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

• 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 parent space group transforms in general the distorted structure into a different structure:

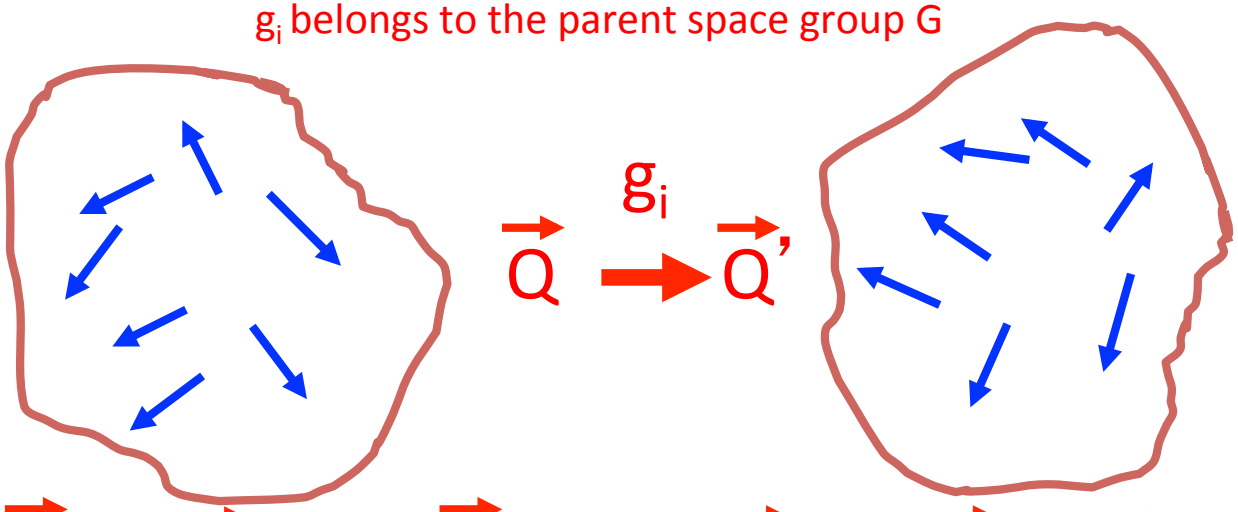
a distorted structure with a different distortion (domain-related), except for the operations that are maintained in the MSG, which keep it invariant or only change to opposite spins

• 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

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

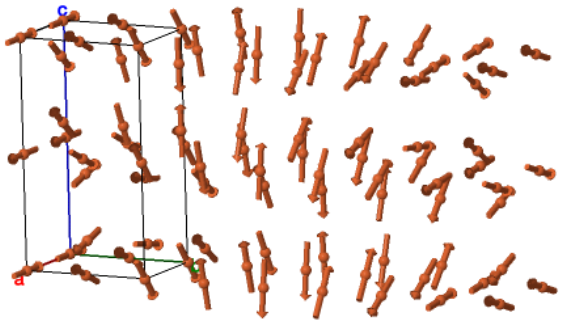
***for all g***

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**

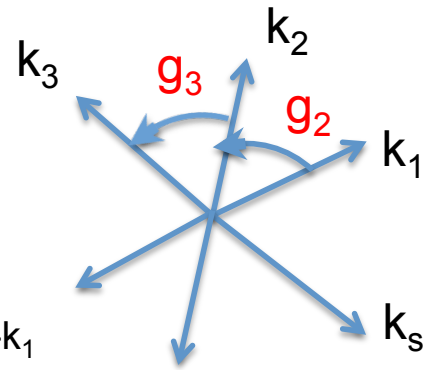


wave vector: $k_1$

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 staris

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 $-k_1$ is not in the star $*k_1$ this dimension is doubled)

## The Magnetic Representation is in general reducible:

First reduction: **WAVES**

subspaces of arrangements with different sets of propagation vectors:

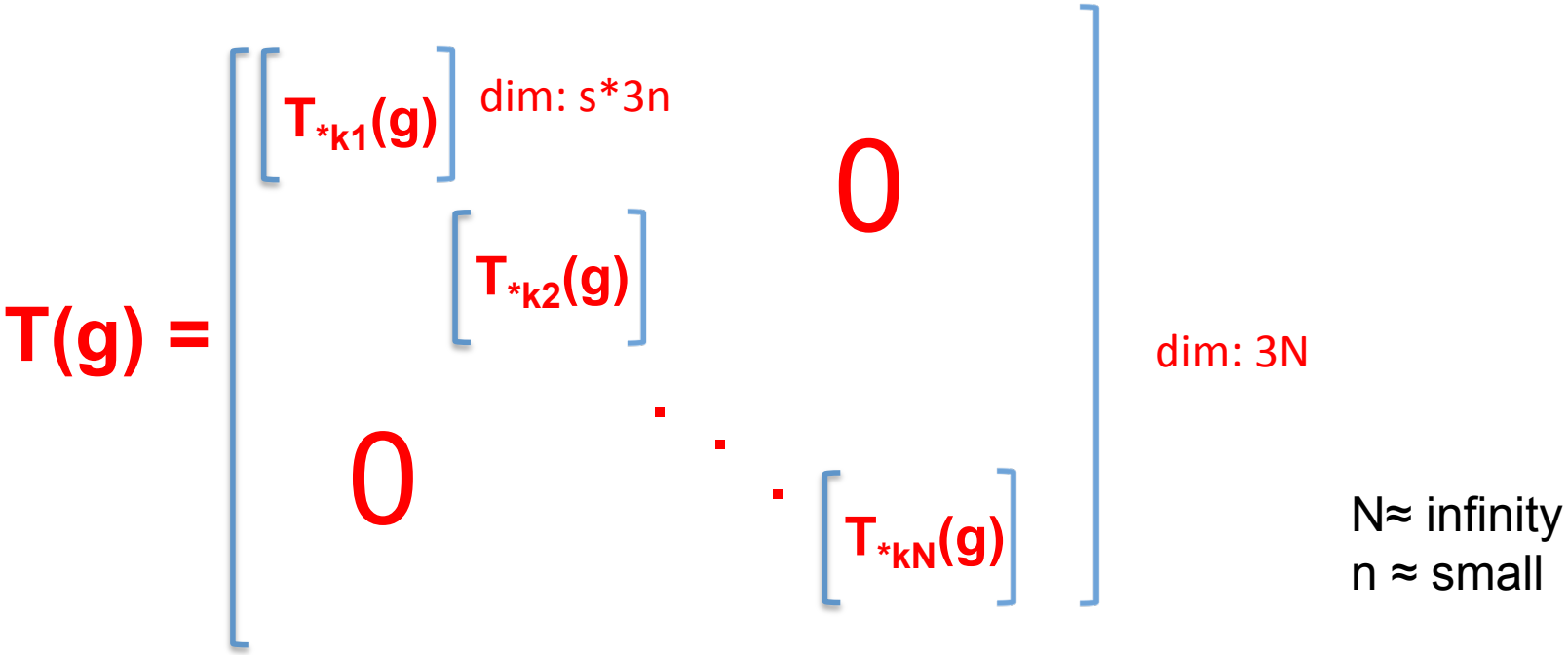
$$T(g) = \sum_{*\mathbf{k}} T_{*\mathbf{k}}(g)$$ **ALL *k within the BZ**

$*\mathbf{k} = \{\mathbf{k}_1,\ldots,\mathbf{k}_s\}$ 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

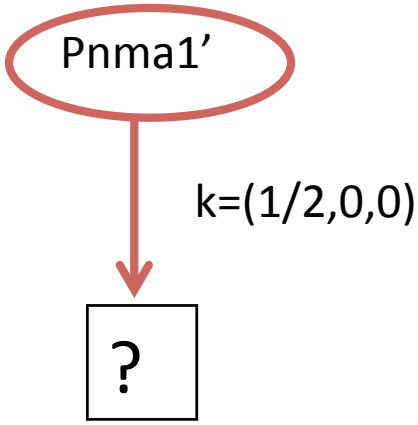
n: number of magnetic atoms in the ***primitive*** unit cell


T(g) =
T*k1(g)
dim: s*3n
T*k2(g)
0
0
T*kN(g)
dim: 3N
N≈ infinity
n ≈ small

# 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)?

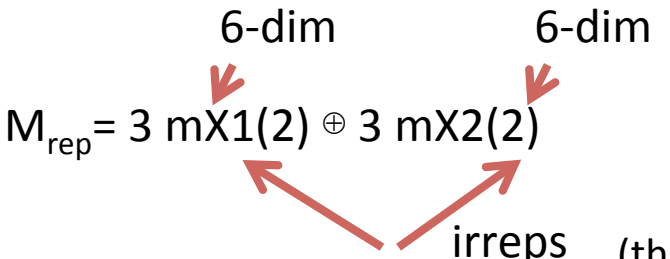
star: only one k!




$HoMnO_3$

*Mn at WP 4b*

Magnetic representation reduced to this k: dim 3x4=12. Further reducible in general




Decomposition into irreps

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

# Magnetic REP. : Decomposition of the magnetic representation into irreps

| Magnetic Symmetry and Applications | |
|---|---|
| MGENPOS | General Positions of Magnetic Space Groups |
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**MAGNETIC REP**: Decomposition of the magnetic representation into irreps.
(*for any 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

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

6-dim 6-dim

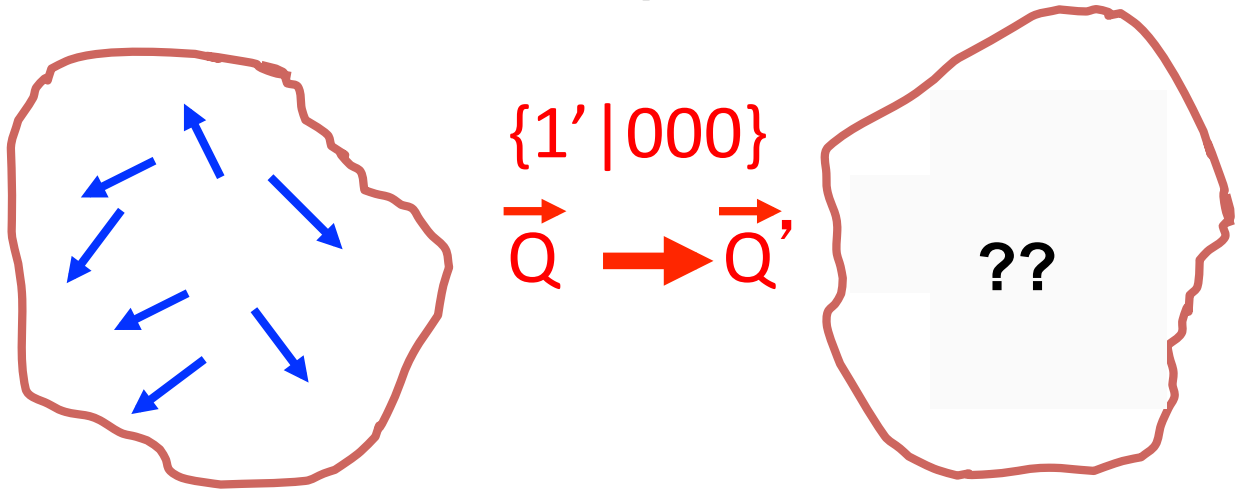
$M_{rep}$= 3 mX1(2) ⊕ 3 mX2(2)

irreps

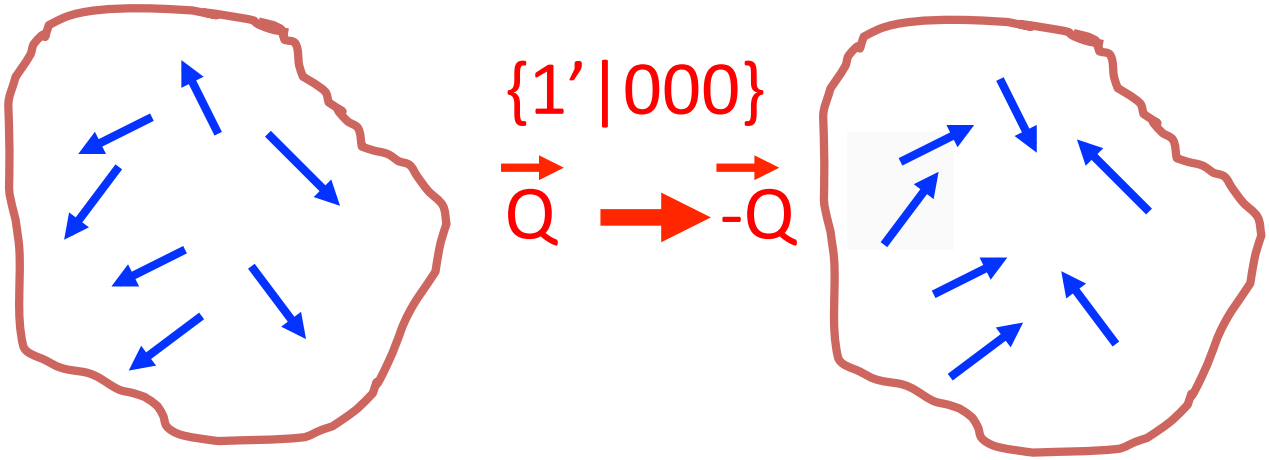
Decomposition into irreps

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

**The reason for the "m" in the irrep label:**



Why an "m" in the irrep label:




