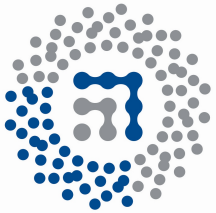

ZTF-FCT
Zientzia eta Teknologia Fakultatea
Facultad de Ciencia y Tecnología

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Universidad del País Vasco
Euskal Herriko Unibertsitatea

III. Magnetic symmetry groups vs. irreducible representations and the Bilbao Crystallographic Server

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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)

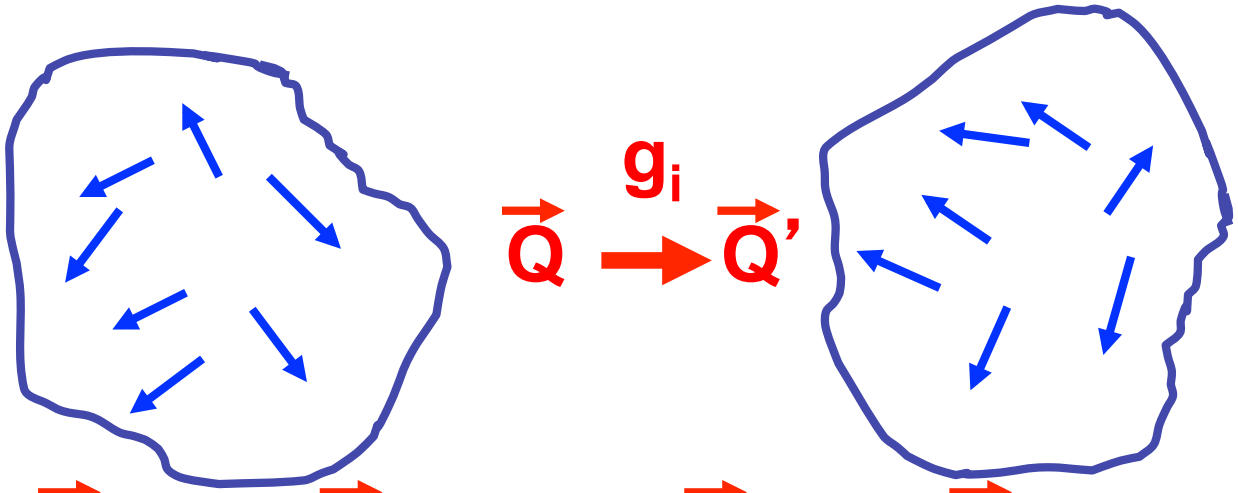
• Lost symmetry operations transform the distorted structure into something different:

a distorted structure with a different distortion.

• Relation with the original distortion?:

•Through 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



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

$\vec{Q}' = Q'_1\vec{d}_1 + \ldots + Q'_n\vec{d}_n$

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

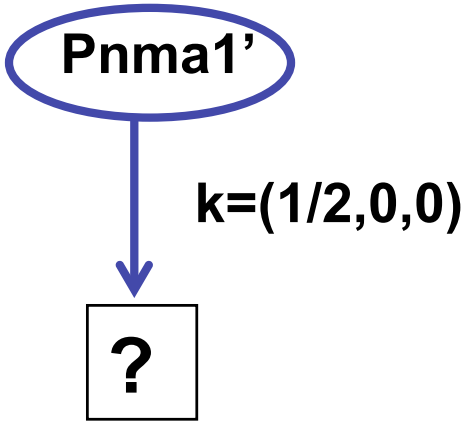
representation of G (matrices)

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

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

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

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

irreps

Decomposition into irreps

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

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)

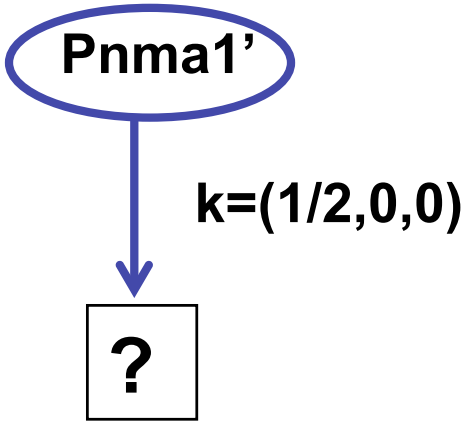
Wyckoff position	Decomposition into irreps
4b:(0,0,1/2)	3 mX1(2) ⊕ 3 mX2(2)

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

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

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

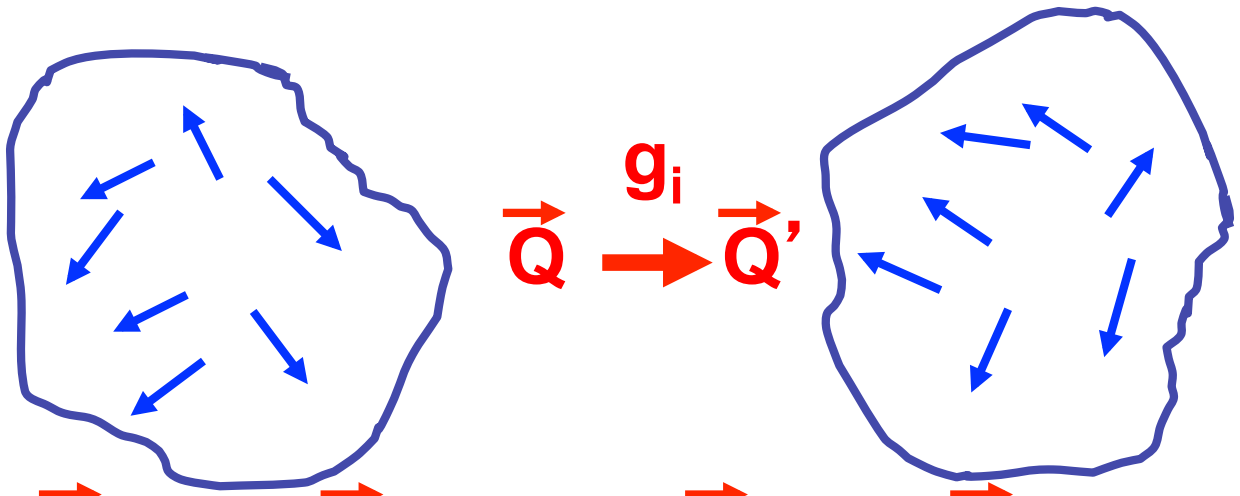
6-dim 6-dim

M_{rep}= 3 mX1(2) ⊕ 3 mX2(2)

irreps

Decomposition into irreps

LANDAU Theory: If transition continuous , then T(g) must be 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

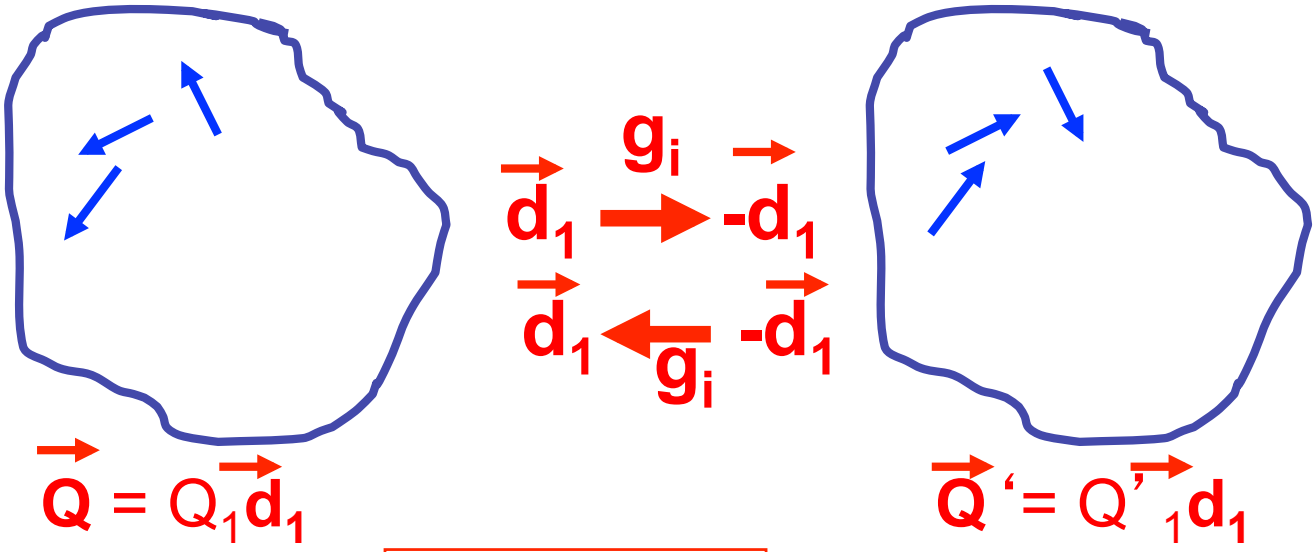
Even if the transition is not continuous, in most cases T(g) is also IRREDUCIBLE, and in the most complex cases only involves a few irreps

Distortions transforming according to representations of the symmetry group of the undistorted structure

Simplest example: some lost operations keep it invariant, some change its sign **(1-dim irrep)**

Distortion in the structure **Distortion after application of g_i**

g_i belongs to the symmetry group G of the parent structure



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

$T(g_i) = -1$

representation of G (irrep) (matrices)

1x1 matrices

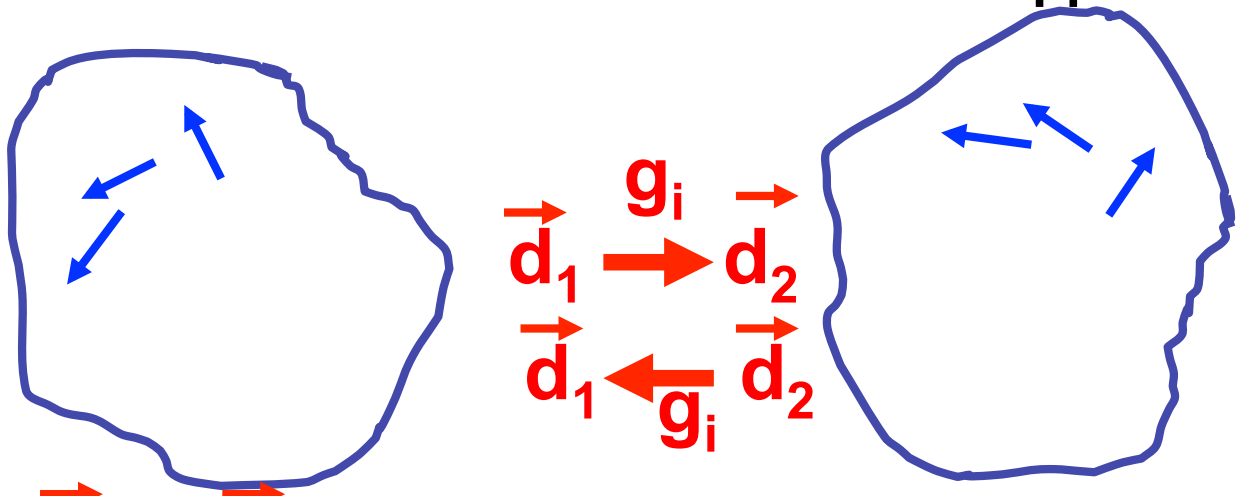
$T(g) = +/-1$

$T(g_1)T(g_2) = T(g_1g_2)$

Distortions transforming according to representations of the symmetry group of the undistorted structure

more complex example: some operations transform the distortion into another independent one, or in a linear combination with it

Distortion in the structure **Distortion after application of g_i**



$\vec{Q} = Q_1\vec{d}_1 + Q_2\vec{d}_2$

$\vec{Q}' = Q'_1\vec{d}_1 + Q'_2\vec{d}_2$

representation of G (irrep) (matrices)

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

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

$T(g_1)T(g_2) = T(g_1g_2)$

2-dim irrep

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: also a mathematical problem.

