complex!)

The general expressions of the Fourier coefficients Sk(j) of the atoms non-related by lattice translations are the following:

SYMM x,y,z Atom: Tm11_1 0.1741 0.6741 0.5000
Sk(1): (0,0,u)

SYMM -y+3/2,-x+1/2,-z+1 Atom: Tm11_2 0.8259 0.3259 0.5000
Sk(2): i.(0,0,-u)

CALCULATIONS FOR SITE : 2

```
==========================================================================
    Sym.Op.     Atoms Numbers, phases and returning Vectors
   Vector Rep.   Character(V)   Character(Perm)(r,i)  ChM
==========================================================================
SYMM_K( 1): x,y,z                 :  1         ->  h1
    Atoms:        1
    Phase:     0.0000
```

```
    Vector:     0.0 0.0 0.0
    Vector Representation: ( Mx, My, Mz)
    Ch(V):  3.000 Chr(P):  1.000 Chi(P):  0.000 Chr(T):  3.000 Chi(T):  0.000
-------------------------------------------------------------------------------
 SYMM_K( 2): -y+1/2,-x+1/2,-z             :  2 ( x,-x, 0) -> h13
     Atoms:         1
     Phase:     -0.5000
    Vector:     0.0 0.0 1.0
    Vector Representation: (-My,-Mx,-Mz)
    Ch(V): -1.000 Chr(P): -1.000 Chi(P):  0.000 Chr(T):  1.000 Chi(T): -0.000
-------------------------------------------------------------------------------
 SYMM_K( 3): x,y,-z                       :  m ( x, y, 0) -> h28
     Atoms:         1
     Phase:     -0.5000
    Vector:     0.0 0.0 1.0
    Vector Representation: (-Mx,-My, Mz)
    Ch(V): -1.000 Chr(P): -1.000 Chi(P):  0.000 Chr(T):  1.000 Chi(T): -0.000
-------------------------------------------------------------------------------
 SYMM_K( 4): -y+1/2,-x+1/2,z              :  m ( x,-x, z) -> h40
     Atoms:         1
     Phase:      0.0000
    Vector:     0.0 0.0 0.0
    Vector Representation: ( My, Mx,-Mz)
    Ch(V): -1.000 Chr(P):  1.000 Chi(P):  0.000 Chr(T): -1.000 Chi(T):  0.000
-------------------------------------------------------------------------------

 => Decomposition of the Magnetic/Mechanic representation:

 -> Characters of GAMMA and IRreps:

  GAMMA      G( 1)    G( 2)    G( 3)    G( 4)
         3.0 0.0  1.0-0.0  1.0-0.0 -1.0 0.0

Irep_k( 1)    G( 1)    G( 2)    G( 3)    G( 4)
         1.0 0.0  1.0 0.0  1.0 0.0  1.0 0.0

Irep_k( 2)    G( 1)    G( 2)    G( 3)    G( 4)
         1.0 0.0  1.0 0.0 -1.0 0.0 -1.0 0.0

Irep_k( 3)    G( 1)    G( 2)    G( 3)    G( 4)
         1.0 0.0 -1.0 0.0  1.0 0.0 -1.0 0.0

Irep_k( 4)    G( 1)    G( 2)    G( 3)    G( 4)
         1.0 0.0 -1.0 0.0 -1.0 0.0  1.0 0.0

 -> GAMMA(Magnetic):   1 Irep_k( 1) + 1 Irep_k( 2) + 1 Irep_k( 3)

-------------------------------------------------------------------------------

 => Decomposition of the Permutational Representation:

 -> GAMMA(Permutation):   1 Irep_k( 4)

 => Exchange multiplets:

   Representation Irep_k( 4) x Axial:   1 Irep_k( 1) + 1 Irep_k( 2) + 1 Irep_k( 3)
```

General information relating the calculated basis functions with the magnetic structure

----

The fundamental hypothesis of the representational analysis is that the vectorial Fourier coefficients are LINEAR COMBINATIONS of Basis Functions, in a simplified form: Sk(j) = Sum{n}{C(n).BsV(n,j)}
The index 'j' labels the sublatices (j=1,2,...na) of the current site: Tm12_1
The simplified notation for C(n) used below, is given by the symbols: u,v,w,p,q ....(may be complex!)
The Fourier coefficients are written as: Sk(j) = u BsV(1,j)+ v BsV(2,j)+ w BsV(3,j)+ p BsV(4,j)+ q BsV(5,j)+ ...
The atomic components of the basis functions BsV(n,j) are 3D constant vectors (may be complex) written as row matrices
BsV(n,j) represents the basis vector 'n' attached to the atom 'j'
BsV(n,1:na) represents the basis vectors 'n' of the atoms 1 up to na (row of na 3D-vectors)
The magnetic moments should be calculated from the Fourier coefficients using the general formula:

m(L,j) = Sum{k}{ Sk(j) exp[-2pi.i.k.R(L)] }

or for a single pair (k,-k)

m(L,j) = Sk(j) exp{-2pi.i.k.R(L)} + Sk*(j) exp{2pi.i.k.R(L)}

Where R(L) is the LATTICE translation giving the vector position of the cell labelled 'L': R(L) = L1 a + L2 b + L3 c

If the lattice is CENTRED the expression of R(L) contains also fractional indices (L1,L2,L3)
The components of m(L,j), Sk(j) and BsV(n,j) are given with respect to a frame with unit vectors along a,b,c

We consider only the propagation vector pair (k,-k) with k = (-0.25000, 0.25000,-0.50000)

=> Atomic components of the BASIS FUNCTIONS using PROJECTION OPERATORS:
Calculation for SITE number: 2
(Only non-null functions are written)

++
=> Basis functions of Representation IRrep(1) of dimension 1 contained 1 times in GAMMA
++

SYMM x,y,z
Atoms: Tm12_1
BsV(1, 1: 1):Re (1 1 0)

----- The Fourier coefficients are LINEAR COMBINATIONS of Basis Functions: coefficients u,v,w,p,q ....(may be complex!)

The general expressions of the Fourier coefficients Sk(j) of the atoms non-related
by lattice translations are the following:

SYMM x,y,z Atom: Tm12_1 0.3259 0.1741 0.5000
Sk(1): (u,u,0)

++

=> Basis functions of Representation IRrep(2) of dimension 1 contained 1 times in GAMMA
 ++

        SYMM x,y,z
        Atoms: Tm12_1
BsV(1, 1: 1):Re (0   0   1)

----- The Fourier coefficients are LINEAR COMBINATIONS of Basis Functions: coefficients u,v,w,p,q ....(may be complex!)

    The general expressions of the Fourier coefficients Sk(j) of the atoms non-related
    by lattice translations are the following:

    SYMM x,y,z   Atom: Tm12_1   0.3259 0.1741 0.5000
    Sk(1): (0,0,u)

 ++
=> Basis functions of Representation IRrep(3) of dimension 1 contained 1 times in GAMMA
 ++

        SYMM x,y,z
        Atoms: Tm12_1
BsV(1, 1: 1):Re (1   -1   0)

----- The Fourier coefficients are LINEAR COMBINATIONS of Basis Functions: coefficients u,v,w,p,q ....(may be complex!)

    The general expressions of the Fourier coefficients Sk(j) of the atoms non-related
    by lattice translations are the following:

    SYMM x,y,z   Atom: Tm12_1   0.3259 0.1741 0.5000
    Sk(1): (u,-u,0)

   CALCULATIONS FOR SITE : 3

===
    Sym.Op.   Atoms Numbers, phases and returning Vectors
   Vector Rep.   Character(V)   Character(Perm)(r,i) ChM
===
SYMM_K(1): x,y,z   : 1   -> h1
    Atoms: 1
    Phase: 0.0000
   Vector: 0.0 0.0 0.0
   Vector Representation: (Mx, My, Mz)
   Ch(V): 3.000 Chr(P): 1.000 Chi(P): 0.000 Chr(T): 3.000 Chi(T): 0.000

SYMM_K(2): -y+1/2,-x+1/2,-z   : 2 (x,-x, 0) -> h13
    Atoms: 1
    Phase: -0.5000
   Vector: 1.0 1.0 1.0
   Vector Representation: (-My,-Mx,-Mz)
   Ch(V): -1.000 Chr(P): -1.000 Chi(P): 0.000 Chr(T): 1.000 Chi(T): -0.000

```
 SYMM_K( 3): x,y,-z                    :   m ( x, y, 0) -> h28
      Atoms:         1
      Phase:      -0.5000
     Vector:     0.0 0.0 1.0
     Vector Representation: (-Mx,-My, Mz)
     Ch(V): -1.000 Chr(P): -1.000 Chi(P):  0.000 Chr(T):  1.000 Chi(T): -0.000
-------------------------------------------------------------------------------
 SYMM_K( 4): -y+1/2,-x+1/2,z           :   m ( x,-x, z) -> h40
      Atoms:         1
      Phase:       0.0000
     Vector:     1.0 1.0 0.0
     Vector Representation: ( My, Mx,-Mz)
     Ch(V): -1.000 Chr(P):  1.000 Chi(P):  0.000 Chr(T): -1.000 Chi(T):  0.000
-------------------------------------------------------------------------------

 => Decomposition of the Magnetic/Mechanic representation:

 -> Characters of GAMMA and IRreps:

  GAMMA      G( 1)    G( 2)    G( 3)    G( 4)
         3.0 0.0  1.0-0.0  1.0-0.0 -1.0 0.0

Irep_k( 1)    G( 1)    G( 2)    G( 3)    G( 4)
         1.0 0.0  1.0 0.0  1.0 0.0  1.0 0.0

Irep_k( 2)    G( 1)    G( 2)    G( 3)    G( 4)
         1.0 0.0  1.0 0.0 -1.0 0.0 -1.0 0.0

Irep_k( 3)    G( 1)    G( 2)    G( 3)    G( 4)
         1.0 0.0 -1.0 0.0  1.0 0.0 -1.0 0.0

Irep_k( 4)    G( 1)    G( 2)    G( 3)    G( 4)
         1.0 0.0 -1.0 0.0 -1.0 0.0  1.0 0.0

 -> GAMMA(Magnetic):   1 Irep_k( 1) + 1 Irep_k( 2) + 1 Irep_k( 3)

-------------------------------------------------------------------------------

 => Decomposition of the Permutational Representation:

 -> GAMMA(Permutation):   1 Irep_k( 4)

 => Exchange multiplets:

   Representation Irep_k( 4) x Axial:   1 Irep_k( 1) + 1 Irep_k( 2) + 1 Irep_k( 3)

-------------------------------------------------------------------------------

 ------------------------------------------------------------------------------------------------------------------------
              General information relating the calculated basis functions with the magnetic structure
 ------------------------------------------------------------------------------------------------------------------------

     The fundamental hypothesis of the representational analysis is that the vectorial Fourier coefficients are
     LINEAR COMBINATIONS of Basis Functions, in a simplified form: Sk(j) = Sum{n}{C(n).BsV(n,j)}
     The index 'j' labels the sublatices (j=1,2,...na) of the current site: Tm13_1
     The simplified notation for C(n) used below, is given by the symbols: u,v,w,p,q ....(may be complex!)
     The Fourier coefficients are written as: Sk(j) = u BsV(1,j)+ v BsV(2,j)+ w BsV(3,j)+ p BsV(4,j)+ q BsV(5,j)+ ...
```

The atomic components of the basis functions BsV(n,j) are 3D constant vectors (may be complex) written as row matrices

BsV(n,j) represents the basis vector 'n' attached to the atom 'j'

BsV(n,1:na) represents the basis vectors 'n' of the atoms 1 up to na (row of na 3D-vectors)

The magnetic moments should be calculated from the Fourier coefficients using the general formula:

$$m(L,j) = \mathrm{Sum}\{k\}\{ Sk(j) \exp[-2\pi i.k.R(L)] \}$$

or for a single pair (k,-k)

$$m(L,j) = Sk(j) \exp\{-2\pi i.k.R(L)\} + Sk^*(j) \exp\{2\pi i.k.R(L)\}$$

Where R(L) is the LATTICE translation giving the vector position of the cell labelled 'L': $R(L) = L1\ a + L2\ b + L3\ c$

If the lattice is CENTRED the expression of R(L) contains also fractional indices (L1,L2,L3)

The components of m(L,j), Sk(j) and BsV(n,j) are given with respect to a frame with unit vectors along a,b,c

We consider only the propagation vector pair (k,-k) with k = (-0.25000, 0.25000,-0.50000)

=> Atomic components of the BASIS FUNCTIONS using PROJECTION OPERATORS:
Calculation for SITE number: 3
(Only non-null functions are written)

++
=> Basis functions of Representation IRrep(1) of dimension 1 contained 1 times in GAMMA
++

SYMM x,y,z
Atoms: Tm13_1
BsV(1, 1: 1):Re (1 1 0)

----- The Fourier coefficients are LINEAR COMBINATIONS of Basis Functions: coefficients u,v,w,p,q ....(may be complex!)

The general expressions of the Fourier coefficients Sk(j) of the atoms non-related
by lattice translations are the following:

SYMM x,y,z Atom: Tm13_1 0.6741 0.8259 0.5000
Sk(1): (u,u,0)

++
=> Basis functions of Representation IRrep(2) of dimension 1 contained 1 times in GAMMA
++

SYMM x,y,z
Atoms: Tm13_1
BsV(1, 1: 1):Re (0 0 1)

----- The Fourier coefficients are LINEAR COMBINATIONS of Basis Functions: coefficients u,v,w,p,q ....(may be complex!)

The general expressions of the Fourier coefficients Sk(j) of the atoms non-related
by lattice translations are the following:

SYMM x,y,z Atom: Tm13_1 0.6741 0.8259 0.5000
Sk(1): (0,0,u)

++
=> Basis functions of Representation IRrep(3) of dimension 1 contained 1 times in GAMMA
++

SYMM x,y,z
Atoms: Tm13_1
BsV(1, 1: 1):Re (1 -1 0)

----- The Fourier coefficients are LINEAR COMBINATIONS of Basis Functions: coefficients u,v,w,p,q ....(may be complex!)

The general expressions of the Fourier coefficients Sk(j) of the atoms non-related
by lattice translations are the following:

SYMM x,y,z Atom: Tm13_1 0.6741 0.8259 0.5000
Sk(1): (u,-u,0)

---

3. Symmetry analysis for the *4h* Wyckoff site and $\boldsymbol{k_2} = \left[0.31, 0.31, \frac{1}{2}\right]$

```
 +++++++++++++++++++++++++++++++++++++++++++++++++++++++
 +++ PROGRAM:BasIreps (Version 4.10, November 2012)+++
 +++              (JRC- ILL)               +++
 +++++++++++++++++++++++++++++++++++++++++++++++++++++++

 The calculation of the IRREPS of the little group is based in
 the procedure of ZAK provided within the program KAREP
 E. Hovestreydt, I. Aroyo et al, J.Appl.Cryst. 25, 544 (1992)
 Program based in CrysFML (Crystallographic Fortran-95 Modules Library)
 BasIreps -> (Version 4.10, November 2012), ILL-Juan Rodriguez-Carvajal

=> Title:Test of new BASIREPS
=> Symbol of the space group: P 4/m b m
=> The given space group P 4/m b m is standard, IT generators will be used
=> List of space group generators:  -x,-y,z; -y,x,z; -x+1/2,y+1/2,-z; -x,-y,-z
=> Propagation vector:   0.3074  0.3074  0.5000
=> BZ-point labelled as  G
=> The representations of Gk will be calculated



      Information on Space Group:
      ---------------------------

=>   Number of Space group: 127
=>  Hermann-Mauguin Symbol: P 4/m b m
=>           Hall Symbol: -P 4 2ab
=>          Setting Type: Generated from explicit IT generators
=>         Crystal System: Tetragonal
=>            Laue Class: 4/mmm
=>           Point Group: 4/mmm
=>        Bravais Lattice: P
=>         Lattice Symbol: tP
=>  Reduced Number of S.O.:   8
=>    General multiplicity:  16
=>         Centrosymmetry: Centric (-1 at origin)
=>  Generators (exc. -1&L):   3
=>        Asymmetric unit:  0.000 <= x <=  0.500
                            0.000 <= y <=  0.500
                            0.000 <= z <=  0.500
=> Centring vectors:  0


=> List of all Symmetry Operators and Symmetry Symbols

=> SYMM(  1): x,y,z                    Symbol: 1
=> SYMM(  2): -x,-y,z                  Symbol: 2 0,0,z
=> SYMM(  3): -y,x,z                   Symbol: 4+ 0,0,z
=> SYMM(  4): -x+1/2,y+1/2,-z          Symbol: 2 (0,1/2,0) 1/4,y,0
=> SYMM(  5): y,-x,z                   Symbol: 4- 0,0,z
=> SYMM(  6): x+1/2,-y+1/2,-z          Symbol: 2 (1/2,0,0) x,1/4,0
=> SYMM(  7): -y+1/2,-x+1/2,-z         Symbol: 2 x,-x+1/2,0
=> SYMM(  8): y+1/2,x+1/2,-z           Symbol: 2 (1/2,1/2,0) x,x,0
```

=> SYMM(9): -x,-y,-z Symbol: -1 0,0,0
=> SYMM(10): x,y,-z Symbol: m x,y,0
=> SYMM(11): y,-x,-z Symbol: -4+ 0,0,z; 0,0,0
=> SYMM(12): x+1/2,-y+1/2,z Symbol: a x,1/4,z
=> SYMM(13): -y,x,-z Symbol: -4- 0,0,z; 0,0,0
=> SYMM(14): -x+1/2,y+1/2,z Symbol: b 1/4,y,z
=> SYMM(15): y+1/2,x+1/2,z Symbol: n (1/2,1/2,0) x,x,z
=> SYMM(16): -y+1/2,-x+1/2,z Symbol: m x,-x+1/2,z

=> Special Wyckoff Positions for P 4/m b m

Multp	Site	Representative Coordinates (centring translations excluded)
8	k	x,x+1/2,z -x,-x+1/2,z -x+1/2,x,z -x+1/2,x,-z x+1/2,-x,z x+1/2,-x,-z -x,-x+1/2,-z x,x+1/2,-z
8	j	x,y,1/2 -x,-y,1/2 -y,x,1/2 -x+1/2,y+1/2,1/2 y,-x,1/2 x+1/2,-y+1/2,1/2 -y+1/2,-x+1/2,1/2 y+1/2,x+1/2,1/2
8	i	x,y,0 -x,-y,0 -y,x,0 -x+1/2,y+1/2,0 y,-x,0 x+1/2,-y+1/2,0 -y+1/2,-x+1/2,0 y+1/2,x+1/2,0
4	h	x,x+1/2,1/2 -x,-x+1/2,1/2 -x+1/2,x,1/2 x+1/2,-x,1/2
4	g	x,x+1/2,0 -x,-x+1/2,0 -x+1/2,x,0 x+1/2,-x,0
4	f	0,1/2,z 1/2,0,z 1/2,0,-z 0,1/2,-z
4	e	0,0,z 1/2,1/2,-z 0,0,-z 1/2,1/2,z
2	d	0,1/2,0 1/2,0,0
2	c	0,1/2,1/2 1/2,0,1/2
2	b	0,0,1/2 1/2,1/2,1/2
2	a	0,0,0 1/2,1/2,0

=> Number of generators of space group: 4

GEN(1): -x,-y,z
GEN(2): -y,x,z
GEN(3): -x+1/2,y+1/2,-z
GEN(4): -x,-y,-z

TRANSLATIONAL COSET REPRESENTATIVES OF SPACE GROUP: P 4/m b m

Num	Symmetry-Element	Eqv. Positions
(1)	1	x,y,z

```
(  2)   2 0,0,z                    -x,-y,z
(  3)   4+ 0,0,z                    -y,x,z
(  4)   2 (0,1/2,0) 1/4,y,0            y,-x,z
(  5)   4- 0,0,z                    -x+1/2,y+1/2,-z
(  6)   2 (1/2,0,0) x,1/4,0            x+1/2,-y+1/2,-z
(  7)   2 x,-x+1/2,0                  y+1/2,x+1/2,-z
(  8)   2 (1/2,1/2,0) x,x,0            -y+1/2,-x+1/2,-z
(  9)   -1 0,0,0                    -x,-y,-z
( 10)   m x,y,0                     x,y,-z
( 11)   -4+ 0,0,z; 0,0,0               y,-x,-z
( 12)   a x,1/4,z                   -y,x,-z
( 13)   -4- 0,0,z; 0,0,0               x-1/2,-y-1/2,z
( 14)   b 1/4,y,z                   -x-1/2,y-1/2,z
( 15)   n (1/2,1/2,0) x,x,z            -y-1/2,-x-1/2,z
( 16)   m x,-x+1/2,z                  y-1/2,x-1/2,z


=> The lattice symbol is tP


 The conventional k-vector is
   0.30740     0.30740     0.50000

THE GENERATORS OF THE LITTLE GROUP OF BRILLOUIN ZONE POINT  G

The little group can be generated from the following 2 elements:-

 => GENk(1): y+1/2,x+1/2,-z
 => GENk(2): x,y,-z

REPRESENTATIVE ELEMENTS OF THE LITTLE GROUP OF BRILLOUIN ZONE POINT  G

 Operator of Gk Number( 1): x,y,z
 Operator of Gk Number( 2): y+1/2,x+1/2,-z
 Operator of Gk Number( 3): x,y,-z
 Operator of Gk Number( 4): y+1/2,x+1/2,z

------------------------------------------------------------
=> Number of elements of G_k:   4
=> Number of irreducible representations of G_k:   4
=> Dimensions:  1 1 1 1

=> Symmetry elements of G_k and irreps:
   Symmetry elements reduced to the standard form (positive translations < 1)
   The matrices of IRreps have been multiplied by the appropriate phase factor

-> SYMM_K( 1):  x,y,z                :  1         ->  h1         Int. symbol: 1
   Phase factor for correcting input data:  0.0000
   Matrix of IRrep( 1):
                1
   Matrix of IRrep( 2):
                1
   Matrix of IRrep( 3):
                1
   Matrix of IRrep( 4):
                1
-> SYMM_K( 2):  y+1/2,x+1/2,-z       :  2 ( x, x, 0) -> h16         Int. symbol: 2 (1/2,1/2,0) x,x,0
```

Phase factor for correcting input data: 0.0000
Matrix of IRrep(1):
-0.3529+0.9357i
Matrix of IRrep(2):
-0.3529+0.9357i
Matrix of IRrep(3):
0.3529-0.9357i
Matrix of IRrep(4):
0.3529-0.9357i
-> SYMM_K(3): x,y,-z : m (x, y, 0) -> h28 Int. symbol: m x,y,0
Phase factor for correcting input data: 0.0000
Matrix of IRrep(1):
1
Matrix of IRrep(2):
-1
Matrix of IRrep(3):
1
Matrix of IRrep(4):
-1
-> SYMM_K(4): y+1/2,x+1/2,z : m (x, x, z) -> h37 Int. symbol: n (1/2,1/2,0) x,x,z
Phase factor for correcting input data: 0.0000
Matrix of IRrep(1):
-0.3529+0.9357i
Matrix of IRrep(2):
0.3529-0.9357i
Matrix of IRrep(3):
0.3529-0.9357i
Matrix of IRrep(4):
-0.3529+0.9357i

==========
Writing of Irreps matrices in symbolic form: Module:Phase (fractions of 2pi)
Numeric values of symbols a,b,c,d, ... are given at the end of the table
==========

In this section the translations associated to Seitz symbols are simplified as
1/2 1/3 2/3 1/4 3/4 1/6 5/6 1/8 3/8 5/8 7/8
p q r s t u v w x y z

The rotational part of Seitz symbols contains information about the orientation as defined in Kovalev. The international symbols may be truncated (for format reasons) in the table below. The complete international symbols can be found in the previous list.

Ireps Symmetry operators ->
v 1 2 (1/2,1/2,0) m x,y,0 n (1/2,1/2,0)
v {1|000} {2_xx0|pp0} {m_xy0|000} {m_xxz|pp0}
v Symm(1) Symm(2) Symm(3) Symm(4)

IRrep(1): 1 a 1 a

IRrep(2): 1 a -1 -a

IRrep(3): 1 -a 1 -a

IRrep(4): 1 -a -1 a

List of constants and phase factors defined in the above table
---

The propagation vector is k=(0.30740, 0.30740, 0.50000)
Phase factor: a = exp{2.pi.i. 0.30740} = (-0.35289, 0.93567) Exponent(fraction 2pi) = 4/13
Phase factor: -a = exp{2.pi.i. 0.80740} = (0.35289,-0.93567) Exponent(fraction 2pi) = 0.8074

=> Alternative evaluation of the propagation vector group.
The ordering of the symmetry operators may be different
than the sequence numbering given above

PROPAGATION VECTOR GROUP INFORMATION
==========

=> The input propagation vector is: K=(0.3074 0.3074 0.5000)
=> K .. IS NOT .. equivalent to -K
=> The operators following the k-vectors constitute the co-set decomposition G[Gk]
The list of equivalent k-vectors are also given on the right of operators.
=> The star of K is formed by the following 4 vectors:

k_1 = (0.3074 0.3074 0.5000) Op: (1) x,y,z
Op: (8) y+1/2,x+1/2,-z -> (0.3074 0.3074 -0.5000)
Op: (10) x,y,-z -> (0.3074 0.3074 -0.5000)
Op: (15) y+1/2,x+1/2,z -> (0.3074 0.3074 0.5000)

Eqv. -K: k_2 = (-0.3074 -0.3074 0.5000) Op: (2) -x,-y,z
Op: (7) -y+1/2,-x+1/2,-z -> (-0.3074 -0.3074 -0.5000)
Op: (9) -x,-y,-z -> (-0.3074 -0.3074 -0.5000)
Op: (16) -y+1/2,-x+1/2,z -> (-0.3074 -0.3074 0.5000)

k_3 = (0.3074 -0.3074 0.5000) Op: (3) -y,x,z
Op: (6) x+1/2,-y+1/2,-z -> (0.3074 -0.3074 -0.5000)
Op: (12) x+1/2,-y+1/2,z -> (0.3074 -0.3074 0.5000)
Op: (13) -y,x,-z -> (0.3074 -0.3074 -0.5000)

k_4 = (-0.3074 0.3074 -0.5000) Op: (4) -x+1/2,y+1/2,-z
Op: (5) y,-x,z -> (-0.3074 0.3074 0.5000)
Op: (11) y,-x,-z -> (-0.3074 0.3074 -0.5000)
Op: (14) -x+1/2,y+1/2,z -> (-0.3074 0.3074 0.5000)

=> G_k has the following symmetry operators:

1 SYMM(1) = x,y,z
2 SYMM(8) = y+1/2,x+1/2,-z
3 SYMM(10) = x,y,-z
4 SYMM(15) = y+1/2,x+1/2,z

```
   DATA ABOUT ATOMS
   ================

 -> The atom site: Ho1   is split in  3 orbits
 -> The total number of sites has been increased consequently

=> No. of sites:    3

=> Calculation for axial vectors

=> List of atoms within a primitive unit cell:
           X      Y      Z         for site:  1
-> Ho11_1  :   0.1758  0.6758  0.5000  : (x,y,z)
           X      Y      Z         for site:  2
-> Ho12_1  :   0.8242  0.3242  0.5000  : (x,y,z)
           X      Y      Z         for site:  3
-> Ho13_1  :   0.3242  0.1758  0.5000  : (x,y,z)
-> Ho13_2  :   0.6758  0.8242  0.5000  : (y+1/2,x+1/2,-z) + (0,0,1)


   CALCULATIONS FOR SITE : 1

================================================================================
    Sym.Op.     Atoms Numbers, phases and returning Vectors
   Vector Rep.    Character(V)    Character(Perm)(r,i)  ChM
================================================================================
 SYMM_K( 1): x,y,z                    :  1          ->  h1
     Atoms:         1
     Phase:       0.0000
    Vector:     0.0 0.0 0.0
    Vector Representation: ( Mx, My, Mz)
    Ch(V):  3.000 Chr(P):  1.000 Chi(P):  0.000 Chr(T):  3.000 Chi(T):  0.000
--------------------------------------------------------------------------------
 SYMM_K( 2): y+1/2,x+1/2,-z           :  2 ( x, x, 0) -> h16
     Atoms:         1
     Phase:       0.1926
    Vector:    -1.0 0.0 1.0
    Vector Representation: ( My, Mx,-Mz)
    Ch(V): -1.000 Chr(P):  0.353 Chi(P): -0.936 Chr(T): -0.353 Chi(T):  0.936
--------------------------------------------------------------------------------
 SYMM_K( 3): x,y,-z                   :  m ( x, y, 0) -> h28
     Atoms:         1
     Phase:       0.5000
    Vector:     0.0 0.0 1.0
    Vector Representation: (-Mx,-My, Mz)
    Ch(V): -1.000 Chr(P): -1.000 Chi(P): -0.000 Chr(T):  1.000 Chi(T):  0.000
--------------------------------------------------------------------------------
 SYMM_K( 4): y+1/2,x+1/2,z            :  m ( x, x, z) -> h37
     Atoms:         1
     Phase:      -0.3074
    Vector:    -1.0 0.0 0.0
    Vector Representation: (-My,-Mx,-Mz)
    Ch(V): -1.000 Chr(P): -0.353 Chi(P):  0.936 Chr(T):  0.353 Chi(T): -0.936
--------------------------------------------------------------------------------

 => Decomposition of the Magnetic/Mechanic representation:
```

-> Characters of GAMMA and IRreps:

```
 GAMMA      G( 1)   G( 2)   G( 3)   G( 4)
        3.0 0.0 -0.4 0.9  1.0 0.0  0.4-0.9

Irep_k( 1)   G( 1)   G( 2)   G( 3)   G( 4)
        1.0 0.0 -0.4 0.9  1.0 0.0 -0.4 0.9

Irep_k( 2)   G( 1)   G( 2)   G( 3)   G( 4)
        1.0 0.0 -0.4 0.9 -1.0 0.0  0.4-0.9

Irep_k( 3)   G( 1)   G( 2)   G( 3)   G( 4)
        1.0 0.0  0.4-0.9  1.0 0.0  0.4-0.9

Irep_k( 4)   G( 1)   G( 2)   G( 3)   G( 4)
        1.0 0.0  0.4-0.9 -1.0 0.0 -0.4 0.9
```

-> GAMMA(Magnetic): 1 Irep_k(1) + 1 Irep_k(2) + 1 Irep_k(3)

=> Decomposition of the Permutational Representation:

-> GAMMA(Permutation): 1 Irep_k(4)

=> Exchange multiplets:

Representation Irep_k(4) x Axial: 1 Irep_k(1) + 1 Irep_k(2) + 1 Irep_k(3)

General information relating the calculated basis functions with the magnetic structure

---

The fundamental hypothesis of the representational analysis is that the vectorial Fourier coefficients are LINEAR COMBINATIONS of Basis Functions, in a simplified form: Sk(j) = Sum{n}{C(n).BsV(n,j)}
The index 'j' labels the sublatices (j=1,2,...na) of the current site: Ho11_1
The simplified notation for C(n) used below, is given by the symbols: u,v,w,p,q ....(may be complex!)
The Fourier coefficients are written as: Sk(j) = u BsV(1,j)+ v BsV(2,j)+ w BsV(3,j)+ p BsV(4,j)+ q BsV(5,j)+ ...
The atomic components of the basis functions BsV(n,j) are 3D constant vectors (may be complex) written as row matrices
BsV(n,j) represents the basis vector 'n' attached to the atom 'j'
BsV(n,1:na) represents the basis vectors 'n' of the atoms 1 up to na (row of na 3D-vectors)
The magnetic moments should be calculated from the Fourier coefficients using the general formula:

$$m(L,j) = \mathrm{Sum}\{k\}\{ Sk(j) \exp[-2\pi i.k.R(L)] \}$$

or for a single pair (k,-k)

$$m(L,j) = Sk(j) \exp\{-2\pi i.k.R(L)\} + Sk^*(j) \exp\{2\pi i.k.R(L)\}$$

Where R(L) is the LATTICE translation giving the vector position of the cell labelled 'L': R(L) = L1 a + L2 b + L3 c

If the lattice is CENTRED the expression of R(L) contains also fractional indices (L1,L2,L3)

The components of m(L,j), Sk(j) and BsV(n,j) are given with respect to a frame with unit vectors along a,b,c

We consider only the propagation vector pair (k,-k) with k = (0.30740, 0.30740, 0.50000)

=> Atomic components of the BASIS FUNCTIONS using PROJECTION OPERATORS:
Calculation for SITE number: 1
(Only non-null functions are written)

++
=> Basis functions of Representation IRrep(1) of dimension 1 contained 1 times in GAMMA
++

SYMM x,y,z
Atoms: Ho11_1
BsV(1, 1: 1):Re (1 -1 0)

----- The Fourier coefficients are LINEAR COMBINATIONS of Basis Functions: coefficients u,v,w,p,q ....(may be complex!)

The general expressions of the Fourier coefficients Sk(j) of the atoms non-related
by lattice translations are the following:

SYMM x,y,z Atom: Ho11_1 0.1758 0.6758 0.5000
Sk(1): (u,-u,0)

++
=> Basis functions of Representation IRrep(2) of dimension 1 contained 1 times in GAMMA
++

SYMM x,y,z
Atoms: Ho11_1
BsV(1, 1: 1):Re (0 0 1)

----- The Fourier coefficients are LINEAR COMBINATIONS of Basis Functions: coefficients u,v,w,p,q ....(may be complex!)

The general expressions of the Fourier coefficients Sk(j) of the atoms non-related
by lattice translations are the following:

SYMM x,y,z Atom: Ho11_1 0.1758 0.6758 0.5000
Sk(1): (0,0,u)

++
=> Basis functions of Representation IRrep(3) of dimension 1 contained 1 times in GAMMA
++

SYMM x,y,z
Atoms: Ho11_1
BsV(1, 1: 1):Re (1 1 0)

----- The Fourier coefficients are LINEAR COMBINATIONS of Basis Functions: coefficients u,v,w,p,q ....(may be complex!)

The general expressions of the Fourier coefficients Sk(j) of the atoms non-related by lattice translations are the following:

SYMM x,y,z Atom: Ho11_1 0.1758 0.6758 0.5000
Sk(1): (u,u,0)

CALCULATIONS FOR SITE : 2

==========

Sym.Op. Atoms Numbers, phases and returning Vectors
Vector Rep. Character(V) Character(Perm)(r,i) ChM

==========

SYMM_K(1): x,y,z : 1 -> h1
Atoms: 1
Phase: 0.0000
Vector: 0.0 0.0 0.0
Vector Representation: (Mx, My, Mz)
Ch(V): 3.000 Chr(P): 1.000 Chi(P): 0.000 Chr(T): 3.000 Chi(T): 0.000

SYMM_K(2): y+1/2,x+1/2,-z : 2 (x, x, 0) -> h16
Atoms: 1
Phase: 0.1926
Vector: 0.0-1.0 1.0
Vector Representation: (My, Mx,-Mz)
Ch(V): -1.000 Chr(P): 0.353 Chi(P): -0.936 Chr(T): -0.353 Chi(T): 0.936

SYMM_K(3): x,y,-z : m (x, y, 0) -> h28
Atoms: 1
Phase: 0.5000
Vector: 0.0 0.0 1.0
Vector Representation: (-Mx,-My, Mz)
Ch(V): -1.000 Chr(P): -1.000 Chi(P): -0.000 Chr(T): 1.000 Chi(T): 0.000

SYMM_K(4): y+1/2,x+1/2,z : m (x, x, z) -> h37
Atoms: 1
Phase: -0.3074
Vector: 0.0-1.0 0.0
Vector Representation: (-My,-Mx,-Mz)
Ch(V): -1.000 Chr(P): -0.353 Chi(P): 0.936 Chr(T): 0.353 Chi(T): -0.936

=> Decomposition of the Magnetic/Mechanic representation:

-> Characters of GAMMA and IRreps:

GAMMA G(1) G(2) G(3) G(4)
3.0 0.0 -0.4 0.9 1.0 0.0 0.4-0.9

Irep_k(1) G(1) G(2) G(3) G(4)
1.0 0.0 -0.4 0.9 1.0 0.0 -0.4 0.9

Irep_k(2) G(1) G(2) G(3) G(4)

```
        1.0 0.0 -0.4 0.9 -1.0 0.0  0.4-0.9

Irep_k( 3)    G( 1)    G( 2)    G( 3)    G( 4)
        1.0 0.0  0.4-0.9  1.0 0.0  0.4-0.9

Irep_k( 4)    G( 1)    G( 2)    G( 3)    G( 4)
        1.0 0.0  0.4-0.9 -1.0 0.0 -0.4 0.9

 -> GAMMA(Magnetic):   1 Irep_k( 1) + 1 Irep_k( 2) + 1 Irep_k( 3)

-------------------------------------------------------------------------------

 => Decomposition of the Permutational Representation:

 -> GAMMA(Permutation):   1 Irep_k( 4)

 => Exchange multiplets:

   Representation Irep_k( 4) x Axial:   1 Irep_k( 1) + 1 Irep_k( 2) + 1 Irep_k( 3)

-------------------------------------------------------------------------------

 ------------------------------------------------------------------------------------------------------------------------
                General information relating the calculated basis functions with the magnetic structure
 ------------------------------------------------------------------------------------------------------------------------

     The fundamental hypothesis of the representational analysis is that the vectorial Fourier coefficients are
     LINEAR COMBINATIONS of Basis Functions, in a simplified form: Sk(j) = Sum{n}{C(n).BsV(n,j)}
     The index 'j' labels the sublatices (j=1,2,...na) of the current site: Ho12_1
     The simplified notation for C(n) used below, is given by the symbols: u,v,w,p,q ....(may be complex!)
     The Fourier coefficients are written as: Sk(j) = u BsV(1,j)+ v BsV(2,j)+ w BsV(3,j)+ p BsV(4,j)+ q BsV(5,j)+ ...
     The atomic components of the basis functions BsV(n,j) are 3D constant vectors (may be complex) written as
row matrices
     BsV(n,j) represents the basis vector 'n' attached to the atom 'j'
     BsV(n,1:na) represents the basis vectors 'n' of the atoms 1 up to na (row of na 3D-vectors)
     The magnetic moments should be calculated from the Fourier coefficients using the general formula:

                        m(L,j) = Sum{k}{ Sk(j) exp[-2pi.i.k.R(L)] }

     or for a single pair (k,-k)

                        m(L,j) = Sk(j) exp{-2pi.i.k.R(L)} +  Sk*(j) exp{2pi.i.k.R(L)}

     Where R(L) is the LATTICE translation giving the vector position of the cell labelled 'L':  R(L) = L1 a + L2 b + L3
c

     If the lattice is CENTRED the expression of R(L) contains also fractional indices (L1,L2,L3)
     The components of m(L,j), Sk(j) and BsV(n,j) are given with respect to a frame with unit vectors along a,b,c

     We consider only the propagation vector pair (k,-k) with k = ( 0.30740, 0.30740, 0.50000)

-------------------------------------------------------------------------------

 => Atomic components of the BASIS FUNCTIONS using PROJECTION OPERATORS:
              Calculation for SITE number:  2
            (Only non-null functions are written)
```

++
=> Basis functions of Representation IRrep(1) of dimension 1 contained 1 times in GAMMA
++

SYMM x,y,z
Atoms: Ho12_1
BsV(1, 1: 1):Re (1 -1 0)

----- The Fourier coefficients are LINEAR COMBINATIONS of Basis Functions: coefficients u,v,w,p,q ....(may be complex!)

The general expressions of the Fourier coefficients Sk(j) of the atoms non-related
by lattice translations are the following:

SYMM x,y,z Atom: Ho12_1 0.8242 0.3242 0.5000
Sk(1): (u,-u,0)

++
=> Basis functions of Representation IRrep(2) of dimension 1 contained 1 times in GAMMA
++

SYMM x,y,z
Atoms: Ho12_1
BsV(1, 1: 1):Re (0 0 1)

----- The Fourier coefficients are LINEAR COMBINATIONS of Basis Functions: coefficients u,v,w,p,q ....(may be complex!)

The general expressions of the Fourier coefficients Sk(j) of the atoms non-related
by lattice translations are the following:

SYMM x,y,z Atom: Ho12_1 0.8242 0.3242 0.5000
Sk(1): (0,0,u)

++
=> Basis functions of Representation IRrep(3) of dimension 1 contained 1 times in GAMMA
++

SYMM x,y,z
Atoms: Ho12_1
BsV(1, 1: 1):Re (1 1 0)

----- The Fourier coefficients are LINEAR COMBINATIONS of Basis Functions: coefficients u,v,w,p,q ....(may be complex!)

The general expressions of the Fourier coefficients Sk(j) of the atoms non-related
by lattice translations are the following:

SYMM x,y,z Atom: Ho12_1 0.8242 0.3242 0.5000
Sk(1): (u,u,0)

```
   CALCULATIONS FOR SITE : 3

================================================================================
     Sym.Op.     Atoms Numbers, phases and returning Vectors
    Vector Rep.    Character(V)    Character(Perm)(r,i)  ChM
================================================================================
 SYMM_K( 1): x,y,z                  :  1          ->  h1
     Atoms:        1            2
     Phase:      0.0000       0.0000
    Vector:    0.0 0.0 0.0    0.0 0.0 0.0
    Vector Representation: ( Mx, My, Mz)
    Ch(V):  3.000 Chr(P):  2.000 Chi(P):  0.000 Chr(T):  6.000 Chi(T):  0.000
--------------------------------------------------------------------------------
 SYMM_K( 2): y+1/2,x+1/2,-z            :  2 ( x, x, 0) -> h16
     Atoms:        2            1
     Phase:      0.5000       -0.1148
    Vector:    0.0 0.0 1.0   -1.0-1.0 1.0
    Vector Representation: ( My, Mx,-Mz)
    Ch(V): -1.000 Chr(P):  0.000 Chi(P):  0.000 Chr(T):  0.000 Chi(T):  0.000
--------------------------------------------------------------------------------
 SYMM_K( 3): x,y,-z                 :  m ( x, y, 0) -> h28
     Atoms:        1            2
     Phase:      0.5000       0.5000
    Vector:    0.0 0.0 1.0    0.0 0.0 1.0
    Vector Representation: (-Mx,-My, Mz)
    Ch(V): -1.000 Chr(P): -2.000 Chi(P): -0.000 Chr(T):  2.000 Chi(T):  0.000
--------------------------------------------------------------------------------
 SYMM_K( 4): y+1/2,x+1/2,z              :  m ( x, x, z) -> h37
     Atoms:        2            1
     Phase:      0.0000       -0.6148
    Vector:    0.0 0.0 0.0   -1.0-1.0 0.0
    Vector Representation: (-My,-Mx,-Mz)
    Ch(V): -1.000 Chr(P):  0.000 Chi(P):  0.000 Chr(T):  0.000 Chi(T):  0.000
--------------------------------------------------------------------------------

 => Decomposition of the Magnetic/Mechanic representation:

 -> Characters of GAMMA and IRreps:

  GAMMA      G( 1)   G( 2)   G( 3)   G( 4)
        6.0 0.0  0.0 0.0  2.0 0.0  0.0 0.0

Irep_k( 1)   G( 1)   G( 2)   G( 3)   G( 4)
        1.0 0.0 -0.4 0.9  1.0 0.0 -0.4 0.9

Irep_k( 2)   G( 1)   G( 2)   G( 3)   G( 4)
        1.0 0.0 -0.4 0.9 -1.0 0.0  0.4-0.9

Irep_k( 3)   G( 1)   G( 2)   G( 3)   G( 4)
        1.0 0.0  0.4-0.9  1.0 0.0  0.4-0.9

Irep_k( 4)   G( 1)   G( 2)   G( 3)   G( 4)
        1.0 0.0  0.4-0.9 -1.0 0.0 -0.4 0.9

 -> GAMMA(Magnetic):   2 Irep_k( 1) + 1 Irep_k( 2) + 2 Irep_k( 3) + 1 Irep_k( 4)

--------------------------------------------------------------------------------
```

=> Decomposition of the Permutational Representation:

-> GAMMA(Permutation): 1 Irep_k(2) + 1 Irep_k(4)

=> Exchange multiplets:

Representation Irep_k(2) x Axial: 1 Irep_k(1) + 1 Irep_k(3) + 1 Irep_k(4)

Representation Irep_k(4) x Axial: 1 Irep_k(1) + 1 Irep_k(2) + 1 Irep_k(3)

General information relating the calculated basis functions with the magnetic structure

----

The fundamental hypothesis of the representational analysis is that the vectorial Fourier coefficients are LINEAR COMBINATIONS of Basis Functions, in a simplified form: Sk(j) = Sum{n}{C(n).BsV(n,j)}
The index 'j' labels the sublatices (j=1,2,...na) of the current site: Ho13_1 Ho13_2
The simplified notation for C(n) used below, is given by the symbols: u,v,w,p,q ....(may be complex!)
The Fourier coefficients are written as: Sk(j) = u BsV(1,j)+ v BsV(2,j)+ w BsV(3,j)+ p BsV(4,j)+ q BsV(5,j)+ ...
The atomic components of the basis functions BsV(n,j) are 3D constant vectors (may be complex) written as row matrices
BsV(n,j) represents the basis vector 'n' attached to the atom 'j'
BsV(n,1:na) represents the basis vectors 'n' of the atoms 1 up to na (row of na 3D-vectors)
The magnetic moments should be calculated from the Fourier coefficients using the general formula:

m(L,j) = Sum{k}{ Sk(j) exp[-2pi.i.k.R(L)] }

or for a single pair (k,-k)

m(L,j) = Sk(j) exp{-2pi.i.k.R(L)} + Sk*(j) exp{2pi.i.k.R(L)}

Where R(L) is the LATTICE translation giving the vector position of the cell labelled 'L': R(L) = L1 a + L2 b + L3 c

If the lattice is CENTRED the expression of R(L) contains also fractional indices (L1,L2,L3)
The components of m(L,j), Sk(j) and BsV(n,j) are given with respect to a frame with unit vectors along a,b,c

We consider only the propagation vector pair (k,-k) with k = (0.30740, 0.30740, 0.50000)

=> Atomic components of the BASIS FUNCTIONS using PROJECTION OPERATORS:
Calculation for SITE number: 3
(Only non-null functions are written)

+++
=> Basis functions of Representation IRrep(1) of dimension 1 contained 2 times in GAMMA
+++

```
      SYMM  x,y,z   y+1/2,x+1/2,-z+1
      Atoms:      Ho13_1           Ho13_2
BsV( 1, 1: 2):Re ( 1.00 0.00 0.00) ( 0.00 0.35 0.00)
       Im ( 0.00 0.00 0.00) ( 0.00 0.94 0.00)
```

BsV(2, 1: 2):Re (0.00 1.00 0.00) (0.35 0.00 0.00)
Im (0.00 0.00 0.00) (0.94 0.00 0.00)

----- The Fourier coefficients are LINEAR COMBINATIONS of Basis Functions: coefficients u,v,w,p,q ....(may be complex!)

The general expressions of the Fourier coefficients Sk(j) of the atoms non-related
by lattice translations are the following:

SYMM x,y,z Atom: Ho13_1 0.3242 0.1758 0.5000
Sk(1): (u,v,0)

SYMM y+1/2,x+1/2,-z+1 Atom: Ho13_2 0.6758 0.8242 0.5000
Sk(2): (r0+i.r1).(v,u,0) = (v,u,0) . exp{ 2.pi.i. 0.1926000}

Values of real constants r0,r1,...
r0 = 0.352887 r1 = 0.935666

To simplify the expressions of the Fourier vector coefficients Sk(j), check combinations of values by pairs
Usually these real constants are related to k-vector, they can constitute real and/or imaginary parts of exp{+/-2.pi.i.K.T },
being T the translation associated to a symmetry operator
In many simple cases r0=cos(2.pi.k.t) and r1=sin(2.pi.k.t), etc ...
Look for common factors and conjugation operations to further simplify the expressions

++
=> Basis functions of Representation IRrep(2) of dimension 1 contained 1 times in GAMMA
++

SYMM x,y,z y+1/2,x+1/2,-z+1
Atoms: Ho13_1 Ho13_2
BsV(1, 1: 2):Re (0.00 0.00 1.00) (0.00 0.00-0.35)
Im (0.00 0.00 0.00) (0.00 0.00-0.94)

----- The Fourier coefficients are LINEAR COMBINATIONS of Basis Functions: coefficients u,v,w,p,q ....(may be complex!)

The general expressions of the Fourier coefficients Sk(j) of the atoms non-related
by lattice translations are the following:

SYMM x,y,z Atom: Ho13_1 0.3242 0.1758 0.5000
Sk(1): (0,0,u)

SYMM y+1/2,x+1/2,-z+1 Atom: Ho13_2 0.6758 0.8242 0.5000
Sk(2): (r0+i.r1).(0,0,-u) = (0,0,-u) . exp{ 2.pi.i. 0.1925999}

Values of real constants r0,r1,...
r0 = 0.352887 r1 = 0.935666

To simplify the expressions of the Fourier vector coefficients Sk(j), check combinations of values by pairs
Usually these real constants are related to k-vector, they can constitute real and/or imaginary parts of exp{+/-2.pi.i.K.T },
being T the translation associated to a symmetry operator

In many simple cases r0=cos(2.pi.k.t) and r1=sin(2.pi.k.t), etc ...
Look for common factors and conjugation operations to further simplify the expressions

++
=> Basis functions of Representation IRrep(3) of dimension 1 contained 2 times in GAMMA
++

SYMM x,y,z y+1/2,x+1/2,-z+1
Atoms: Ho13_1 Ho13_2
BsV(1, 1: 2):Re (1.00 0.00 0.00) (0.00-0.35 0.00)
Im (0.00 0.00 0.00) (0.00-0.94 0.00)
BsV(2, 1: 2):Re (0.00 1.00 0.00) (-0.35 0.00 0.00)
Im (0.00 0.00 0.00) (-0.94 0.00 0.00)

----- The Fourier coefficients are LINEAR COMBINATIONS of Basis Functions: coefficients u,v,w,p,q ....(may be complex!)

The general expressions of the Fourier coefficients Sk(j) of the atoms non-related
by lattice translations are the following:

SYMM x,y,z Atom: Ho13_1 0.3242 0.1758 0.5000
Sk(1): (u,v,0)

SYMM y+1/2,x+1/2,-z+1 Atom: Ho13_2 0.6758 0.8242 0.5000
Sk(2): (r0+i.r1).(-v,-u,0) = (-v,-u,0) . exp{ 2.pi.i. 0.1926000}

Values of real constants r0,r1,...
r0 = 0.352887 r1 = 0.935666

To simplify the expressions of the Fourier vector coefficients Sk(j), check combinations of values by pairs
Usually these real constants are related to k-vector, they can constitute real and/or imaginary parts of exp{+/-2.pi.i.K.T },
being T the translation associated to a symmetry operator
In many simple cases r0=cos(2.pi.k.t) and r1=sin(2.pi.k.t), etc ...
Look for common factors and conjugation operations to further simplify the expressions

++
=> Basis functions of Representation IRrep(4) of dimension 1 contained 1 times in GAMMA
++

SYMM x,y,z y+1/2,x+1/2,-z+1
Atoms: Ho13_1 Ho13_2
BsV(1, 1: 2):Re (0.00 0.00 1.00) (0.00 0.00 0.35)
Im (0.00 0.00 0.00) (0.00 0.00 0.94)

----- The Fourier coefficients are LINEAR COMBINATIONS of Basis Functions: coefficients u,v,w,p,q ....(may be complex!)

The general expressions of the Fourier coefficients Sk(j) of the atoms non-related
by lattice translations are the following:

SYMM x,y,z Atom: Ho13_1 0.3242 0.1758 0.5000
Sk(1): (0,0,u)

SYMM y+1/2,x+1/2,-z+1 Atom: Ho13_2 0.6758 0.8242 0.5000
Sk(2): (r0+i.r1).(0,0,u) = (0,0,u) . exp{ 2.pi.i. 0.1926000}

Values of real constants r0,r1,...
r0 = 0.352887 r1 = 0.935666

To simplify the expressions of the Fourier vector coefficients Sk(j), check combinations of values by pairs
Usually these real constants are related to k-vector, they can constitute real and/or imaginary parts of exp{+/-2.pi.i.K.T },
being T the translation associated to a symmetry operator
In many simple cases r0=cos(2.pi.k.t) and r1=sin(2.pi.k.t), etc ...
Look for common factors and conjugation operations to further simplify the expressions
---

4. FP Studio input .fst files of magnetic structures

$TbNi_{1.78}In_2$, T = 1.6 K

```
BKG  0.996  0.996  0.996  1.000
CELL    7.3510    7.3510    3.6727   90.0000   90.0000   90.0000 COLOR  0.500  0.500  0.500  1.000 MULTIPLE
BOX  -0.150   4.150  -0.150   4.150  -1.150   1.150
ROTAX    22.166  0.72958 -0.68354  0.02193
SPACEG P 1
ATOM Tb1_1    Tb  0.17484  0.67484  0.50000 COLOR 1.000 0.000 0.000 1.000 RADIUS 1.120
ATOM Tb1_2    Tb  0.17484  0.67484  0.50000 COLOR 1.000 0.000 0.000 1.000 RADIUS 1.120
ATOM Tb3_1    Tb  0.32516  0.17484  0.50000 COLOR 1.000 1.000 0.000 1.000 RADIUS 1.120
ATOM Tb3_2    Tb  0.67484  0.82516  0.50000 COLOR 0.000 0.000 0.000 1.000 RADIUS 1.120
ATOM Tb4_1    Tb  0.82516  0.32516  0.50000 COLOR 0.000 0.650 0.270 1.000 RADIUS 1.120
ATOM Tb4_2    Tb  0.82516  0.32516  0.50000 COLOR 0.000 0.650 0.270 1.000 RADIUS 1.120
{
LATTICE P
K   0.2500  0.2500  0.5000
SYMM x,y,z
MSYM u,v,w,0.0
MATOM Tb1_1    Tb  0.17484  0.67484  0.50000 SCALE  0.60 GROUP
SKP   1  1    0.000    0.000   10.675    0.000    0.000    0.000    0.125 COLOR  1.000 0.000 0.000 1.000
MATOM Tb1_2    Tb  0.17484  0.67484  0.50000 SCALE  0.60 GROUP
SKP   1  1    0.000    0.000    0.000    0.000    0.000    0.000   -0.125 COLOR  1.000 0.000 0.000 1.000
MATOM Tb3_1    Tb  0.32516  0.17484  0.50000 SCALE  0.60 GROUP
SKP   1  1    0.000    0.000   10.675    0.000    0.000    0.000    0.375 COLOR  1.000 1.000 0.000 1.000
MATOM Tb3_2    Tb  0.67484  0.82516  0.50000 SCALE  0.60 GROUP
SKP   1  1    0.000    0.000    0.000    0.000    0.000  -10.675    0.375 COLOR  0.000 0.000 0.000 1.000
MATOM Tb4_1    Tb  0.82516  0.32516  0.50000 SCALE  0.60 GROUP
SKP   1  1    0.000    0.000  -10.675    0.000    0.000    0.000    0.375 COLOR  0.000 0.650 0.270 1.000
MATOM Tb4_2    Tb  0.82516  0.32516  0.50000 SCALE  0.60 GROUP
SKP   1  1    0.000    0.000    0.000    0.000    0.000    0.000    0.125 COLOR  0.000 0.650 0.270 1.000
}
```

$HoNi_{1.78}In_2$, T = 1.6 K

```
BKG  0.900  0.900  0.900  1.000
CELL    7.3195    7.3195    3.6055   90.0000   90.0000   90.0000 COLOR  0.500  0.500  0.500  1.000 MULTIPLE
BOX  -0.150   4.150  -0.150   4.150  -1.150   1.150
ROTAX    22.166  0.72958 -0.68354  0.02193
SPACEG P 1
ATOM Ho1_1    Ho  0.17579  0.67579  0.50000 COLOR 1.000 0.000 0.000 1.000 RADIUS 1.100
ATOM Ho1_2    Ho  0.17579  0.67579  0.50000 COLOR 1.000 0.000 0.000 1.000 RADIUS 1.100
ATOM Ho3_1    Ho  0.32421  0.17579  0.50000 COLOR 1.000 1.000 0.000 1.000 RADIUS 1.100
ATOM Ho3_2    Ho  0.67579  0.82421  0.50000 COLOR 0.000 0.000 0.000 1.000 RADIUS 1.100
ATOM Ho4_1    Ho  0.82421  0.32421  0.50000 COLOR 0.000 0.650 0.270 1.000 RADIUS 1.100
ATOM Ho4_2    Ho  0.82421  0.32421  0.50000 COLOR 0.000 0.650 0.270 1.000 RADIUS 1.100
{
LATTICE P
K   0.3074  0.3074  0.5000
SYMM x,y,z
MSYM u,v,w,0.0
MATOM Ho1_1    Ho  0.17579  0.67579  0.50000 SCALE  1.00 GROUP
SKP   1 1    0.000    0.000    7.930    0.000    0.000    0.000   -0.000 COLOR  1.000 0.000 0.000 1.000
MATOM Ho1_2    Ho  0.17579  0.67579  0.50000 SCALE  1.00 GROUP
SKP   1 1    0.000    0.000    0.000    0.000    0.000    0.000   -0.307 COLOR  1.000 0.000 0.000 1.000
MATOM Ho3_1    Ho  0.32421  0.17579  0.50000 SCALE  1.00 GROUP
SKP   1 1    0.000    0.000    7.930    0.000    0.000    0.000    0.241 COLOR  1.000 1.000 0.000 1.000
MATOM Ho3_2    Ho  0.67579  0.82421  0.50000 SCALE  1.00 GROUP
SKP   1 1    0.000    0.000   -2.799    0.000    0.000   -7.420    0.241 COLOR  0.000 0.000 0.000 1.000
MATOM Ho4_1    Ho  0.82421  0.32421  0.50000 SCALE  1.00 GROUP
SKP   1 1    0.000    0.000    7.930    0.000    0.000    0.000   -0.296 COLOR  0.000 0.650 0.270 1.000
MATOM Ho4_2    Ho  0.82421  0.32421  0.50000 SCALE  1.00 GROUP
SKP   1 1    0.000    0.000    0.000    0.000    0.000    0.000   -0.604 COLOR  0.000 0.650 0.270 1.000
}
```

$ErNi_{1.78}In_2$, T = 1.6 K

```
BKG  0.900  0.900  0.900  1.000
CELL    7.3005    7.3005    3.5911   90.0000   90.0000   90.0000 COLOR  0.500  0.500  0.500  1.000 MULTIPLE
BOX  -0.150   4.150  -0.150   4.150  -1.150   1.150
ROTAX    22.166  0.72958 -0.68354  0.02193
SPACEG P 1
ATOM Er1_1    Er  0.17381  0.67381  0.50000 COLOR 1.000 0.000 0.000 1.000 RADIUS 1.080
ATOM Er2_1    Er  0.67381  0.82619  0.50000 COLOR 0.000 0.000 0.000 1.000 RADIUS 1.080
ATOM Er3_1    Er  0.32619  0.17381  0.50000 COLOR 1.000 1.000 0.000 1.000 RADIUS 1.080
ATOM Er4_1    Er  0.82619  0.32619  0.50000 COLOR 0.000 0.650 0.270 1.000 RADIUS 1.080
{
LATTICE P
K   0.2500  0.2500  0.5000
K  -0.2500  0.2500 -0.5000
SYMM x,y,z
MSYM u,v,w,0.0
MATOM Er1_1    Er  0.17381  0.67381  0.50000 SCALE  0.60 GROUP
SKP   1 1    6.504   -6.504    0.000    0.000    0.000    0.000    0.125 COLOR  1.000 0.000 0.000 1.000
MATOM Er2_1    Er  0.67381  0.82619  0.50000 SCALE  0.60 GROUP
SKP   2 1   -6.504   -6.504    0.000    0.000    0.000    0.000    0.375 COLOR  0.000 0.000 0.000 1.000
MATOM Er3_1    Er  0.32619  0.17381  0.50000 SCALE  0.60 GROUP
SKP   2 1    6.504    6.504    0.000    0.000    0.000    0.000    0.125 COLOR  1.000 1.000 0.000 1.000
MATOM Er4_1    Er  0.82619  0.32619  0.50000 SCALE  0.60 GROUP
SKP   1 1   -6.504    6.504    0.000    0.000    0.000    0.000    0.375 COLOR  0.000 0.650 0.270 1.000
}
```

$TmNi_{1.78}In_2$, T = 1.6 K

```
BKG  0.996  0.996  0.996  1.000
CELL    7.2760    7.2760    3.5691   90.0000   90.0000   90.0000 COLOR  0.500  0.500  0.500  1.000 MULTIPLE
BOX  -0.150   4.150  -0.150   4.150  -1.150   1.150
ROTAX    22.166  0.72958 -0.68354  0.02193
SPACEG P 1
ATOM Tm1_1    Tm  0.17386  0.67386  0.50000 COLOR 1.000 0.000 0.000 1.000 RADIUS 1.070
ATOM Tm2_1    Tm  0.67386  0.82614  0.50000 COLOR 0.000 0.000 0.000 1.000 RADIUS 1.070
ATOM Tm3_1    Tm  0.32614  0.17386  0.50000 COLOR 1.000 1.000 0.000 1.000 RADIUS 1.070
ATOM Tm4_1    Tm  0.82614  0.32614  0.50000 COLOR 0.000 0.650 0.270 1.000 RADIUS 1.070
{
LATTICE P
K   0.2500  0.2500  0.5000
K  -0.2500  0.2500 -0.5000
SYMM x,y,z
MSYM u,v,w,0.0
MATOM Tm1_1    Tm  0.17386  0.67386  0.50000 SCALE  0.60 GROUP
SKP   1 1    6.086   -6.086    0.000    0.000    0.000    0.000    0.125 COLOR  1.000 0.000 0.000 1.000
MATOM Tm2_1    Tm  0.67386  0.82614  0.50000 SCALE  0.60 GROUP
SKP   2 1   -6.086   -6.086    0.000    0.000    0.000    0.000    0.375 COLOR  0.000 0.000 0.000 1.000
MATOM Tm3_1    Tm  0.32614  0.17386  0.50000 SCALE  0.60 GROUP
SKP   2 1    6.086    6.086    0.000    0.000    0.000    0.000    0.125 COLOR  1.000 1.000 0.000 1.000
MATOM Tm4_1    Tm  0.82614  0.32614  0.50000 SCALE  0.60 GROUP
SKP   1 1   -6.086    6.086    0.000    0.000    0.000    0.000    0.375 COLOR  0.000 0.650 0.270 1.000
}
```

5. Parts of FullProf input .pcr files regarding magnetic structures

$TbNi_{1.78}In_2$, T = 1.6 K

```
Tb2Ni1.78In
!
!Nat Dis Ang Pr1 Pr2 Pr3 Jbt Irf Isy Str Furth      ATZ    Nvk Npr More
  3   0   0 0.0 0.0 1.0   1  -1  -2   0   0      1133.480  -1   7   0
!
!
P -1                  <--Space group symbol for hkl generation
! Nsym   Cen  Laue Ireps N_Bas
    2     1     1    -1     2
! Real(0)-Imaginary(1) indicator for Ci
 0  0
!
SYMM x,y,z
BASR   0  0  1   0  0  1
BASI   0  0  0   0  0  0
SYMM y+1/2,x+1/2,-z+1
BASR   0  0  0   0  0  0
BASI   0  0  0   0  0 -1
!
!Atom   Typ  Mag Vek   X      Y      Z      Biso    Occ      C1      C2      C3
!    C4     C5     C6     C7     C8     C9     MagPh
Tb1    JTB3  1  0  0.17484 0.67484 0.50000 0.00000  1.00000  10.675   0.000   0.000
                0.00    0.00    0.00    0.00    0.00  111.00    0.00    0.00
   0.000   0.000   0.000   0.000   0.000   0.000  0.12500
    0.00    0.00    0.00    0.00    0.00    0.00    0.00
Tb3    JTB3  1  0  0.32516 0.17484 0.50000 0.00000  1.00000   0.000  10.675   0.000
                0.00    0.00    0.00    0.00    0.00    0.00  111.00    0.00
   0.000   0.000   0.000   0.000   0.000   0.000  0.37500
    0.00    0.00    0.00    0.00    0.00    0.00    0.00
Tb4    JTB3  1  0  0.82516 0.32516 0.50000 0.00000  1.00000 -10.675   0.000   0.000
                0.00    0.00    0.00    0.00    0.00 -111.00    0.00    0.00
   0.000   0.000   0.000   0.000   0.000   0.000  0.37500
    0.00    0.00    0.00    0.00    0.00    0.00    0.00
!-------> Profile Parameters for Pattern #  1
!  Scale      Shape1      Bov      Str1      Str2      Str3   Strain-Model
 78.863      0.00000   0.00000   0.00000   0.00000   0.00000      0
   0.00000     0.000     0.000     0.000     0.000     0.000
!      U         V         W         X         Y       GauSiz   LorSiz Size-Model
  1.508438  -1.079667   0.704022   0.000000   0.000000   0.000000   0.000000    0
    51.000    61.000    21.000     0.000     0.000     0.000     0.000
!    a         b         c       alpha      beta       gamma      #Cell Info
  7.350958   7.350964   3.672695  90.000000  90.000000  90.000000
  31.00000   31.00000   41.00000   0.00000   0.00000   0.00000
!  Pref1    Pref2     Asy1     Asy2     Asy3     Asy4     S_L      D_L
 1.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000
   0.00     0.00     0.00     0.00     0.00     0.00     0.00     0.00
! Propagation vectors:
  0.2500000   0.2500000   0.5000000         Propagation Vector  1
   0.000000    0.000000    0.000000
```

$HoNi_{1.78}In_2$, T = 1.6 K

```
Ho2Ni1.78In
!
!Nat Dis Ang Pr1 Pr2 Pr3 Jbt Irf Isy Str Furth      ATZ    Nvk Npr More
  3   0   0 0.0 0.0 1.0   1  -1  -2   0   0      1133.480  -1   7   0
!
!
P -1                 <--Space group symbol for hkl generation
! Nsym   Cen  Laue Ireps N_Bas
    2     1     1    -1     2
! Real(0)-Imaginary(1) indicator for Ci
 0  0
!
SYMM x,y,z
BASR   0  0  1   0  0  1
BASI   0  0  0   0  0  0
SYMM y+1/2,x+1/2,-z+1
BASR   0  0  0   0.0000  0.0000 -0.3529
BASI   0  0  0   0.0000  0.0000 -0.9357
!
!Atom   Typ  Mag Vek    X      Y      Z      Biso    Occ      C1      C2      C3
!    C4     C5     C6     C7     C8     C9     MagPh
Ho1    JHO3  1  0  0.17579 0.67579 0.50000 0.00000  1.00000   7.930   0.000   0.000
                0.00    0.00    0.00    0.00    0.00  101.00    0.00    0.00
    0.000   0.000   0.000   0.000   0.000   0.000  0.00000
     0.00    0.00    0.00    0.00    0.00    0.00     0.00
Ho3    JHO3  1  0  0.32421 0.17579 0.50000 0.00000  1.00000   0.000   7.930   0.000
                0.00    0.00    0.00    0.00    0.00    0.00  101.00    0.00
    0.000   0.000   0.000   0.000   0.000   0.000  0.24127
     0.00    0.00    0.00    0.00    0.00    0.00    91.00
Ho4    JHO3  1  0  0.82421 0.32421 0.50000 0.00000  1.00000   7.930   0.000   0.000
                0.00    0.00    0.00    0.00    0.00  101.00    0.00    0.00
    0.000   0.000   0.000   0.000   0.000   0.000 -0.29650
     0.00    0.00    0.00    0.00    0.00    0.00   111.00
!-------> Profile Parameters for Pattern #  1
!  Scale      Shape1      Bov      Str1      Str2      Str3   Strain-Model
 9.9668       0.00000   0.00000   0.60000   0.00000   0.00000       0
    0.00000     0.000     0.000     0.000     0.000     0.000
!      U         V         W         X         Y       GauSiz   LorSiz Size-Model
  1.505845  -2.498452   1.473595   1.095095   0.000000   0.000000   0.000000    0
    51.000     61.000     21.000     81.000      0.000      0.000      0.000
!    a         b         c        alpha      beta       gamma      #Cell Info
  7.319465   7.319464   3.605520  90.000000  90.000000  90.000000
  31.00000   31.00000   41.00000    0.00000    0.00000    0.00000
!  Pref1    Pref2      Asy1      Asy2      Asy3      Asy4      S_L      D_L
 0.98386  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000
    0.00     0.00     0.00     0.00     0.00     0.00     0.00     0.00
! Propagation vectors:
  0.3073780   0.3073780   0.5000000         Propagation Vector  1
  71.000000   71.000000    0.000000
```

$ErNi_{1.78}In_2$, T = 1.6 K

```
Er2Ni1.78In
!
!Nat Dis Ang Pr1 Pr2 Pr3 Jbt Irf Isy Str Furth      ATZ    Nvk Npr More
  4   0   0 0.0 0.0 1.0   1  -1  -2   0   0      1133.480  -2   7   0
!
!
P -1                 <--Space group symbol for hkl generation
! Nsym   Cen  Laue Ireps N_Bas
    1     1     1    -1     2
! Real(0)-Imaginary(1) indicator for Ci
 0  0
!
SYMM x,y,z
BASR   1 -1  0   1  1  0
BASI   0  0  0   0  0  0
!
!Atom   Typ  Mag Vek    X      Y      Z      Biso    Occ      C1      C2      C3
!    C4     C5     C6     C7     C8     C9     MagPh
Er1    JER3  1 -1  0.17381 0.67381 0.50000 0.00000  1.00000   6.504   0.000   0.000
              111.00  111.00    0.00    0.00    0.00   71.00    0.00    0.00
    0.000   0.000   0.000   0.000   0.000   0.000  0.12500
     0.00    0.00    0.00    0.00    0.00    0.00    0.00
Er2    JER3  1 -2  0.67381 0.82619 0.50000 0.00000  1.00000   0.000  -6.504   0.000
              111.00 -111.00    0.00    0.00    0.00    0.00  -71.00    0.00
    0.000   0.000   0.000   0.000   0.000   0.000  0.37500
     0.00    0.00    0.00    0.00    0.00    0.00    0.00
Er3    JER3  1 -2  0.32619 0.17381 0.50000 0.00000  1.00000   0.000   6.504   0.000
             -111.00  111.00    0.00    0.00    0.00    0.00   71.00    0.00
    0.000   0.000   0.000   0.000   0.000   0.000  0.12500
     0.00    0.00    0.00    0.00    0.00    0.00    0.00
Er4    JER3  1 -1  0.82619 0.32619 0.50000 0.00000  1.00000  -6.504   0.000   0.000
             -111.00 -111.00    0.00    0.00    0.00  -71.00    0.00    0.00
    0.000   0.000   0.000   0.000   0.000   0.000  0.37500
     0.00    0.00    0.00    0.00    0.00    0.00    0.00
!-------> Profile Parameters for Pattern #  1
!  Scale      Shape1      Bov      Str1      Str2      Str3   Strain-Model
  8.1893      0.00000   0.00000   0.00000   0.00000   0.00000      0
    0.00000     0.000     0.000     0.000     0.000     0.000
!      U         V         W         X         Y       GauSiz   LorSiz Size-Model
   2.890530  -3.129514   1.426328   0.000000   0.000000   0.000000   0.000000    0
     51.000    61.000    21.000     0.000     0.000     0.000     0.000
!    a         b         c       alpha      beta       gamma     #Cell Info
   7.300467   7.300467   3.591078  90.000000  90.000000  90.000000
   31.00000   31.00000   41.00000    0.00000    0.00000    0.00000
!  Pref1    Pref2     Asy1     Asy2     Asy3     Asy4     S_L     D_L
  1.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000
    0.00     0.00     0.00     0.00     0.00     0.00     0.00     0.00
! Propagation vectors:
   0.2500000   0.2500000   0.5000000         Propagation Vector  1
    0.000000    0.000000    0.000000
  -0.2500000   0.2500000  -0.5000000         Propagation Vector  2
    0.000000    0.000000    0.000000
```

$TmNi_{1.78}In_2$, T = 1.6 K

```
Tm2Ni1.78In
!
!Nat Dis Ang Pr1 Pr2 Pr3 Jbt Irf Isy Str Furth       ATZ    Nvk Npr More
  4   0   0 0.0 0.0 1.0   1  -1  -2   0   0      1133.480  -2   7   0
!
!
P -1                  <--Space group symbol for hkl generation
! Nsym   Cen  Laue Ireps N_Bas
    1     1     1    -1     2
! Real(0)-Imaginary(1) indicator for Ci
 0  0
!
SYMM x,y,z
BASR   1 -1  0   1  1  0
BASI   0  0  0   0  0  0
!
!Atom   Typ  Mag Vek    X      Y      Z      Biso    Occ      C1      C2      C3
!    C4     C5     C6     C7     C8     C9     MagPh
Tm1    JTM3  1 -1  0.17386 0.67386 0.50000 0.00000  1.00000   6.086   0.000   0.000
               0.00    0.00    0.00    0.00    0.00   21.00    0.00    0.00
    0.000   0.000   0.000   0.000   0.000   0.000  0.12500
     0.00    0.00    0.00    0.00    0.00    0.00     0.00
Tm2    JTM3  1 -2  0.67386 0.82614 0.50000 0.00000  1.00000   0.000  -6.086   0.000
               0.00    0.00    0.00    0.00    0.00    0.00  -21.00    0.00
    0.000   0.000   0.000   0.000   0.000   0.000  0.37500
     0.00    0.00    0.00    0.00    0.00    0.00     0.00
Tm3    JTM3  1 -2  0.32614 0.17386 0.50000 0.00000  1.00000   0.000   6.086   0.000
               0.00    0.00    0.00    0.00    0.00    0.00   21.00    0.00
    0.000   0.000   0.000   0.000   0.000   0.000  0.12500
     0.00    0.00    0.00    0.00    0.00    0.00     0.00
Tm4    JTM3  1 -1  0.82614 0.32614 0.50000 0.00000  1.00000  -6.086   0.000   0.000
               0.00    0.00    0.00    0.00    0.00  -21.00    0.00    0.00
    0.000   0.000   0.000   0.000   0.000   0.000  0.37500
     0.00    0.00    0.00    0.00    0.00    0.00     0.00
!-------> Profile Parameters for Pattern #  1
!  Scale      Shape1      Bov      Str1      Str2      Str3   Strain-Model
  48.509      0.00000   0.00000   0.00000   0.00000   0.00000      0
    0.00000     0.000     0.000     0.000     0.000     0.000
!      U         V         W         X         Y       GauSiz   LorSiz Size-Model
   2.554342  -2.351642   1.142267   0.000000   0.000000   0.000000   0.000000    0
     51.000    61.000    71.000     0.000     0.000     0.000     0.000
!    a         b         c       alpha      beta       gamma      #Cell Info
   7.275986   7.275986   3.569058  90.000000  90.000000  90.000000
   31.00000   31.00000   41.00000    0.00000    0.00000    0.00000
!  Pref1    Pref2     Asy1     Asy2     Asy3     Asy4     S_L      D_L
  1.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000
    0.00     0.00     0.00     0.00     0.00     0.00     0.00     0.00
! Propagation vectors:
   0.2500000   0.2500000   0.5000000         Propagation Vector  1
    0.000000    0.000000    0.000000
  -0.2500000   0.2500000  -0.5000000         Propagation Vector  2
    0.000000    0.000000    0.000000
```