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

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'!**

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

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

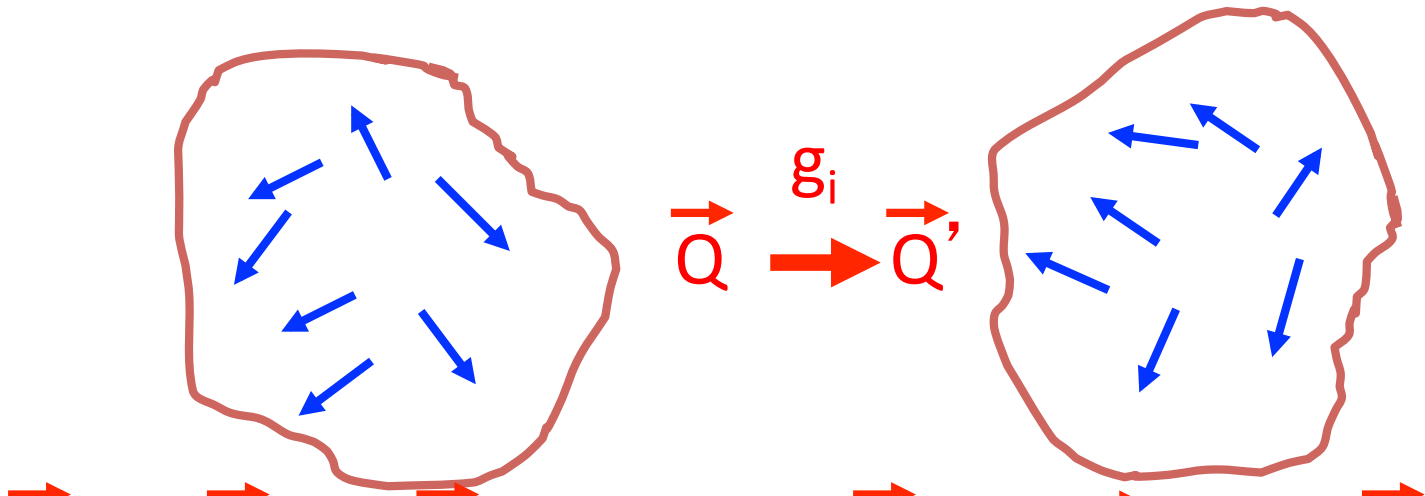
2 x2

12x12

k1=(1/2,0,0)

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

**LANDAU Theory:** If transition continuous , then T(g) must be an **IRREDUCIBLE representation** (irrep) of G




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

**$\{T(g)\}$ : 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 or "**basis vectors**" for each irrep: also a mathematical problem.

## 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.**

# KSUBGROUPSMAG : Filter with Irreps

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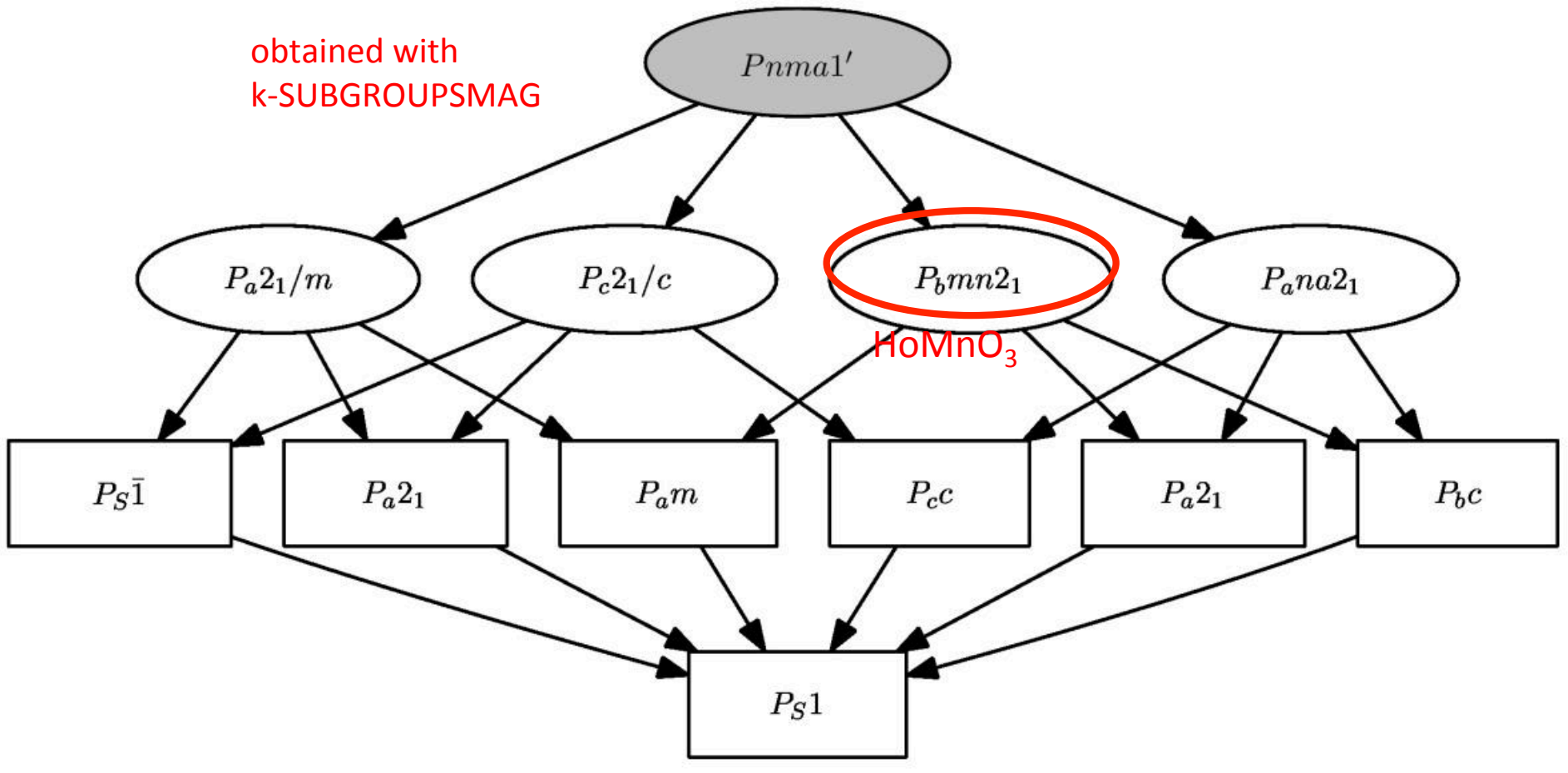
# Symmetry based modeling of magnetic structures

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

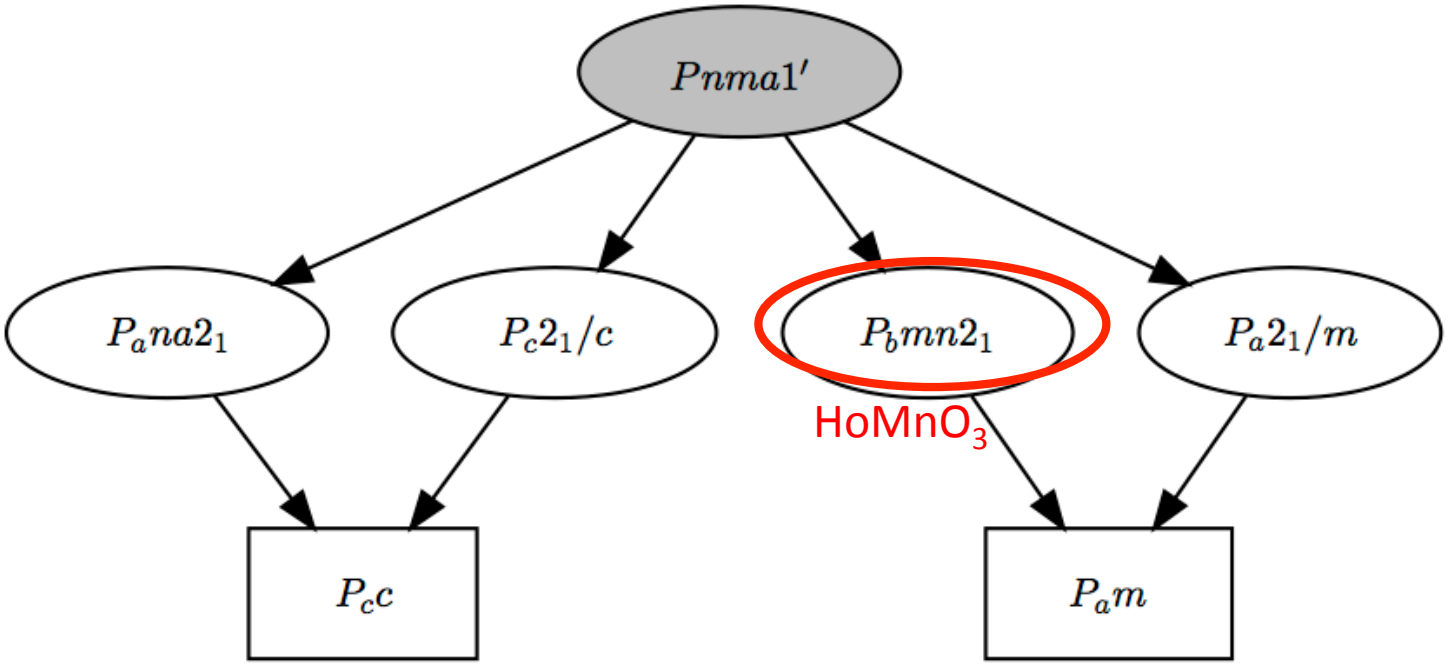



(magnetic cell= ($2a_p$,$b_p$,$c_p$))

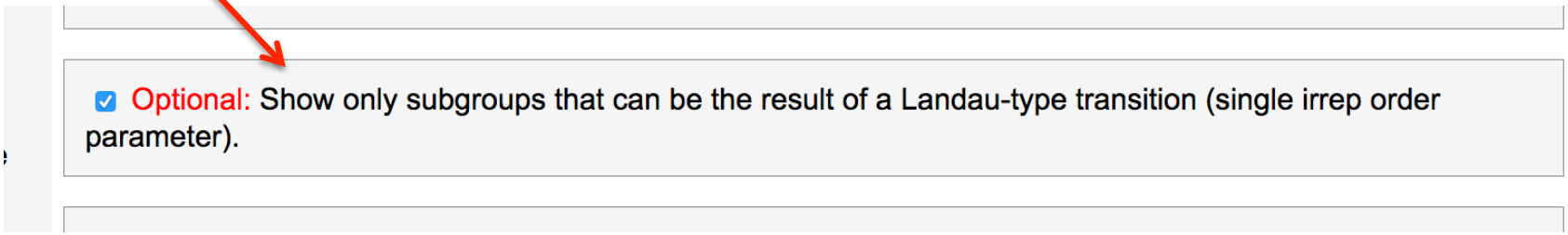
# Symmetry based modeling in magnetic structures

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)




obtained with k-SUBGROUPSMAG:



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 compatible with a given symmetry brea