Representation analysis was taken as a "superior" alternative to magnetic symmetry groups, and it included incommensurate cases

Acta Cryst. (1968). A**24**, 217

Representation Analysis of Magnetic Structures

BY E. F. BERTAUT

Abstract:

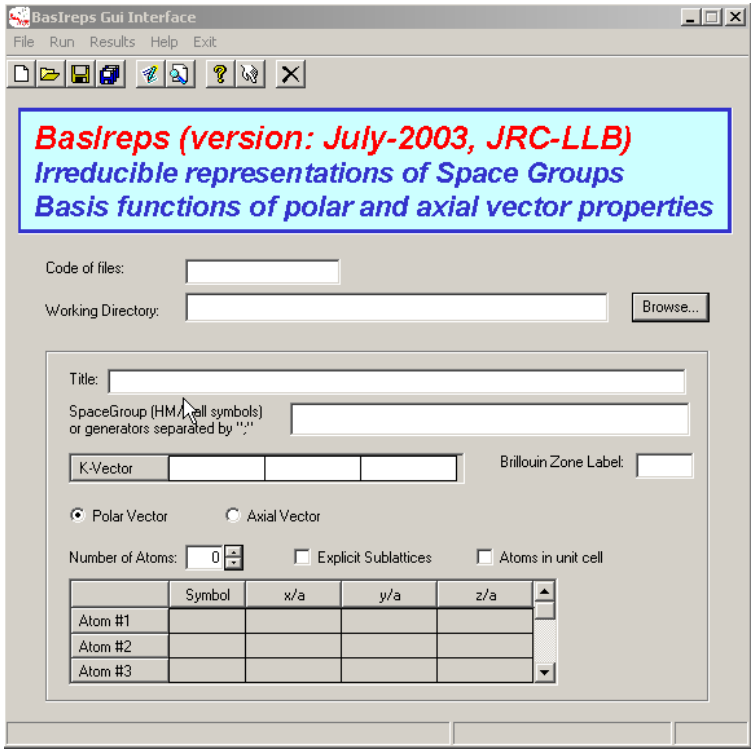
In the analysis of spin structures a 'natural' point of view looks for the set of symmetry operations which leave the magnetic structure invariant and has led to the development of magnetic or Shubnikov groups. A second point of view presented here simply asks for the transformation properties of a magnetic structure under the classical symmetry operations of the 230 conventional space groups and allows one to assign irreducible representations of the actual space group to all known magnetic structures. The superiority of representation theory over symmetry invariance under Shubnikov groups is already demonstrated by the fact proven here that the only invariant magnetic structures describable by magnetic groups belong to real one-dimensional representations of the 230 space groups. Representation theory on the other hand is richer because the number of representations is infinite, *i.e.* it can deal not only with magnetic structures belonging to one-dimensional real representations, but also with those belonging to one-dimensional complex and even to two-dimensional and three-dimensional representations associated with any **k** vector in or on the first Brillouin zone.

We generate from the transformation matrices of the spins a representation Γ of the space group

It includes incommensurate magnetic structures…

Appropriate SOFTWARE for the calculations were soon developed…

Appropriate SOFTWARE for REPRESENTATION ANALYSIS were soon developed…



Basirreps from J. Rodriguez-Carvajal

SARA*h* Representational Analysis -
Performs the calculations of Representational Analysis. These allow the determination of atomic displacements or magnetic structures that can accompany a second-order phase transition. Output files includes a tailored summary with cut-and-paste tables written in LaTeX. (Win9x, 2000, Vista and Windows 7) [1]

Sarah from A.S. Wills

The representation method became the most used method of analysis, most magnetic structures were determined and reported without the assignment of a space (or superspace) group symmetry, not even point-group symmetry.

What is the problem of using "only" irreps?

Commensurate magnetic structures:

Representation Analysis (irreducible representations, basis functions...)

Magnetic Symmetry (Shubnikov groups, ...)

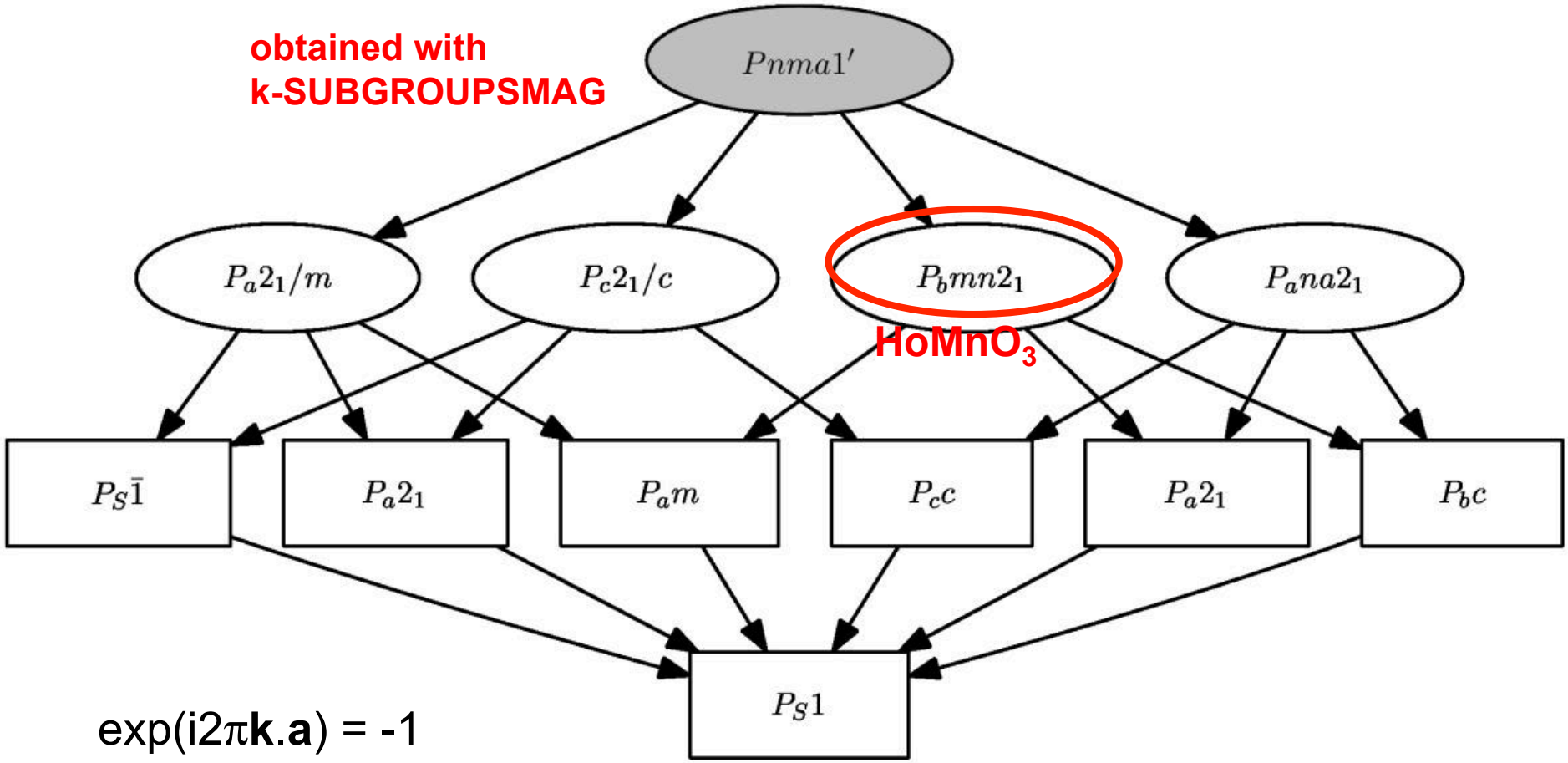
Identifying the active irrep(s) or the MSG are not alternative equivalent methods:

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

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



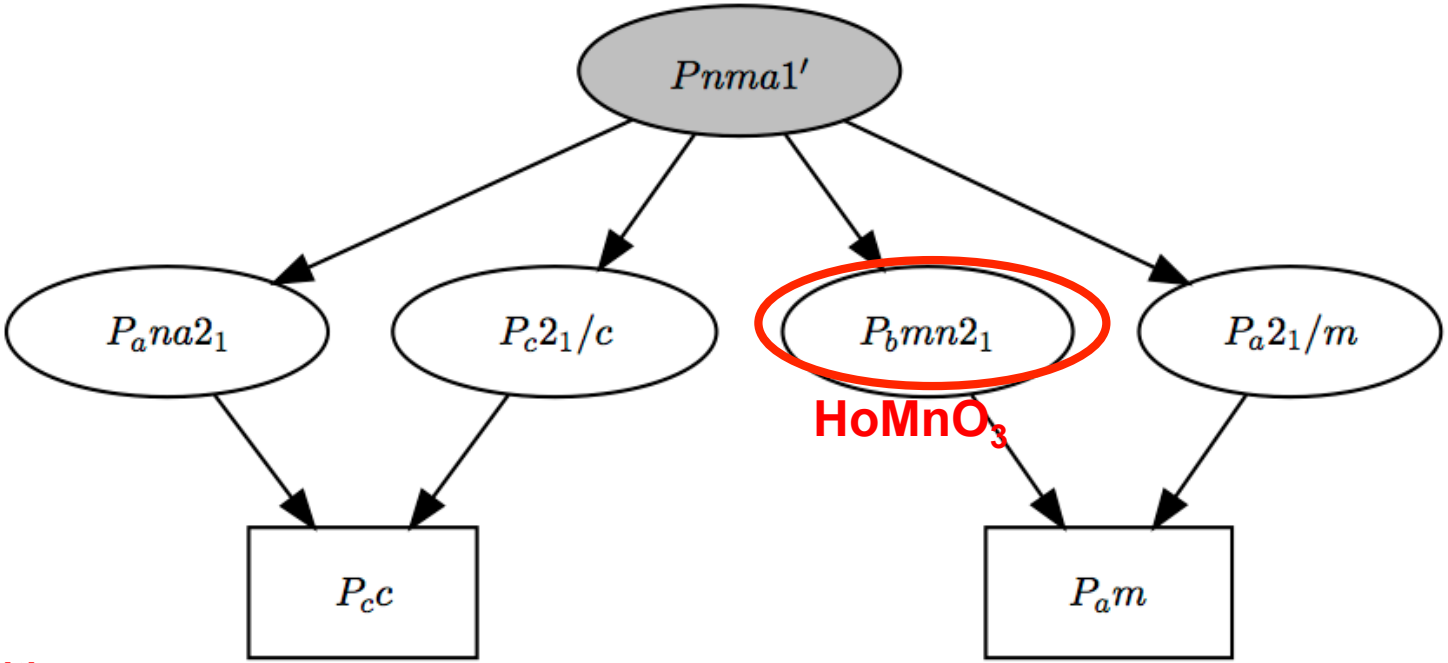
$\exp(i2\pi \mathbf{k}.\mathbf{a}) = -1$

(magnetic cell= $(2\mathbf{a}_p,\mathbf{b}_p,\mathbf{c}_p)$)

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:

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

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

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

primary irrep

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_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)	$P2_1/m1'$ (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

Phase Transition / Symmetry break / Order Parameter

High symmetry group G = {g}

Irreducible representation of G (irrep) (matrices)

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

g belongs to F

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

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

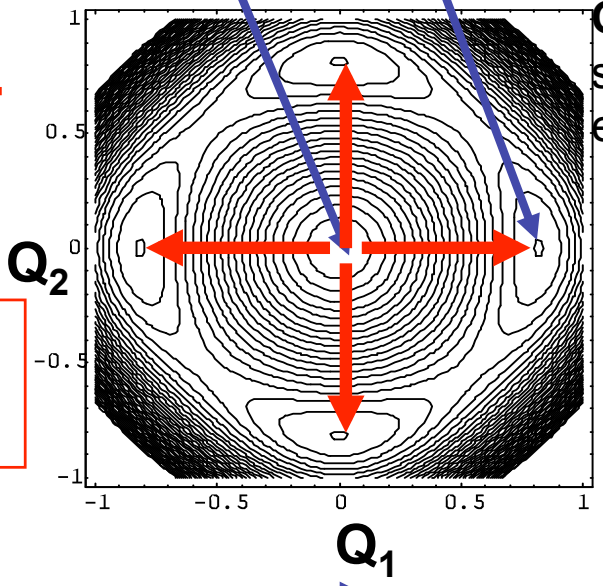
group-subgroup relation:

G → F **F: isotropy subgroup**

High symmetry **Low symmetry**

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,…)

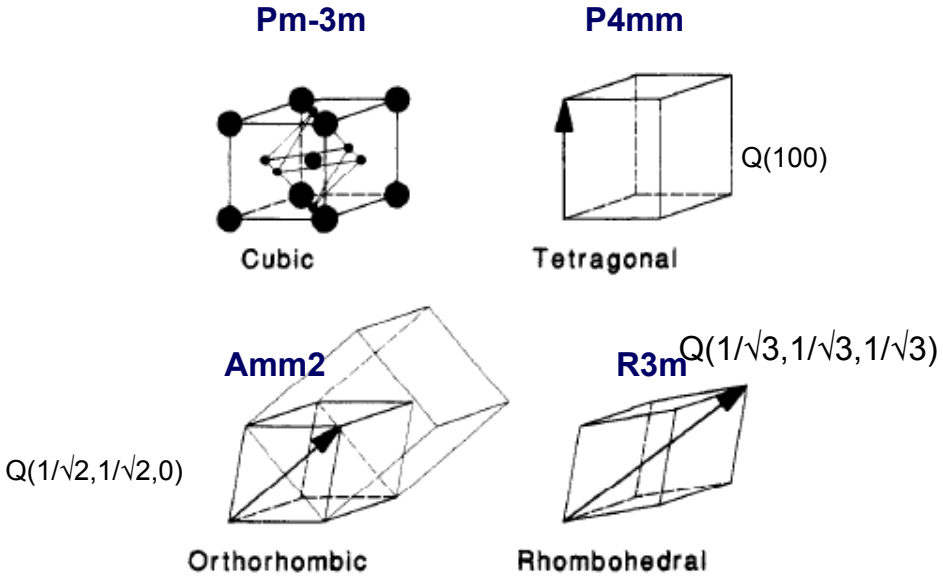
Example: $g_i = \{\mathbf{R},\theta|\mathbf{t}\}$

