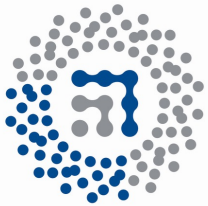


ZTF-FCT
Zientzia eta Teknologia Fakultatea
Facultad de Ciencia y Tecnología

eman ta zabal zazu

Universidad del País Vasco
Euskal Herriko Unibertsitatea

Magnetic symmetry groups vs. irreducible representations

J. Manuel Perez-Mato
Facultad de Ciencia y Tecnología
Universidad del País Vasco, UPV-EHU
BILBAO, SPAIN

Acta Cryst. (2024). B80, 370–376

feature articles

STRUCTURAL SCIENCE
CRYSTAL ENGINEERING
MATERIALS

ISSN 2052-5206

Magnetic space groups *versus* representation analysis in the investigation of magnetic structures: the happy end of a strained relationship

J. Rodriguez-Carvajal[a] and J. M. Perez-Mato[b]*

[a]Diffraction Group, Institut Laue-Langevin, 38054 Grenoble Cedex 9, France, and [b]Facultad de Ciencia y Tecnología, Universidad del País Vasco, UPV/EHU, Apartado 644, 48080 Bilbao, Spain. *Correspondence e-mail: jm.perezmato@gmail.com

Received 6 June 2024
Accepted 29 July 2024

Edited by V. Garlea, Oak Ridge National Laboratory, USA

This article is part of a focused issue on Magnetic Structures.

Keywords: magnetic space groups; representation analysis; magnetic structures; irreducible representations; mode decomposition.

In recent decades, sustained theoretical and software developments have clearly established that representation analysis and magnetic symmetry groups are complementary concepts that should be used together in the investigation and description of magnetic structures. Historically, they were considered alternative approaches, but currently, magnetic space groups and magnetic superspace groups can be routinely used together with representation analysis, aided by state-of-the-art software tools. After exploring the historical antagonism between these two approaches, we emphasize the significant advancements made in understanding and formally describing magnetic structures by embracing their combined use.

- Magnetic ordering is a symmetry break process

- We talk of a "distorted structure" and a "distortion".

- The paramagnetic structure is the "parent" structure and it has a higher symmetry: group-subgroup relation. (magnetic groups)

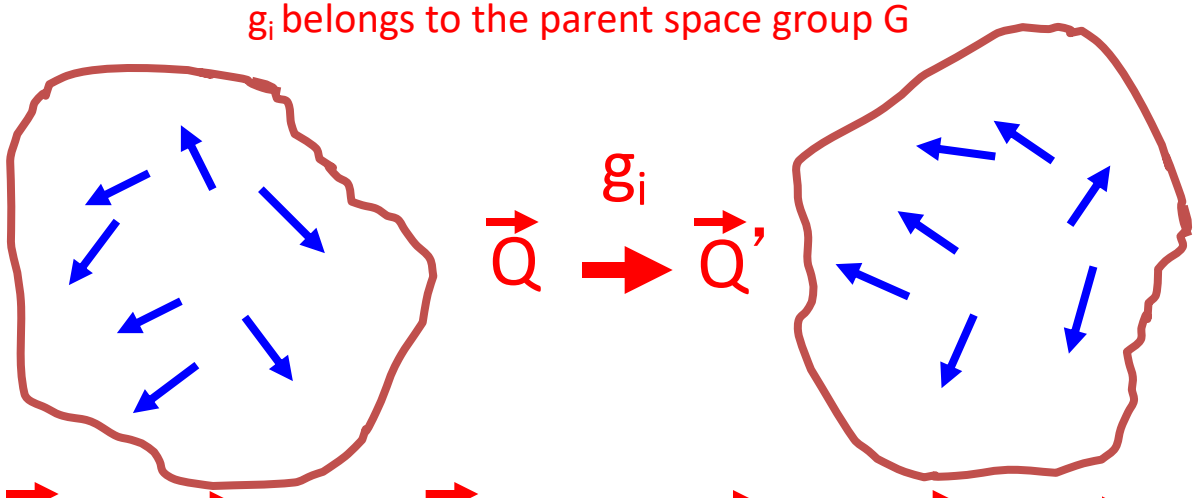
- a symmetry operation of the GRAY parent space group transforms in general the distorted structure into a different structure: a distorted structure with a different distortion (domain-related), except for the operations that are maintained in the MSG.

- **Relation with the original distortion?:**

- **The relation is described by a "REPRESENTATION" of the symmetry group of the paramagnetic phase: A matrix for each operation describes the corresponding transformation of the distortion.**

The Magnetic Representation: an arbitrary spin arrangement transforms according to a representation of the parent symmetry group

g_i belongs to the parent space group G



$\vec{Q} = Q_1\vec{s}_{1x}+Q_2\vec{s}_{1y} \ldots +Q_{3N}\vec{s}_{Nz}$

$\vec{Q}' = Q'_1\vec{s}_{1x}+Q'_2\vec{s}_{1y} \ldots + Q'_{3N}\vec{s}_{Nz}$

representation of G (matrices)

$T(g)\vec{Q} = \vec{Q}'$

$T(g)$: one nxn matrix for each operation g of G

n= 3N, N: total number of magnetic atoms

$\{\vec{s}_1,\ldots\ldots,\vec{s}_n\}$ orthonormal basis of spin modes

$T(g_1g_2) = T(g_1)\,T(g_2)$ Representation

The Magnetic Representation is in general ***reducible***:

$T(g)$: one nxn matrix for each operation g of **G** (parent space group)

$T(g_1 g_2) = T(g_1)\, T(g_2)$ Representation

invariant subspaces in the 3N-dim space

$$T(g) = \begin{bmatrix} [T_1(g)] & & & 0 \\ & [T_2(g)] & & \\ & & \ddots & \\ 0 & & & [T_n(g)] \end{bmatrix}$$

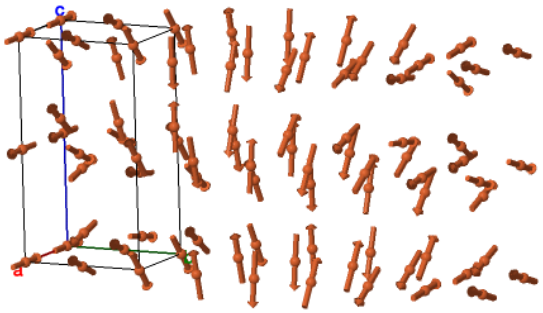
for all g

The magnetic representation is *reduced* to representations of smaller dimension:

$$T = T_1 + T_2 + \ldots + T_n$$

The Magnetic Representation is in general reducible:

First reduction: **WAVES**

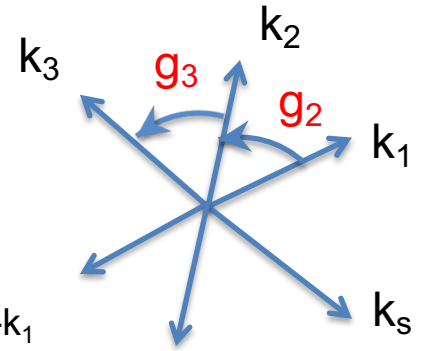


wave vector: k_1

n: number of magnetic atoms in the ***primitive*** unit cell

number of spin variables: 3n if $k_1 == -k_1$

6n if $k_1 \neq\neq -k_1$



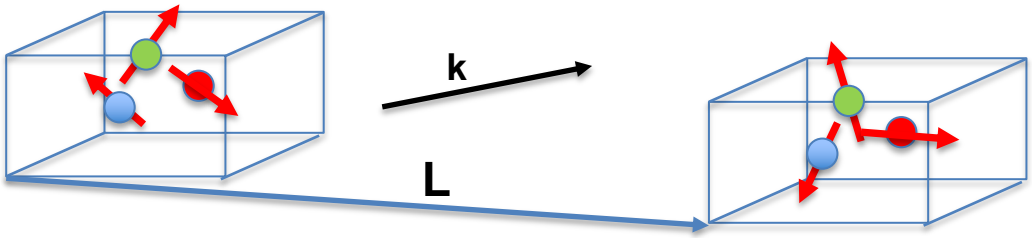
$*\mathbf{k_1} = \{\mathbf{k_1},\ldots,\mathbf{k_s}\}$ set of k-vectors related by the operations of G (star)

s: number of k-vectors in the star

A spin wave with wave vector k_1 transforms into waves with other wave vectors of its star…. Necessarily the set of wave vectors $*k_1$ "go together" in the reduced representation:

Dimension of $T_{*\mathbf{k1}}(g) = s*3n \times s*3n$

(if $-\mathbf{k_1}$ is not in the star $*\mathbf{k_1}$ this dimension is doubled)



The spin of each atom **i** in the primitive unit cell varies along the crystal according to a modulation wave with the propagation vector **k.**

Two alternative equivalent expressions for this modulation :

real vector (3 var.)

complex vector (6 var.)

$$\mathbf{m}^{(i)}(\mathbf{L}) = \mathbf{S}^{(i)}_{\mathbf{k}}\, e^{-i2\pi \mathbf{k}.\mathbf{L}} + \mathbf{S}^{(i)}_{-\mathbf{k}}\, e^{i2\pi \mathbf{k}.\mathbf{L}} \qquad \mathbf{S}^{(i)}_{-\mathbf{k}} = \mathbf{S}^{(i)}_{\mathbf{k}}{}^{*}$$

$$\mathbf{m}^{(i)}(\mathbf{L}) = \mathbf{m}^{(i)}_{c} \cos[2\pi(\mathbf{k}.\mathbf{L}+\mathbf{r}^{(i)})] + \mathbf{m}^{(i)}_{s} \sin[2\pi(\mathbf{k}.\mathbf{L}+\mathbf{r}^{(i)})]$$

atom position

6 degr. freedom per magnetic atoms in the prim. unit cell for {**k**,-**k**}

If **k == -k : k= k+G**

$$e^{-i2\pi \mathbf{k}.\mathbf{L}} = e^{i2\pi \mathbf{k}.\mathbf{L}} = \pm 1$$

$\mathbf{S}^{(i)}_{\mathbf{k}}$: real vector (3 var.)

3 degr. freedom per magnetic atoms in the prim. unit cell for a single **k**

The Magnetic Representation is in general reducible:

First reduction: **WAVES**

subspaces of arrangements with different sets of propagation vectors:

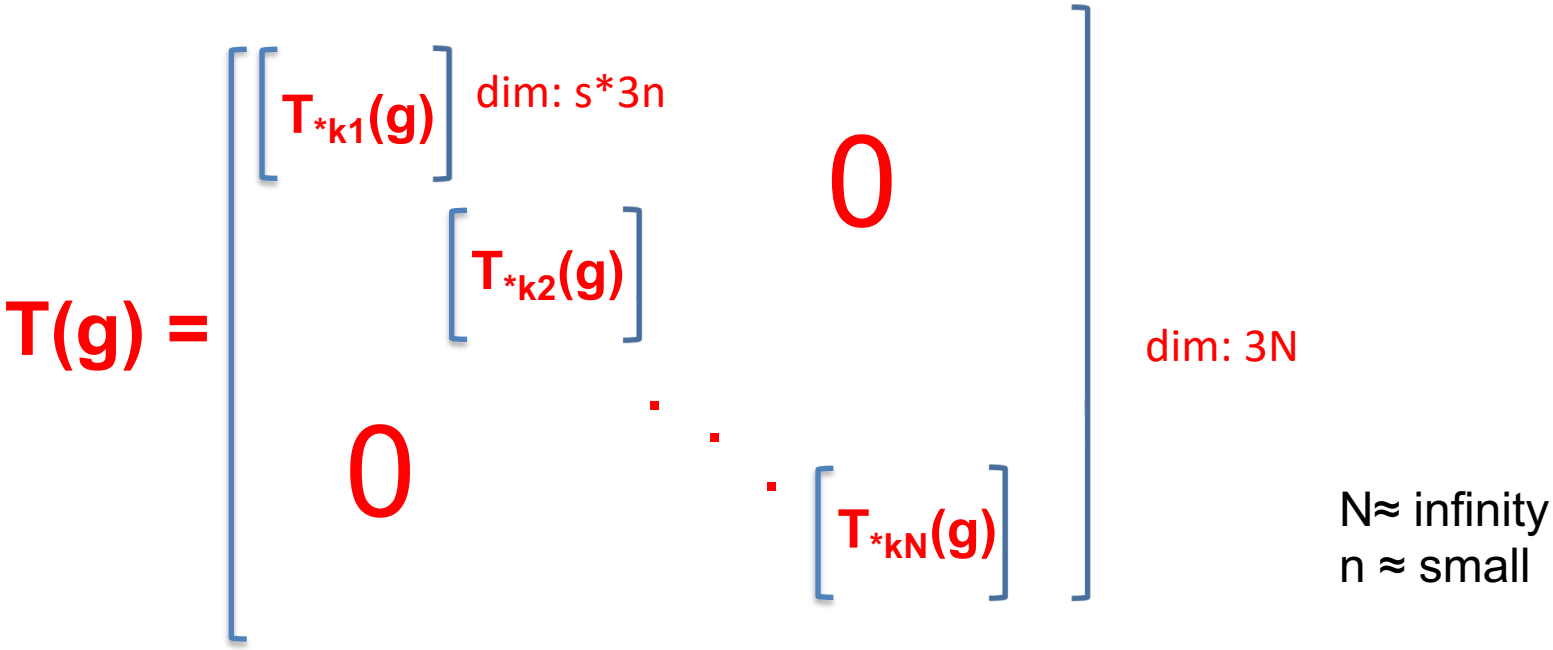
$$T(g) = \sum_{*\mathbf{k}} T_{*\mathbf{k}}(g)$$ **ALL *k within the BZ**

$*\mathbf{k} = \{\mathbf{k}_1,\ldots,\mathbf{k}_s\}$ set of k-vectors related by the operations of G (star)

Dimension of $T_{*\mathbf{k}}(g) = s*3n \times s*3n$

s: number of k-vectors in the star

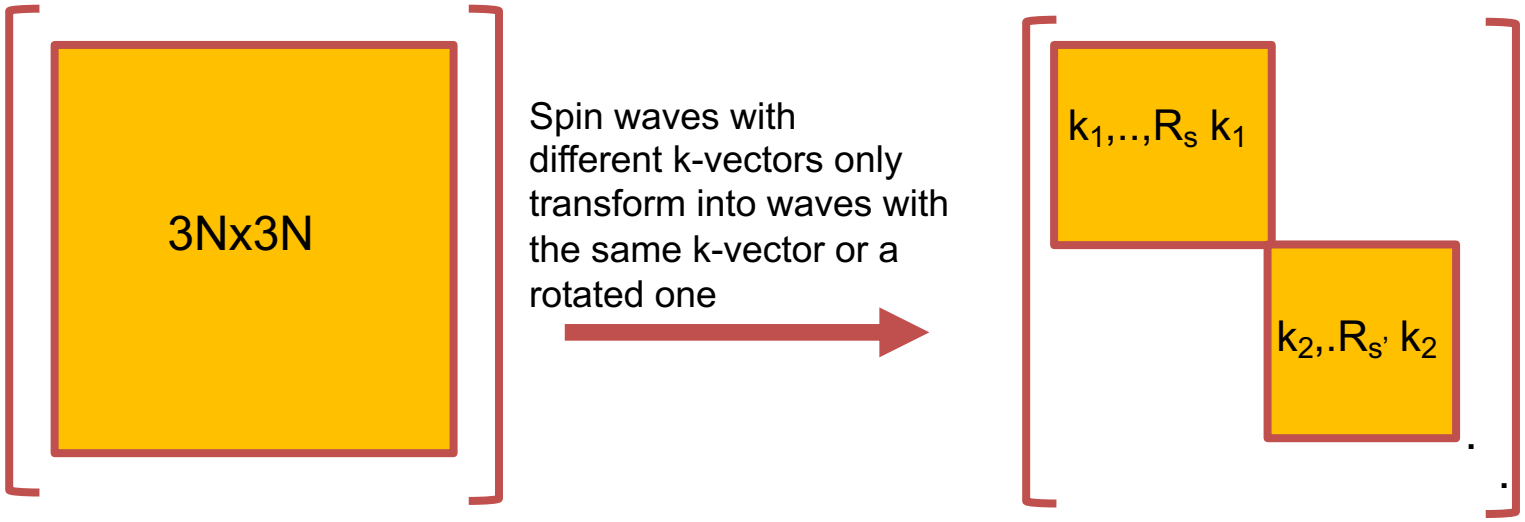
n: number of magnetic atoms in the ***primitive*** unit cell



N≈ infinity
n ≈ small

$Q = (Q_{1x}, Q_{1y}, \ldots Q_{Ny}, Q_{Nz})$ change of basis $Q = (Q1, Q2, Q3, \ldots, Q3N)$

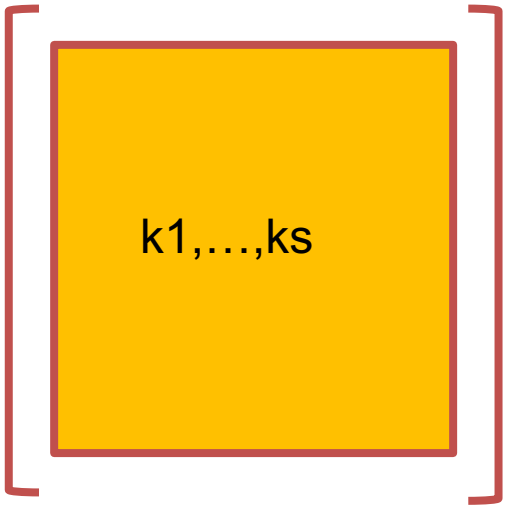
first step: decompositions in waves with different ks:



Representations are first classified according to their k-vector(s)

The infinite N in T goes into the infinite of possible k-vectors!

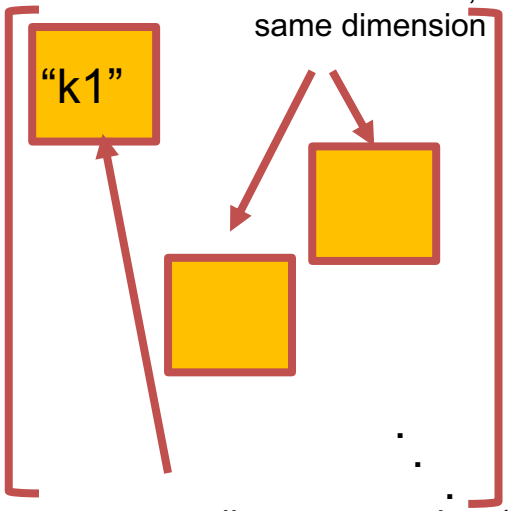
$Q = (Q1_{k1}, Q2_{k1},\ldots Q3s_{k1},\ldots,Q1_{kn}, Q2_{kn},\ldots Q3s_{kn})$



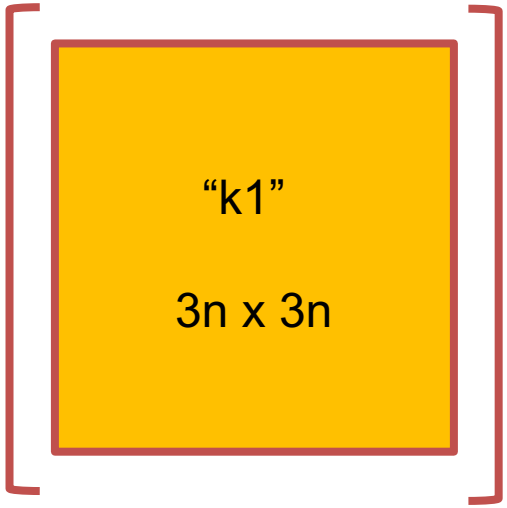
The block of k1 and related ones decomposes into a set of blocks (smaller matrices)

If the operation g keeps k1 invariant

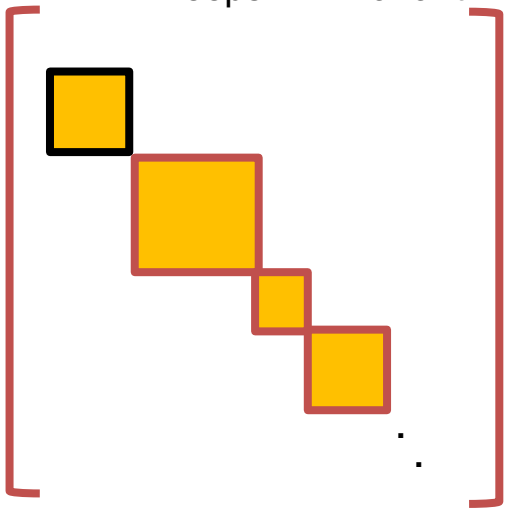
they can be derived from the matrix “k1” , with the same dimension



small representation (reducible!) (only for the little group G_k, which keeps k1 invariant



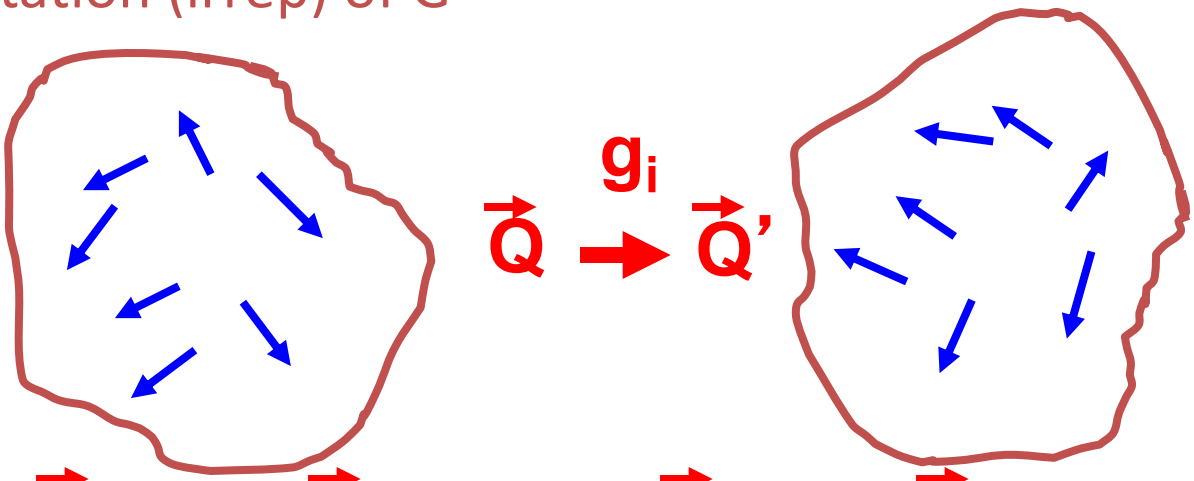
Decomposition of the small rep into irreps transformation to a basis of irrep modes:



if several magnetic atoms in the asymmetric unit- each orbit can be decomposed separately

n=number of magnetic atoms in a primitive unit cell

LANDAU Theory: If transition continuous , then the spin arrangement transforms according to an IRREDUCIBLE representation (irrep) of G



$\vec{Q} = Q_1\vec{d}_1+\ldots+Q_n\vec{d}_n$ $\qquad$ $\vec{Q}\,' = Q'_1\vec{d}_1+\ldots+Q'_n\vec{d}_n$

$$T(g)\,\vec{Q} = \vec{Q}'$$

{T(g)} : **IRREDUCIBLE REPRESENTATION (irrep)**

$\vec{Q} = (Q_1,Q_2,\ldots,Q_n)$ -> Order Parameter of the transition

Even if the transition is not continuous, in most cases T(g) is also IRREDUCIBLE, and in the most complex cases only involves a few irreps

Even if the transition is not continuous, in most cases T(g) is also IRREDUCIBLE, and in the most complex cases only involves a few irreps

This is the basis for the REPRESENTATION METHOD

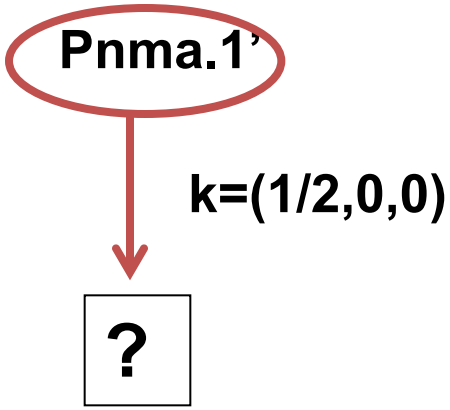
Possible irreps: can be determined mathematically and they are quite limited both in their number and in their dimension.

The determination of the basis of spin modes for each irrep: Is also a pure mathematical problem.

The irreps are mathematical constructs. They are tabulated or calculated by programs. They do not depend on your specific system. **You do not need to know how to calculate them but you need to know how to use them.**

Representation-based modelling of magnetic structures

Possible spin arrangements for a magnetic structure having space group Pnma in the paramagnetic phase and a magnetic ordering with propagation vector k=(1/2,0,0)?



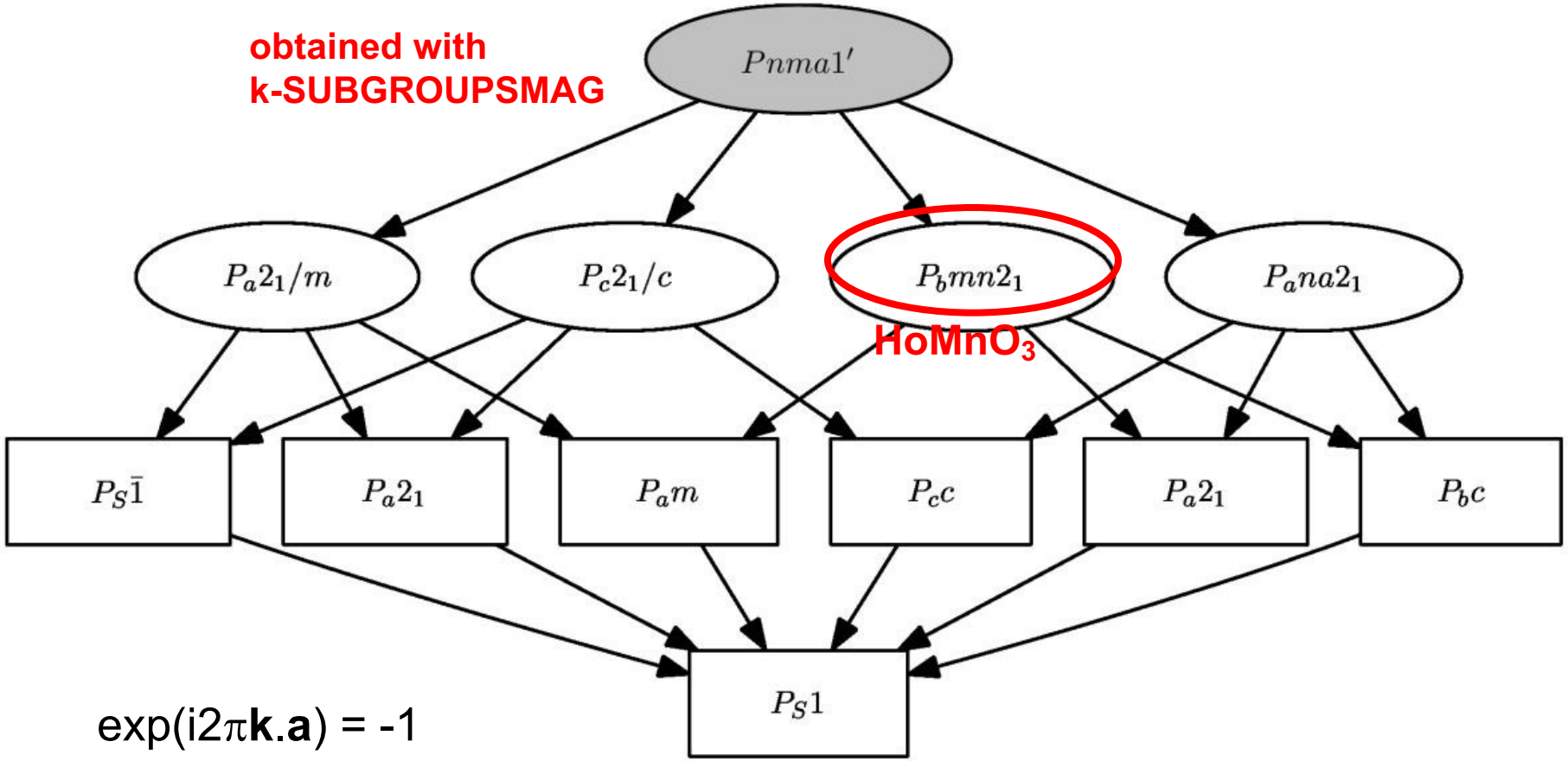
$HoMnO_3$

Mn at WP 4b

Number of Mn atoms in the unit cell =4

Symmetry based modelling of magnetic structures

ALL possible magnetic symmetries for a magnetic phase with propagation vector (1/2,0,0) and parent space group Pnma

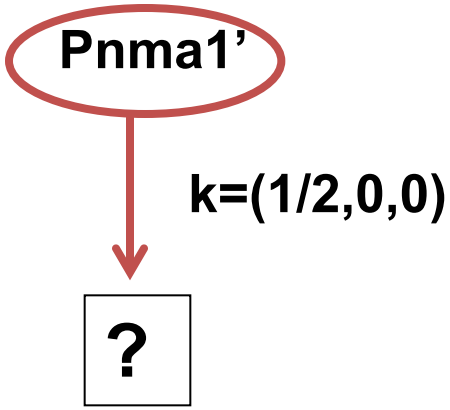


exp(i2π**k**.**a**) = -1

(magnetic cell= (2**a**$_p$,**b**$_p$,**c**$_p$))

Representation based modelling of magnetic structures

Possible spin arrangements for a magnetic structure having space group Pnma in the paramagnetic phase and a magnetic ordering with propagation vector k=(1/2,0,0)?