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# 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*

for $P_amn2_1$

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

## 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,-a,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 |

# 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 $P_am$

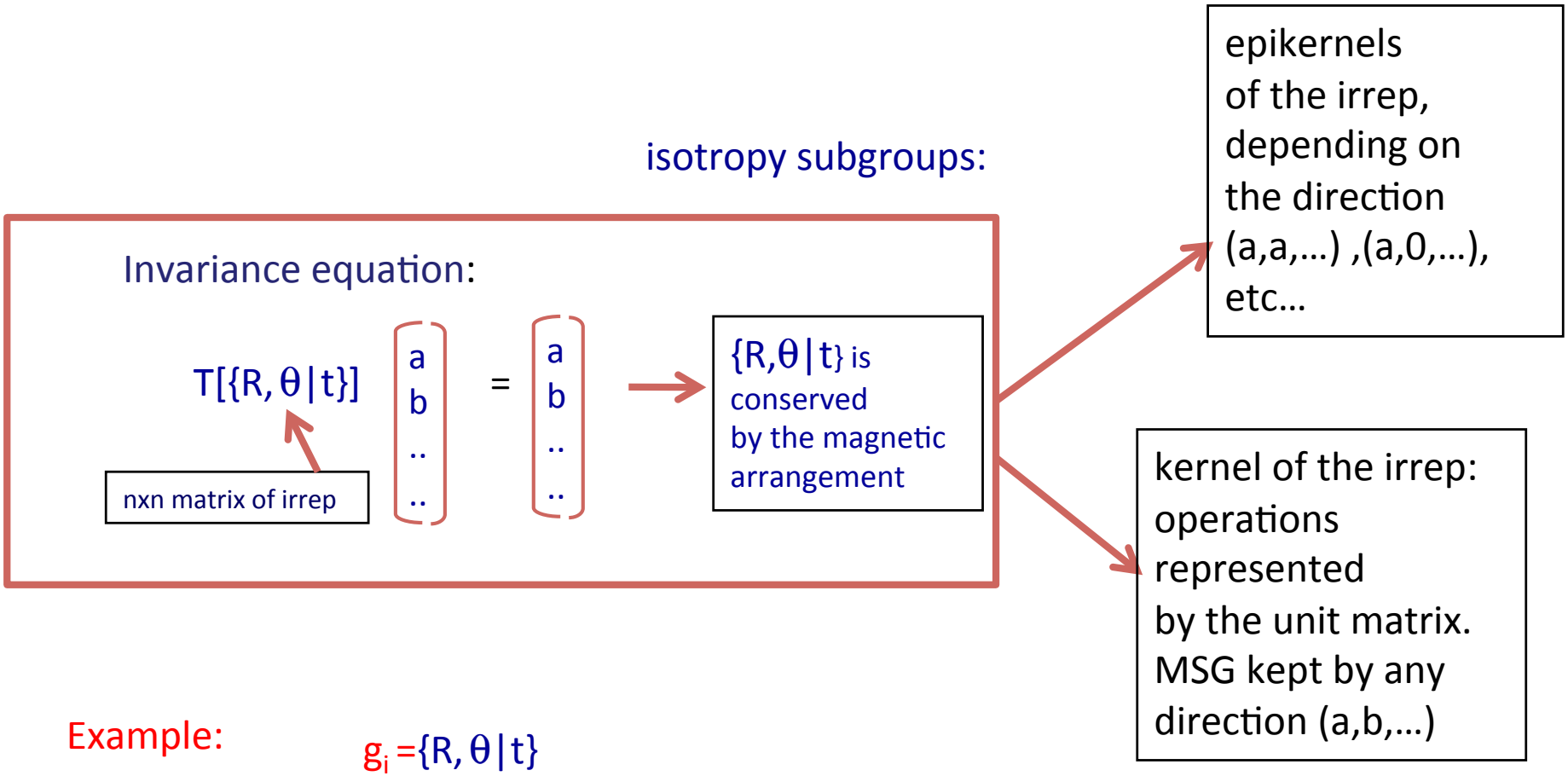
## Representations and order parameters

Show the graph of isotropy subgroups

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 |
| | $GM_4^+$: (a) | $P2_1/m$1' (No. 11.51) a,b,c;0,0,0 | |
| | $GM_2^-$: (a) | $Pmn2_1$1' (No. 31.124) b,-a,c;1/4,1/4,0 | |
| | $GM_3^-$: (a) | $Pmc2_1$1' (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 |

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




Example:

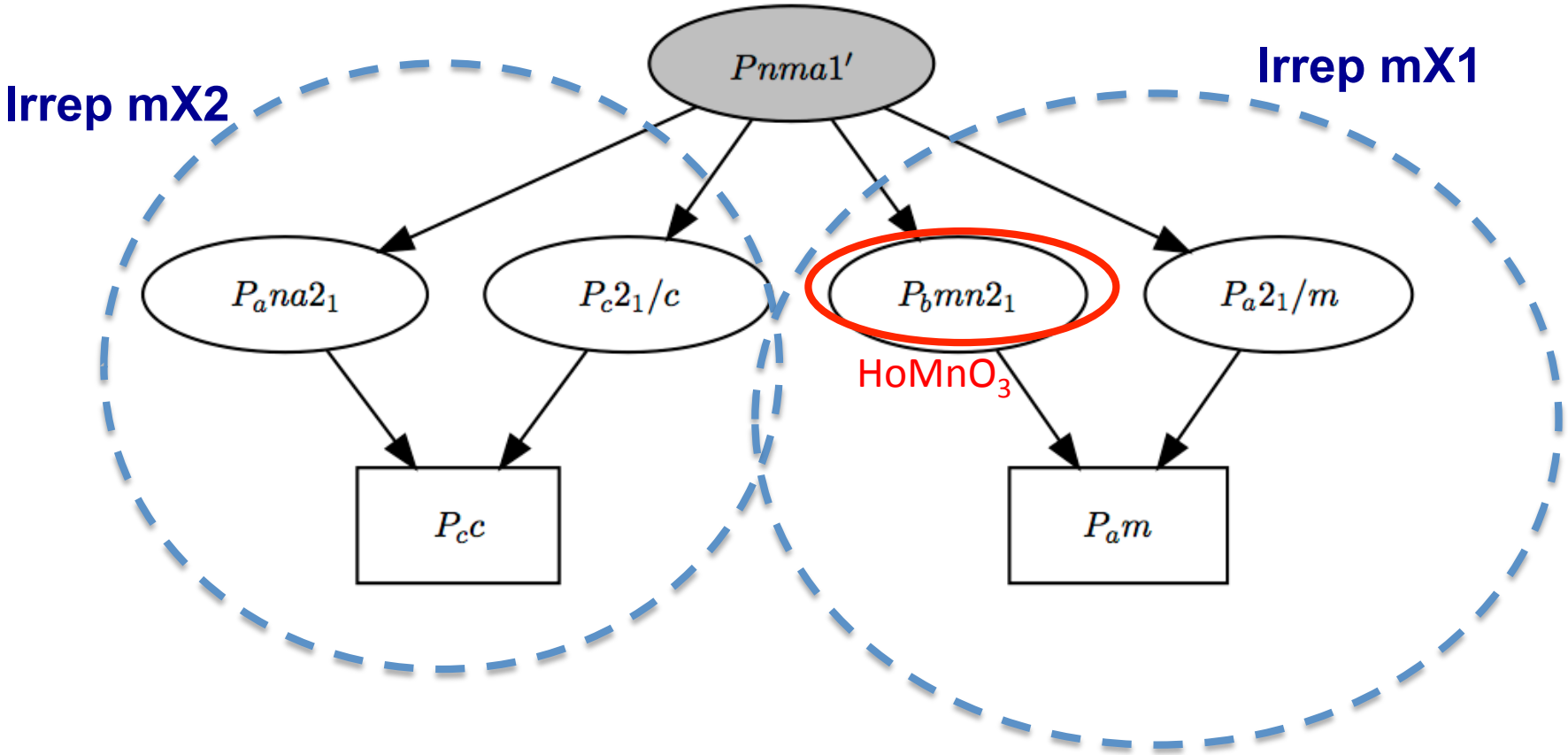
$g_i = \{R, \theta | t\}$

$T(g_i) = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$ $T(g_i) \begin{pmatrix} a \\ a \end{pmatrix} = \begin{pmatrix} a \\ a \end{pmatrix}$ ➔ $g_i$ will belong to the MSG if OP=(a,a)

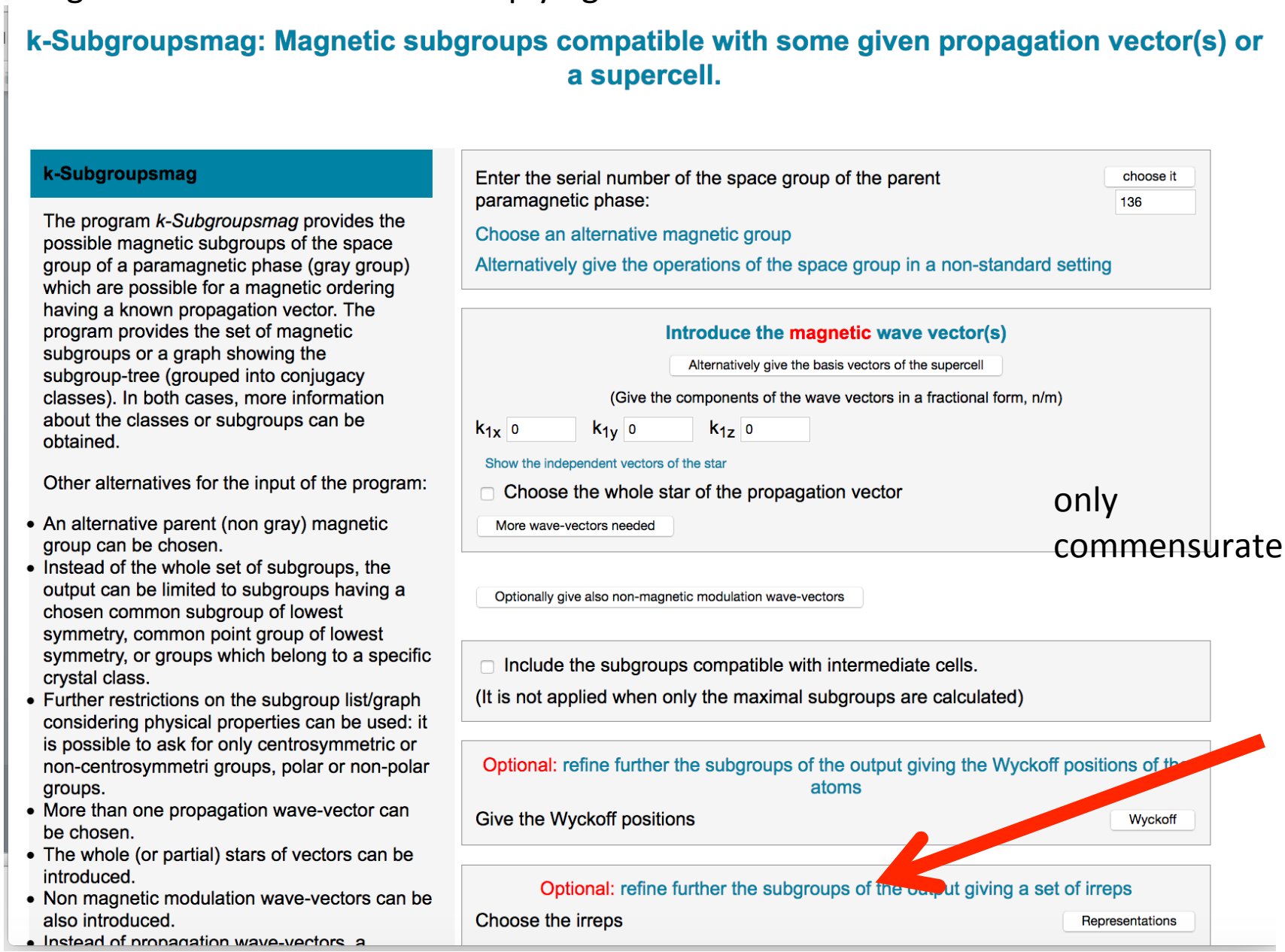
# Symmetry based modeling in magnetic structures

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)