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

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

The different phases of $BaTiO_3$

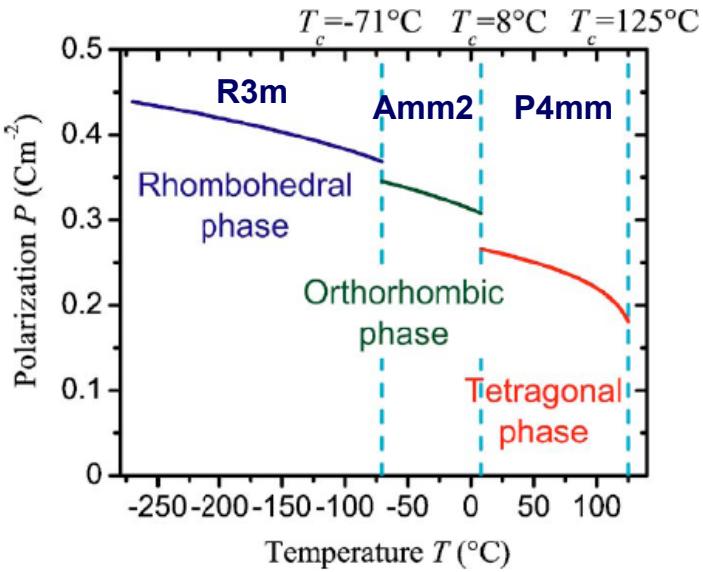
Similar to structural phase transitions: the same irrep can produce different symmetries



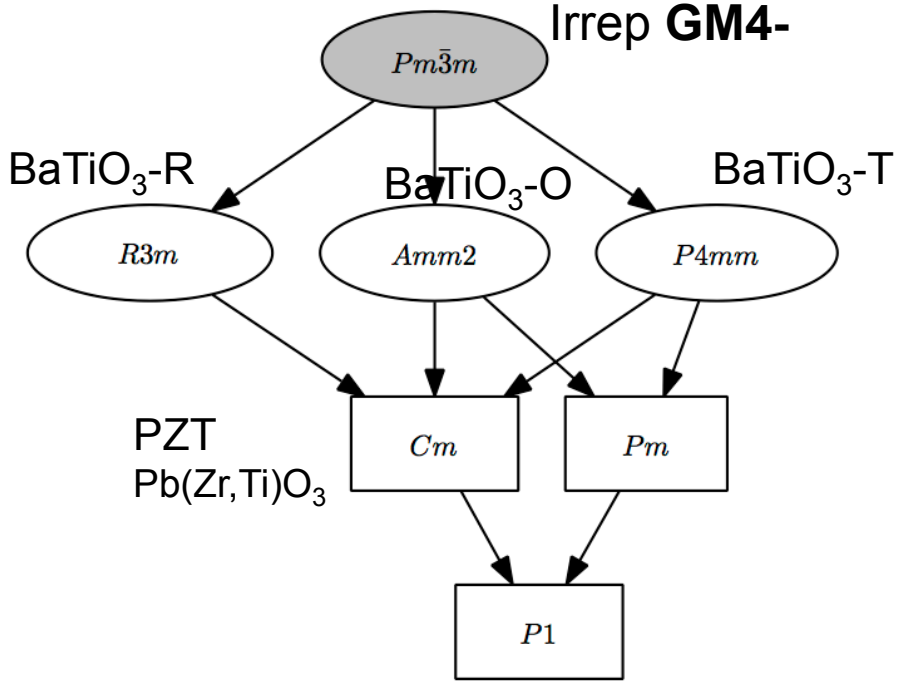
Polar distortion according to the 3-dim irrep GM4-:

3-dim order parameter (OP):

different symmetries depending on the direction of the OP:

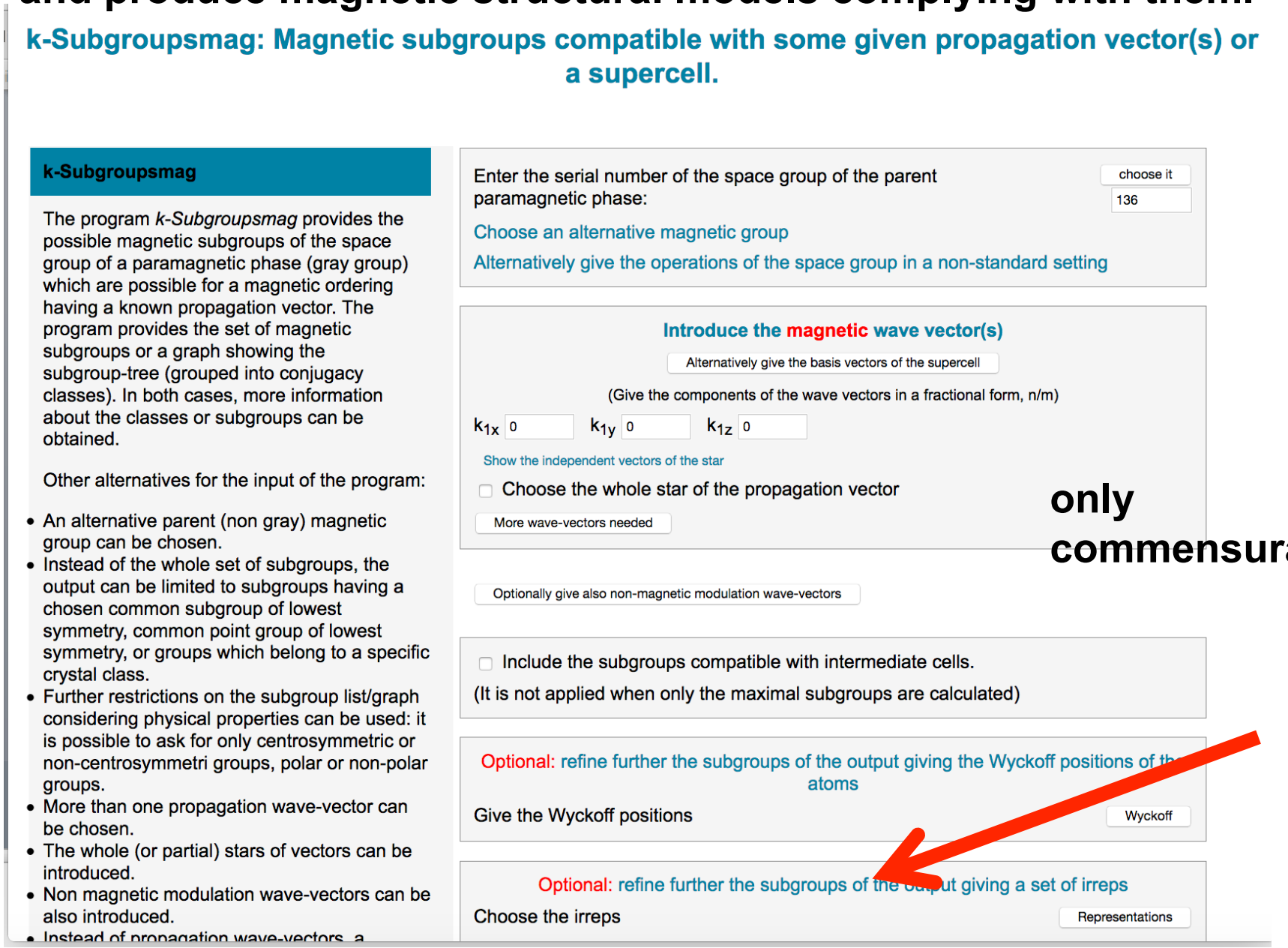


Li et al. J. Appl. Phys. (2005)



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

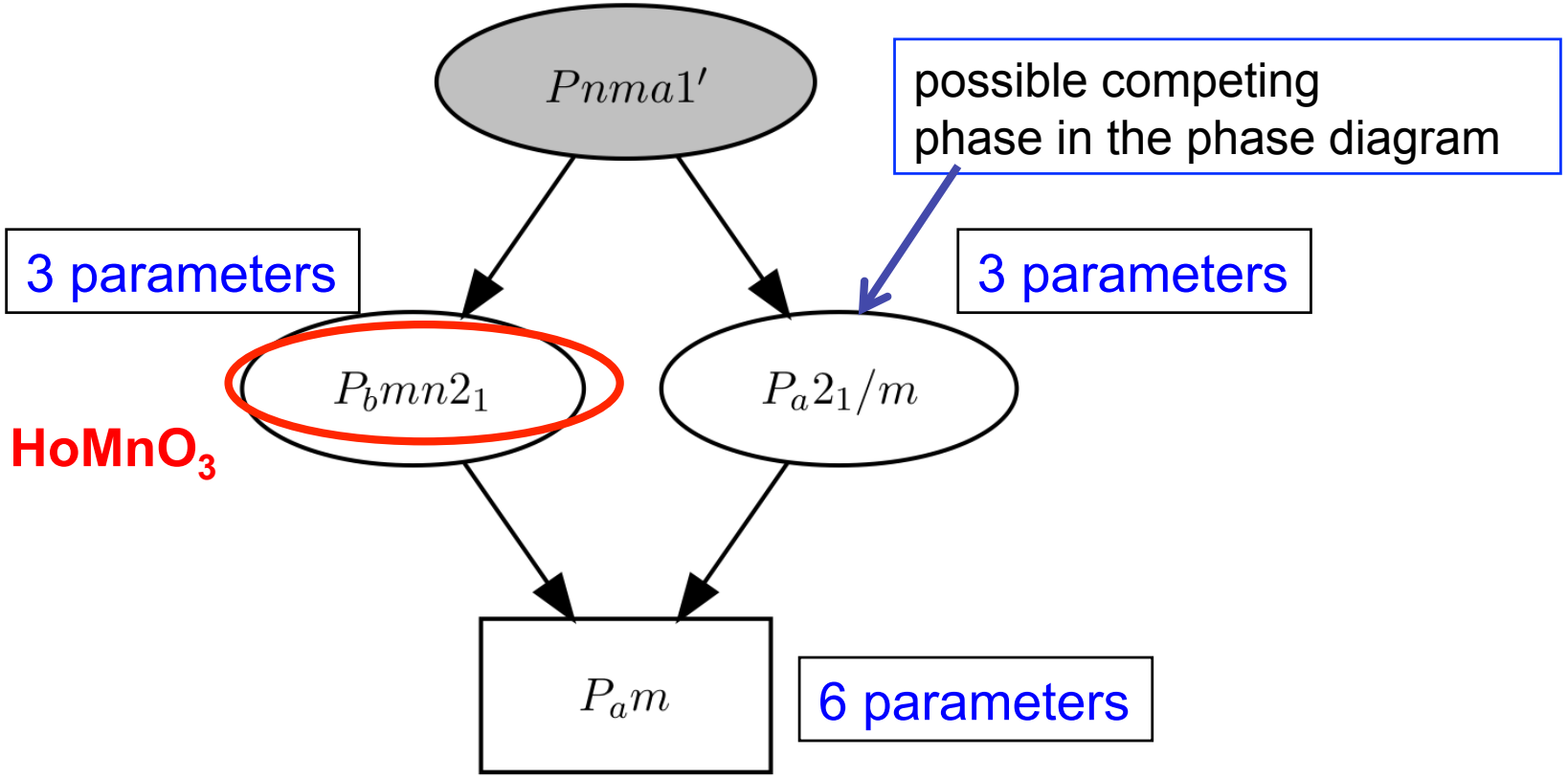
k-Subgroupsmag: Magnetic subgroups compatible with some given propagation vector(s) or a supercell.



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.