$HoMnO_3$

Mn at WP 4b

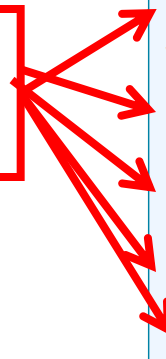
Magnetic representation for this k and this 4b site:

dim: 4 atoms x3 spin components =12. Reducible in general

Decomposition into irreps??

Tutorial_magnetic_section_BCS_2

Only section 2.2



Magnetic Symmetry and Applications	
MGENPOS	General Positions of Magnetic Space Groups
MWYCKPOS	Wyckoff Positions of Magnetic Space Groups
MKVEC ⚠	The k-vector types and Brillouin zones of Magnetic Space Groups
IDENTIFY MAGNETIC GROUP	Identification of a Magnetic Space Group from a set of generators in an arbitrary setting
BNS2OG	Transformation of symmetry operations between BNS and OG settings
mCIF2PCR	Transformation from mCIF to PCR format (FullProf).
MPOINT	Magnetic Point Group Tables
MAGNEXT	Extinction Rules of Magnetic Space Groups
MAXMAGN	Maximal magnetic space groups for a given space group and a propagation vector
MAGMODELIZE	Magnetic structure models for any given magnetic symmetry
STRCONVERT	Convert & Edit Structure Data (supports the CIF, mCIF, VESTA, VASP formats -- with magnetic information where available)
k-SUBGROUPSMAG	Magnetic subgroups consistent with some given propagation vector(s) or a supercell
MAGNDATA	A collection of magnetic structures with portable cif-type files
MVISUALIZE	3D Visualization of magnetic structures with Jmol
MTENSOR ⚠	Symmetry-adapted form of crystal tensors in magnetic phases
MAGNETIC REP.	Decomposition of the magnetic representation into irreps
Get_mirreps	Irreps and order parameters in a paramagnetic space group- magnetic subgroup phase transition

MAGNETIC REP

Magnetic Symmetry and Applications	
MGENPOS	General Positions of Magnetic Space Groups
MWYCKPOS	Wyckoff Positions of Magnetic Space Groups
MKVEC ⚠	The k-vector types and Brillouin zones of Magnetic Space Groups
IDENTIFY MAGNETIC GROUP	Identification of a Magnetic Space Group from a set of generators in an arbitrary setting
BNS2OG	Transformation of symmetry operations between BNS and OG settings
mCIF2PCR	Transformation from mCIF to PCR format (FullProf).
MPOINT	Magnetic Point Group Tables
MAGNEXT	Extinction Rules of Magnetic Space Groups
MAXMAGN	Maximal magnetic space groups for a given space group and a propagation vector
MAGMODELIZE	Magnetic structure models for any given magnetic symmetry
STRCONVERT	Convert & Edit Structure Data (supports the CIF, mCIF, VESTA, VASP formats -- with magnetic information where available)
k-SUBGROUPSMAG	Magnetic subgroups consistent with some given propagation vector(s) or a supercell
MAGNDATA	A collection of magnetic structures with portable cif-type files
MVISUALIZE	3D Visualization of magnetic structures with Jmol
MTENSOR ⚠	Symmetry-adapted form of crystal tensors in magnetic phases
MAGNETIC REP.	Decomposition of the magnetic representation into irreps
Get_mirreps	Irreps and order parameters in a paramagnetic space group- magnetic subgroup phase transition

MAGNETIC REP: Decomposition of the magnetic representation into irreps.

(*for some input wave vector(s) and chosen Wyckoff positions*)

Decomposition of the magnetic representation of the magnetic space group *Pnma*1' (No. 62.442)

(gray group of the paramagnetic phase)

Wave-vector: X:(1/2,0,0)

Wave-vectors of the star (1 vector):

X:(1/2,0,0)

Wyckoff position	Decomposition into irreps
4b:(0,0,1/2)	3 mX1(2) ⊕ 3 mX2(2)

In parentheses the dimensions of the irreducible representations of the little group of k

(small irreps)

(the m in the irrep label means "odd" for time reversal)

CDML notation for the irrep labels: the corresponding irreps are listed in the Bilbao Crystallographic Server and in the ISOTROPY webpage

Decomposition of the magnetic representation of the magnetic space group *Pnma*1' (No. 62.442)

(gray group of the paramagnetic phase)

Wave-vector: X:(1/2,0,0)

Wave-vectors of the star (1 vector):

X:(1/2,0,0)

Wyckoff position	Decomposition into irreps
4b:(0,0,1/2)	3 mX1(2) ⊕ 3 mX2(2)

In parentheses the dimensions of the irreducible representations of the little group of k

Output of Basirreps

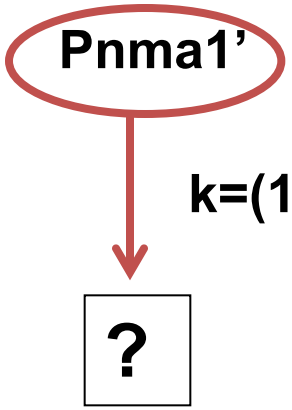
```
-------------------------------------------------------------------------------

 => Decomposition of the Magnetic/Mechanic representation:

 -> Characters of GAMMA and IRreps:

  GAMMA        G( 1)     G( 2)     G( 3)     G( 4)     G( 5)     G( 6)     G( 7)     G( 8)
            12.0 0.0  0.0 0.0  0.0 0.0  0.0 0.0  0.0 0.0  0.0 0.0  0.0 0.0  0.0 0.0

Irep_k( 1)     G( 1)     G( 2)     G( 3)     G( 4)     G( 5)     G( 6)     G( 7)     G( 8)
             2.0 0.0  0.0 0.0  0.0 0.0  0.0 0.0  0.0 0.0  2.0 0.0  0.0 0.0  0.0 0.0

Irep_k( 2)     G( 1)     G( 2)     G( 3)     G( 4)     G( 5)     G( 6)     G( 7)     G( 8)
             2.0 0.0  0.0 0.0  0.0 0.0  0.0 0.0  0.0 0.0 -2.0 0.0  0.0 0.0  0.0 0.0

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

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

mX1

mX2

Representation based modeling of magnetic structures

Possible spin arrangements for a magnetic structure having space group Pnma in the paramagnetic phase and a magnetic ordering with propagation vector k=(1/2,0,0)?



$HoMnO_3$

Mn at WP 4b

Magnetic representation: dim 4x3=12. Reducible in general

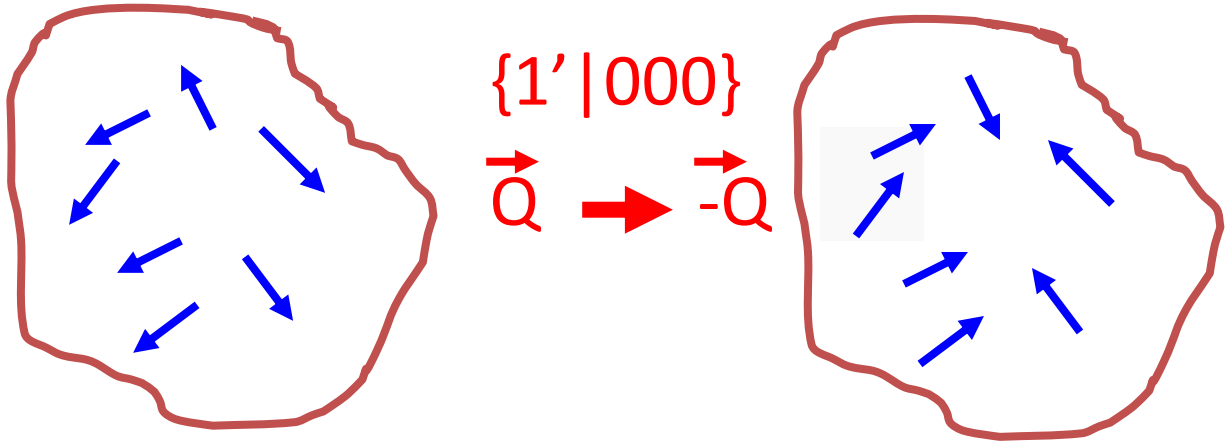
6-dim 6-dim

M_{rep}= 3 mX1(2) $\oplus$ 3 mX2(2)

irreps

Decomposition into irreps

Why an "m" in the irrep label:



$$T_{*k1}(\{1'|000\}) = \begin{bmatrix} -1 & & & & & 0 \\ & -1 & & & & \\ & & \ddots & & & \\ & & & \ddots & & \\ 0 & & & & \ddots & \\ & & & & & -1 \end{bmatrix}$$

12x12

$k_1=(1/2,0,0)$

The representation is "odd" for time reversal when considered for the parent grey group G1'

To distinguish from distortions that are even for time reversal: Phonons modes in the parent phase also transform according to irreps of G, but they are EVEN for time reversal when considered for the grey group G1'!

$$T(g) = \begin{bmatrix} [T_{*k1}(g)] & & & 0 \\ & [T_{*k2}(g)] & & \\ & & \ddots & \\ 0 & & & [T_{*kN}(g)] \end{bmatrix}$$

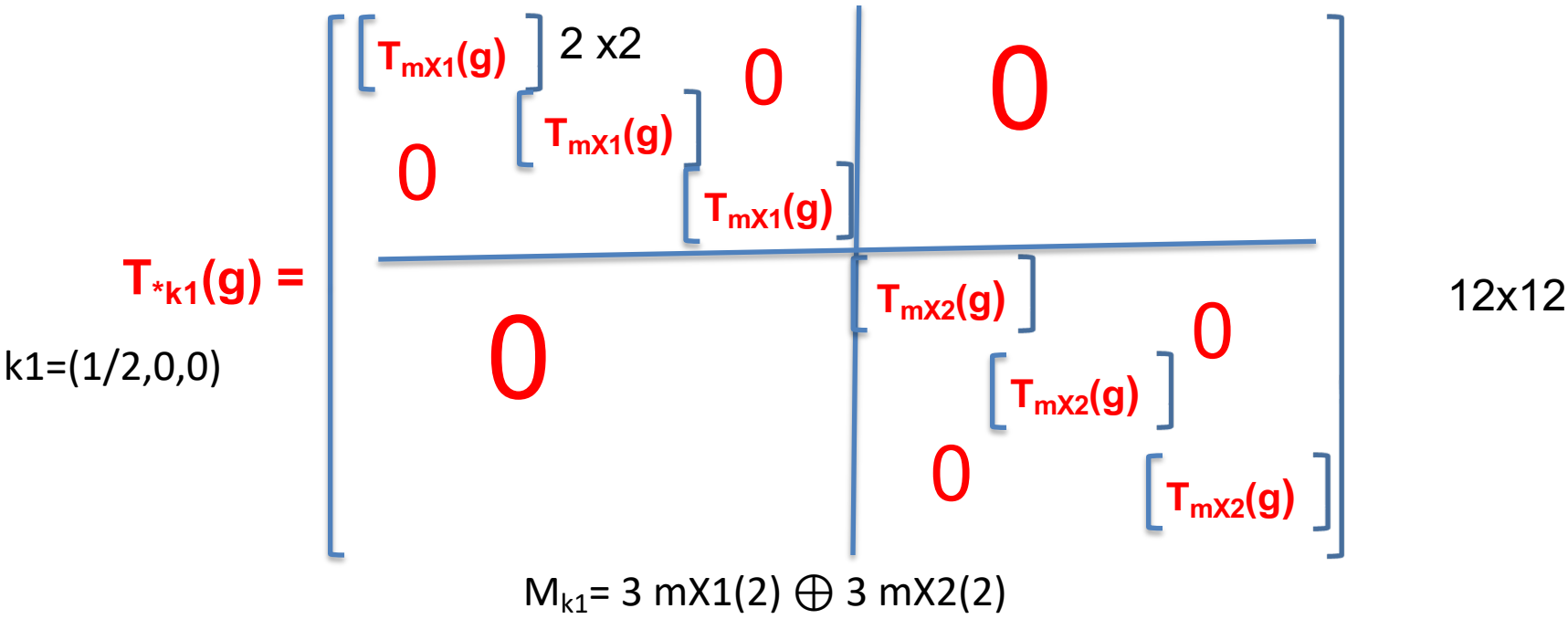
$$T_{*k1}(g) = \left[\begin{array}{cc|c} [T_{mX1}(g)] & 0 & 0 \\ 0 & [T_{mX1}(g)] & \\ & & [T_{mX1}(g)] \\ \hline 0 & & [T_{mX2}(g)] \\ & 0 & [T_{mX2}(g)] \\ & & 0 \\ & & [T_{mX2}(g)] \end{array}\right]$$

2 x2

12x12

k1=(1/2,0,0)

M_{k1}= 3 mX1(2) $\oplus$ 3 mX2(2)



(1) $\left[T_{mX1}(g)\right]$ 2 x2 → $\{f^{(1)}_1, f^{(1)}_2\}$

(2) $\left[T_{mX1}(g)\right]$ 2 x2 → $\{f^{(2)}_1, f^{(2)}_2\}$

(3) $\left[T_{mX1}(g)\right]$ 2 x2 → $\{f^{(3)}_1, f^{(3)}_2\}$

→ Basis vectors or Basis Functions

determined by mathematics only!

determined by program Basirreps (also Sarah, …)

choice is not unique! : $\{a_1 f^{(1)}_1 + a_2 f^{(2)}_1 + a_3 f^{(3)}_1 \ , \ a_1 f^{(1)}_2 + a_2 f^{(2)}_2 + a_3 f^{(3)}_2\}$

(1) $\left[T_{mX1}(g) \right]$ 2 x2 $\longrightarrow$ $\{f^{(1)}{}_1, f^{(1)}{}_2\}$

(2) $\left[T_{mX1}(g) \right]$ 2 x2 $\longrightarrow$ $\{f^{(2)}{}_1, f^{(2)}{}_2\}$

(3) $\left[T_{mX1}(g) \right]$ 2 x2 $\longrightarrow$ $\{f^{(3)}{}_1, f^{(3)}{}_2\}$

choice is not unique! : $\{a_1 f^{(1)}{}_1 + a_2 f^{(2)}{}_1 + a_3 f^{(3)}{}_1 \ , \ a_1 f^{(1)}{}_2 + a_2 f^{(2)}{}_2 + a_3 f^{(3)}{}_2\}$

Output of Basirreps

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

            SYMM  x,y,z    -x,-y,z+1/2    x+1/2,-y+1/2,-z    -x+1/2,y+1/2,-z+1/2
            Atoms:      Mn_1               Mn_2               Mn_3               Mn_4
BsV( 1, 1: 4):Re (    1    0    0) (   -1    0    0) (    0    0    0) (    0    0    0)
BsV( 2, 1: 4):Re (    0    1    0) (    0   -1    0) (    0    0    0) (    0    0    0)
BsV( 3, 1: 4):Re (    0    0    1) (    0    0    1) (    0    0    0) (    0    0    0)
BsV( 4, 1: 4):Re (    0    0    0) (    0    0    0) (    1    0    0) (   -1    0    0)
BsV( 5, 1: 4):Re (    0    0    0) (    0    0    0) (    0   -1    0) (    0    1    0)
BsV( 6, 1: 4):Re (    0    0    0) (    0    0    0) (    0    0   -1) (    0    0   -1)
```

$f^{(1)}{}_1$ $f^{(2)}{}_1$ $f^{(3)}{}_1$ $f^{(1)}{}_2$ $f^{(2)}{}_2$ $f^{(3)}{}_2$

```
----- 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: Mn_1      0.0000  0.0000  0.0000
      Sk(1): (u,v,w)

      SYMM -x,-y,z+1/2                                              Atom: Mn_2      0.0000  0.0000  0.5000
      Sk(2): (-u,-v,w)

      SYMM x+1/2,-y+1/2,-z                                          Atom: Mn_3      0.5000  0.5000  0.0000
      Sk(3): (p,-q,-r)

      SYMM -x+1/2,y+1/2,-z+1/2                                      Atom: Mn_4      0.5000  0.5000  0.5000
      Sk(4): (-p,q,-r)

 ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
```

Output of Basirreps

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

             SYMM  x,y,z    -x,-y,z+1/2    x+1/2,-y+1/2,-z    -x+1/2,y+1/2,-z+1/2
             Atoms:      Mn_1               Mn_2                Mn_3               Mn_4
BsV( 1, 1: 4):Re (    1    0    0) (   -1    0    0) (    0    0    0) (    0    0    0)
BsV( 2, 1: 4):Re (    0    1    0) (    0   -1    0) (    0    0    0) (    0    0    0)
BsV( 3, 1: 4):Re (    0    0    1) (    0    0    1) (    0    0    0) (    0    0    0)
BsV( 4, 1: 4):Re (    0    0    0) (    0    0    0) (    1    0    0) (   -1    0    0)
BsV( 5, 1: 4):Re (    0    0    0) (    0    0    0) (    0   -1    0) (    0    1    0)
BsV( 6, 1: 4):Re (    0    0    0) (    0    0    0) (    0    0   -1) (    0    0   -1)
```

$f^{(1)}_1$ $f^{(2)}_1$ $f^{(3)}_1$ $f^{(1)}_2$ $f^{(2)}_2$ $f^{(3)}_2$

```
----- 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: Mn_1      0.0000  0.0000  0.0000
      Sk(1): (u,v,w)

      SYMM -x,-y,z+1/2                                            Atom: Mn_2      0.0000  0.0000  0.5000
      Sk(2): (-u,-v,w)

      SYMM x+1/2,-y+1/2,-z                                        Atom: Mn_3      0.5000  0.5000  0.0000
      Sk(3): (p,-q,-r)

      SYMM -x+1/2,y+1/2,-z+1/2                                    Atom: Mn_4      0.5000  0.5000  0.5000
      Sk(4): (-p,q,-r)

 ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
```

Basis of subspace mX1 for the order parameter ordering :

$$\{c_1 f^{(1)}_1 + c_2 f^{(2)}_1 + c_3 f^{(3)}_1 \ , \ c_1 f^{(1)}_2 + c_2 f^{(2)}_2 + c_3 f^{(3)}_2\} = (F_1, F_2)$$

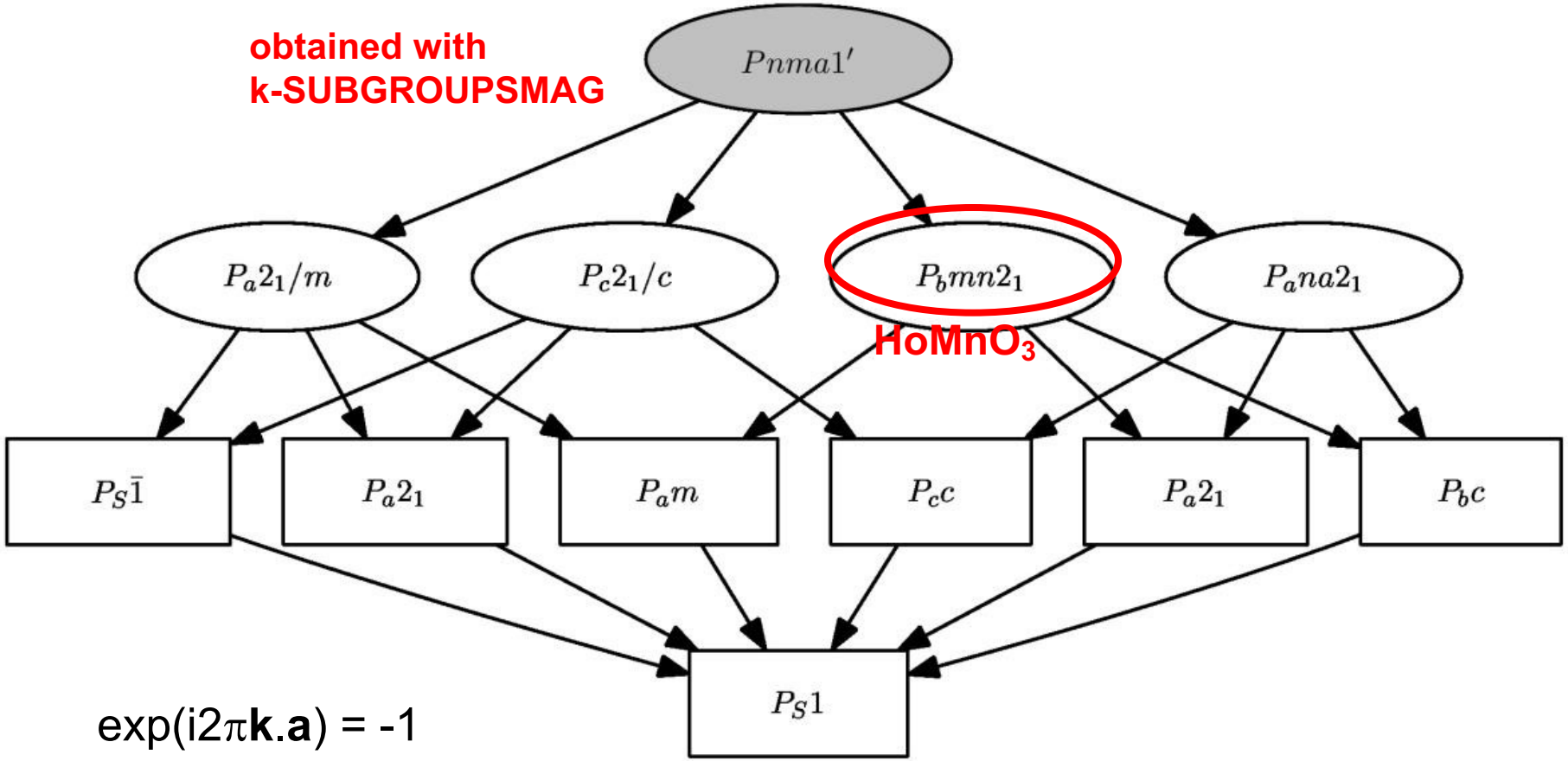
spin arrangement: $\mathbf{a}\, F_1 + \mathbf{b} F_2$: order parameter direction (a,b)

To be determined from exp. data!

possible different MSGs for special directions

Symmetry based modelling of magnetic structures

ALL possible magnetic symmetries for a magnetic phase with propagation vector (1/2,0,0) and parent space group Pnma



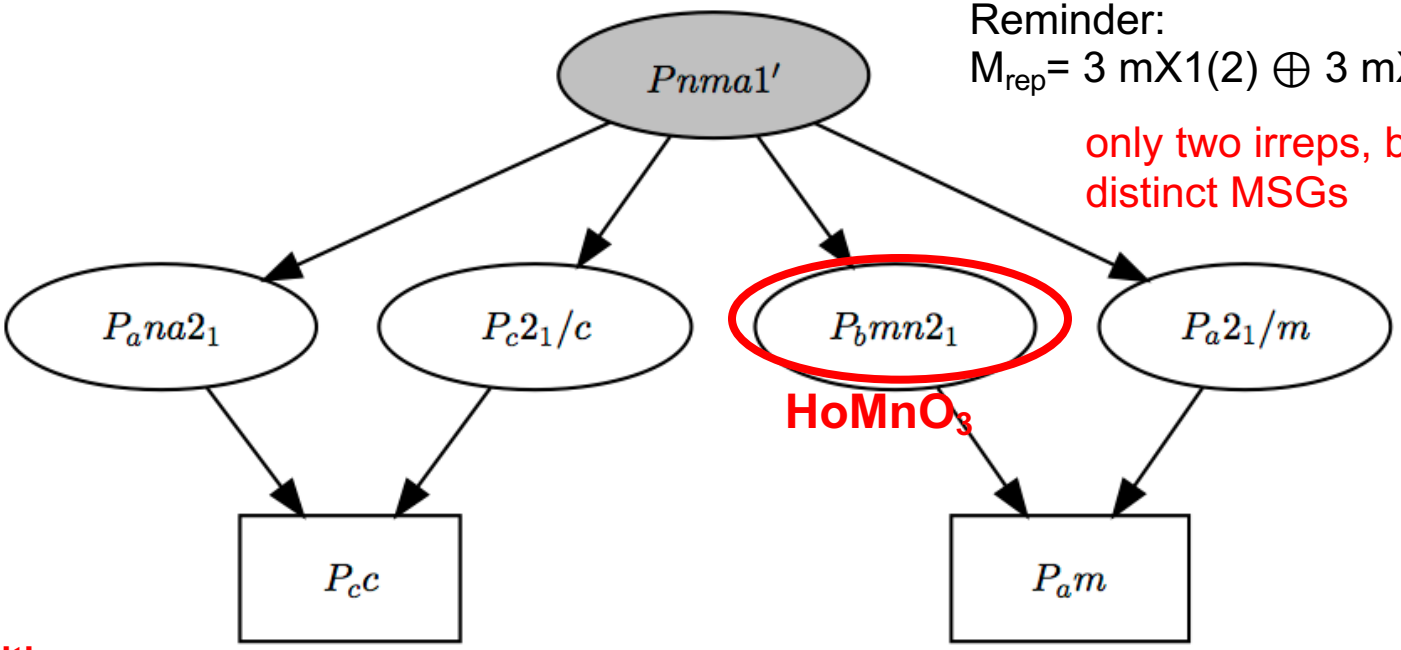
exp(i2π**k**.**a**) = -1

(magnetic cell= (2**a**$_p$,**b**$_p$,**c**$_p$))

Symmetry based modeling in magnetic structures

Possible magnetic symmetries for a magnetic phase with propagation vector (1/2,0,0) and parent space group Pnma

BUT only those that can be the result of a Landau-type transition (single irrep order parameter)



Reminder:
M_{rep}= 3 mX1(2) ⊕ 3 mX2(2)

only two irreps, but 6 possible distinct MSGs

$HoMnO_3$

obtained with k-SUBGROUPSMAG:

☑ Optional: Show only subgroups that can be the result of a Landau-type transition (single irrep order parameter).

Phase Transition / Symmetry break / Order Parameter

group-subgroup relation:

G → F **F: isotropy subgroup**

High symmetry **Low symmetry**

High symmetry group G = {g}

$T(g)\,\vec{Q} = \vec{Q}$

g belongs to F

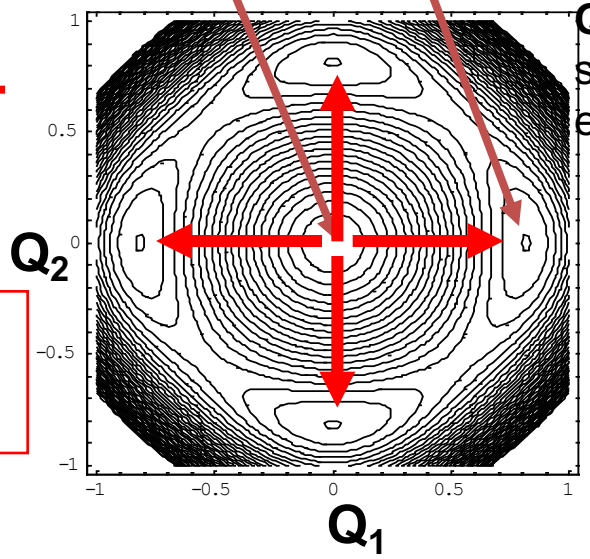
Irreducible representation of G (irrep) (matrices)

$T(g)\,\vec{Q} = \vec{Q}' \neq \vec{Q}$

g does not belong to F: $\vec{Q}'$ equivalent but distinguishable state (domain)

For special directions of **Q**. F of higher symmetry: epikernels

For general direction of **Q**, the lowest F: kernel



amplitude

Key concept of a symmetry break

← Order parameter $\vec{Q} = (Q_1, Q_2) = \rho\,(a_1, a_2)$

$a_1^2 + a_2^2 = 1$

Possible Magnetic Space Groups (MSGs) for a single irrep:

isotropy subgroups:

Invariance equation:

$$T[\{\mathbf{R}, \theta|\mathbf{t}\}] \begin{pmatrix} a \\ b \\ .. \\ .. \end{pmatrix} = \begin{pmatrix} a \\ b \\ .. \\ .. \end{pmatrix}$$

nxn matrix of irrep

$\{\mathbf{R},\theta|\mathbf{t}\}$ is conserved by the magnetic arrangement

epikernels of the irrep, depending on the direction (a,a,…) ,(a,0,…), etc…

kernel of the irrep: operations represented by the unit matrix. MSG kept by any direction (a,b,…)

Example: $g_i = \{R, -1|t\}$

$$T(g_i) = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \qquad T(g_i) \begin{pmatrix} a \\ a \end{pmatrix} = \begin{pmatrix} a \\ a \end{pmatrix}$$

➔ **g_i will belong to the MSG if OP=(a,a)**

K-SUBGROUPSMAG output:

List of subgroups that can be the result of a Landau-type transition

Get the subgroup-graph

N	Group Symbol	Transformation matrix	Group-Subgroup index	Other members of the Conjugacy Class	irreps	Magnetic structure models (MAGMODELIZE)
1	P_ana2_1 (No. 33.149)	$\begin{pmatrix} 2 & 0 & 0 & -1/4 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps	☐
2	P_bmn2_1 (No. 31.129)	$\begin{pmatrix} 0 & -2 & 0 & -1/4 \\ 1 & 0 & 0 & 1/4 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps	☐
3	P_c2_1/c (No. 14.82)	$\begin{pmatrix} 0 & 0 & 2 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps	☐
4	P_a2_1/m (No. 11.55)	$\begin{pmatrix} 2 & 0 & 0 & 1/2 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps	☐
5	P_cc (No. 7.28)	$\begin{pmatrix} 0 & 0 & 2 & 0 \\ 0 & 1 & 0 & 1/4 \\ -1 & 0 & 0 & 0 \end{pmatrix}$	8=2x4	Conjugacy Class	Get irreps	☐
6	P_am (No. 6.21)	$\begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1/4 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	8=2x4	Conjugacy Class	Get irreps	☐

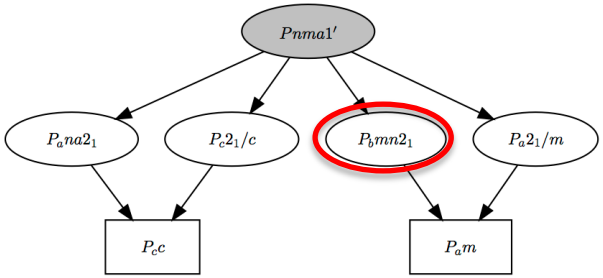
Link to Get_mirreps

Get_mirreps: Irreps that are compatible with a given magnetic phase transition

Input: SG of the paramagnetic phase + MSG of the magnetic phase and their relation

Group→subgroup	Transformation matrix
*Pnma*1' (N. 62.442)→P_bmn2_1 (N. 31.129)	$\begin{pmatrix} 0 & -2 & 0 & -1/4 \\ 1 & 0 & 0 & 1/4 \\ 0 & 0 & 1 & 0 \end{pmatrix}$

for P_amn2_1



Representations and order parameters

Show the graph of isotropy subgroups

primary irrep

k-vectors	irreps and order parameters	isotropy subgroup transformation matrix	link to the irreps
GM: **(0,0,0)**	GM_1^+: (a)	*Pnma*1' (No. 62.442) a,b,c;0,0,0	matrices of the irreps
	GM_2^-: (a)	$Pmn2_1$1' (No. 31.124) b,-2a,c;1/4,1/4,0	
X: **(1/2,0,0)**	mX_1: (a,a)	P_bmn2_1 (No. 31.129) b,-2a,c;-1/4,1/4,0	matrices of the irreps

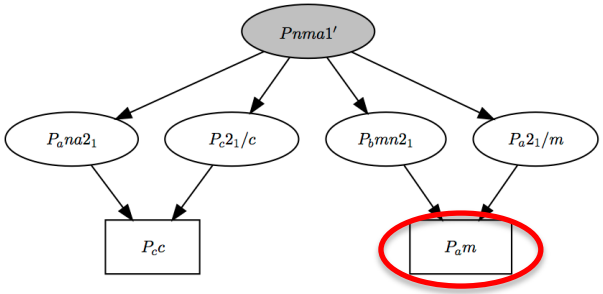
special direction

Get_mirreps: Irreps that are compatible with a given magnetic phase transition

Input data

Group→subgroup	Transformation matrix
*Pnma*1' (N. 62.442)→P_am (N. 6.21)	$\begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1/4 \\ 0 & 0 & 1 & 0 \end{pmatrix}$

for P_am



Representations and order parameters

Show the graph of isotropy subgroups

k-vectors	irreps and order parameters	isotropy subgroup transformation matrix	link to the irreps
GM: **(0,0,0)**	GM_1^+: (a)	*Pnma*1' (No. 62.442) a,b,c;0,0,0	matrices of the irreps
	GM_4^+: (a)	$P2_1/m1'$ (No. 11.51) a,b,c;0,0,0	
	GM_2^-: (a)	$Pmn2_11'$ (No. 31.124) b,-a,c;1/4,1/4,0	
	GM_3^-: (a)	$Pmc2_11'$ (No. 26.67) b,c,a;0,1/4,1/4	
X: **(1/2,0,0)**	mX_1: (a,b)	P_am (No. 6.21) 2a,b,c;0,1/4,0	matrices of the irreps

primary irrep

general direction

k-SUBGROUPSMAG determine the epikernels and kernel of any irrep and produce magnetic structural models complying with them.

k-Subgroupsmag: Magnetic subgroups compatible with some given propagation vector(s) or a supercell.

k-Subgroupsmag

The program *k-Subgroupsmag* provides the possible magnetic subgroups of the space group of a paramagnetic phase (gray group) which are possible for a magnetic ordering having a known propagation vector. The program provides the set of magnetic subgroups or a graph showing the subgroup-tree (grouped into conjugacy classes). In both cases, more information about the classes or subgroups can be obtained.

Other alternatives for the input of the program:

- An alternative parent (non gray) magnetic group can be chosen.
- Instead of the whole set of subgroups, the output can be limited to subgroups having a chosen common subgroup of lowest symmetry, common point group of lowest symmetry, or groups which belong to a specific crystal class.
- Further restrictions on the subgroup list/graph considering physical properties can be used: it is possible to ask for only centrosymmetric or non-centrosymmetri groups, polar or non-polar groups.
- More than one propagation wave-vector can be chosen.
- The whole (or partial) stars of vectors can be introduced.
- Non magnetic modulation wave-vectors can be also introduced.
- Instead of propagation wave-vectors, a

Enter the serial number of the space group of the parent paramagnetic phase: choose it 136

Choose an alternative magnetic group

Alternatively give the operations of the space group in a non-standard setting

Introduce the magnetic wave vector(s)

Alternatively give the basis vectors of the supercell

(Give the components of the wave vectors in a fractional form, n/m)

k_{1x} 0 k_{1y} 0 k_{1z} 0

Show the independent vectors of the star

Choose the whole star of the propagation vector

More wave-vectors needed

only commensurate

Optionally give also non-magnetic modulation wave-vectors

Include the subgroups compatible with intermediate cells.

(It is not applied when only the maximal subgroups are calculated)

Optional: refine further the subgroups of the output giving the Wyckoff positions of the atoms

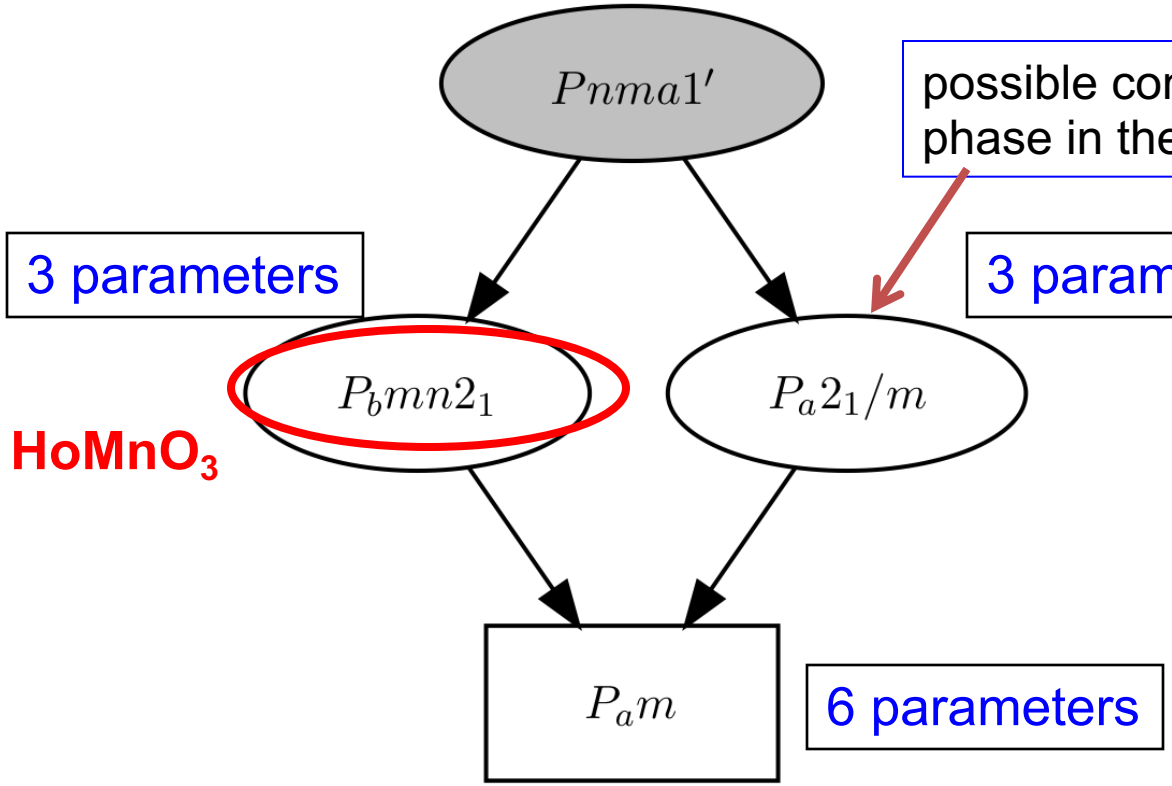
Give the Wyckoff positions Wyckoff

Optional: refine further the subgroups of the output giving a set of irreps

Choose the irreps Representations

filter by irreps

Possible MSGs for a magnetic structure with space group Pnma, with propagation vector k=(1/2,0,0), and a magnetic ordering according to the irrep mX1.



M_{rep}= 3 mX1(2) $\oplus$ 3 mX2(2)

6 basis spin modes: 6 parameters

Other programs that determine the epikernels and kernel of any irrep, and produce magnetic structural models complying with them.

Program for mode analysis: (with irrep mode decomposition!)

ISODISTORT http://stokes.byu.edu/iso/isotropy.php Stokes & Campbell, Provo

Version 6.1.8, November 2014

Harold T. Stokes. Branton J. Campbell, and Dorian M. Hatch, Department of Physics and Astronomy, Brigham Young University, Provo, Utah, 84602, USA, stokesh@byu.edu

Description: ISODISTORT is a tool for exploring the structural distortion modes of crystalline materials. It provides a user-friendly interface to many of the algorithms used by the **Isotropy Software Suite**, allowing one to generate and explore distortion modes induced by irreducible representations of the parent space-group symmetry. It also provides a Java applet for visualizing and interactively manipulating the free parameters associated with these modes.

Help, Tutorials, Version History

NOTICE: Version 6.1 is a major new release. We appreciate your bug reports -- please send relevant input files along with the html page showing the failed output.

Legacy copy of ISODISTORT version 5.6.1, August 2013

Begin by entering the structure of parent phase: (?)

Get started quickly with a cubic perovskite parent.

Import parent structure from a CIF structure file: OK | Browse... | No file selected.

Both programs also support incommensurate cases, deriving epikernels and kernel of the irreps in the form of MSSGs, and corresponding magnetic models

Program for structure refinement:

JANA

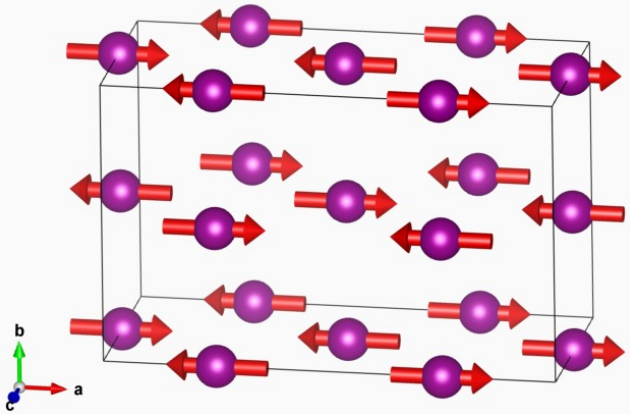
Institute of Physics http://jana.fzu.cz/ V. Petricek, Prague
Department of Structure Analysis
Cukrovarnicka 10
16253 Praha 6
Czech Republic

Academy of Sciences | Institute of Physics
Dept of Structure Analysis | Laboratory of Crystallography
ECA-SIG#3 | Contact Us

CRYSTALLOGRAPHIC COMPUTING SYSTEM FOR STANDARD AND MODULATED STRUCTURES

Vaclav Petricek, Michal Dusek & Lukas Palatinus

News



$HoMnO_3$ (*Magndata #1.20*)

parent space group: *Pnma*, k=(1/2,0,0)

transformation from parent structure: (2a,b,c;0,0,0)

BNS magnetic space group: P_bmn2_1 (#29.104) (non-standard)

Transformation to standard setting: (-b,a,c;1/8,1/4,0)

k-maximal symmetry

Label	Atom type	x	y	z	Multiplicity	Symmetry constraints on M	M_x	M_y	M_z	|M|
Mn	Mn	0.00000	0.00000	0.50000	8	m_x,m_y,m_z	3.87	0.0	0.0	3.87

NOT symmetry forced

magnetic space group:

N	(x,y,z)	Seitz notation
1	x,y,z,+1	{ 1 | 0 }
2	-x+1/4,-y,z+1/2,+1	{ 2_{001} | 1/4 0 1/2 }
3	x,-y+1/2,z,+1	{ m_{010} | 0 1/2 0 }
4	-x+1/4,y+1/2,z+1/2,+1	{ m_{100} | 1/4 1/2 1/2 }
5	x+1/2,y,z,-1	{ 1' | 1/2 0 0 }
6	-x+3/4,-y,z+1/2,-1	{ $2'_{001}$ | 3/4 0 1/2 }
7	x+1/2,-y+1/2,z,-1	{ m'_{010} | 1/2 1/2 0 }
8	-x+3/4,y+1/2,z+1/2,-1	{ m'_{100} | 3/4 1/2 1/2 }

2-dim irrep mX1 but restricted to a special direction:

fixed combination of each pair of spin basis functions => **half number of degrees of freedom with respect to only restricting to the irrep mX1**

Does the identification of the irrep bring some additional knowledge or constraint? …NO

(Because the MSG of structure is only compatible with a single irrep…)

ABOUT LABELS OF IRREDUCIBLE REPRESENTATIONS (IRREPS)

- **The irrep notation lacks a standard, but there is a couple of alternative unambiguous irrep labeling systems, supported with computer listings, that can be recommended:**
  - **CDML notation (**A. P. Cracknell, B. L. Davies, S. C. Miller and W. F. Love (1979)):
    software: ISOTROPY, Bilbao Crystallographic Server, JANA, FullProf (Basirreps)
  - **Kovalev notation** (O.V. Kovalev 1965-1993)**:**
    software: SARAh
- **It is strongly advised against using arbitrary irrep labels (like those of traditional software), but if done, then full unambiguous listings of the irrep characters must be necessarily included. Otherwise the irrep labels mean NOTHING!**

Last version of Basirreps gives the CDML labels of the listed irreps!

The irreps are mathematical constructs. They are tabulated or calculated by programs. They do not depend on you specific system.

You do not need to know how to calculate them but you need to know what they mean and how to use them.

MSGs vs. Irreps

Commensurate magnetic structures:

Representation Analysis (irreducible representations, basis functions...)	?	Magnetic Symmetry (Shubnikov groups, superspace groups...)

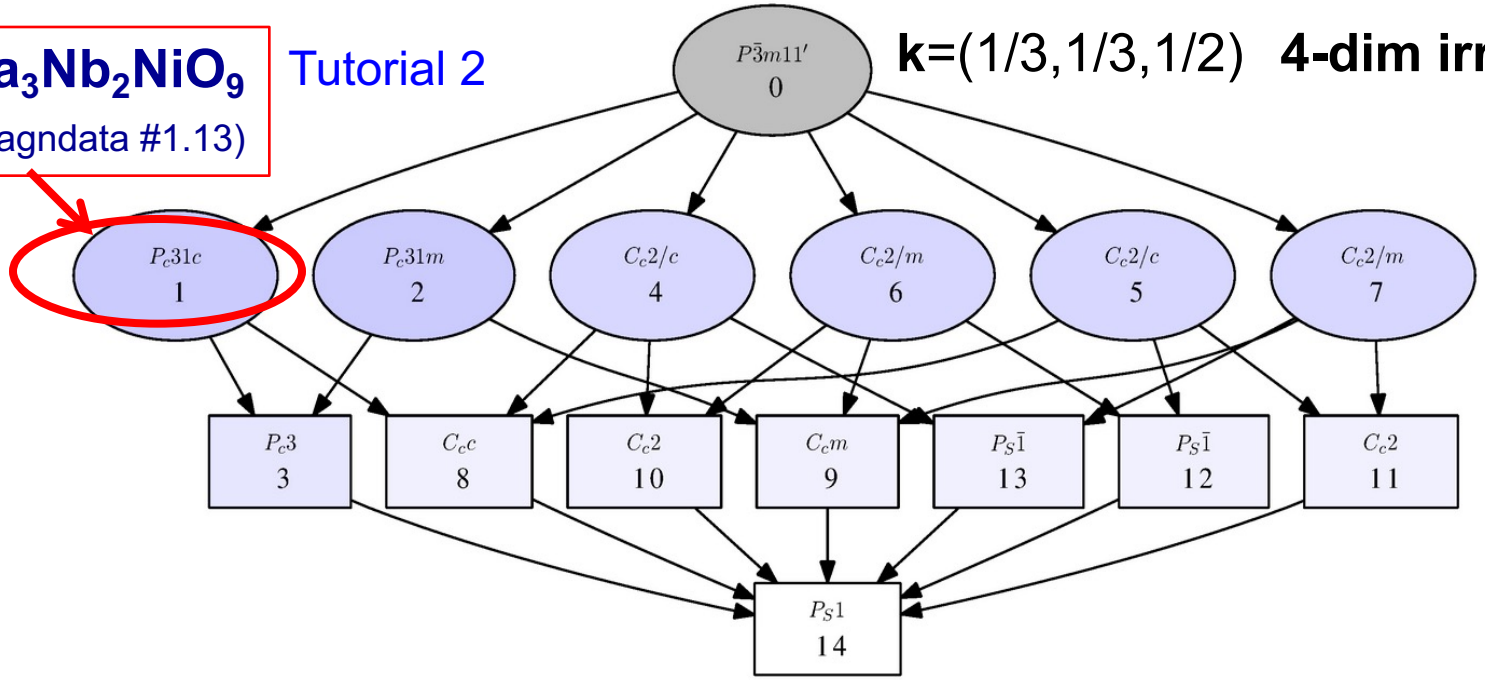
Identifying the active irrep(s) or the MSG are not alternative equivalent methods:

In the case of N-dim irreps several MSGs are in general possible for the same irrep

Only in the case of 1-dim irreps there is a one to one relation

The number of possible epikernels for an irrep increases wih the dimension of the irrep:

$Ba_3Nb_2NiO_9$ Tutorial 2
(magndata #1.13)



k=(1/3,1/3,1/2) 4-dim irrep mH3

13 distinct epikernels for 4-dim irrep mH3 of P-3m1 (some k-maximal and some not)

MSGs vs. Irreps

Case 1 : the structure is only compatible with a single irrep (the majority of cases):

In this case a description using irrep spin basis vectors does bring advantage:

- If the irrep is 1-dim, the two descriptions will be fully equivalent: the irrep basis functions will reproduce the same moment constraints and relationships among the magnetic atoms as the MSG.

- If the irrep is multidimensional, in most cases several alternative MSGs can realized for the same irrep and the description using the actual MSG automatically introduces additional constraints that are not included when only restricting to the basis vectors of the irrep.

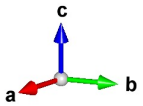
Case 2: the MSG is compatible with more than one irrep

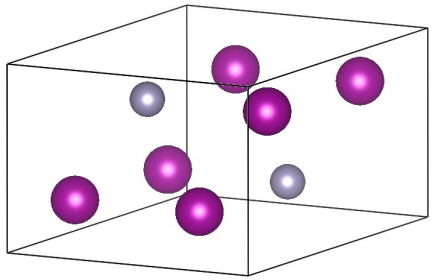
Mn_3Sn

k=(0,0,0)

$P6_3/mmc.1'$ → *Cmc'm'*(-**b**,2**a**,**c**;0,0,0)

Mn Wyckoff position: 6h (x,2x,1/4)

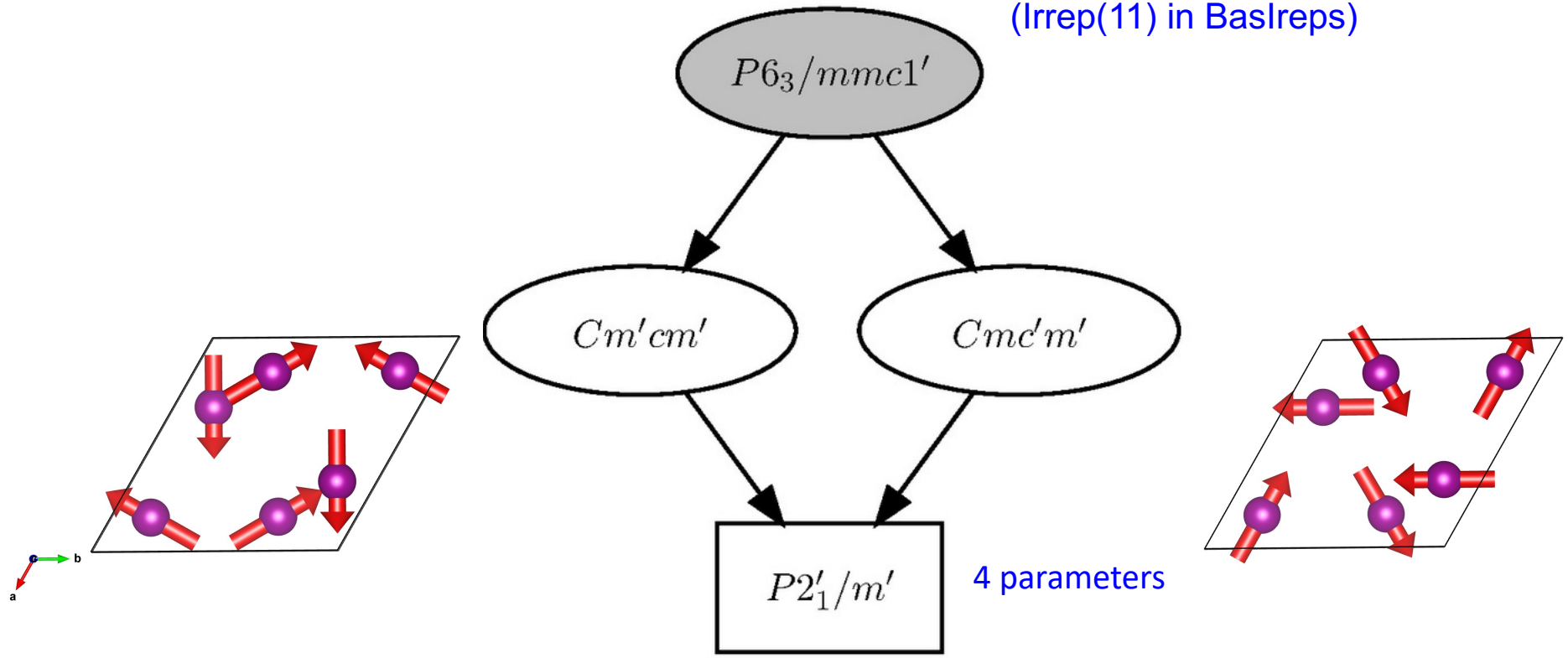




194
5.665 5.665 4.531 90 90 120
2
Mn1 6h 0.8388 0.6776 0.25
Sn1 2d 0.33333 0.66667 0.25

Mn_3Sn k=(0,0,0)

2-dim irrep mGM6+
(Irrep(11) in BasIreps)



MAGNETIC REP output:

Wave-vectors of the star (1 vector):

GM:(0,0,0)

4 basis functions/vectors

Wyckoff position	Decomposition into irreps
6h:(x,2*x,1/4)	mGM1-(1) ⊕ mGM2+(1) ⊕ mGM2-(1) ⊕ mGM3+(1) ⊕ mGM3-(1) ⊕ mGM4+(1) ⊕ mGM5+(2) ⊕ 2 mGM5-(2) ⊕ 2 mGM6+(2) ⊕ mGM6-(2)

In parentheses the dimensions of the irreducible representations of the little group of k

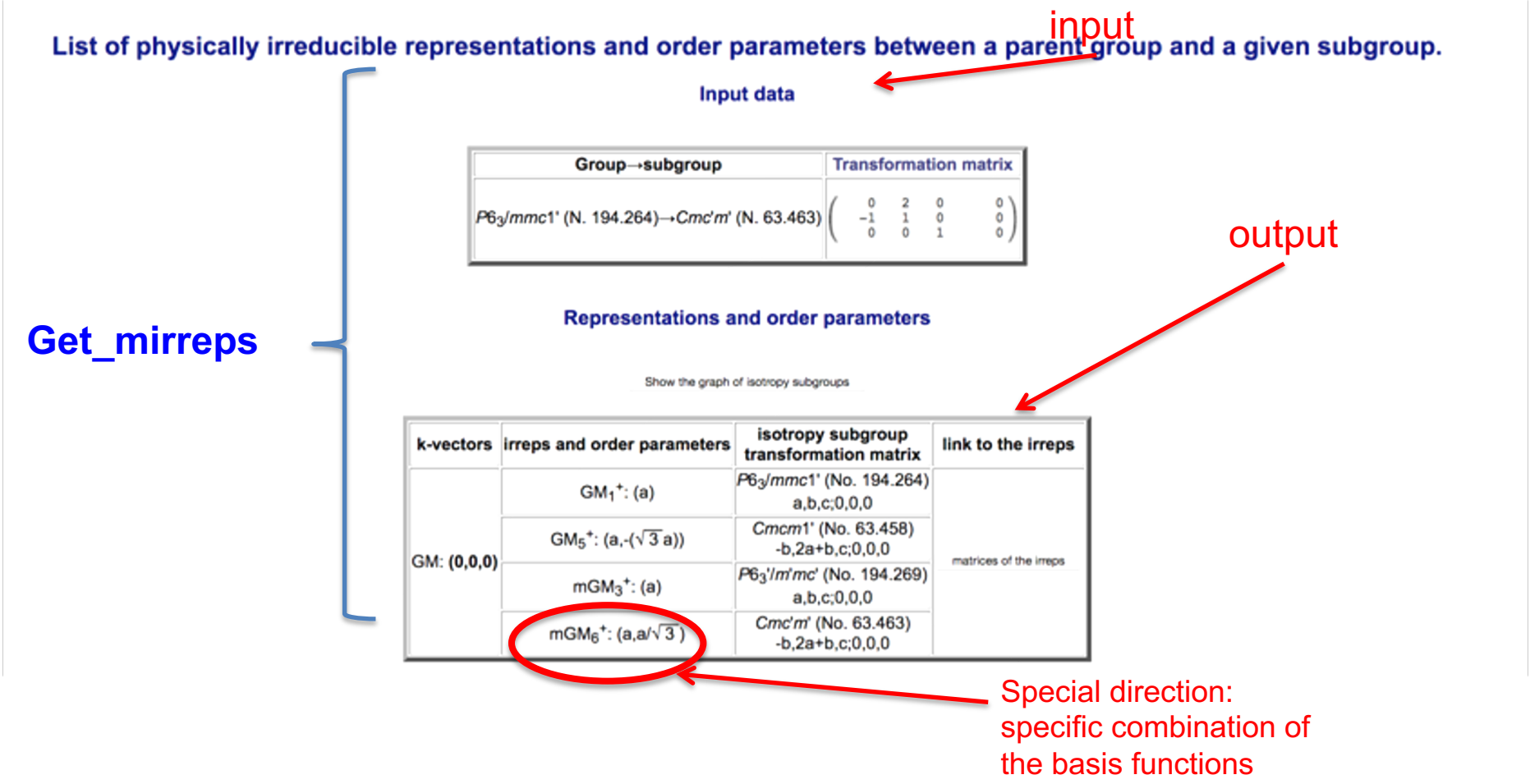
```
+
 => Basis functions of Representation IRrep( 12) of dimension   2 contained  2 times in GAMMA
   ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

+
              SYMM  x,y,z   -x,-y,z+1/2   -y,x-y,z   y,-x+y,z+1/2
              Atoms:      Mn_1              Mn_2              Mn_3              Mn_4
 BsV( 1, 1: 4):Re ( 1.00 0.00 0.00) ( 1.00 0.00 0.00) ( 0.00-0.50 0.00) ( 0.00-0.50 0.00)
               Im ( 0.00 0.00 0.00) ( 0.00 0.00 0.00) ( 0.00-0.87 0.00) ( 0.00-0.87 0.00)
 BsV( 2, 1: 4):Re ( 0.00 1.00 0.00) ( 0.00 1.00 0.00) ( 0.50 0.50 0.00) ( 0.50 0.50 0.00)
               Im ( 0.00 0.00 0.00) ( 0.00 0.00 0.00) ( 0.87 0.87 0.00) ( 0.87 0.87 0.00)
 BsV( 3, 1: 4):Re ( 0.50 0.00 0.00) ( 0.50 0.00 0.00) ( 0.00-1.00 0.00) ( 0.00-1.00 0.00)
               Im ( 0.87 0.00 0.00) ( 0.87 0.00 0.00) ( 0.00-0.00 0.00) ( 0.00-0.00 0.00)
 BsV( 4, 1: 4):Re (-0.50-0.50 0.00) (-0.50-0.50 0.00) (-1.00 0.00 0.00) (-1.00 0.00 0.00)
               Im (-0.87-0.87 0.00) (-0.87-0.87 0.00) (-0.00 0.00 0.00) (-0.00 0.00 0.00)