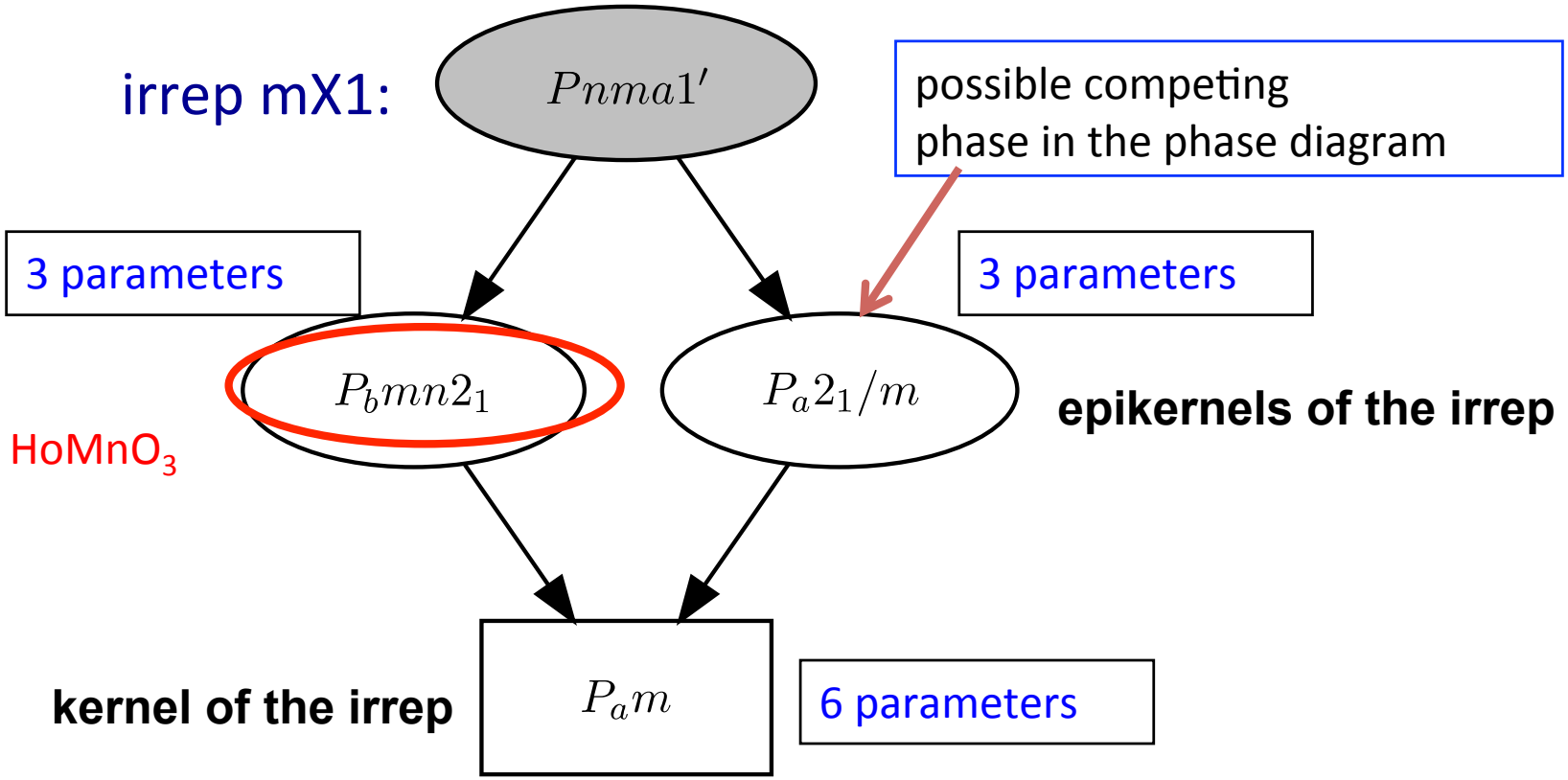
k-SUBGROUPSMAG determine the epikernels and kernel of any irrep and produce magnetic structural models complying with them.




only commensurate

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 vectors: 6 parameters

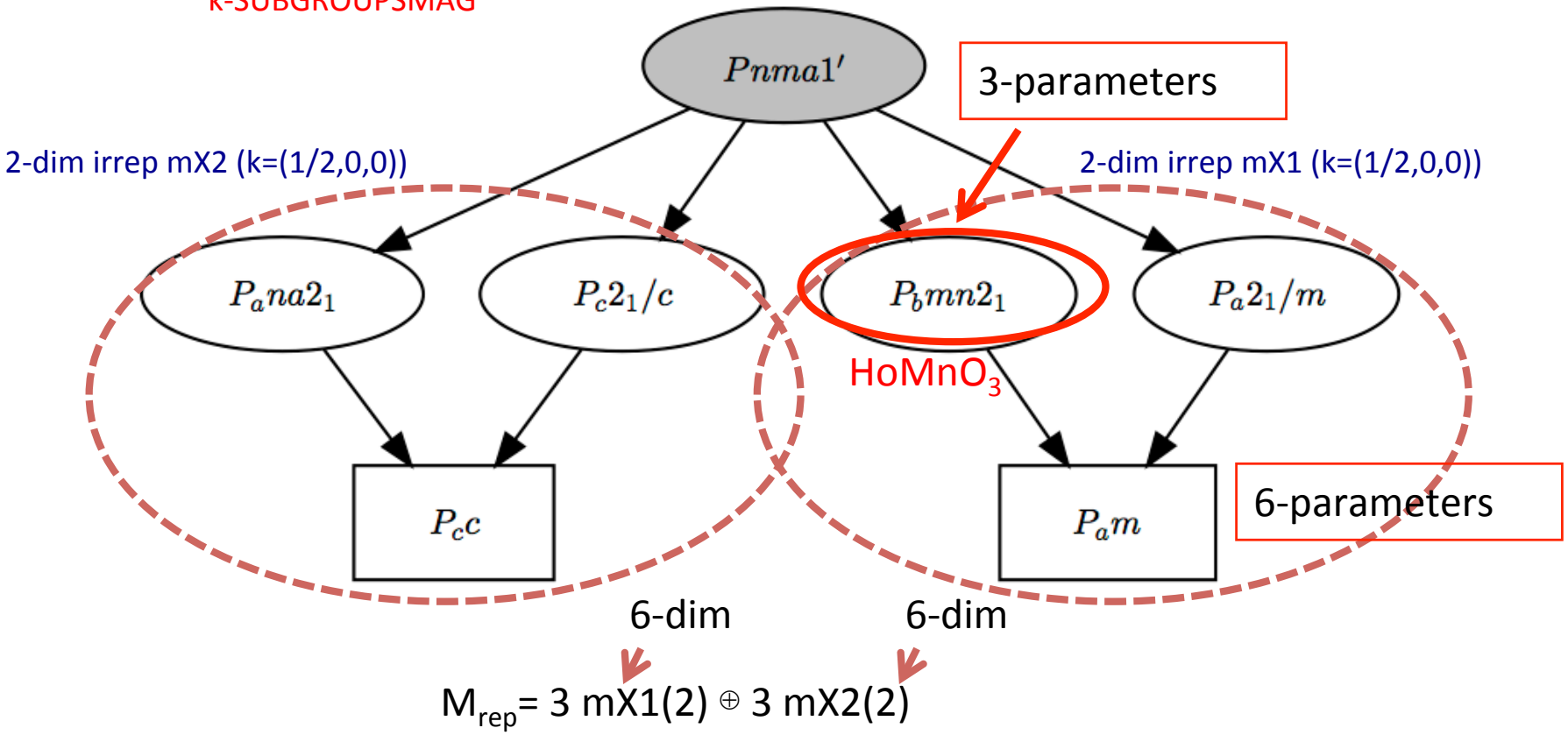
# Symmetry based modeling in magnetic structures

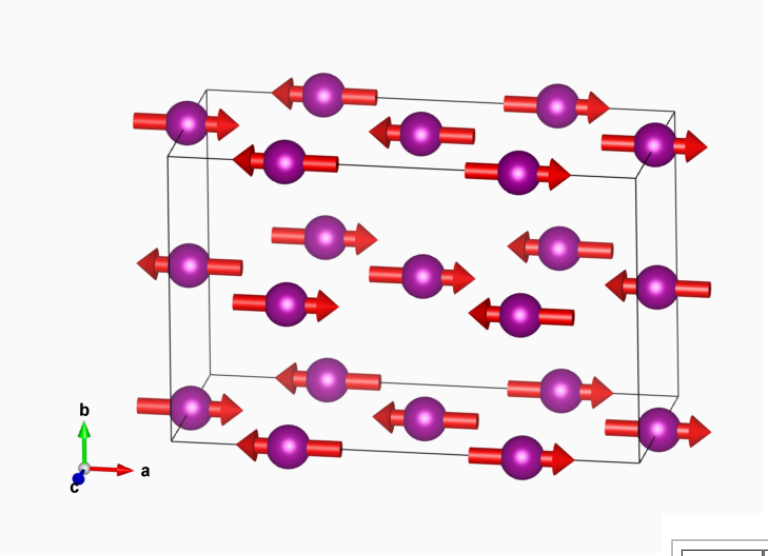
Possible magnetic symmetries for a magnetic phase with propagation vector (1/2,0,0) and parent space group Pnma

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

obtained with k-SUBGROUPSMAG

case 1: The MSG of structure is only compatible with a single irrep.






$HoMnO_3$ (*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: $P_b mn2_1$ (#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 |

3 free parameters

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 } |

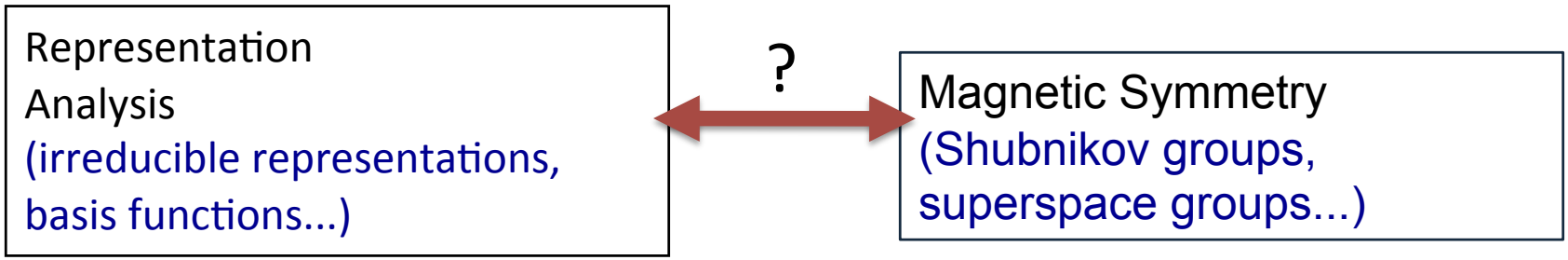
2-dim irrep mX1 but restricted to a special direction: fixed combination of each pair of spin basis functions => half number of degrees of freedom with respect to the only restriction to the irrep

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

**(case 1: The MSG of structure is only compatible with with a single irrep)**

# MSGs vs. Irreps

Commensurate magnetic structures:

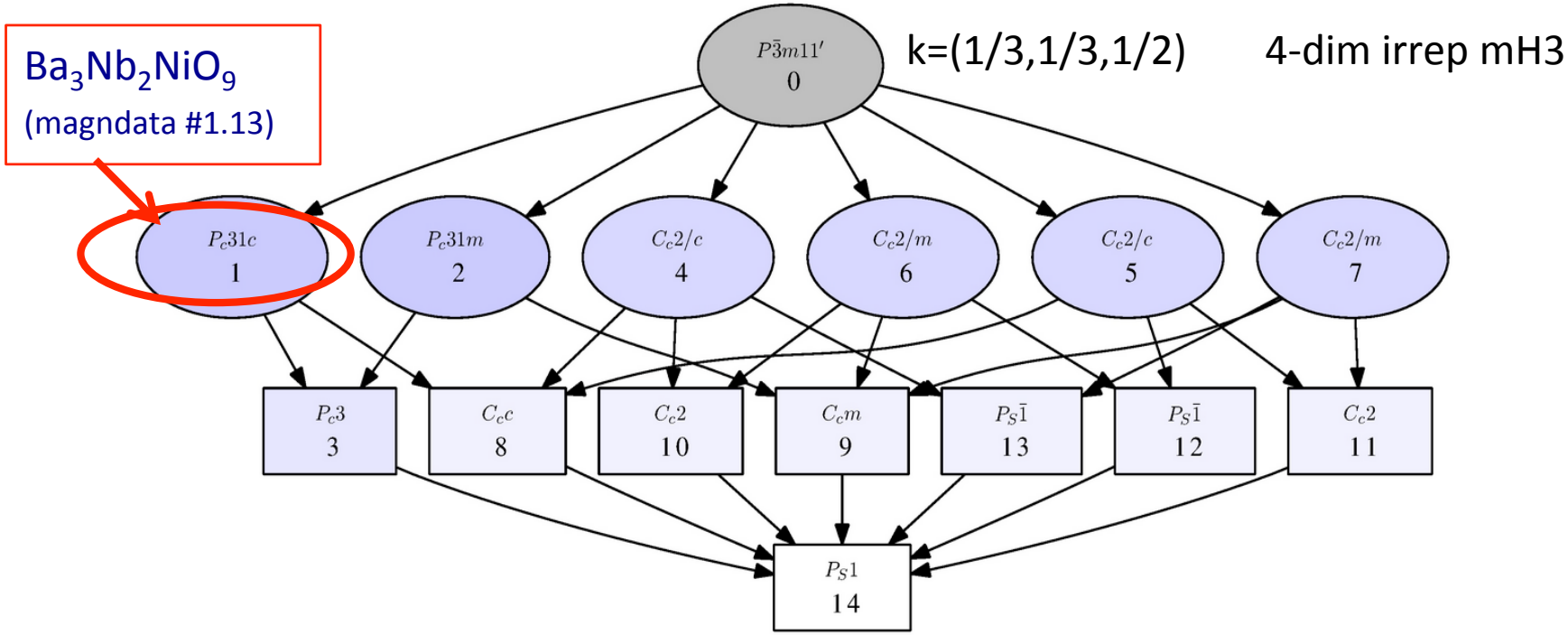



Identifying the active irrep(s) or the MSG are not alternative equivalent methods:

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:




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

## On the use of irreps as an "alternative" description to the use of the MSG for Case 1 structures

- **if the MSG of the structure is only compatible with a single irrep (the majority of cases): A description using irrep spin basis vectors does NOT bring any 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)