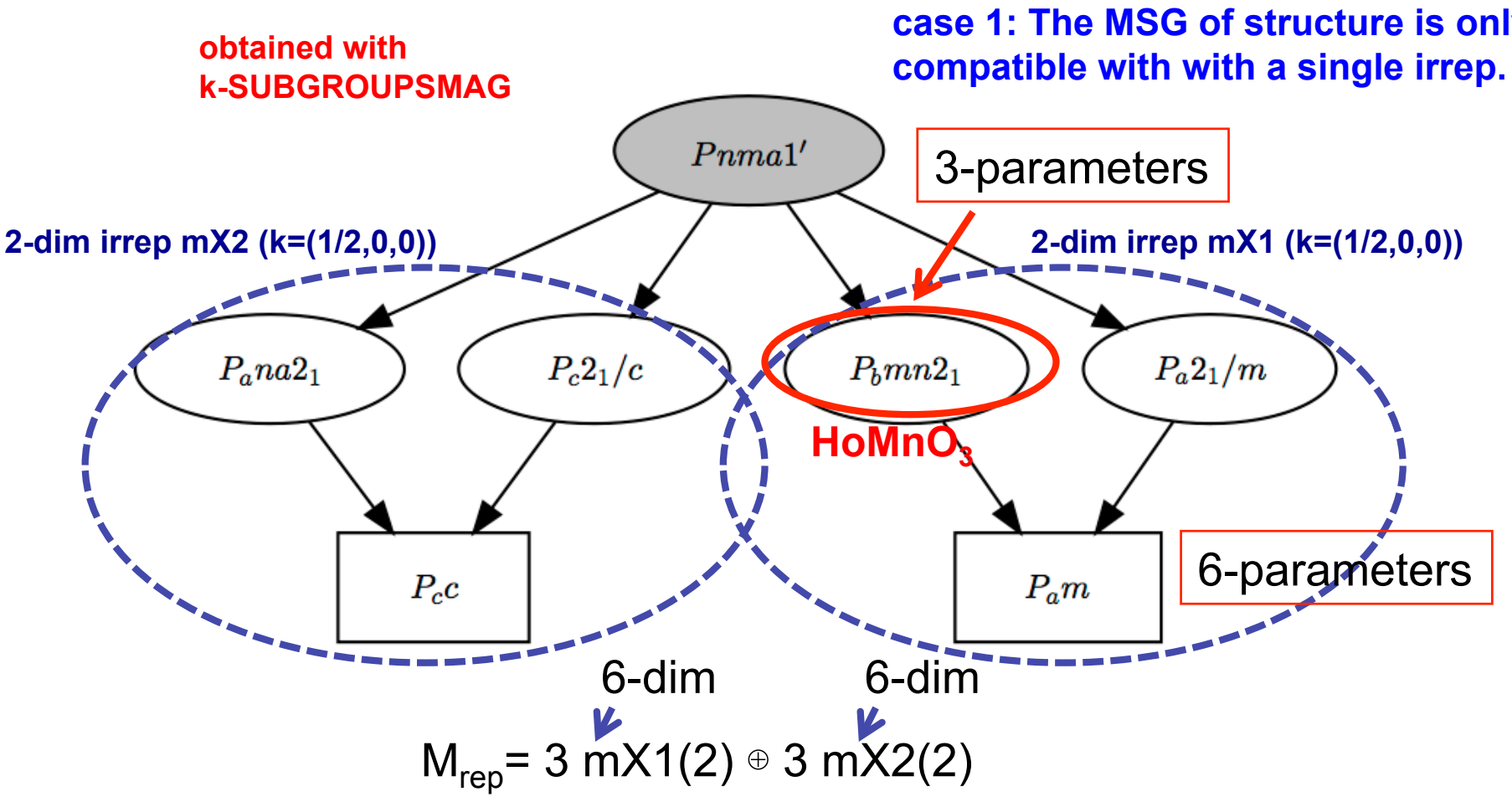
M_{rep}= 3 mX1(2) ⊕ 3 mX2(2)

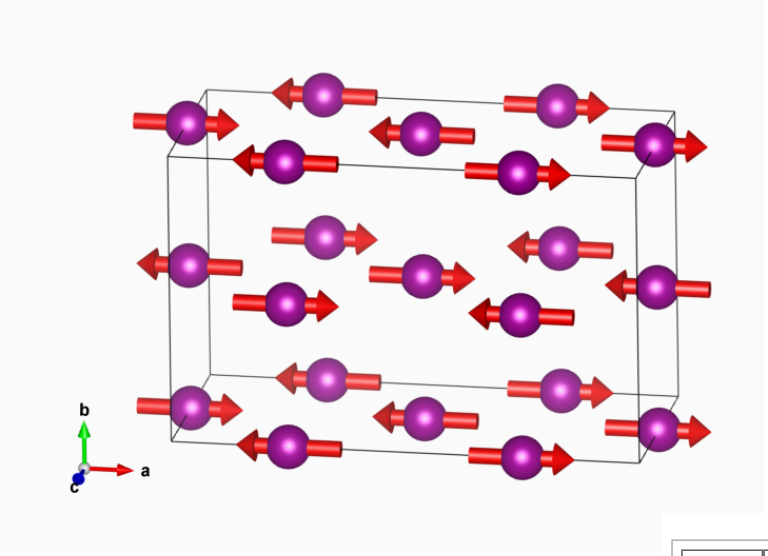
6 basis spin modes: 6 parameters

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)





$HoMnO_3$ (*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 }

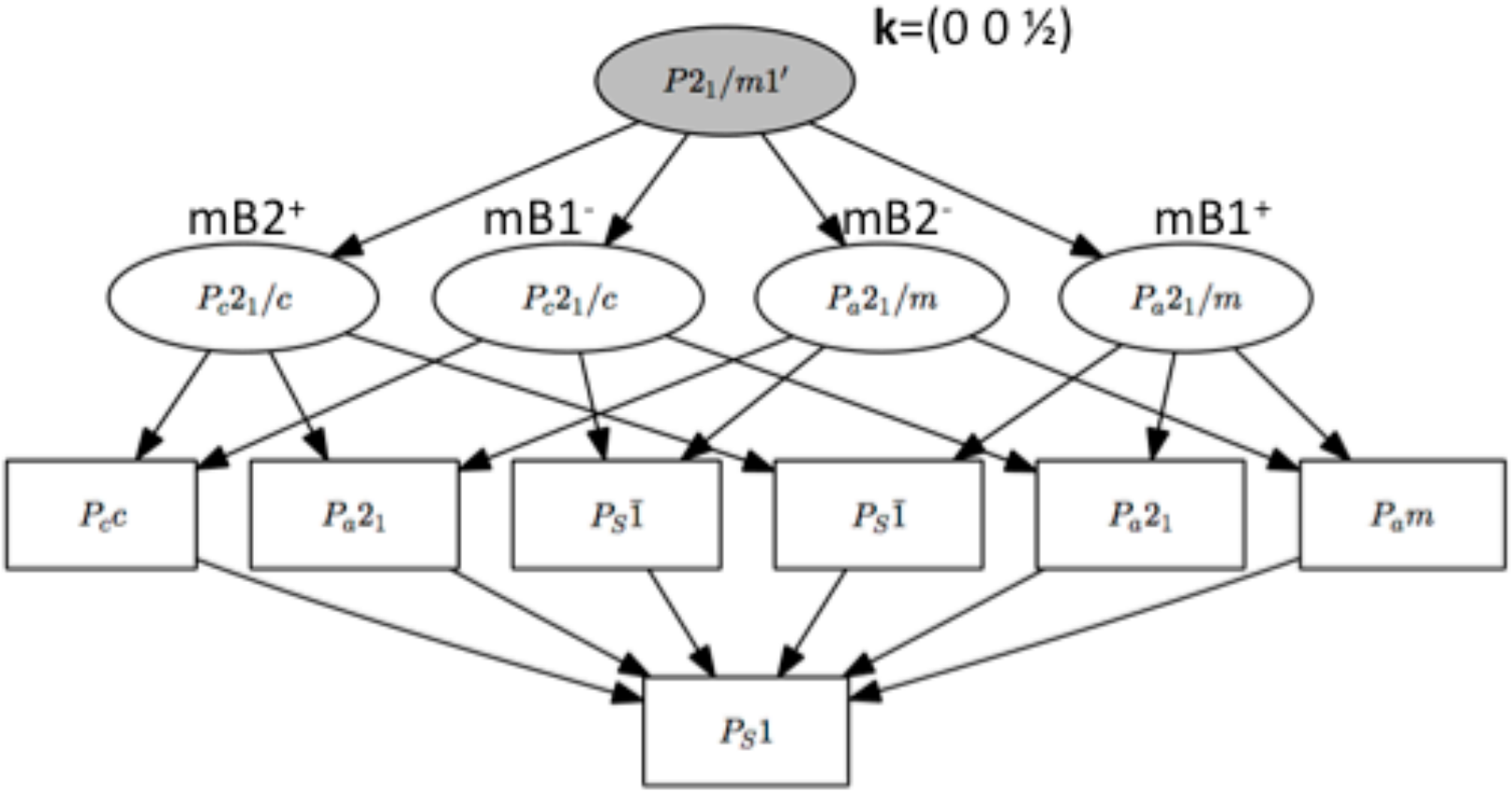
2-dim irrep mX1 but restricted to a special direction:
fixed combination of each pair of spin basis functions => **half number of degrees of freedom with respect to the only restriction to the irrep**

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)

Only for 1-dim (full) irreps there is a one to one correspondence between a MSG and the irrep

Possible MSGs for magnetic ordering with propagation vector (0,0,1/2) on a structure with space group $P2_1/m$:



Another example irreps vs MSG with some more complications:

Mn_3Sn

k=(0,0,0)

$P6_3/mmc1'$ ⟶ *??*

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

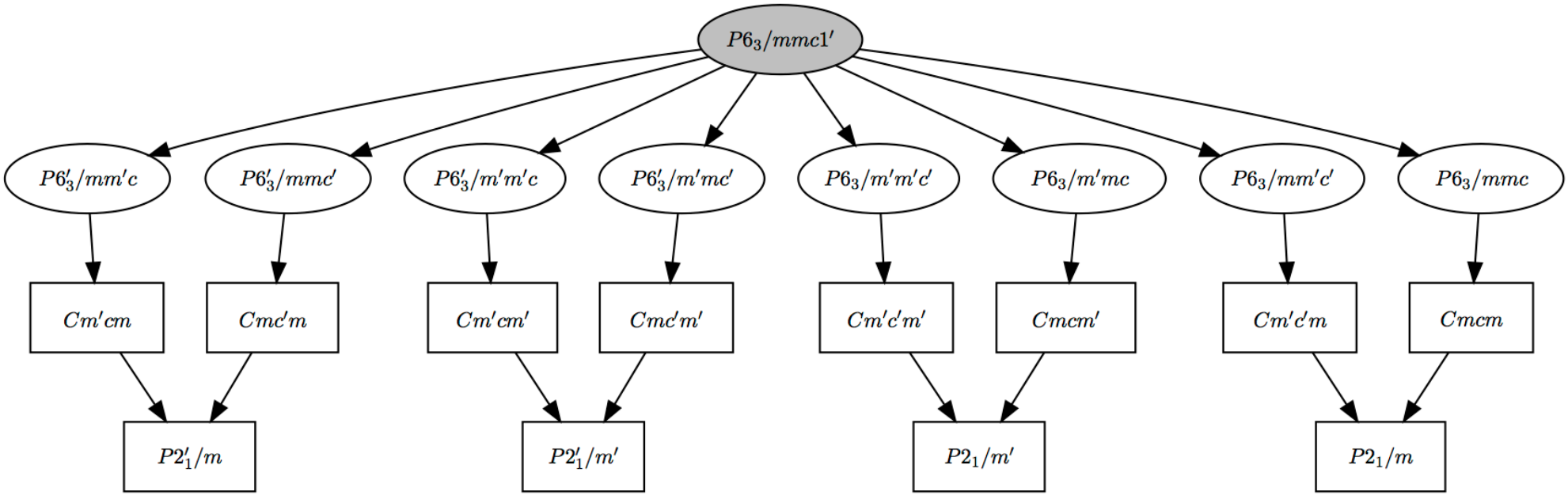
Mn_3Sn

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):



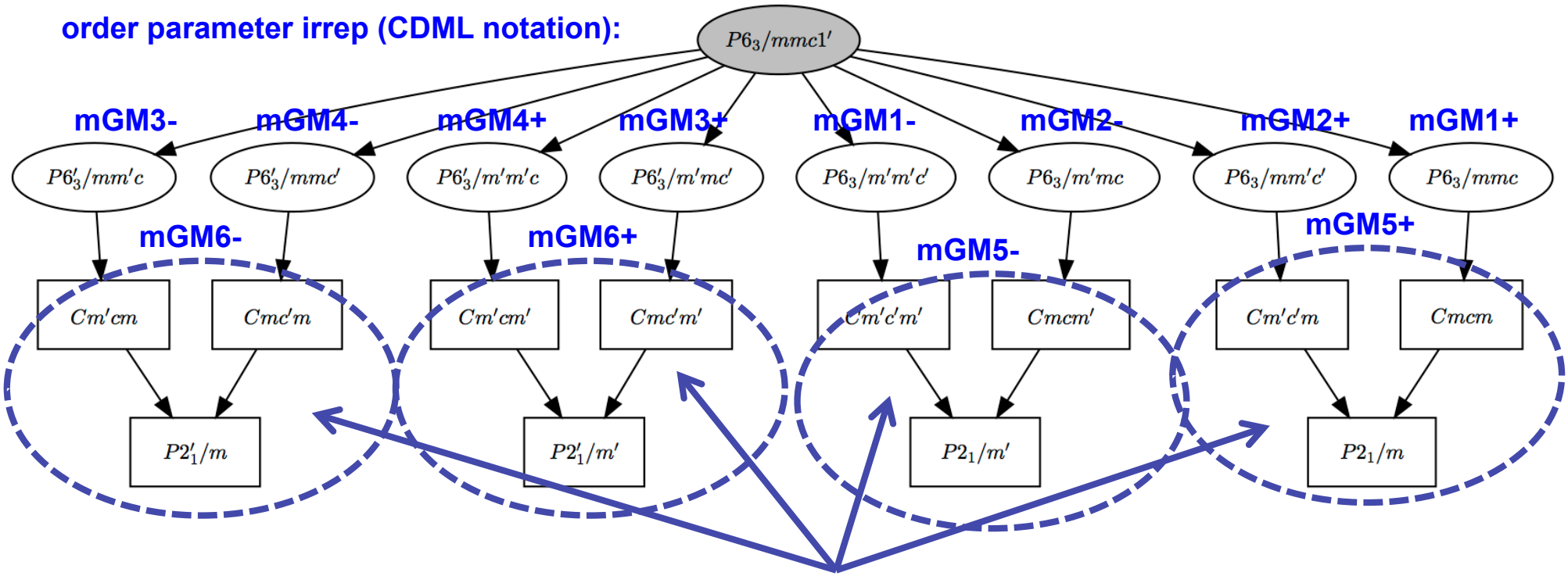
Mn_3Sn

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):