              SYMM  -x+y,-x,z   x-y,x,z+1/2
              Atoms:      Mn_5              Mn_6
 BsV( 1, 5: 6):Re ( 0.50 0.50 0.00) ( 0.50 0.50 0.00)
               Im (-0.87-0.87 0.00) (-0.87-0.87 0.00)
 BsV( 2, 5: 6):Re (-0.50 0.00 0.00) (-0.50 0.00 0.00)
               Im ( 0.87 0.00 0.00) ( 0.87 0.00 0.00)
 BsV( 3, 5: 6):Re (-0.50-0.50 0.00) (-0.50-0.50 0.00)
               Im ( 0.87 0.87 0.00) ( 0.87 0.87 0.00)
 BsV( 4, 5: 6):Re ( 0.00 0.50 0.00) ( 0.00 0.50 0.00)
               Im ( 0.00-0.87 0.00) ( 0.00-0.87 0.00)


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

       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: Mn_1      0.8300  0.6600  0.2500
       Sk(1): (u+r0.w-r0.p,v-r0.p,0)+i.r1.(w-p,-p,0)

       SYMM -x,-y,z+1/2                                              Atom: Mn_2     -0.8300 -0.6600  0.7500
       Sk(2): (u+r0.w-r0.p,v-r0.p,0)+i.r1.(w-p,-p,0)

       SYMM -y,x-y,z                                                 Atom: Mn_3     -0.6600  0.1700  0.2500
       Sk(3): (r0.v-p,-r0.u+r0.v-w,0)+i.r1.(v,-u+v,0)
```

4 basis functions

4 parameters

Get_mirreps in the Bilbao Server

Input: Parent SG and MSG as a subgroup



for each pair of basis functions a single parameter

Mn_3Sn (MAGNDATA #0.199)

$P6_3/mmc1'$ → *$Cmc'm'$* (-b, 2a+b, c; 0,0,0)

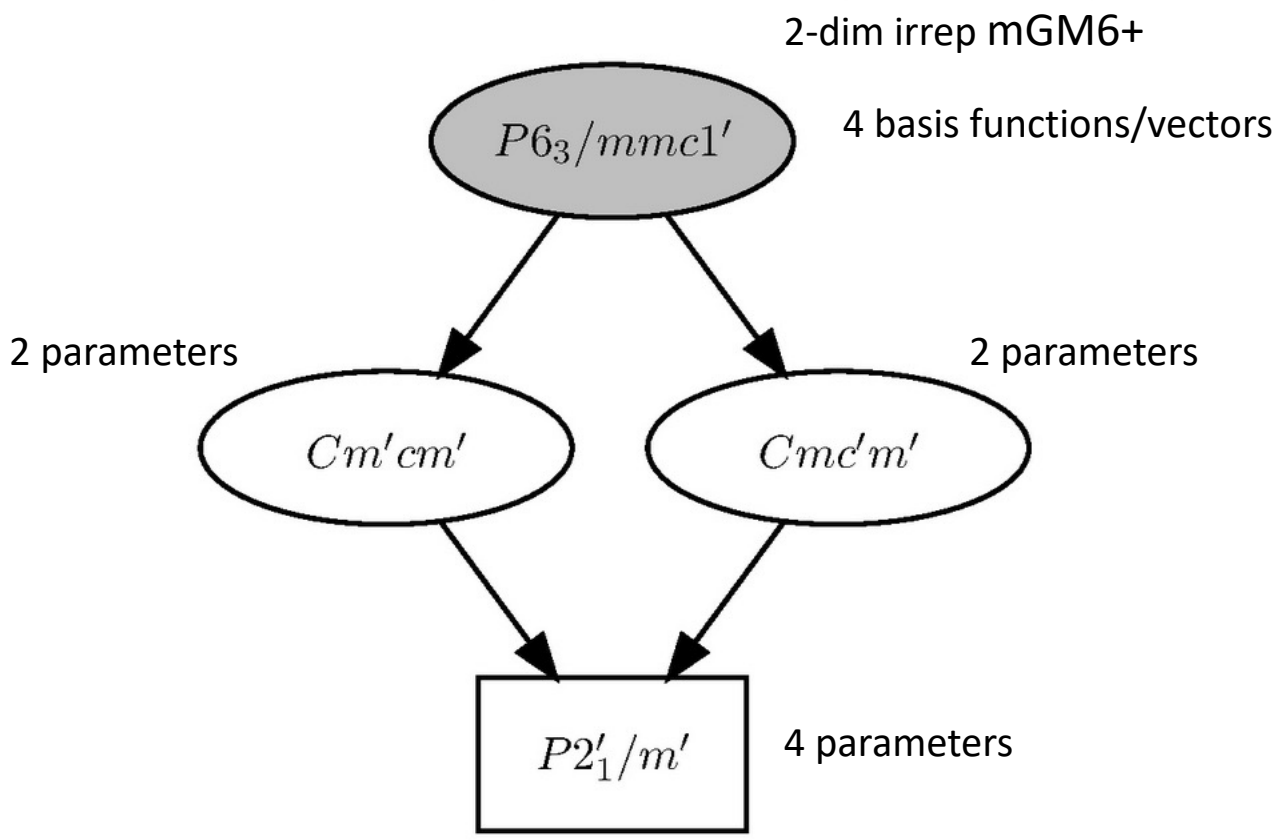
```
_space_group_magn.transform_BNS_Pp_abc  '-b,2a+b,c;0,0,0'
_space_group_magn.number_BNS  63.463
_space_group_magn.name_BNS  "C m c' m'"
_cell_length_a          5.66500
_cell_length_b          5.66500
_cell_length_c          4.53100
_cell_angle_alpha       90.00
_cell_angle_beta        90.00
_cell_angle_gamma       120.00

loop_
_space_group_symop_magn_operation.id
_space_group_symop_magn_operation.xyz
1 x,y,z,+1
2 -x,-x+y,-z,+1
3 -x,-y,-z,+1
4 x,x-y,z,+1
5 x,x-y,-z+1/2,-1
6 -x,-y,z+1/2,-1
7 -x,-x+y,z+1/2,-1
8 x,y,-z+1/2,-1

loop_
_space_group_symop_magn_centering.id
_space_group_symop_magn_centering.xyz
1 x,y,z,+1
```

```
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
Mn1_1 Mn 0.83880 0.67760 0.25000
Mn1_2 Mn  0.32240 0.16120 0.25000
Sn1 Sn 0.333333 0.666667 0.25000

loop_
_atom_site_moment.label
_atom_site_moment.crystalaxis_x
_atom_site_moment.crystalaxis_y
_atom_site_moment.crystalaxis_z
_atom_site_moment.symmform
Mn1_1 3.00(1) 3.00 0.00000 mx,my,0
Mn1_2 0.00000 -3.00 0.00000 0,my,0
```

3 free parameters

k=(0,0,0) 2-dim irrep mGM6+

$P6_3/mmc1'$ ⟶ $Cmc'm'$ (-b, 2a+b, c; 0,0,0)



Why 3 free parameters when described using the MSG Cmc’m’ instead of 2 parameters?

MAGNETIC REP output:

Wave-vectors of the star (1 vector):

GM:(0,0,0)

Wyckoff position	Decomposition into irreps
6h:(x,2*x,1/4)	mGM1-(1) ⊕ mGM2+(1) ⊕ mGM2-(1) ⊕ mGM3+(1) ⊕ mGM3-(1) ⊕ mGM4+(1) ⊕ mGM5+(2) ⊕ 2 mGM5-(2) ⊕ 2 mGM6+(2) ⊕ mGM6-(2)

In parentheses the dimensions of the irreducible representations of the little group of k

List of physically irreducible representations and order parameters between a parent group and a given subgroup.

Get_mirreps

Input data

input

Group→subgroup	Transformation matrix
$P6_3/mmc1'$ (N. 194.264)→$Cmc'm'$ (N. 63.463)	$\begin{pmatrix} 0 & 2 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$

Representations and order parameters

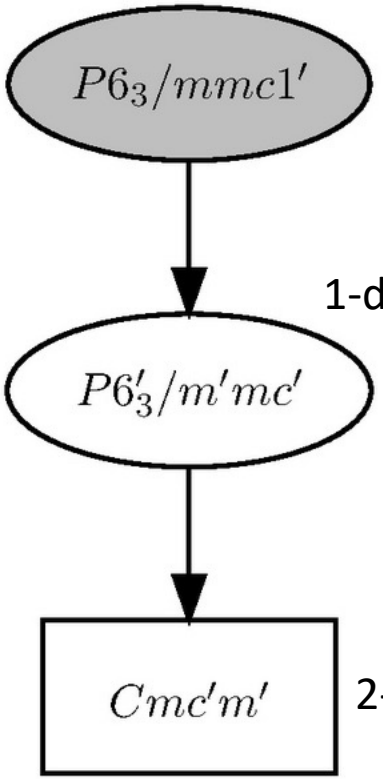
output

Show the graph of isotropy subgroups

k-vectors	irreps and order parameters	isotropy subgroup transformation matrix	link to the irreps
GM: (0,0,0)	GM_1^+: (a)	$P6_3/mmc1'$ (No. 194.264) a,b,c;0,0,0	matrices of the irreps
	GM_5^+: (a, a/√3)	$Cmcm1'$ (No. 63.458) -b,2a+b,c;0,0,0	
	mGM_3^+: (a)	$P6_3'/m'mc'$ (No. 194.269) a,b,c;0,0,0	
	mGM_6^+: (a,a/√3)	$Cmc'm'$ (No. 63.463) -b,2a+b,c;0,0,0	

2 magn. irreps allowed

Case 2: the MSG of the structure is compatible with more than one irrep



1-dim irrep mGM3+

2-dim irrep mGM6+

Von Neumann principle:
Everything that keeps the symmetry Cmc’ m’ is allowed and can happen…
Anything that keeps the symmetry P6’$_3$/m’ mc’ keeps the symmetry of its subgroup Cmc’ m’
THEREFORE…. a spin arrangement according to the irrep mGM3+ is also allowed in the structure with MSG Cmc’ m’

FullProf can refine under a MSG the amplitudes of the irrep modes compatible with the MSG using output of ISODISTORT

Part of the pcr file created with ISODISTORT:

This is the future and is already available!

```
!-------------------------------------------------------------------------------
AMPLIMODES for FullProf          FIX xyz
!
!Nat Dis Ang Pr1 Pr2 Pr3 Jbt Irf Isy Str Furth       ATZ    Nvk Npr More
  3   0   0   0.0 0.0 1.0  -6   0   2   0    3       1000.0  0   7   0
Cmc'm'  number:  63.463   <--Magnetic Space Group Symbol (UNI symbol and BNS number)
Transform to standard:  b,-2a-b,c;0,0,0  <--Basis transformation from alt setting to standard BNS
Parent space group:  P6_3/mmc  IT_number:  194  <--Nonmagnetic Parent Group
Transform from Parent:  a,b,c;0,0,0  <--Basis transformation from parent to current setting
!
! Atom Typ    Mag Vec      X         Y         Z        Biso      Occ  N_type  Spc/Fftype
!       Rx        Ry        Rz        Ix        Iy        Iz     MagPh
Mn1_1  MMN2     1    0  -0.16120  0.67760   0.25000   0.50000  0.50000      1    1
                           0.00      0.00      0.00      0.00     0.00
     0.00000   0.00000   0.00000   0.00000   0.00000   0.00000  0.00000
                           0.00      0.00      0.00      0.00     0.00
Mn1_2  MMN2     1    0  -1.67760 -0.83880   0.25000   0.50000  0.25000      1    1
                           0.00      0.00      0.00      0.00     0.00
     0.00000   0.00000   0.00000   0.00000   0.00000   0.00000  0.00000
                           0.00      0.00      0.00      0.00     0.00
Sn1    SN       0    0  -0.66667 -0.33333   0.25000   0.50000  0.25000      0    2
                           0.00      0.00      0.00      0.00     0.00
! Basis vectors of magnetic symmetry modes for each atom
M_MODES   6
! Nm Atom  Irrep      Mx       My       Mz       Coeff
  1 Mn1_1  mGM3+      0.0721   0.0000   0.0000   1.00
  1 Mn1_2  mGM3+      0.0000   0.0721   0.0000   1.00
  2 Mn1_1  mGM6+      0.0510   0.1019   0.0000   1.00
  2 Mn1_2  mGM6+      0.0000   0.0000   0.0000   1.00
  3 Mn1_1  mGM6+      0.0510   0.0000   0.0000   1.00
  3 Mn1_2  mGM6+      0.0000  -0.1019   0.0000   1.00
! Amplitudes of Magnetic Symmetry Modes
MA_MODES   3   2
    A1_mGM3+         0.00000    1.00
    A2_mGM6+         0.00000    1.00
    A3_mGM6+         0.00000    1.00
!
```

mode 1 mGM3+

mode 2 mGM6+

mode 3 mGM6+

mode amplitudes to refine

Description of the irrep basis vectors involved

FullProf can refine under a MSG the amplitudes of the irrep modes compatible with the MSG using output of ISODISTORT

Part of the pcr file created with ISODISTORT:

```
! Basis vectors of magnetic symmetry modes for each atom
M_MODES    6
! Nm Atom   Irrep      Mx        My        Mz      Coeff
   1 Mn1_1   mGM3+      0.0721   0.0000   0.0000   1.00
   1 Mn1_2   mGM3+      0.0000   0.0721   0.0000   1.00
   2 Mn1_1   mGM6+      0.0510   0.1019   0.0000   1.00
   2 Mn1_2   mGM6+      0.0000   0.0000   0.0000   1.00
   3 Mn1_1   mGM6+      0.0510   0.0000   0.0000   1.00
   3 Mn1_2   mGM6+      0.0000  -0.1019   0.0000   1.00
! Amplitudes of Magnetic Symmetry Modes
MA_MODES    3    2
     A1_mGM3+          0.00000    1.00
     A2_mGM6+          0.00000    1.00
     A3_mGM6+          0.00000    1.00
!
```

mode 1 mGM3+ → Mn1_1 (a,0,0); Mn1_2 (0,a,0)

mode 2 mGM6+ → Mn1_1 (a,2a,0); Mn1_2 (0,0,0)

mode 3 mGM6+ → Mn1_1 (a,0,0); Mn1_2 (0,-2a,0)

Refinement in terms of the amplitudes of the three irrep basis modes/vectors compatible with the MSG

Description of the posible irrep basis vectors involved in the structure under a fixed MSG: The spins of all atoms in the unit are NOT needed! Only those in the asymmetric unit. The MSG operations takes care of rest.

When defined under the MSG symmetry of the structure, the description of the basis modes/vectors:

- **does not require complex functions**
- **does not require full listing of the spins in the unit cell.**

FullProf can refine under a MSG the amplitudes of the irrep modes compatible with the MSG using output of ISODISTORT

Part of the pcr file created with ISODISTORT:

```
! Basis vectors of magnetic symmetry modes for each atom
M_MODES    6
! Nm Atom   Irrep      Mx       My       Mz       Coeff
   1 Mn1_1   mGM3+      0.0721   0.0000   0.0000   1.00
   1 Mn1_2   mGM3+      0.0000   0.0721   0.0000   1.00
   2 Mn1_1   mGM6+      0.0510   0.1019   0.0000   1.00
   2 Mn1_2   mGM6+      0.0000   0.0000   0.0000   1.00
   3 Mn1_1   mGM6+      0.0510   0.0000   0.0000   1.00
   3 Mn1_2   mGM6+      0.0000  -0.1019   0.0000   1.00
! Amplitudes of Magnetic Symmetry Modes
MA_MODES    3   2
     A1_mGM3+          0.00000    1.00
     A2_mGM6+          0.00000    1.00
     A3_mGM6+          0.00000    1.00
!
```

mode 1 mGM3+ → Mn1_1 (a,0,0); Mn1_2 (0,a,0)

mode 2 mGM6+ → Mn1_1 (a,2a,0); Mn1_2 (0,0,0)

mode 3 mGM6+ → Mn1_1 (a,0,0); Mn1_2 (0,-2a,0)

param. to refine

Refinement solution in terms of the amplitudes of the three irrep basis modes:

A1_mGM3+ = 0 A2_mGM6+ = A_3mGM6+ ≠0

Choice of basis modes for each irrep is not unique, if several ones. Alternative linear combinations are posible modes:

Mn1_1 (a,2a,0) Mn1_2 (0,0,0)	+	Mn1_1 (a,0,0) Mn1_2 (0,-2a,0)	=	Mn1_1 (2a,2a,0) Mn1_2 (0,-2a,0)	==	Mn1_1 (1,1,0) Mn1_2 (0,-1,0)
Mn1_1 (a,2a,0) Mn1_2 (0,0,0)	-	Mn1_1 (a,0,0) Mn1_2 (0,-2a,0)	=	Mn1_1 (0,2a,0) Mn1_2 (0,2a,0)	==	Mn1_1 (0,1,0) Mn1_2 (0,1,0)

from the mCIF file of the structure:

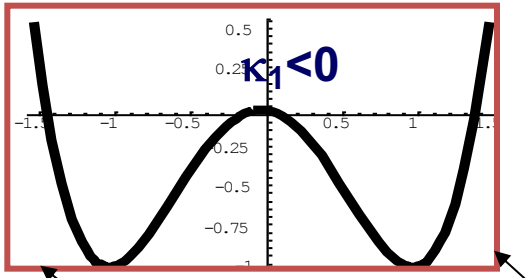
```
loop_
_atom_site_moment.label
_atom_site_moment.crystalaxis_x
_atom_site_moment.crystalaxis_y
_atom_site_moment.crystalaxis_z
_atom_site_moment.symmform
Mn1_1 3.00(1) 3.00 0.00000 mx,my,0
Mn1_2 0.00000 -3.00 0.00000 0,my,0
```

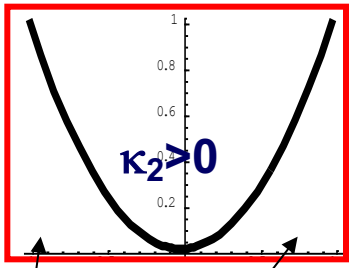
- The secondary irrep mGM3+ spin mode is absent.
- Only the irrep mGM6+ mode is present, but the model includes an additional constraint (c_2=0), which is not forced by the restriction to this single irrep. It is a FM mode along b (weak Ferromagnetism).

Magnetic moment components (μ_B) of magnetic atoms, symmetry constraints and moment magnitudes	Mn1_1 3.00(1) 3.00 0.0 (mx,my,0) 3.00(1) Mn1_2 0.0 -3.00 0.0 (0,my,0) 3.00(1)

Primary basis mode(s) and amplitude(s) C_i (in μ_B)	mGM6+, mode 1: Mn1_1 (1, 1 , 0) C_1= 3.00(1) Mn1_2 (0, -1, 0) mGM6+, mode 2: C_2=0.0 Mn1_1 (0, 1, 0) Mn1_2 (0, 1, 0)
Secondary basis mode(s) and amplitude(s) C_i (in μ_B)	mGM3+, mode 3: Mn1_1 (1, 0, 0) C_3=0.0 Mn1_2 (0, 1, 0)

Why secondary modes



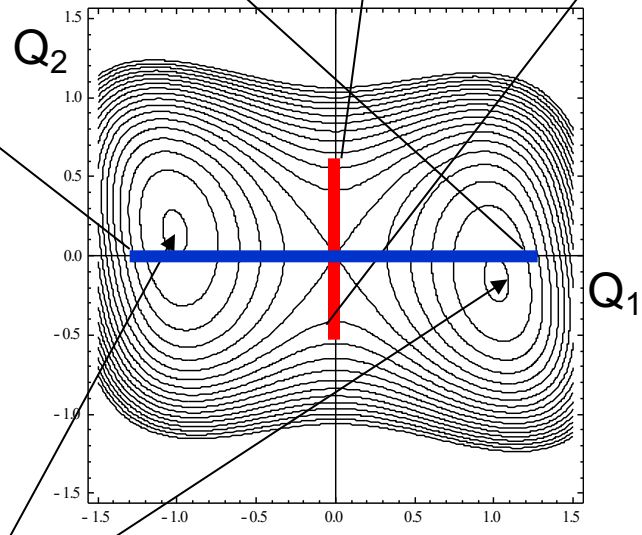


Example of an energy map with primary (Q_1) and secondary (Q_2) distortion modes:

$$E = E_o + \tfrac{1}{2}\,\kappa_1 Q_1^2 + \tfrac{1}{2}\,\kappa_2 Q_2^2 + \gamma\, Q_1^3\, Q_2 + \ldots$$

($\kappa_1 < 0$, $\kappa_2 > 0$)

Anharmonic allowed coupling



Equivalent ferroic stable structures

We do not have to worry about the coupled secondary irreps, they are automatically included in the description under the MSG…..

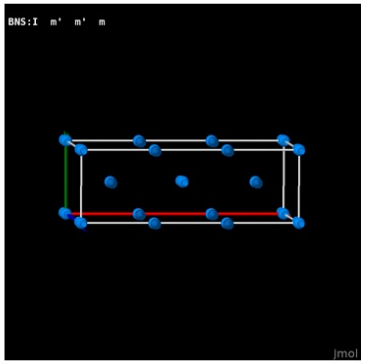
is it an advantage or a nuisance?

It depends …..

- In many cases these induced effects are negligible (weak spin-orbit coupling effects) and we would like to have these secondary degrees of freedom set to zero from the start, and then some additional restrictions in the model have to be added to describe only the primary mode.

- In other cases, we want to be aware of all possible degrees of freedom which are set free by the primary magnetic ordering and the MSG takes care of all of them automatically.

A simple example where the automatic inclusion of secondary irreps by the MSG is advantageous:



UAu_2Si_2 (#1.0.12) **Im’m’m**

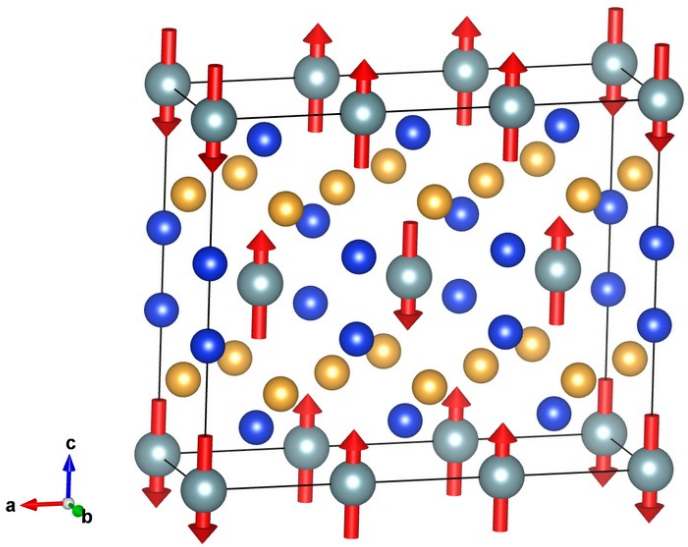
view in Jmol
Download mcif file
Download vesta file (all atoms)
Download vesta file (magnetic atoms only)

submit to STRCONVERT

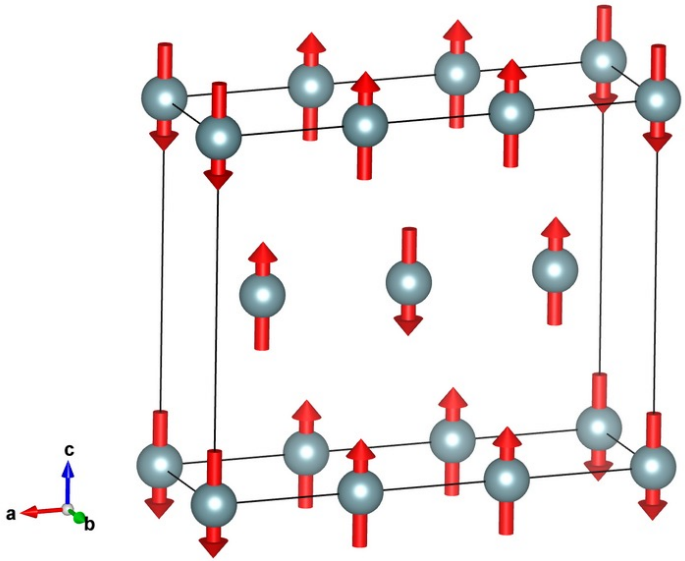
UAu2Si2 (#1.0.12)

k=(2/3,0,0)

Allowed third harmonic with k=0 is automatically included

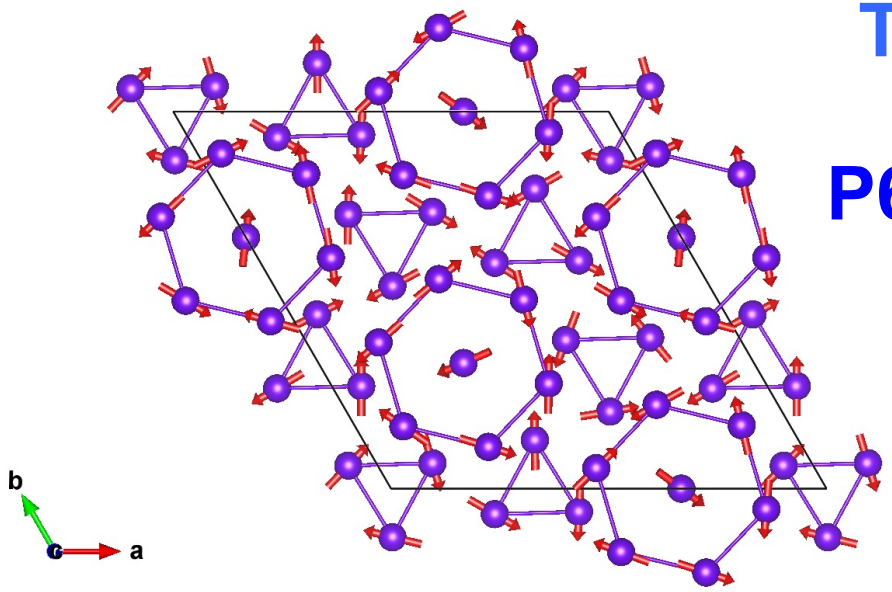


Magnetic structure with all atoms



Magnetic structure with only magnetic atoms

A complex example where the automatic inclusion of secondary irreps by the MSG is an advantage:



$Tb_{14}Ag_{51}$ (Magndata #1.0.52)

P6/m → P-6' (2a+b,-a+b,c;1/3,-1/3,0)

$k_1 = (1/3,1/3,0)$

third harmonic: $k_2 = 3k = (0,0,0)$

Active Irreps: *Irrep decomposition via* Get_mirreps

label	dim. full irrep	dim. small irrep	direction	action	number of modes	presence
mK4K6	4	2	special	primary	18	
mGM2+	1	1		secondary	4	yes
mGM1-	1	1		secondary	5	yes

Conclusions 1:

- **The assignment of MSG is a must:** Whatever method is employed to determine a commensurate magnetic structure, the final model has necessarily a certain symmetry that must be given by a MSG, which should be identified.

- **The description using the MSG in a crystallographic form is the best "way":** The simpler, more robust and unambiguous form of describing a commensurate magnetic structure is to use consistently its MSG and only give the atomic positions and magnetic moments of a set of symmetry independent atoms with respect to this MSG.

- **The MSG is relevant for all properties:** Properties of commensurate magnetic phases are constrained by their MSG, including their atomic positions. Any possible magneto-structural induced effect is constrained by the MSG.

Conclusions 2:

• ***Representation analysis of magnetic structures is NOT in general equivalent to the use of magnetic symmetry*** *(i.e. to give an irrep is not equivalent to give the magnetic space (superspace) group of the system).*

• **Irrep constraints additional to those of the MSG are not needed in most cases:** Only in the case that the MSG of the structure is compatible with more than one irrep for the magnetic arrangement, the restriction to a single irrep introduces additional constraints not taken into account by the MSG, and their existence has to be indicated extra. *In these cases the best approach is to combine magnetic symmetry and representation analysis.*

• **In the case of incommensurate structures similar considerations apply but with MSSGs**: The symmetry of these systems is described by the so-called magnetic superspace groups (MSSGs).