*$P6_3/mmc1'$* ⟶ *??*

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

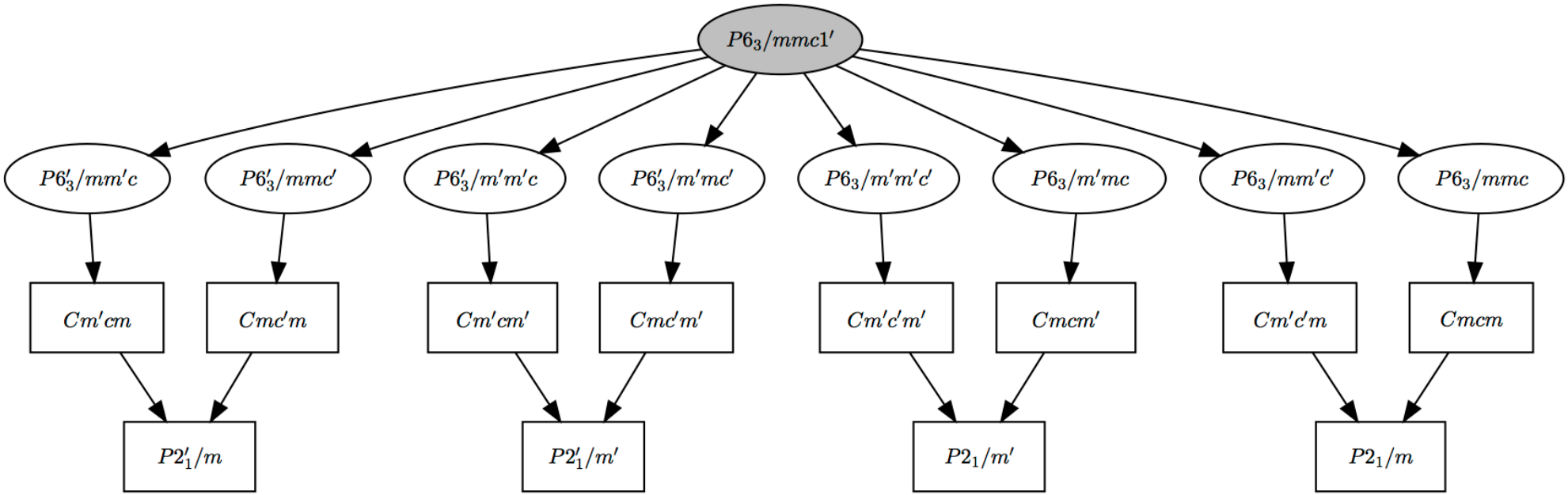
# $Mn_3Sn$

k=(0,0,0)

$P6_3/mmc1'$ ⟶ ??

Possible magnetic symmetries for a magnetic phase with propagation vector (0,0,0) and parent space group $P6_3/mmc$

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



# $Mn_3Sn$

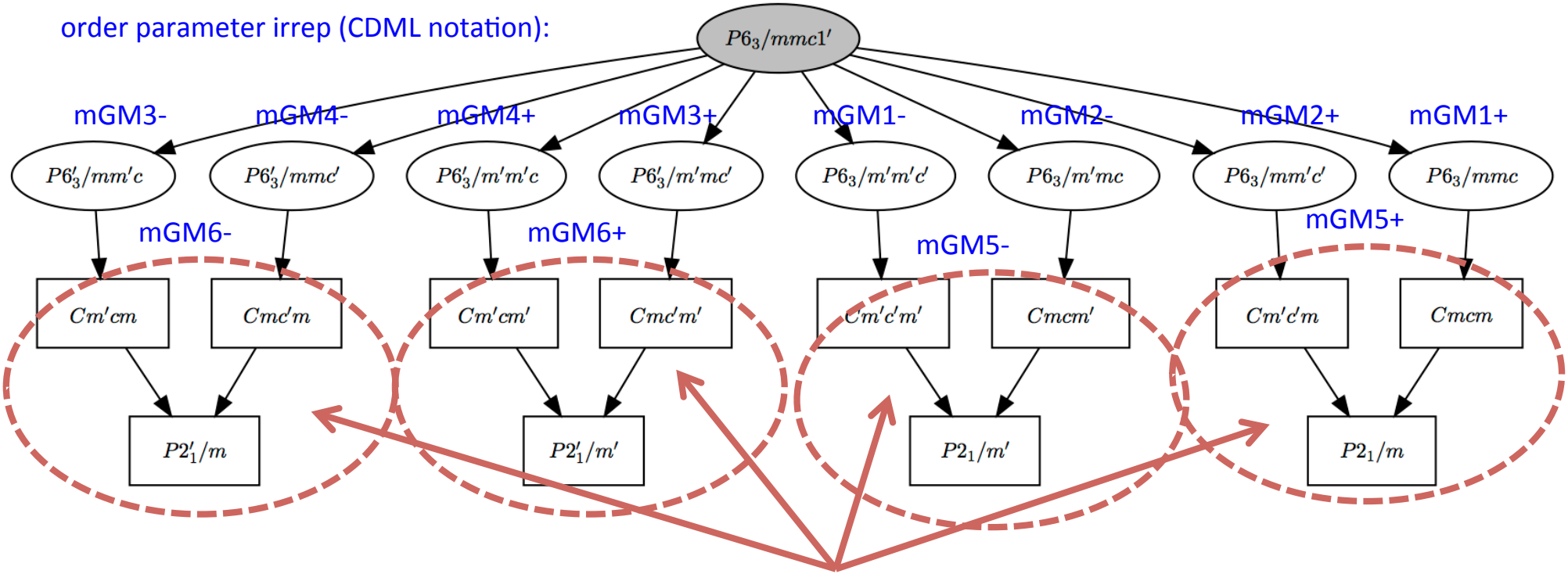
k=(0,0,0)

*$P6_3/mmc1'$* ⟶ *??*

Possible magnetic symmetries for a magnetic phase with propagation vector (0,0,0) and parent space group $P6_3/mmc$

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

order parameter irrep (CDML notation):




not k-maximal but possible as the result of a single active irrep

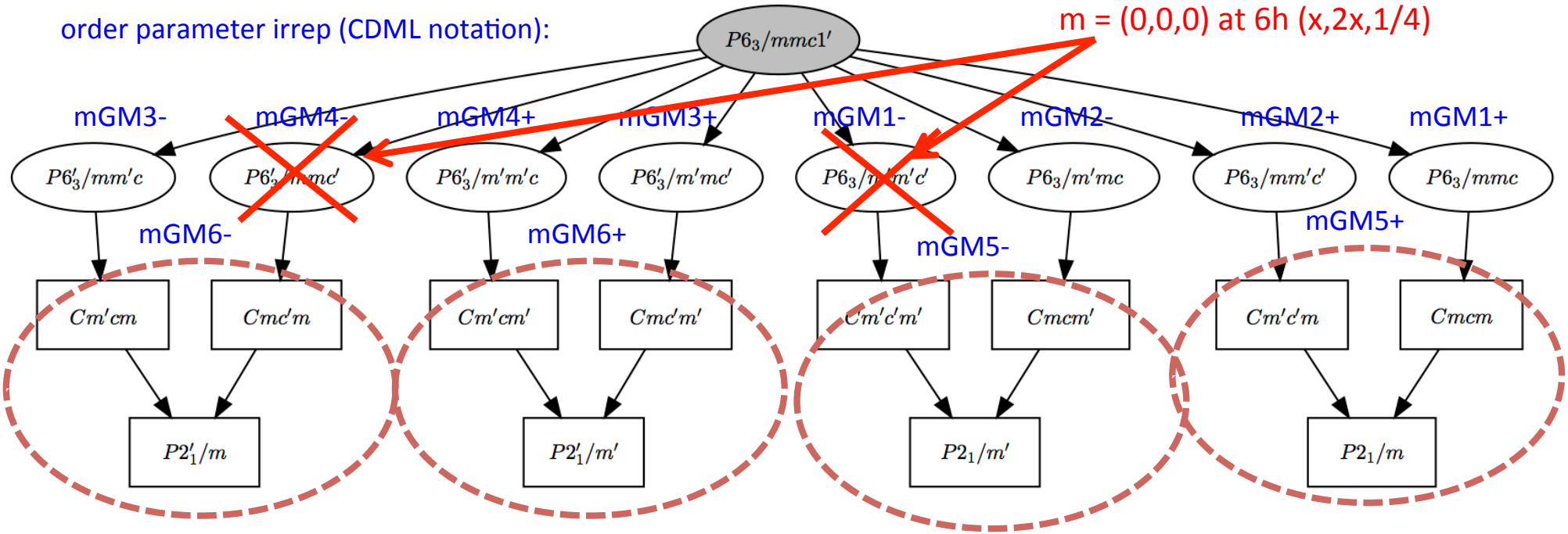
# $Mn_3Sn$

k=(0,0,0)

*$P6_3/mmc1'$* ⟶ *??*

Possible magnetic symmetries for a magnetic phase with propagation vector (0,0,0) and parent space group $P6_3/mmc$

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



$Mn_3Sn$

k=(0,0,0)

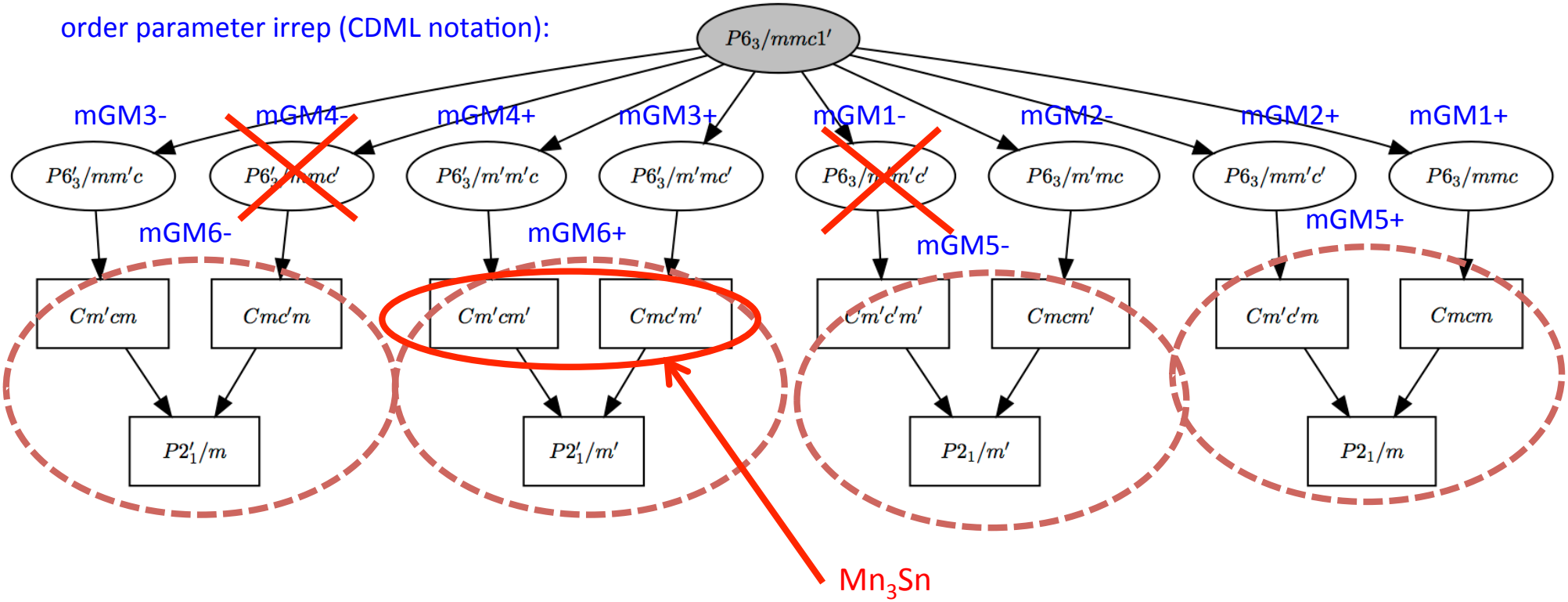
$P6_3/mmc1'$ → 2-dim irrep mGM6+

$Cmc'm'$ (-b, 2a+b, c; 0,0,0)

or

$Cm'cm'$ (-b, 2a+b, c; 0,0,0)

order parameter irrep (CDML notation):



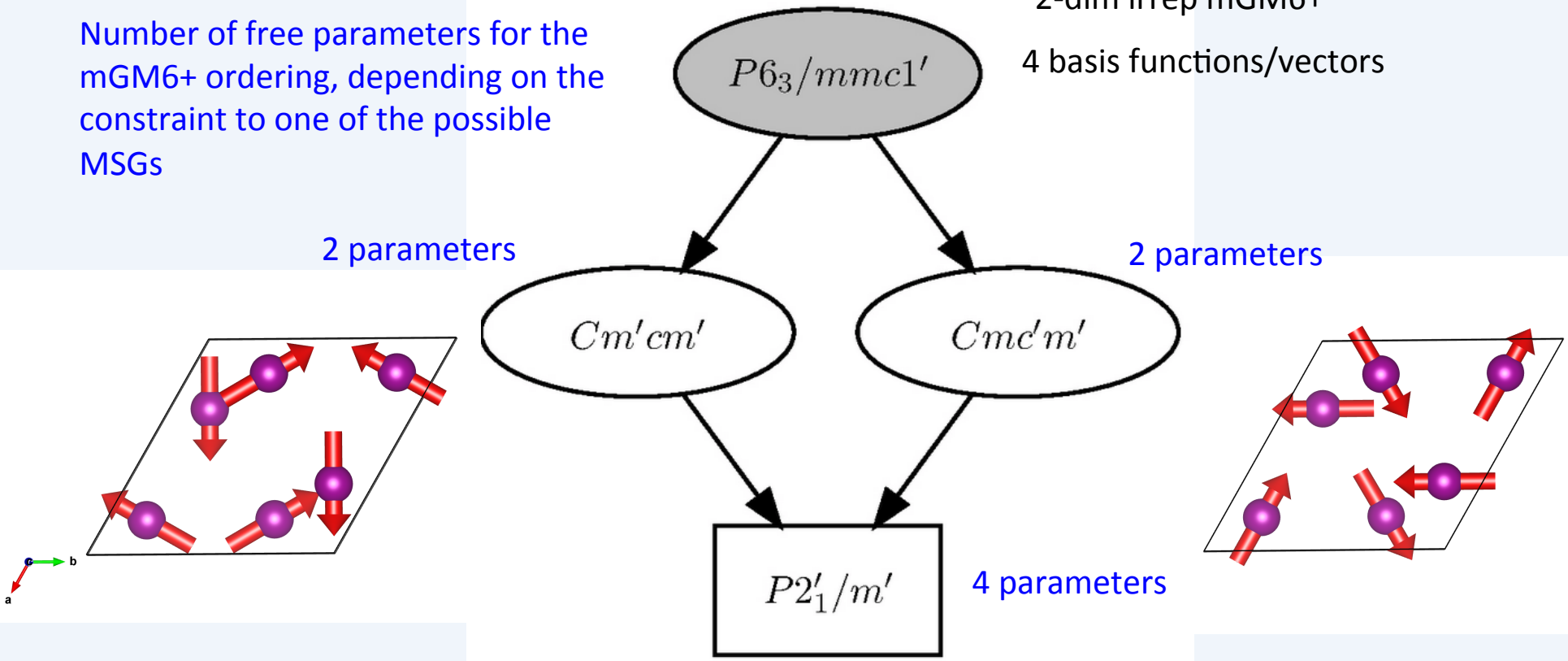
# $Mn_3Sn$

k=(0,0,0)

2-dim irrep mGM6+

4 basis functions/vectors

Number of free parameters for the mGM6+ ordering, depending on the constraint to one of the possible MSGs




**Wave-vectors of the star (1 vector):**

GM:(0,0,0)

**Descomposition of the magnetic representation(s) into irreps.**

6h:(x,2*x,1/4) → 1×mGM1-(1) ⊕ 1×mGM2+(1) ⊕ 1×mGM2-(1) ⊕ 1×mGM3+(1) ⊕

⊕ 1×mGM3-(1) ⊕ 1×mGM4+(1) ⊕ 1×mGM5+(2) ⊕ 2×mGM5-(2) ⊕ 2×mGM6+(2) ⊕ 1×mGM6-(2)

# $Mn_3Sn$ (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
```

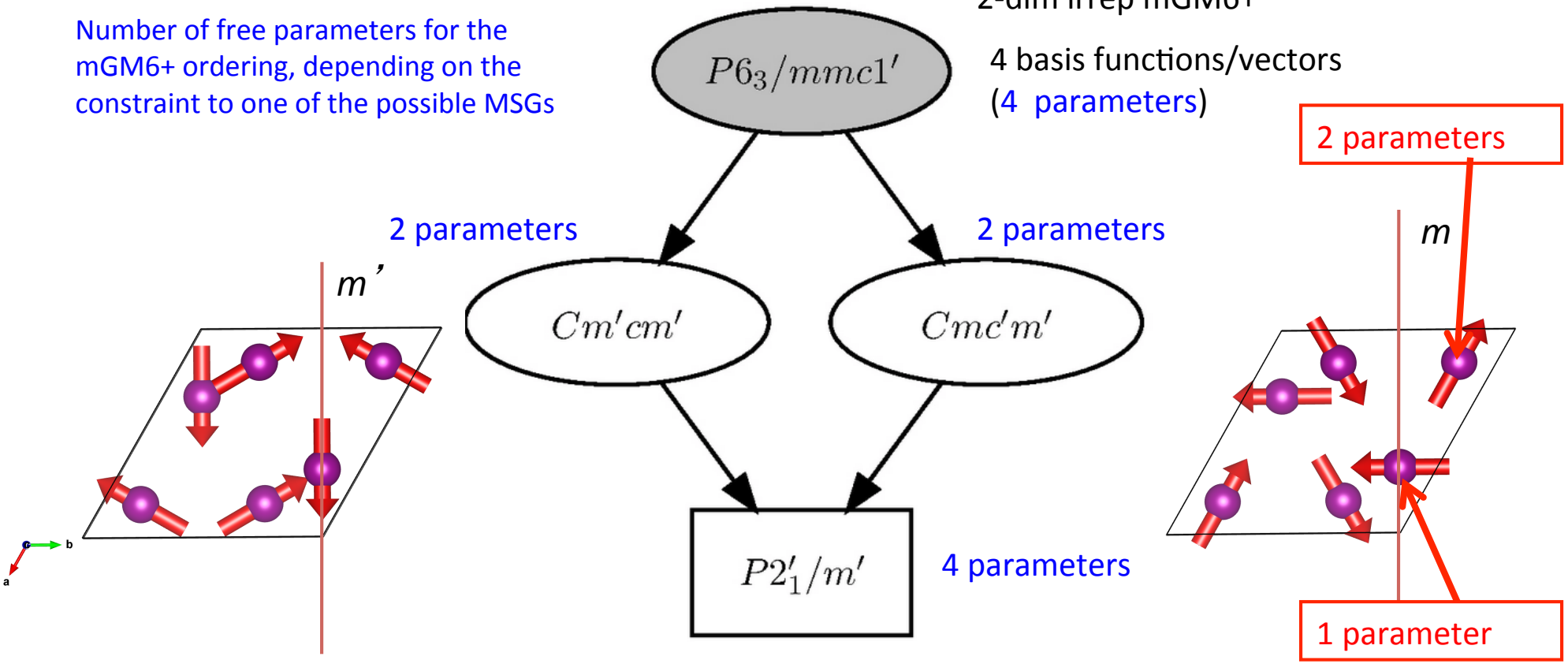
3 free parameters

# $Mn_3Sn$ k=(0,0,0)

Number of free parameters for the mGM6+ ordering, depending on the constraint to one of the possible MSGs

2-dim irrep mGM6+

4 basis functions/vectors
(4 parameters)




**Wave-vectors of the star (1 vector):**

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**Descomposition of the magnetic representation(s) into irreps.**

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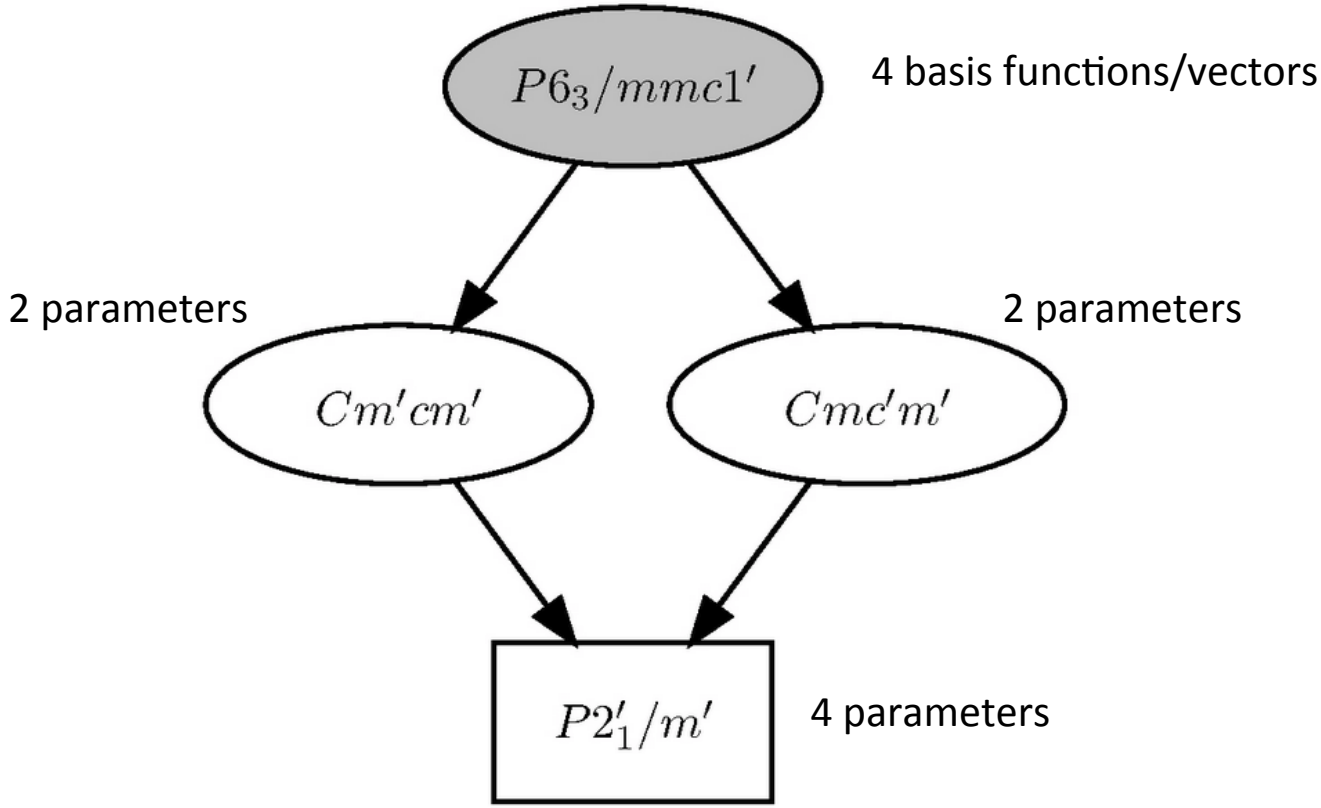
⊕ 1×mGM3-(1) ⊕ 1×mGM4+(1) ⊕ 1×mGM5+(2) ⊕ 2×mGM5-(2) ⊕ 2×mGM6+(2) ⊕ 1×mGM6-(2)

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

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

2-dim irrep mGM6+



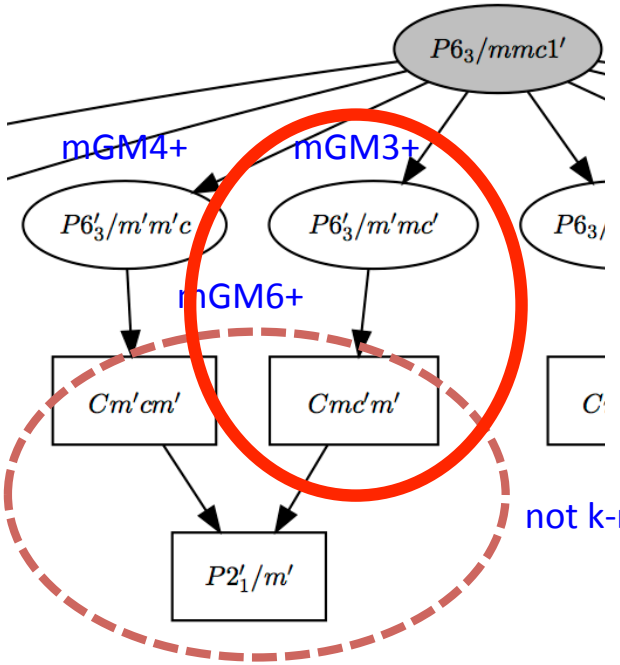

Why 3 free parameters when described using the MSG Cmc'm' instead of 2 parameters?

# $Mn_3Sn$

k=(0,0,0)

$P6_3/mmc1'$ ⟶ ??

Possible magnetic symmetries for a magnetic phase with propagation vector (0,0,0) and parent space group $P6_3/mmc$ (LANDAU)



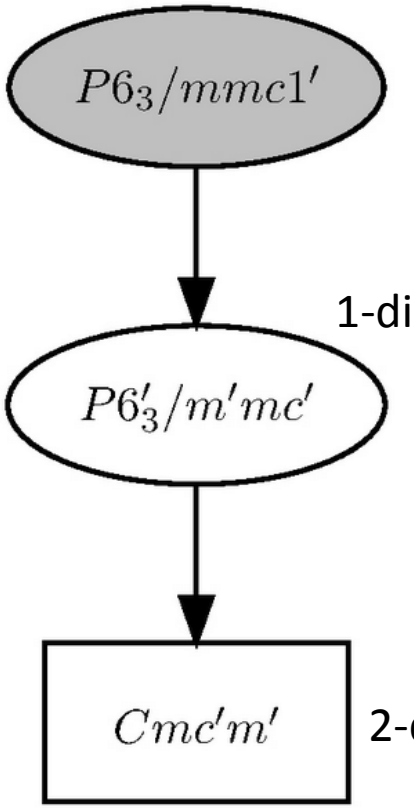

not k-maximal symmetry

**Descomposition of the magnetic representation(s) into irreps.**

6h:(x,2*x,1/4) → 1×mGM1-(1) ⊕ 1×mGM2+(1) ⊕ 1×mGM2-(1) ⊕ 1×mGM3+(1) ⊕

⊕ 1×mGM3-(1) ⊕ 1×mGM4+(1) ⊕ 1×mGM5+(2) ⊕ 2×mGM5-(2) ⊕ 2×mGM6+(2) ⊕ 1×mGM6-(2)

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

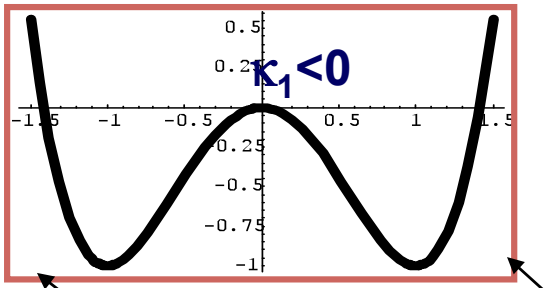


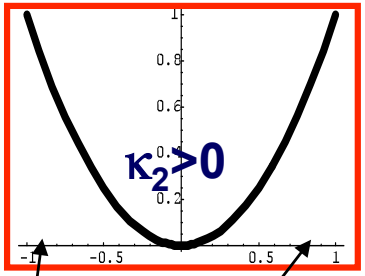

1-dim irrep mGM3+

2-dim irrep mGM6+

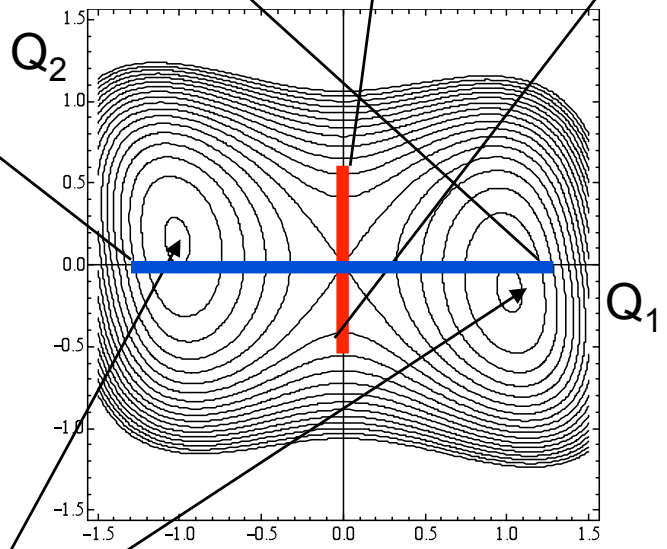
Von Neumann principle:
Everything that keeps the symmetry Cmc’ m’ is allowed and can happen…
Anything that keeps the symmetry P6’ $_3$/m’ mc’ keeps the symmetry of its subgroup Cmc’ m’
THEREFORE…. a spin arrangement according to the irrep mGM3+ is also allowed in the structure with MSG Cmc’ m’

# Why secondary modes




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




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

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

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…..**

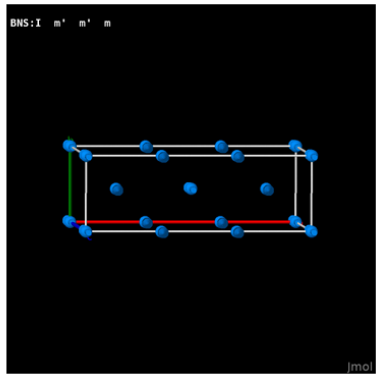
is it an advantage or a nuisance?

It depends …..

- In many cases these induced effects are negligible 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 addedto 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**

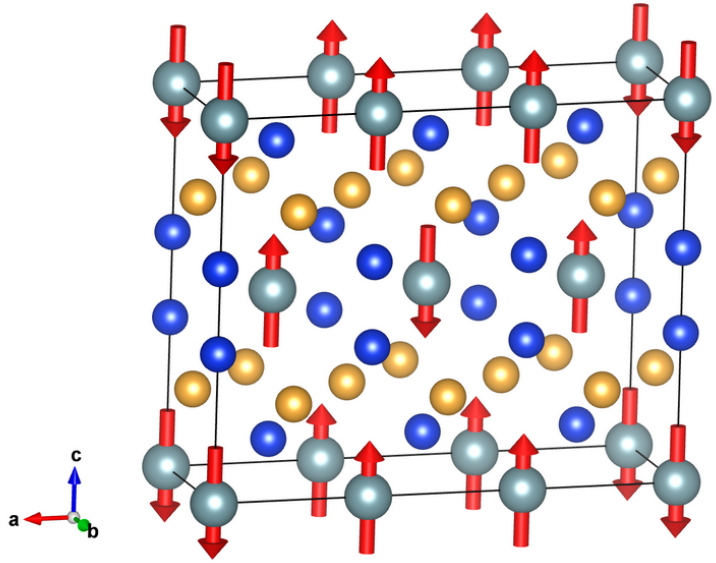
view in Jmol
Download mcif file
Download vesta file (all atoms)
Download vesta file (magnetic atoms only)

submit to STRCONVERT

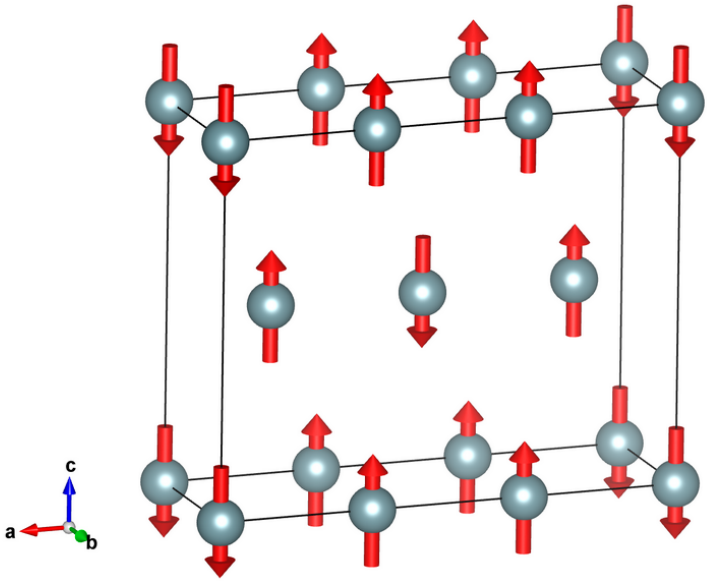
UAu2Si2 (#1.0.12)

**k**=(2/3,0,0)

Allowed third harmonic with k=0 is automatically included

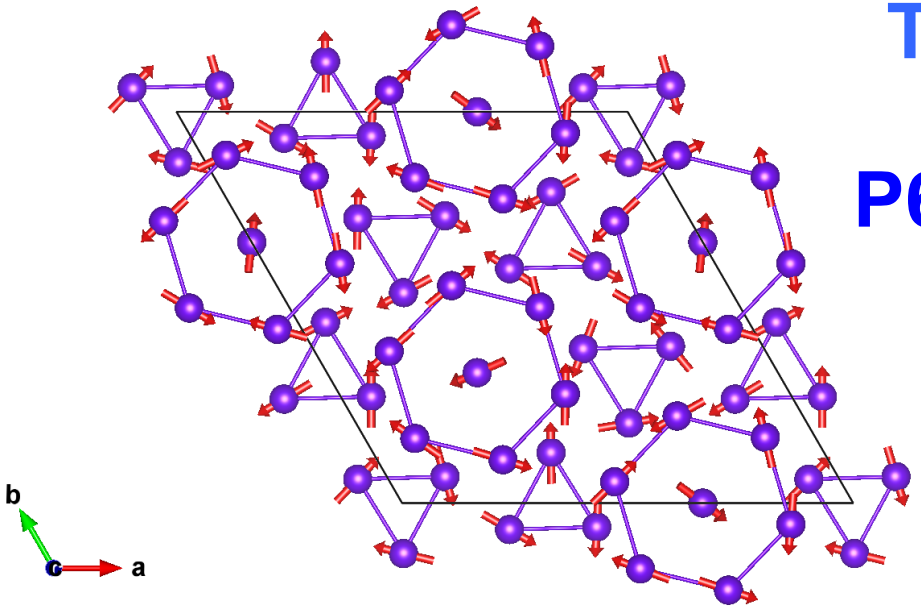



*Magnetic structure with all atoms*




*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

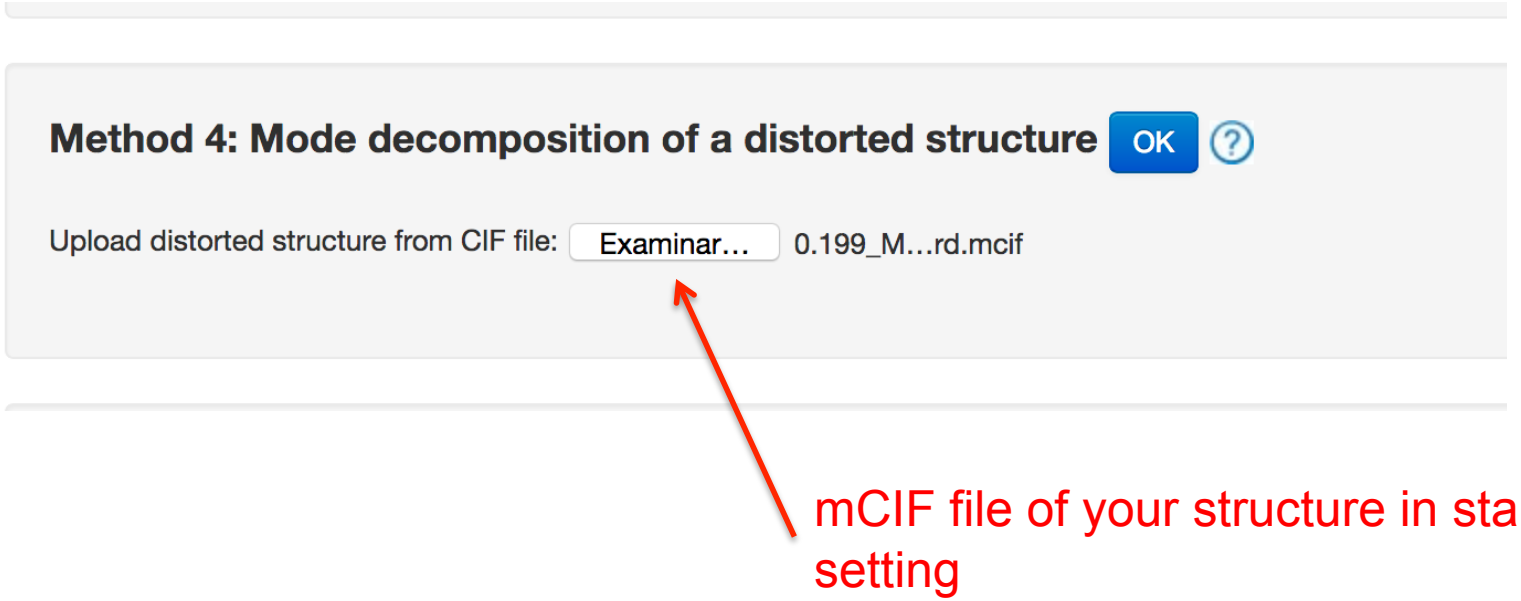
| label | dim. full irrep | dim. small irrep | direction | action | number of modes | presence |
|---|---|---|---|---|---|---|
| mK4K6 | 4 | 2 | special | primary | 18 | |
| mGM2+ | 1 | 1 | | secondary | 4 | yes |
| mGM1- | 1 | 1 | | secondary | 5 | yes |

**How do I know that more than one irrep is compatible with the symmetry of my structure and therefore they are allowed within the phase (Case 2)?**

**Method 1: Use ISODISTORT (Method 4) to decompose your structure in irrep modes (available in the ISOTROPY Software Suite in the web).**

Input: CIF and mCIF files of parent and magnetic structure

*standard setting ! (use ISOCIF to transform to a standard setting if needed)*



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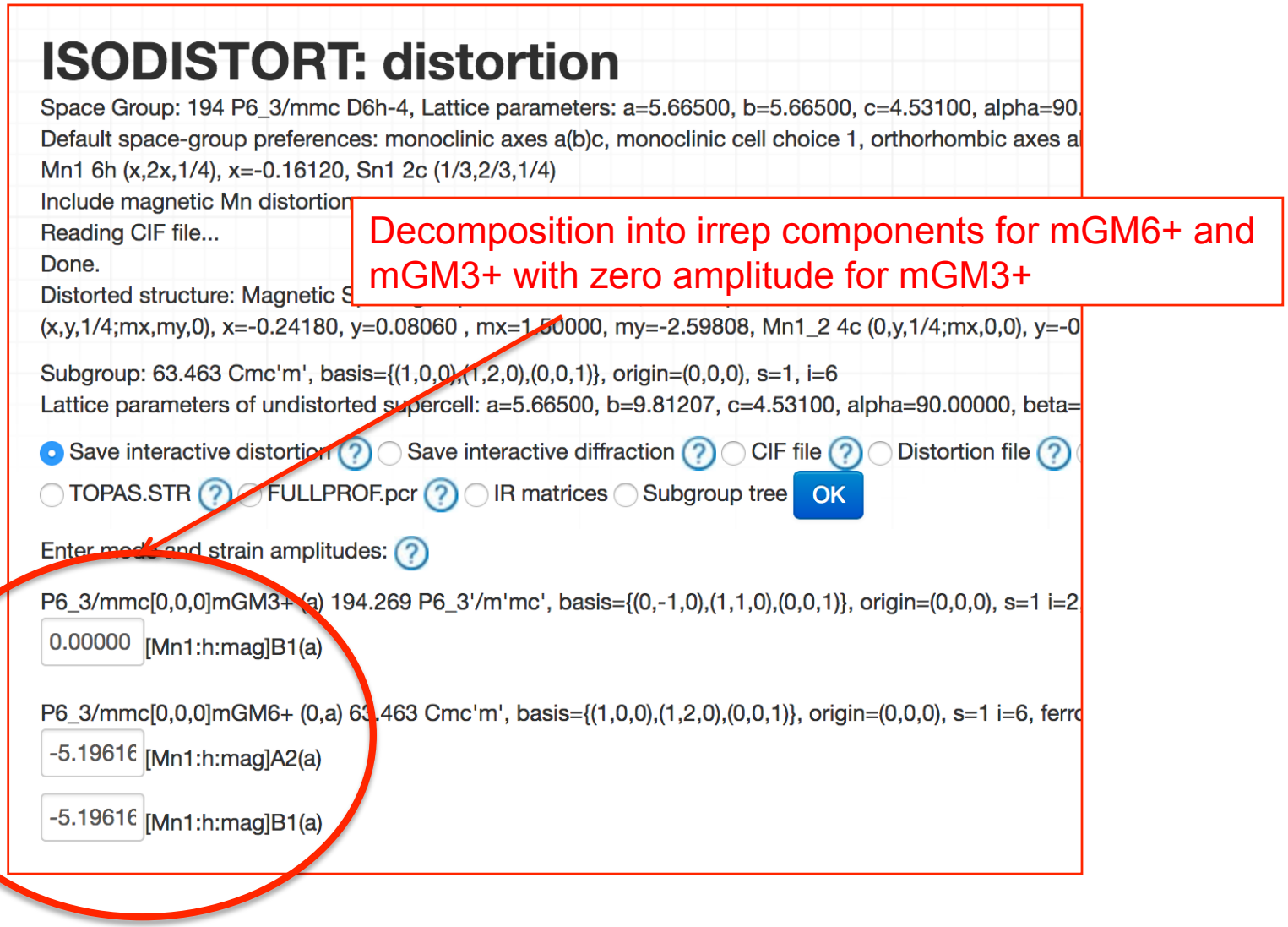

## How do I know that more than one irrep is compatible with the symmetry of my structure and therefore allowed within the phase (Case 2)?

### Method 2: Use Get_mirreps and MAGNETIC REP in the Bilbao Server

Input: Parent SG, Wyckoff position(s) of magnetic atom(s) and MSG

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

**Input data**

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

input

**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) | $P6_3/mmc1'$ (No. 194.264) a,b,c;0,0,0 | matrices of the irreps |
| | $GM_3^+$: (a,-(√3 a)) | $Cmcm1'$ (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 | |

output

2 magn. irreps allowed

## How do I know that more than one irrep is compatible with the symmetry of my structure and therefore allowed within the phase?

**Method 2: Use Get_mirreps and MAGNETIC REP in the Bilbao Server**

Input: Parent SG, Wyckoff position(s) of magnetic atom(s) and MSG

**MAGNETIC REP output:**

**Decomposition of the magnetic representation of the magnetic space group $P6_3/mmc1'$ (No. 194.264)**

**(gray group of the paramagnetic phase)**

**Wave-vector: GM:(0,0,0)**

**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

The 2 irreps are possible for the WP 6h

# How to report combining MSG and irreps in Case 2

## fundamental necessary information **(the same as in case 1)**

| | | | |
|---|---|---|---|
| | | $Mn_3Sn$ (#0.199)<br><br>(BNS setting) | |
| 1.1 | MSG symbol | *Cmc'm'* | |
| 1.2 | MSG number | 63.463 | |
| 1.3 | Transformation to standard setting of MSG | (**-b**,2**a+b**,**c**;0,0,0) | |
| 1.4 | Magnetic point group | *mm21'* (**c**,**a**,**b**) *or m2m1'* | |
| 1.5 | Unit cell parameters (Å) | a=5.665 α=90º<br>b=5.665 β =90º<br>c=4.531 γ =120º | |
| 1.6 | MSG symmetry operations | x,y,z,+1<br>-x,-x<br>-x,-y<br>x,x-y,z,+1<br>x,x-y,-z+1/2,-1<br>-x,-y,z+1/2,-1<br>-x,-x+y,z+1/2,-1<br>x,y,-z+1/2,-1 | {1\|0,0,0}<br><br><br>{$m_{010}$\|0,0,0}<br>{$2'_{210}$\|0,0,½}<br>{$2'_{001}$\|0,0,½}<br>{$m'_{210}$\|0,0,½}<br>{$m'_{001}$\|0,0,½} |
| 1.7 | MSG symmetry centering operations | x,y,z,+1 | {1\|0,0,0} |
| 1.9 | Positions of magnetic atoms | Mn1_1 Mn 0.8388 0.6776 0.25<br>Mn1_2 Mn 0.3224 0.1612 0.25 | |
| 1.10 | Positions of non-magnetic atoms | Sn1 Sn 0.333333 0.666667 0.25 | |
| 1.11 | Magnetic moments ($\mu_B$) of magnetic atoms<br>and their symmetry constraints | Mn1_1 3.00(1) 3.0 0.0 (mx,my,0)<br>Mn1_2 0.0 -3.0 0.0 (0,my,0) | |

**3 free parameters**

# How to report combining MSG and irreps in Case 2

fundamental information **(different than in case 1)**

| | | |
|---|---|---|
| 2.1 | Parent space group | *P63/mmc* (N. 194) |
| 2.2 | Propagation vector(s) | k1=(0,0,0) |
| 2.3 | Transformation from parent setting to the one being used | (**a**,**b**,**c**;0,0,0) |
| 2.4 | Primary irrep(s) labels with dimension | mGM6+(2) |
| 2.5 | Secondary irrep(s) labels with dimension (if symmetry allowed) | mGM3+(1) |
| 2.6 | Description of primary irrep(s) | mGM6+:<br>$\{6_{001}\|0,0,1/2\}$ : ( ½ ,-√3/2 ; √3/2 , ½ )<br>{-1\|0,0,0}: (1, 0 ; 0, 1)<br>$\{m_{010}\|0,0,0\}$: ( ½ ,√3/2 ; √3/2 , -½ ) |
| 2.7 | Description of secondary irrep(s) if allowed | mGM3+:<br>$\{6_{001}\|0,0,1/2\}$: -1<br>{-1\|0,0,0}: 1<br>$\{m_{010}\|0,0,0\}$: 1 |

**Second(ary) irrep allowed by the MSG**

# Description of the irrep basis vectors involved

1 basis vector for **mGM3+**:

Mn1_1 c (1,0,0)
Mn1_2 (0,1,0)

c=0

The form of the moments of all atoms in the unit cell is NOT needed! The MSG operations takes care of that

2 basis vectors for **mGM6+**:

| | basis vector 1: | | basis vector 2: |
|---|---|---|---|
| Mn1_1 | a (1,1,0) | + | b (0,1,0) |
| Mn1_2 | (0,-1,0) | | (0,1,0) |

b=0

The form of the moments of all atoms in the unit is NOT needed! The MSG operations takes care of that

| | | | |
|---|---|---|---|
| 3.1 | Description of primary mode(s) and amplitude(s) (in $\mu_B$) | mGM6+, mode1:<br>Mn1_1 (a, a ,0) a= 3.00(1)<br>Mn1_2 (0,-a,0)<br><br>mGM6+, mode2: b=0.0<br>Mn1_1 (0,b,0)<br>Mn1_2 (0,b,0) | 2 parameters |
| 3.2 | Description of secondary mode(s) and amplitude(s) (in $\mu_B$) | mGM3+, mode 1: c=0.0<br>Mn1_1 (c,0,0)<br>Mn1_2 (0,c,0) | 1 parameter |

**When defined under the MSG symmetry of the structure, the description of the irrep basis functions/vectors does not require complex functions, nor a full listing of the moments in the unit cell.**

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

| | | |
|---|---|---|
| 1.9 | Positions of magnetic atoms | Mn1_1 Mn 0.8388 0.6776 0.25<br>Mn1_2 Mn 0.3224 0.1612 0.25 |
| 1.11 | Magnetic moments ($\mu_B$) of magnetic atoms<br>and their symmetry constraints | Mn1_1 3.00(1) 3.0 0.0 (mx,my,0)<br>Mn1_2 0.0 -3.0 0.0 (0,my,0) |
| 3.1 | Description of<br>primary mode(s) and amplitude(s) (in $\mu_B$) | mGM6+, mode1:<br>Mn1_1 (a, a ,0) a= 3.00(1)<br>Mn1_2 (0,-a,0)<br><br>mGM6+, mode2: b=0.0<br>Mn1_1 (0,b,0)<br>Mn1_2 (0,b,0) |
| 3.2 | Description of<br>secondary mode(s) and amplitude(s) (in $\mu_B$) | mGM3+, mode 1: c=0.0<br>Mn1_1 (c,0,0)<br>Mn1_2 (0,c,0) |

a =3

b =0 FM mode along b

c = 0

# FullProf can refine under a MSG with the amplitudes of the irrep basis functions compatible with the MSG as parameters to refine, using an output file of ISODISTORT

*This is the future already at your disposal !*

```
! Basis vectors of magnetic symmetry modes for each atom
M_MODES    6
! Nm Atom   Irrep      Mx       My       Mz       Coeff
   1 Mn1_1   mGM3+      0.0719   0.0000   0.0000   1.00
   1 Mn1_2   mGM3+      0.0000   0.0719   0.0000   1.00
   2 Mn1_1   mGM6+      0.0508   0.1017   0.0000   1.00
   2 Mn1_2   mGM6+      0.0000   0.0000   0.0000   1.00
   3 Mn1_1   mGM6+      0.0508   0.0000   0.0000   1.00
   3 Mn1_2   mGM6+      0.0000  -0.1017   0.0000   1.00
! Amplitudes of Magnetic Symmetry Modes
MA_MODES    3    2
     A1_mGM3+          0.00000    1.00
     A2_mGM6+         -5.20716    1.00
     A3_mGM6+         -5.20716    1.00
!
```

**mode 1 mGM3+**
**mode 2 mGM6+**
**mode 3 mGM6+**

Mn1_1 (a,2a,0)
Mn1_2 (0,0,0)

linear combination of the two modes chosen here. Choice is not unique

| | | | |
|---|---|---|---|
| 3.1 | Description of primary mode(s) and amplitude(s) (in $\mu_B$) | mGM6+, mode1:<br>Mn1_1 (a, a ,0) a= 3.00(1)<br>Mn1_2 (0,-a,0)<br><br>mGM6+, mode2: b=0.0<br>Mn1_1 (0,b,0)<br>Mn1_2 (0,b,0) | 2 parameters |
| 3.2 | Description of secondary mode(s) and amplitude(s) (in $\mu_B$) | mGM3+, mode 1: c=0.0<br>Mn1_1 (c,0,0)<br>Mn1_2 (0,c,0) | 1 parameter |

# Conclusions:

• The assignment of MSG should be 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:

• *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, as the description of these constraints can be limited to the magnetic atoms in the asymmetric unit*

• 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).