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

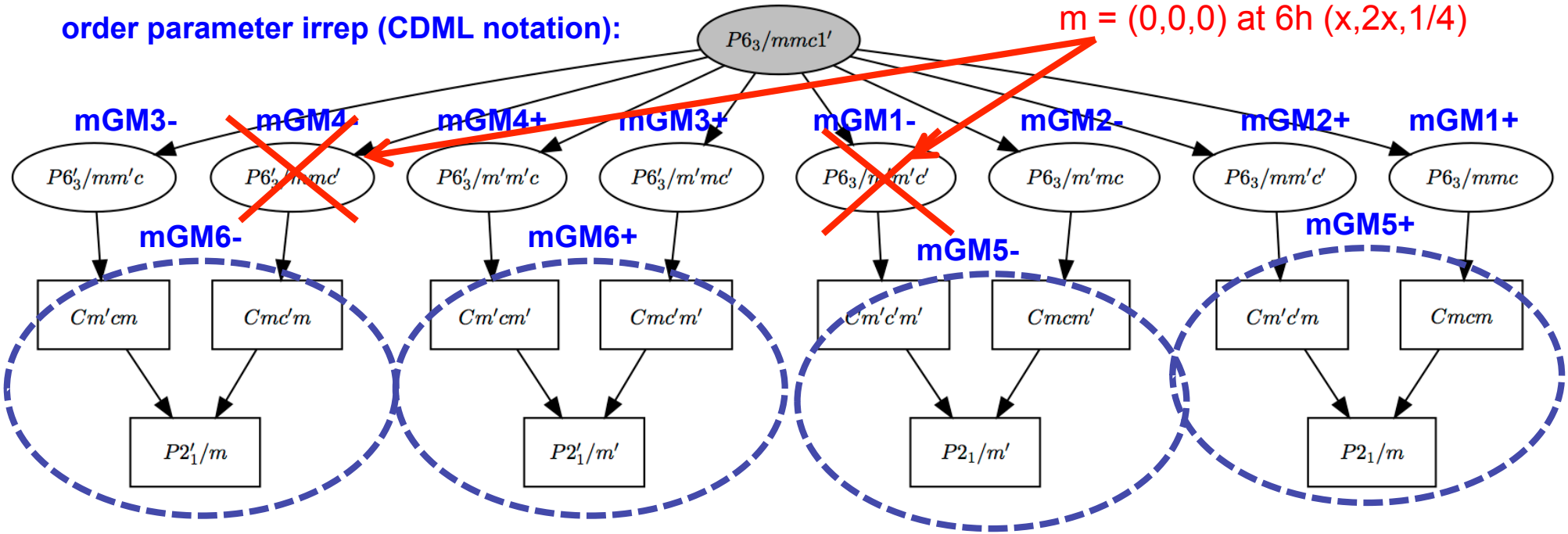
Mn_3Sn

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

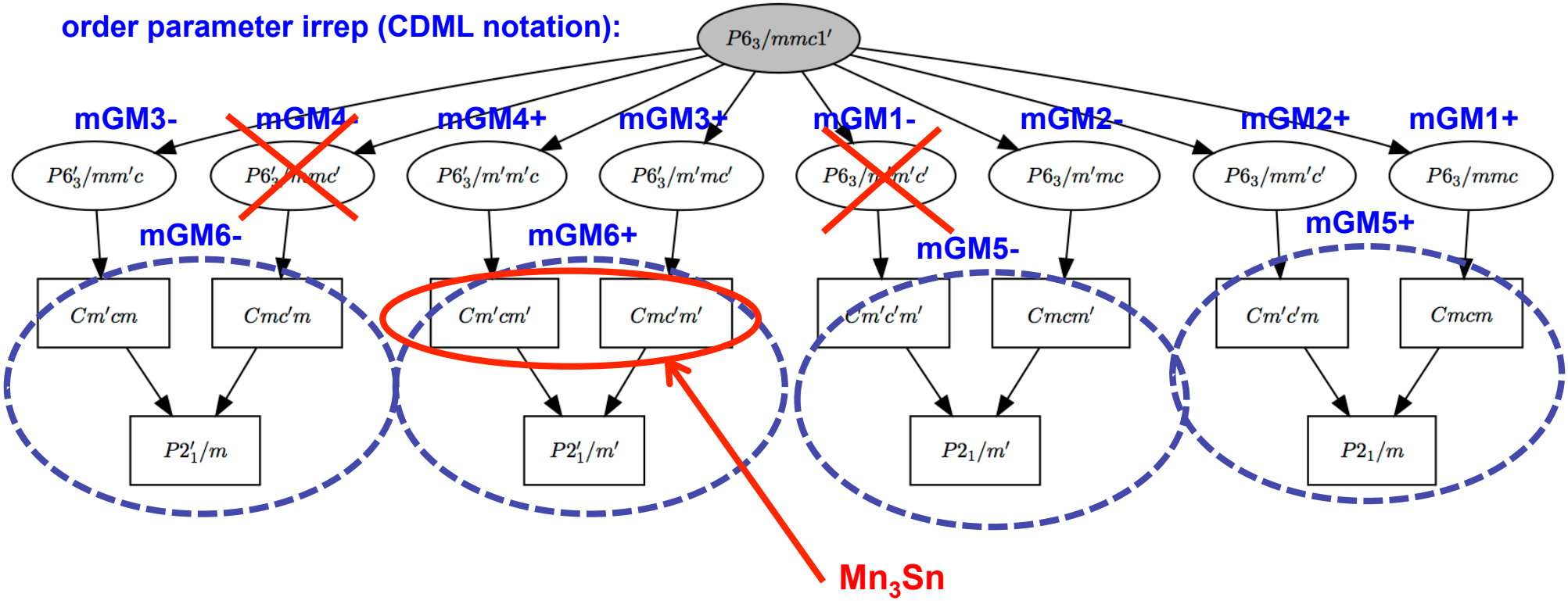
k=(0,0,0)

$P6_3/mmc1'$ ⟶ 2-dim irrep **mGM6+**

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

or

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

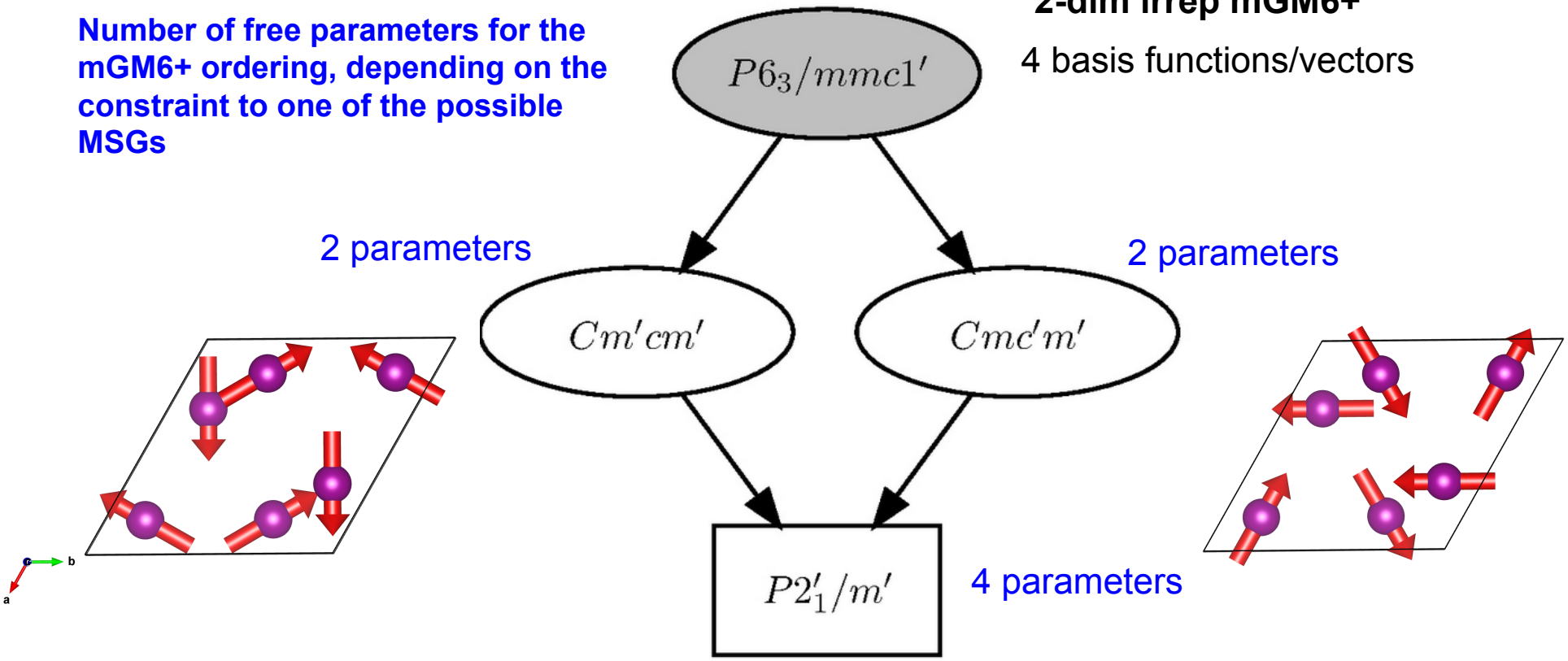


Mn_3Sn k=(0,0,0)

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



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) ⊕

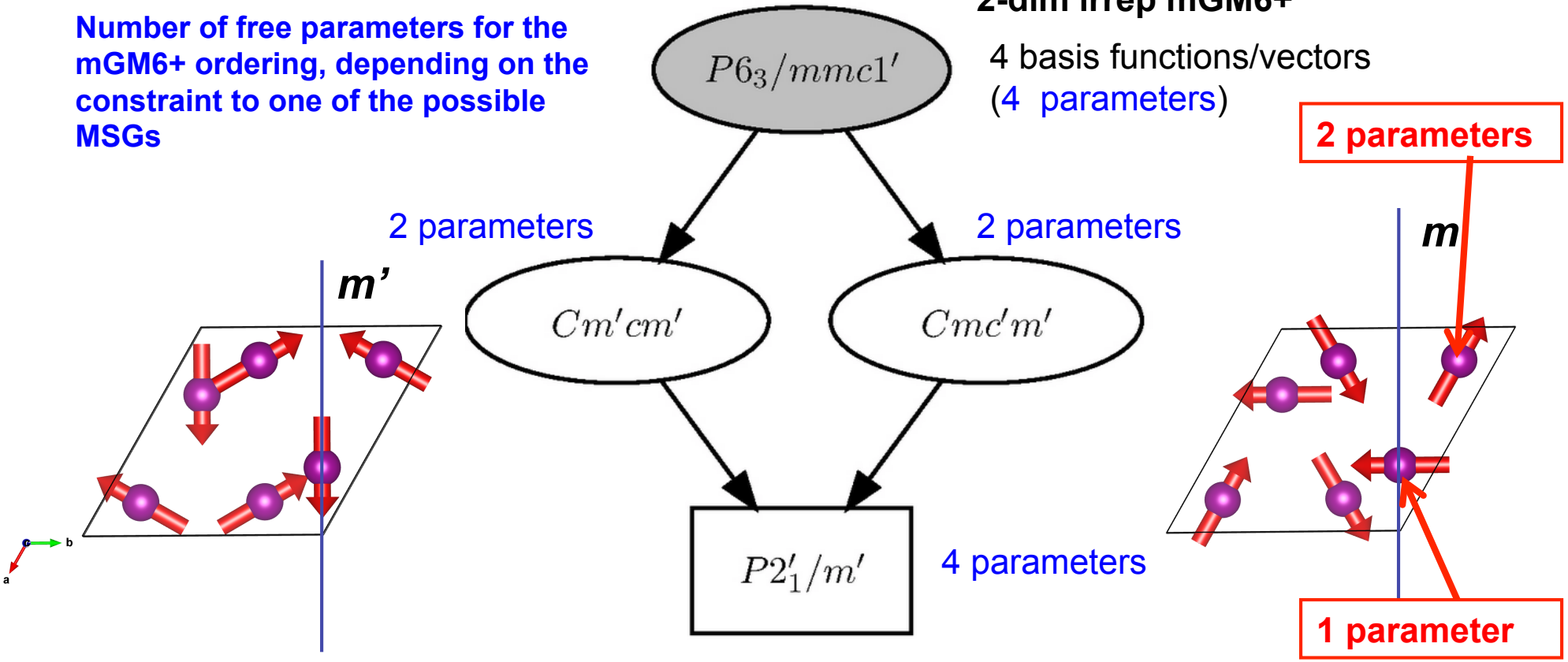
⊕ 1×mGM3-(1) ⊕ 1×mGM4+(1) ⊕ 1×mGM5+(2) ⊕ 2×mGM5-(2) ⊕ 2×mGM6+(2) ⊕ 1×mGM6-(2)

Mn_3Sn 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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⊕ 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
```

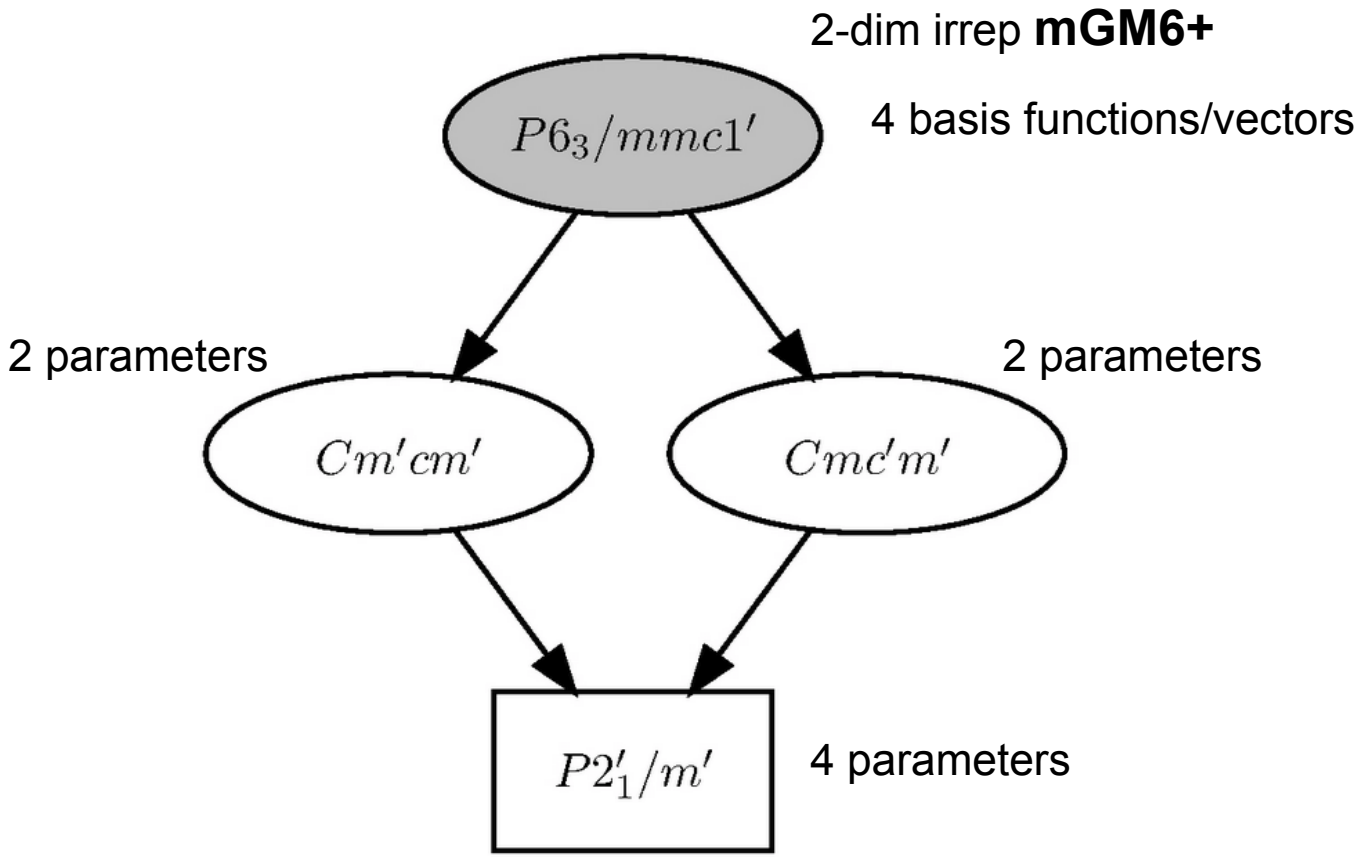
```
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
Mn1_1 Mn 0.83880 0.67760 0.25000
Mn1_2 Mn  0.32240 0.16120 0.25000
Sn1 Sn 0.333333 0.666667 0.25000

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

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

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



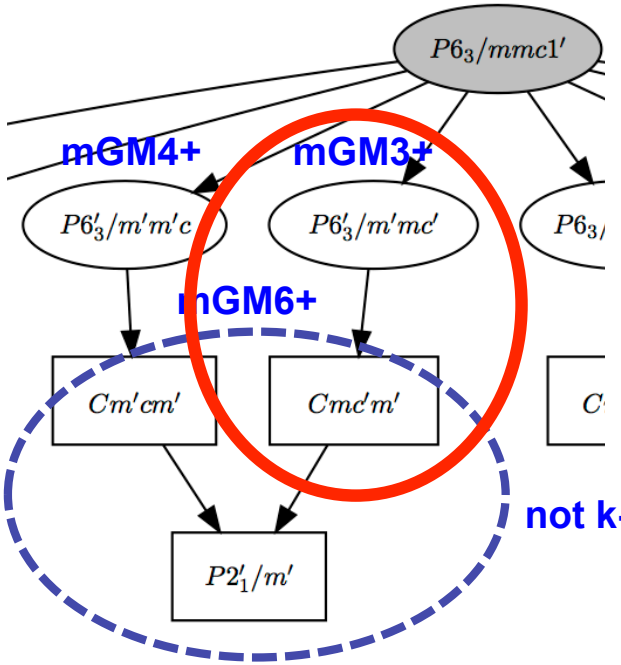
Why 3 free parameters when described using the MSG Cmc'm' instead of 2 parameters?

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)



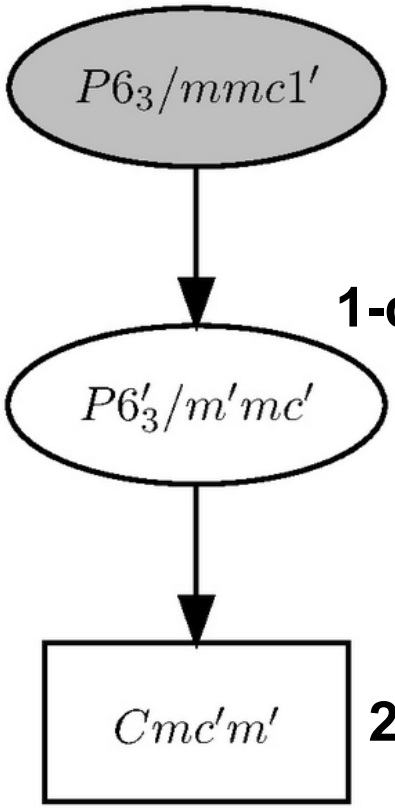
not k-maximal symmetry

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'

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
```

2 parameters if the mGM3+ component is set to zero. Only one parameter because in addition, the two moment magnitudes are forced to be equal.

```
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 parameters because in addition to the constrained mGM6+ arrangement, also a mGM3+ component is also physically possible in the same phase

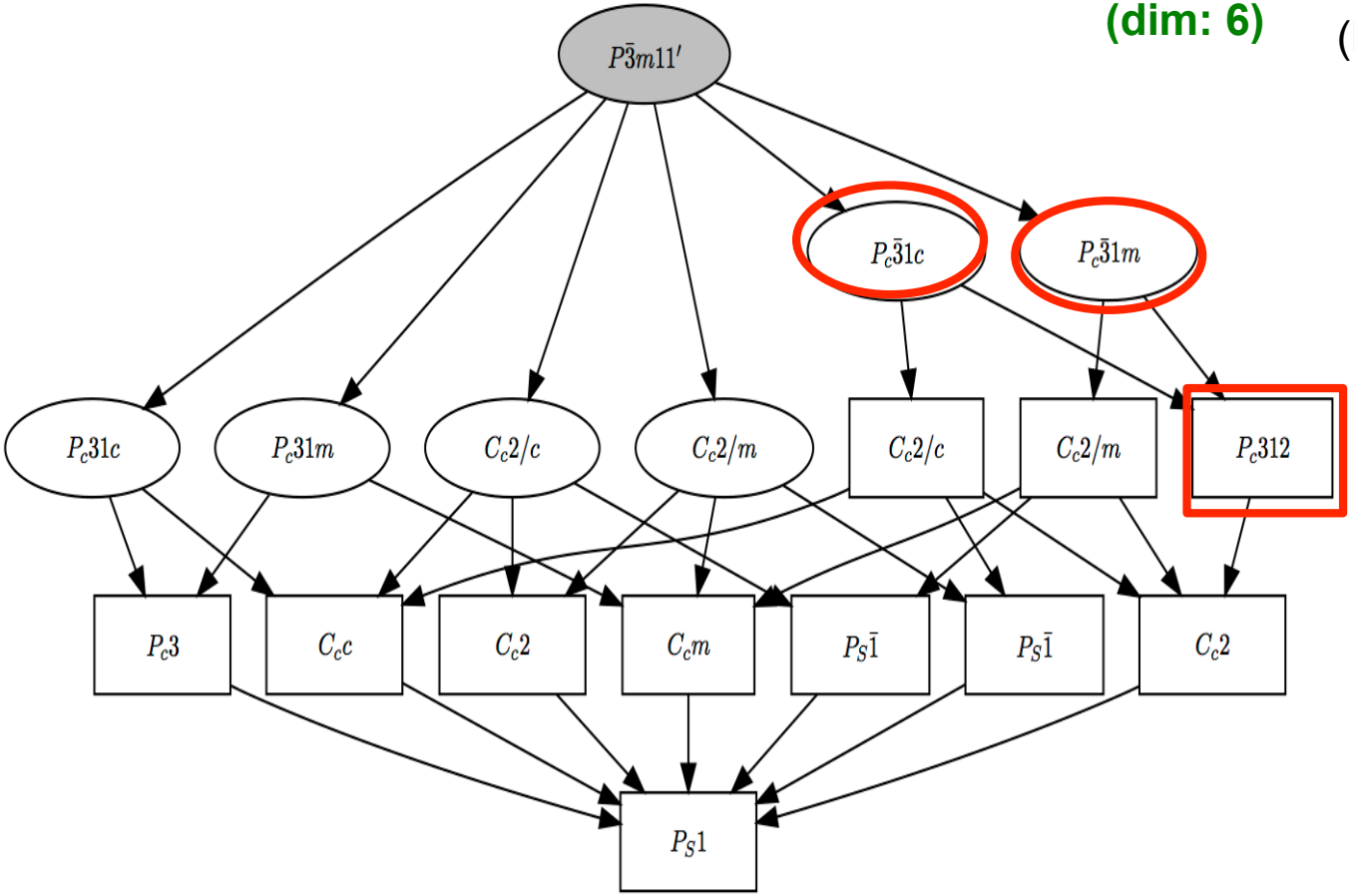
Another example of k-SUBGROUPSMAG with an irrep filter: (Tutorial 2)

Possible magnetic symmetries for a magnetic phase with parent space group P-3m1, propagation vector (1/3,1/3,1/2) and magnetic atom at 1b (0,0,1/2)

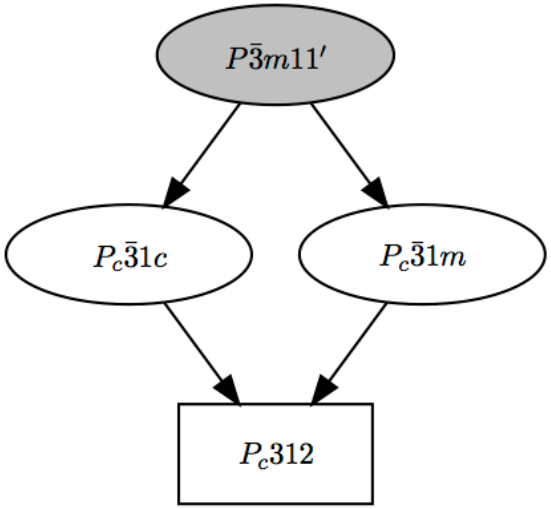
dim
small irrep

Magn_rep (1b)= 1mH1(1)+1mH3(2)

(dim: 6) (k, -k not equivalent)



Restricted to the FULL (k,-k) irrep mH1:



k-SUBGROUPSMAG with an irrep filter:

Possible magnetic symmetries for a magnetic phase with parent space group P-3m1, propagation vector (1/3,1/3,1/2) and magnetic atom at 1b (0,0,1/2)

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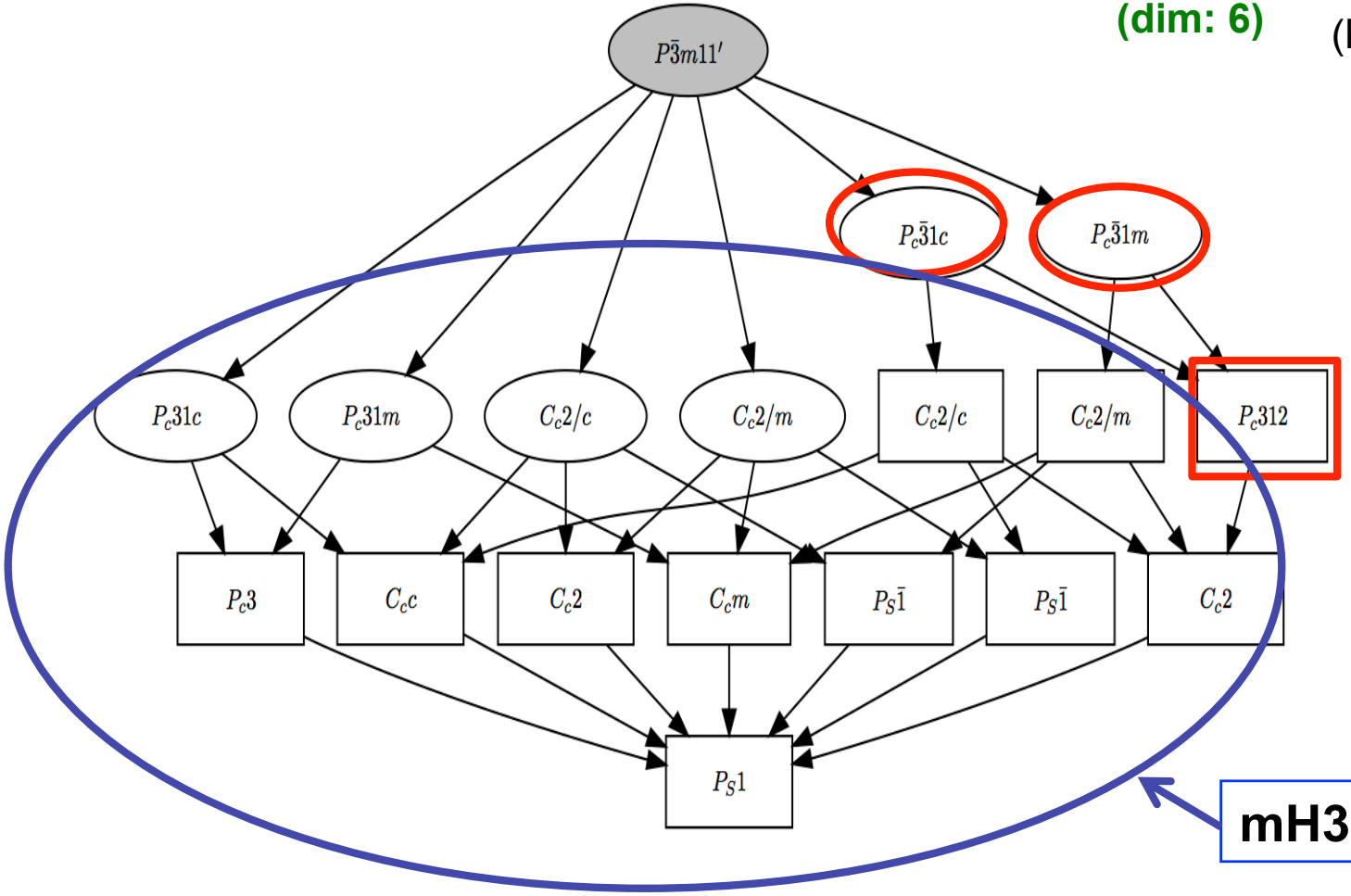
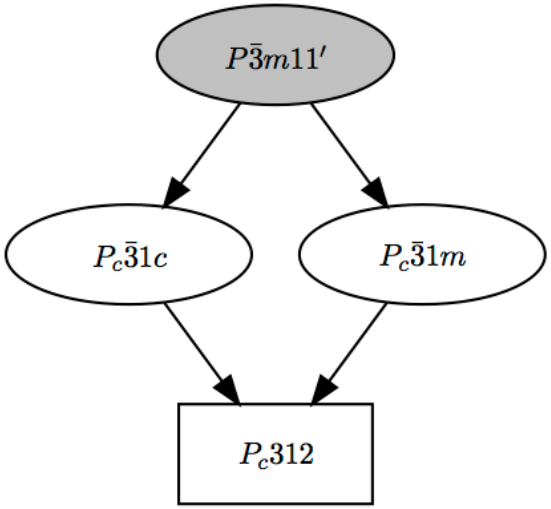
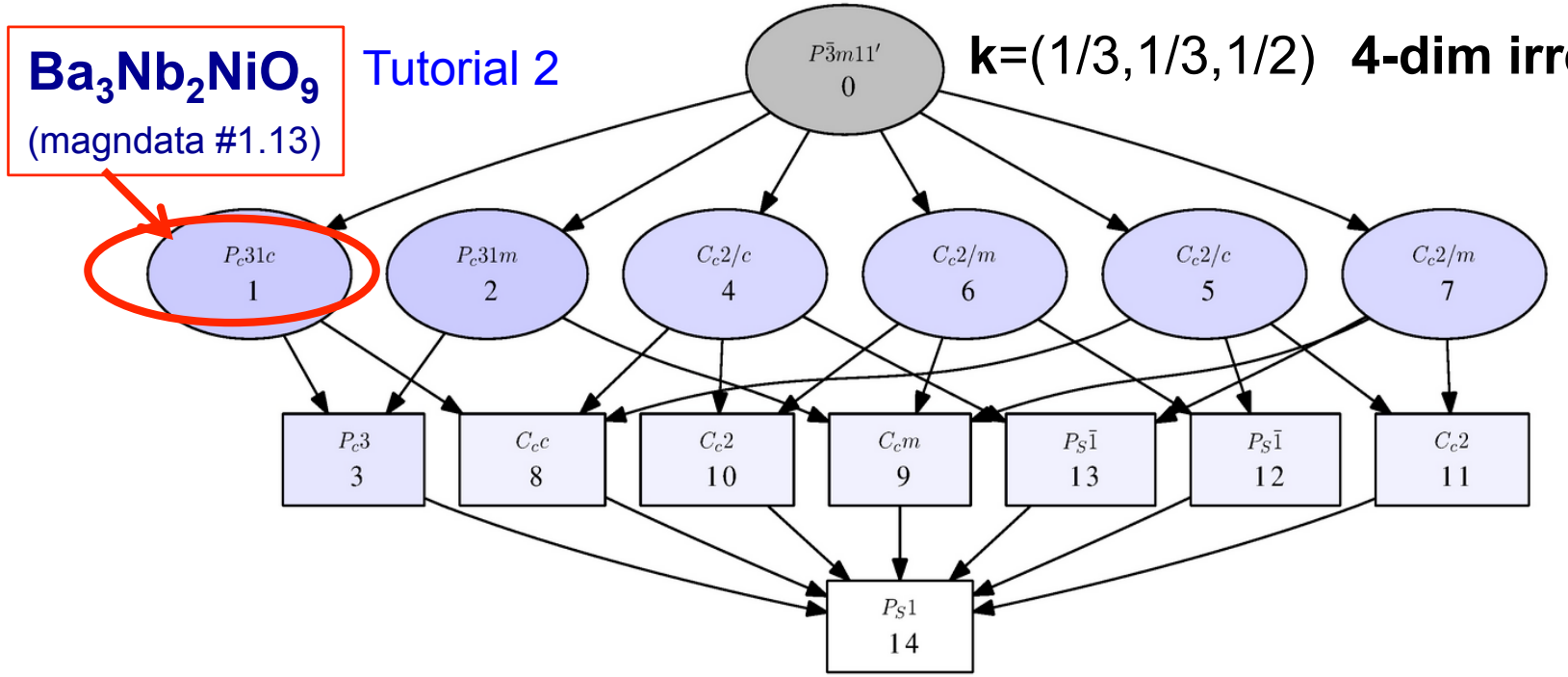


Restricted to the FULL (k,-k) irrep mH1:



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

$Ba_3Nb_2NiO_9$ (magndata #1.13) Tutorial 2



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

Conclusions:

• **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:

• ***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 less frequent 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).

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

Program for mode analysis:

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

January 24, 2015 APERIODIC2015: abstract submission, deadline 30 April

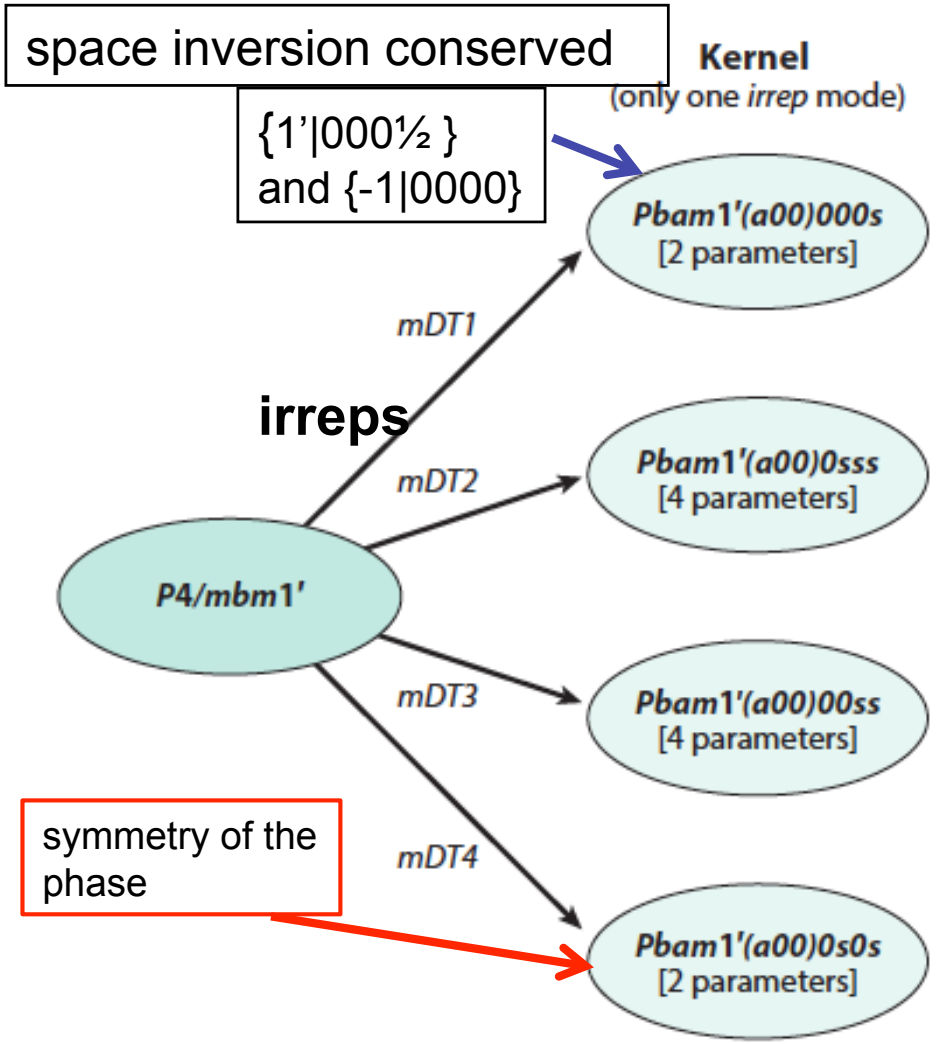
What about magnetic incommensurate structures?

Their symmetry is given by
a magnetic **superspace** group (MSSG)

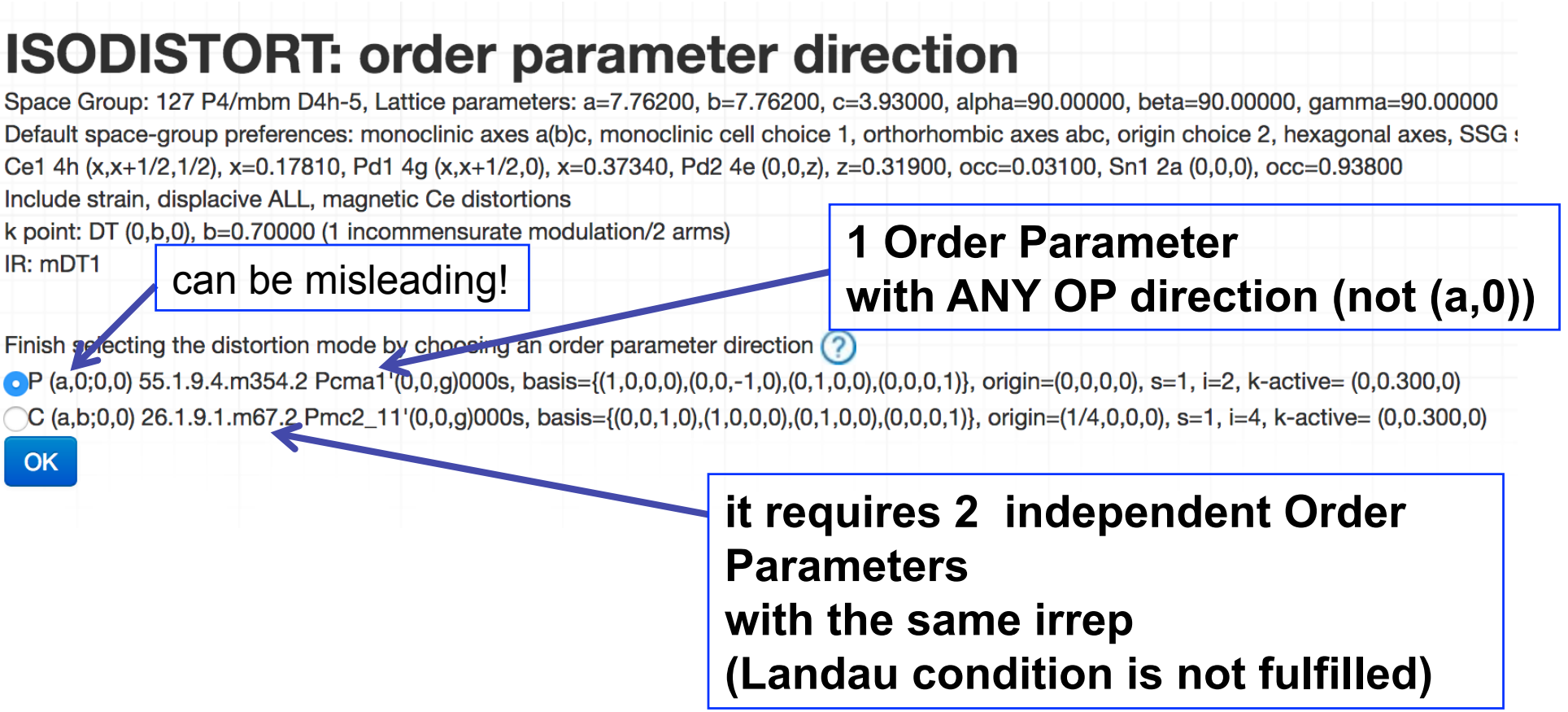
Ce_2Pd_2Sn magndata 1.1.9 space inversion is maintained !

superspace group: Pbam1'(α00)0s0s parent space group: P4/mbm

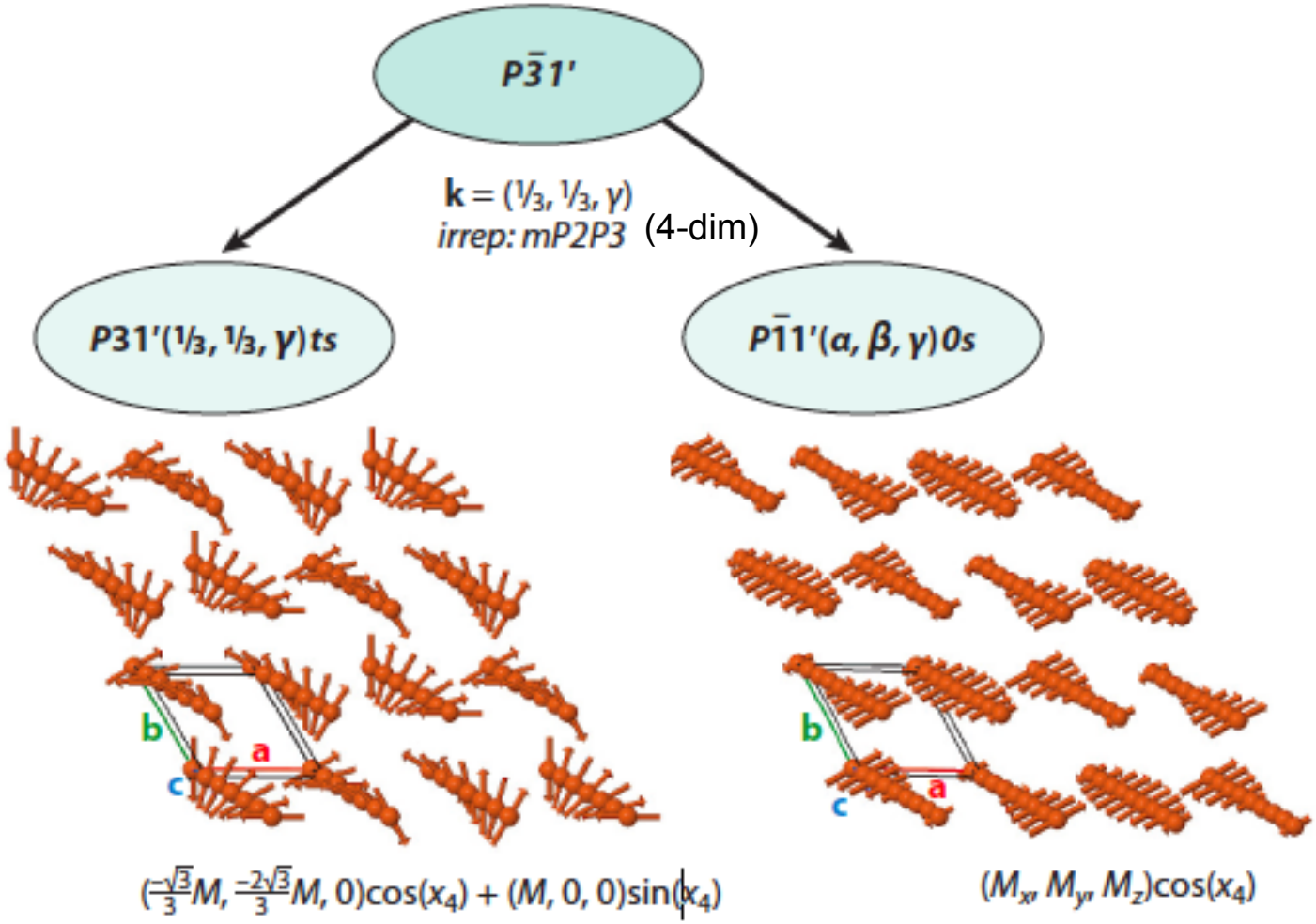
k= (α,0,0)



Beware when interpreting ISODISTORT output:

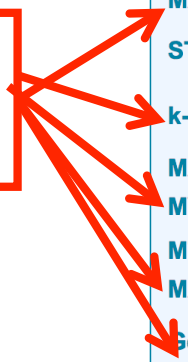


Two possible higher alternative superspace symmetries for the same irrep.



Tutorial to follow:

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

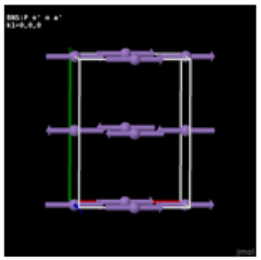
MAGNDATA: A Collection of magnetic structures with portable cif-type files

Element search (separate with space or comma): ◉AND ○OR Search

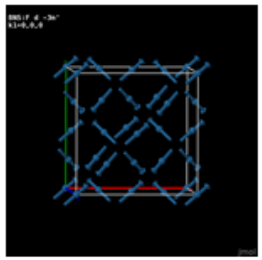
312 structures found

Update: by April 2022 it contains about 1800 structures

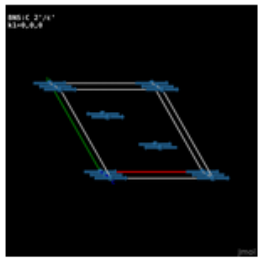
Zero propagation vector



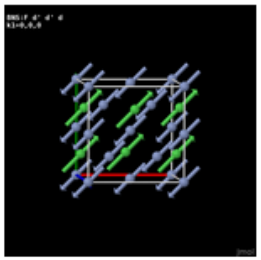
0.1 $LaMnO_3$



0.2 $Cd_2Os_2O_7$



0.3 Ca_3LiOsO_6



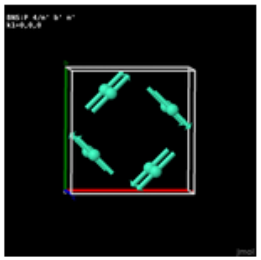
0.4 $NiCr_2O_4$

0.5 Cr_2S_3

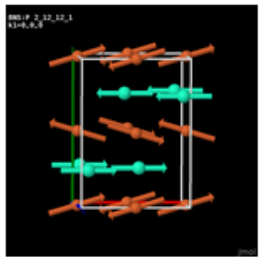
0.6 $YMnO_3$

0.7 $ScMnO_3$

0.8 $ScMnO_3$



0.9 GdB_4



0.10 $DyFeO_3$

$Sr_2F_2Fe_2OS_2$ (MAGNDATA #2.2)

MAGNDATA: A Collection of magnetic structures with portable cif-type files

Log in

MAGNDATA: A collection of magnetic structures with portable cif-type files

A database of more than 1000 published commensurate and incommensurate magnetic structures can be found here. The structures are described using magnetic symmetry (Shubnikov magnetic space groups) in the BNS setting for commensurate structures, and magnetic superspace groups for incommensurate structures. Symmetry is applied both for magnetic moments and atomic positions. The information provided is sufficient to define unambiguously the positions and magnetic moments (if any) of all atoms in the structure. A non-standard setting consistent with the setting of the paramagnetic phase is often used (this setting does not necessarily coincide with the one used in the original reference). A cif-like (.mcif) file of each entry can be downloaded. mcif files are supported by: ISOCIF, ISODISTORT, VESTA, Jmol, JANA2006 and FullProf. ISOCIF can be used to generate an alternative mcif file in a standard setting, as required by ISODISTORT. Vesta files for visualization of a single magnetic unit cell are also available. Any entry can be directly downloaded in StrConvert for editing, visualization,

View Full Database

Element search (separate with space or comma): AND OR Search

Enter the label of the structure: Submit

Advanced Search & Statistics

To upload any published structure click HERE

Now you can help to complete the database and submit your structure(s) or any other published structure that you may fancy.

STRCONVERT: Editor of Structure magCIF files and other formats

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Structure Data Converter & Editor

Please submit a structure file:

Browse... No file selected. Upload the file

[Supported file formats: CIF, mCIF, VESTA, VASP]

Symmetry

Magnetic Space Group # (BNS): 31.129 (P_bmn2_1) *Type: IV*

Lattice Parameters

a: 11.670 Å b: 7.360 Å c: 5.2572 Å

α 90.000° β: 90.000° γ: 90.000°

Symmetry Operations [Show/Hide]

Recognized formats:

1. x,y,z mx,my,mz +1
x,y,z mx,my,mz +1
x,y,z
x,y,z,+1
1 'x, y, z'
1 x,y,z

```
x,y,z,+1
-x+1/4,-y,z+1/2,+1
x,-y+1/2,z,+1
-x+1/4,y+1/2,z+1/2,+1
x+1/2,y,z,-1
-x+3/4,-y,z+1/2,-1
x+1/2,-y+1/2,z,-1
-x+3/4,y+1/2,z+1/2,-1
```

Update the symmetry operators with the above Apply

Symmetry operations have been parsed from the file/form

Populate with operators from database

Structure Data Converter & Editor

Atomic Positions & Magnetic Moments

Switch to the treatment of the vectors as: displacements Go!

	Label	Element	x	y	z	Occ.	m_x	m_y	m_z
☐	Ho	Ho	0.04195	0.25000	0.98250	1.00000	0.00000	0.00000	0.00000
☐	Ho_1	Ho	0.95805	0.75000	0.01750	1.00000	0.00000	0.00000	0.00000
☐	Mn	Mn	0.00000	0.00000	0.50000	1.00000	3.87000	0.00000	0.00000
☐	O1	O	0.23110	0.25000	0.11130	1.00000	0.00000	0.00000	0.00000
☐	O1_1	O	0.76890	0.75000	0.88870	1.00000	0.00000	0.00000	0.00000
☐	O2	O	0.16405	0.05340	0.70130	1.00000	0.00000	0.00000	0.00000
☐	O2_1	O	0.83595	0.55340	0.29870	1.00000	0.00000	0.00000	0.00000

Add atoms more. || Remove selected atoms || Change the selected atoms' symbol to

Select the atoms with the symbol: || Select all atoms || Unselect all atoms

Longest Arrow size: 1.314 [for VESTA format export: Å *(Default: min(a,b,c)/4)*]
[for Jmol visualize: a proportional coefficient]

Export to BCS format | Export to VESTA format
Export to Standard CIF format | Export to MCIF format
Export to VASP format | Transform the structure to P1 setting
Remove the magnetic information | Re-order the sites | Visualize

magCIF file can be produced: