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Magnetic space groups vs. irreducible representations and the Bilbao Crystallographic Server

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- **Magnetic ordering is a symmetry-breaking 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?:

- A matrix for each operation describes the corresponding transformation of the distortion: A REPRESENTATION of the symmetry group of the paramagnetic phase:

Clumsy/primitive way of describing a spin arrangement in a crystal:

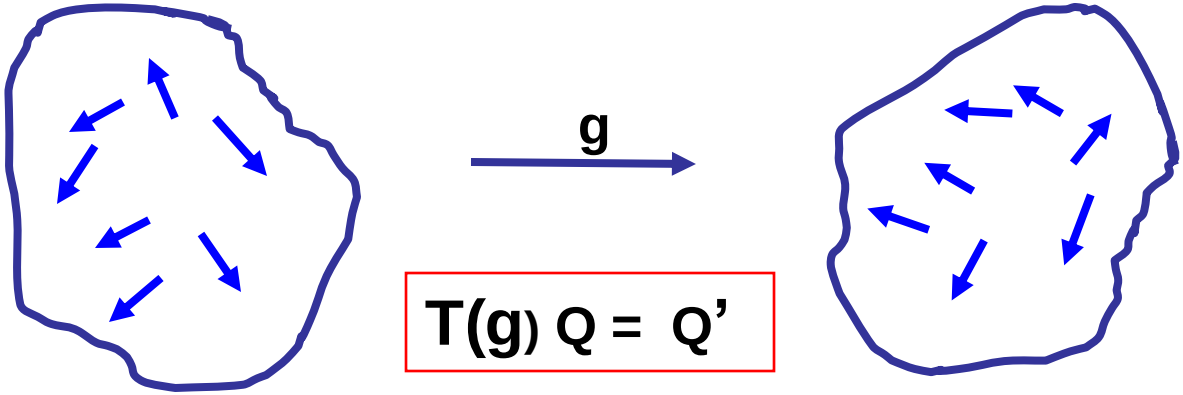
Description atom by atom:
Atomic spins of all magnetic atoms :

$S_{1x} = Q_{1x}\ ex1$
$S_{1y} = Q_{1y}\ ey1$
$S_{1z} = Q_{1z}\ ez1$
$S_{2x} = Q_{2x}\ ex2$
$S_{2y} = Q_{2y}\ ey2$ Atoms 1,...,N
$S_{2z} = Q_{2z}\ ez2$
…
…
$S_{Nx} = Q_{Nx}\ exN$
$S_{Ny} = Q_{Ny}\ eyN$
$S_{Nz} = Q_{Nz}\ ezN$

Distortion:
$Q = (Q_{1x}, Q_{1y}, Q_{1z}, \ldots\ldots, Q_{Nx}, Q_{Ny}, Q_{Nz})$

3N parameters

g operation of the parent space group G

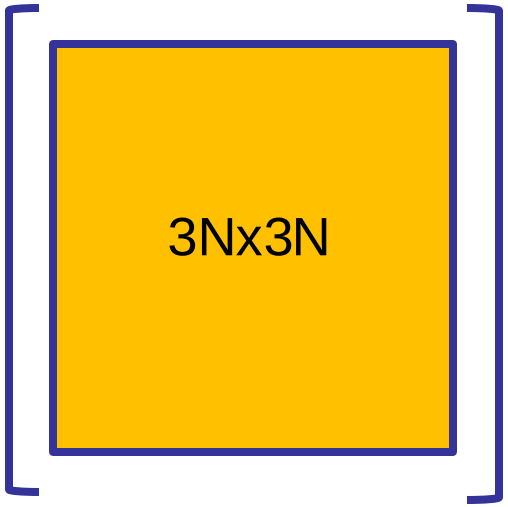


$Q = (Q_{1x}, Q_{1y}, \ldots Q_{Ny}, Q_{Nz})$ $\quad$ $Q' = (Q'_{1x}, Q'_{1y}, \ldots Q'_{Ny}, Q'_{Nz})$

Magnetic representation of the parent space group G:

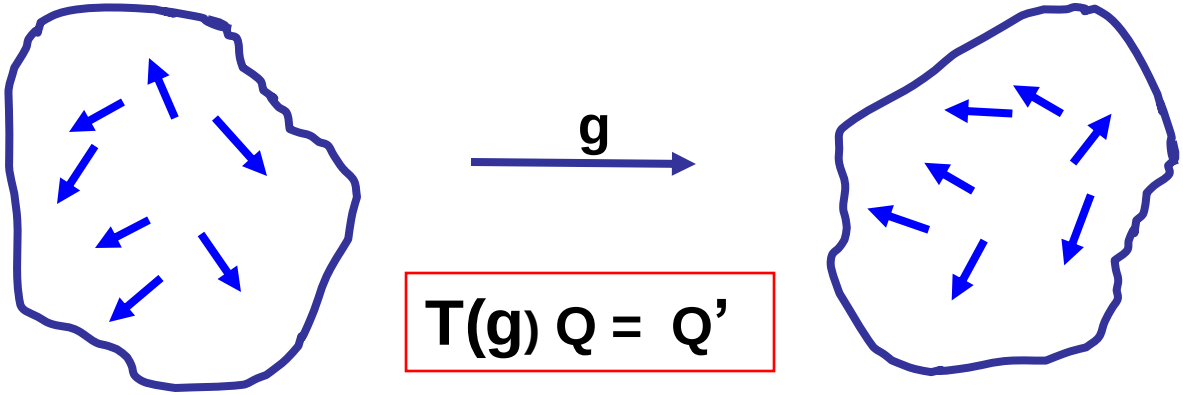
Set of the matrices T(g): 3Nx3N, one for each g of the parent space group:

T(g) =



For a given parent structure the determination of the magnetic representation (the matrices T) is a pure mathematical problem (no physics!)

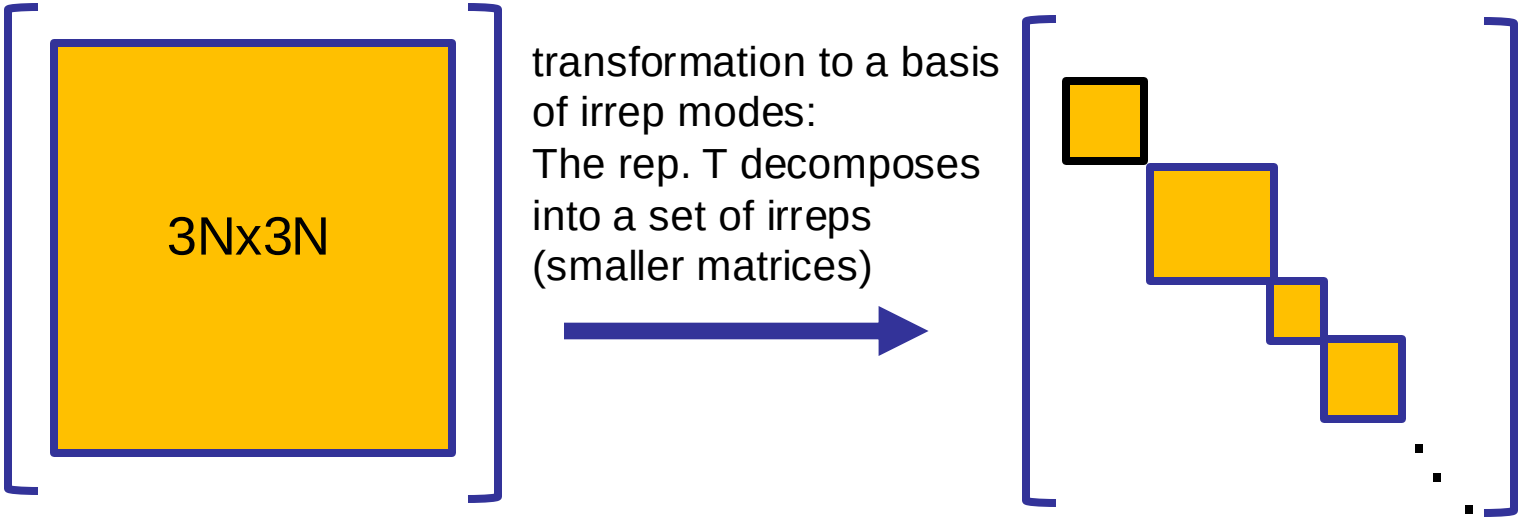
g operation of the parent space group G



Set of matrices T(g): 3Nx3N representation of the parent space group G

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

Irrep decomposition of the magnetic representation: Pure mathematical problem!



We change to a basis of collective modes:

Description atom by atom:
Atomic spins in all magnetic atoms :

$S_{1x} = Q_{1x}\ ex1$
$S_{1y} = Q_{1y}\ ey1$
$S_{1z} = Q_{1z}\ ez1$
$S_{2x} = Q_{2x}\ ex2$
$S_{2y} = Q_{2y}\ ey2$ Atoms 1,...,N
$S_{2z} = Q_{2z}\ ez2$
…
…
$S_{Nx} = Q_{Nx}\ exN$
$S_{Ny} = Q_{Ny}\ eyN$
$S_{Nz} = Q_{Nz}\ ezN$

Distortion:
$Q = (Q_{1x}, Q_{1y}, Q_{1z}, \ldots\ldots, Q_{Nx}, Q_{Ny}, Q_{Nz})$

3N parameters

Change of basis:
Mode basis (orthonormal) :

$\varepsilon 1 = a_{11} ex1 + a_{12} ey1 + a_{13} ex1 \ldots a_{13N} ezN$
$\varepsilon 2 = a_{21} ex1 + a_{22} ey1 + a_{23} ex1 \ldots a_{23} NezN$
$\varepsilon 3 = a_{31} ex1 + a_{32} ey1 + a_{33} ex1 \ldots a_{33N} ezN$
…
…
$\varepsilon 3N = a_{3N1} ex1 + a_{3N2} ey1 + \ldots + a_{3N3N} ezN$

(3N x 3N) matrix transformation

Distortion in the new basis:

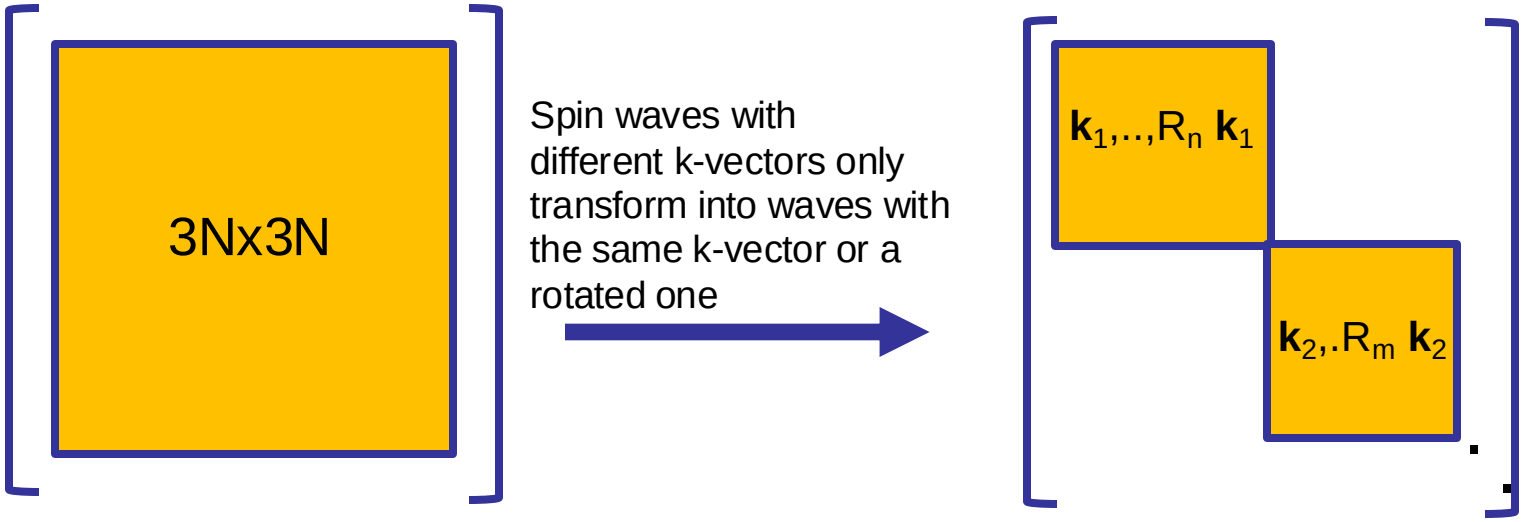
$Q = Q_1\ \varepsilon 1 + Q_2\ \varepsilon 2 + Q3\ \varepsilon 3 + \square . + Q_{3N}\ \varepsilon_{3N}$

Q = (Q1, Q2, Q3, …, Q3N)
3N parameters (mode amplitudes)
(collective coordinates)

N is infinite, but ……

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

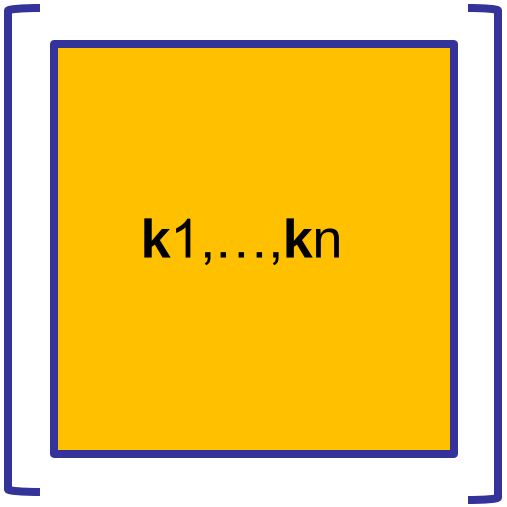
first step: decompositions in waves with different ks:



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

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

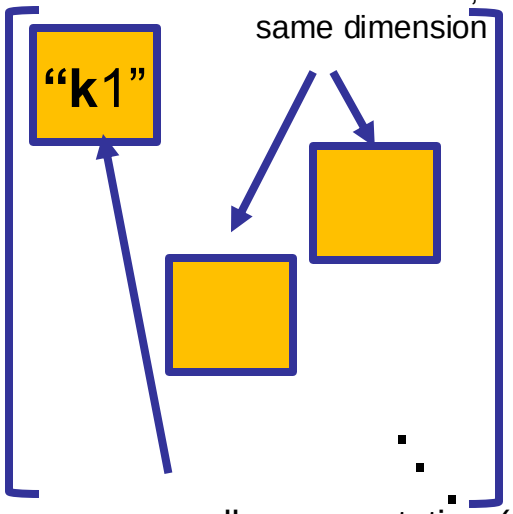
$Q = (Q1_{k1}, Q2_{k1},\ldots Q3s_{k1},\ldots,Q1_{kn}, Q2_{kn},\ldots Q3s_{kn})$



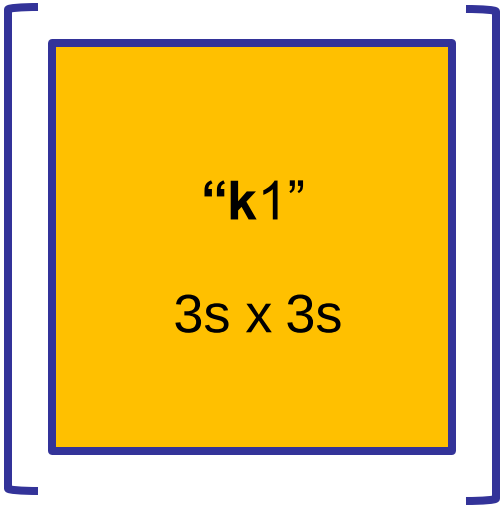
The block of k1 and related ones decomposes into a set of blocks (smaller matrices)

If the operation **g** keeps k1 invariant

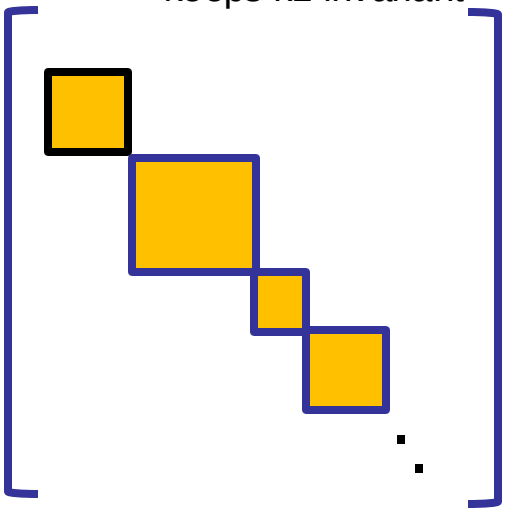
they can be derived from the matrix “k1” , with the same dimension



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:

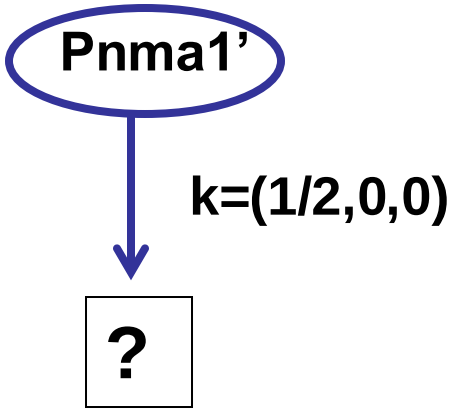


if several magnetic atoms in the asymmetric unit- each orbit can be decomposed separately

s=number of magnetic atoms in a primitive unit cell

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

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 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

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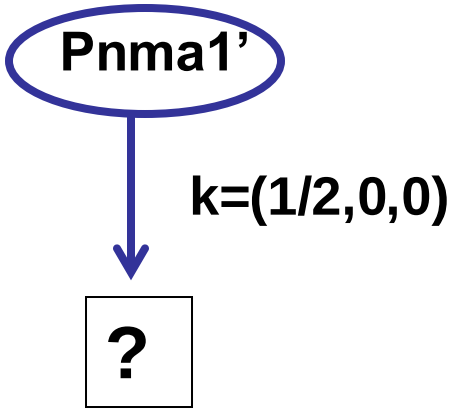
Possible spin arrangements for a magnetic structure having space group Pnma in the paramagnetic phase and a magnetic ordering with propagation vector k=(1/2,0,0)?



$HoMnO_3$

Mn at WP 4b

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

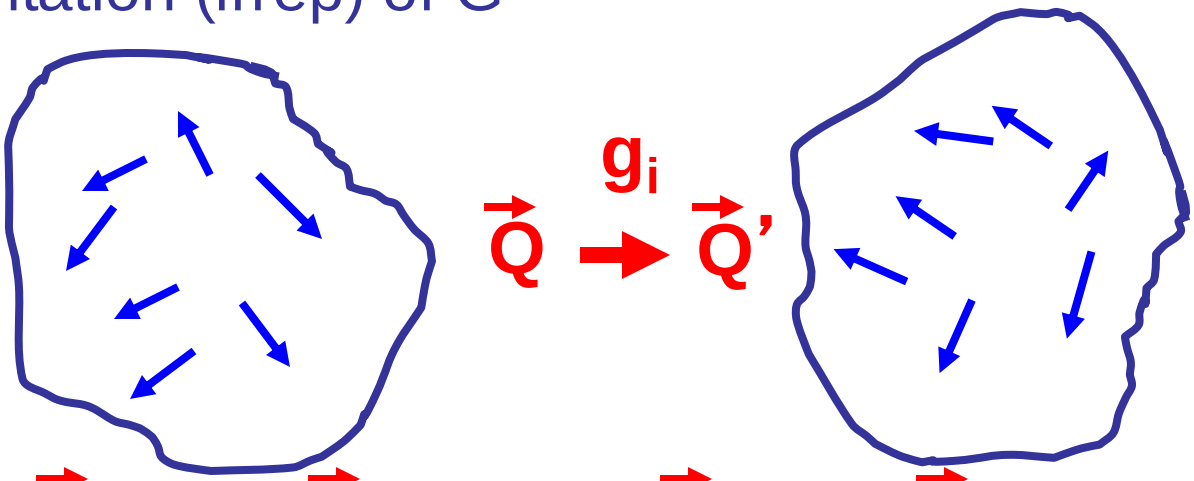
6-dim 6-dim

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

irreps

Decomposition into irreps

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 of modeling magnetic structures

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 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:

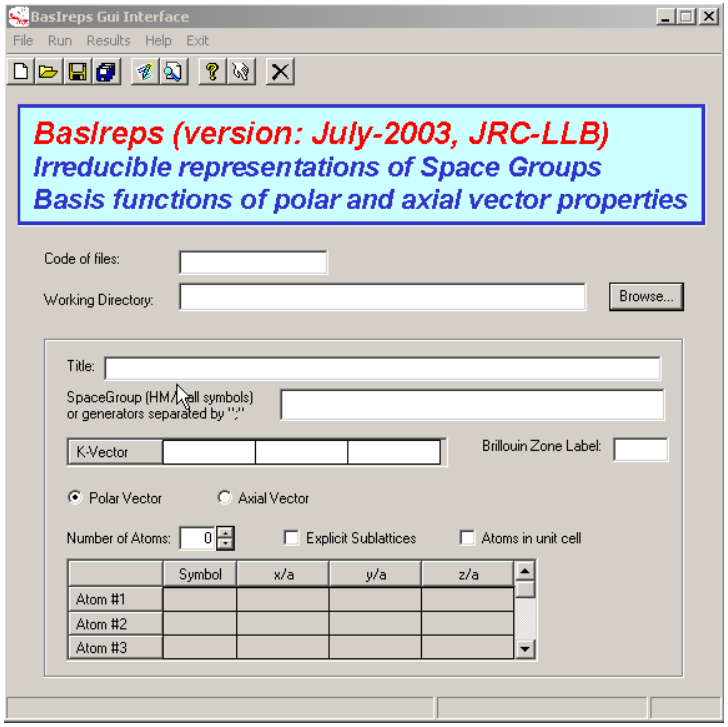
In the analysis of spin structures a 'natural' point of view looks for the set of symmetry operations which leave the magnetic structure invariant and has led to the development of magnetic or Shubnikov groups. A second point of view presented here simply asks for the transformation properties of a magnetic 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, ...)

The use of MSGs and Representation Analysis should not taken as alternative 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

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

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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.

3. How RA and MSGs work together

3.1. General considerations

As previously mentioned, RA and space group symmetry began to be applied in the analysis of structurally distorted structures in the 1970s, not as competing approaches, but as complementary concepts. Following Landau theory, a structurally distorted structure relative to a parent structure of higher symmetry (real or virtual) can be viewed as the outcome of a symmetry-breaking instability. In this scenario, one or more primary order parameters (unstable distortion

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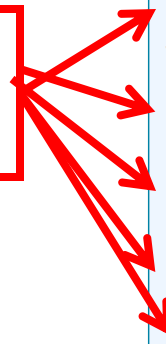
Tutorial_magnetic_section_BCS_2

Only section 2.2



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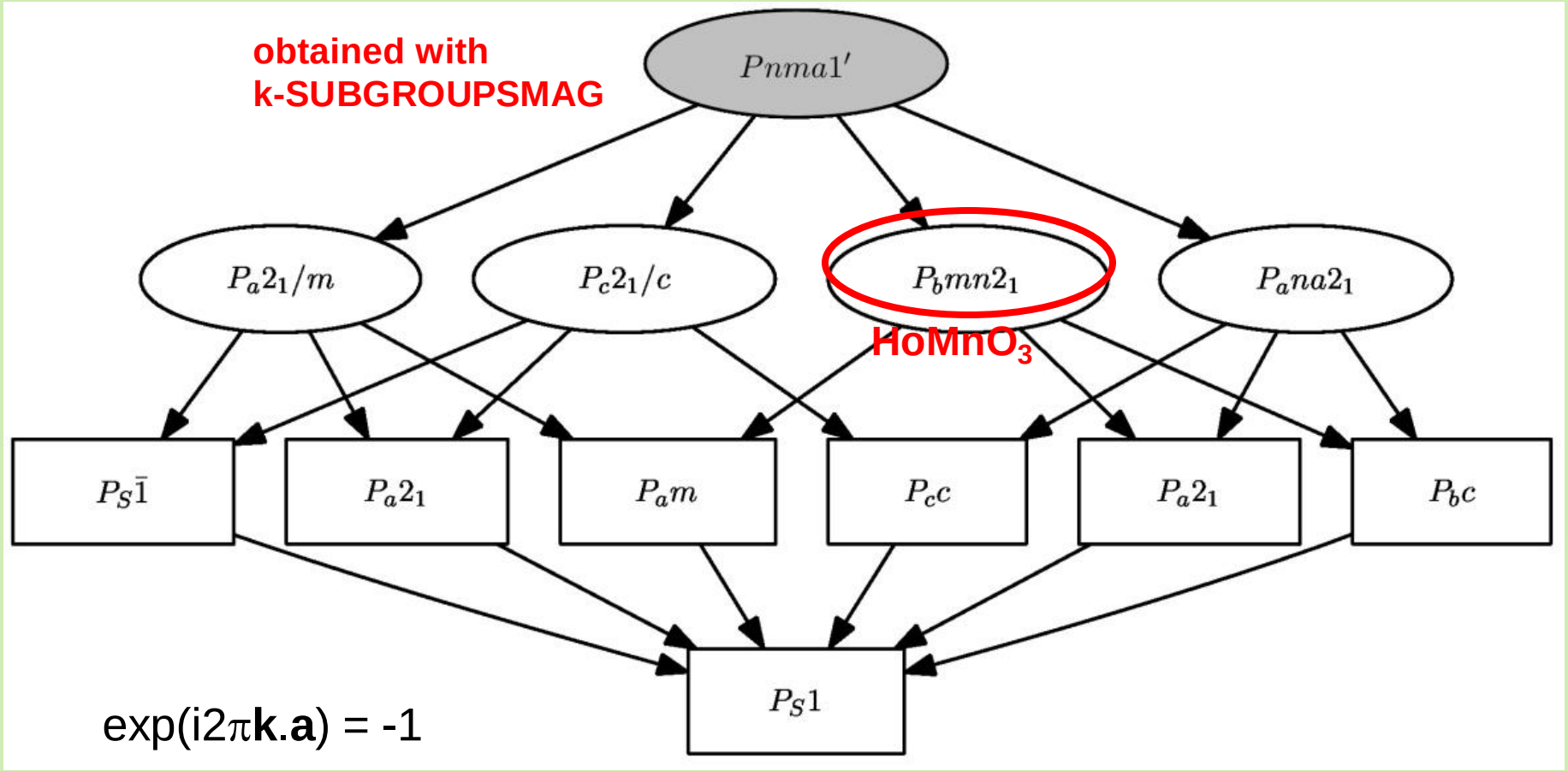
Symmetry based modelling of magnetic structures

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



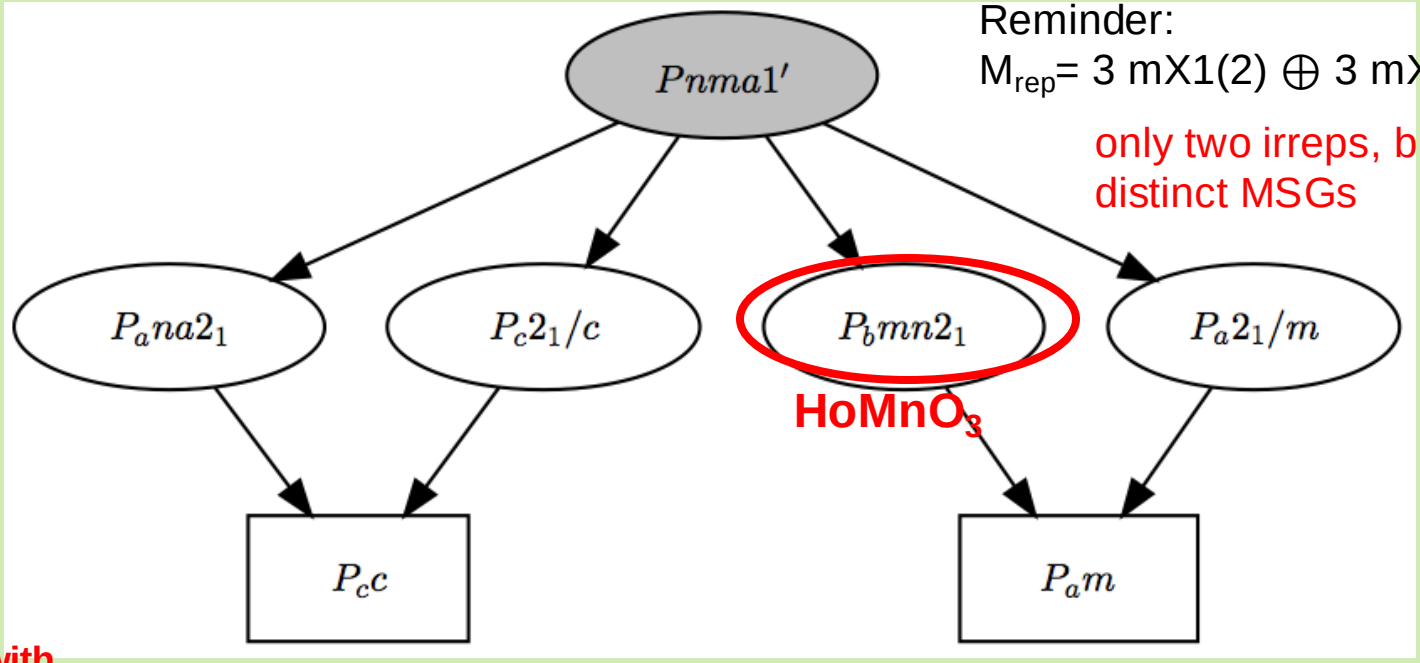
exp(i2π**k**.**a**) = -1

(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

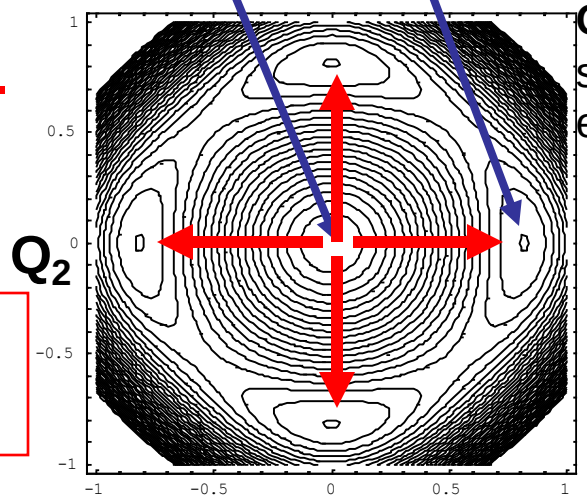
Irreducible representation of G (irrep) (matrices)

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

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:

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

nxn matrix of irrep

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

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

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

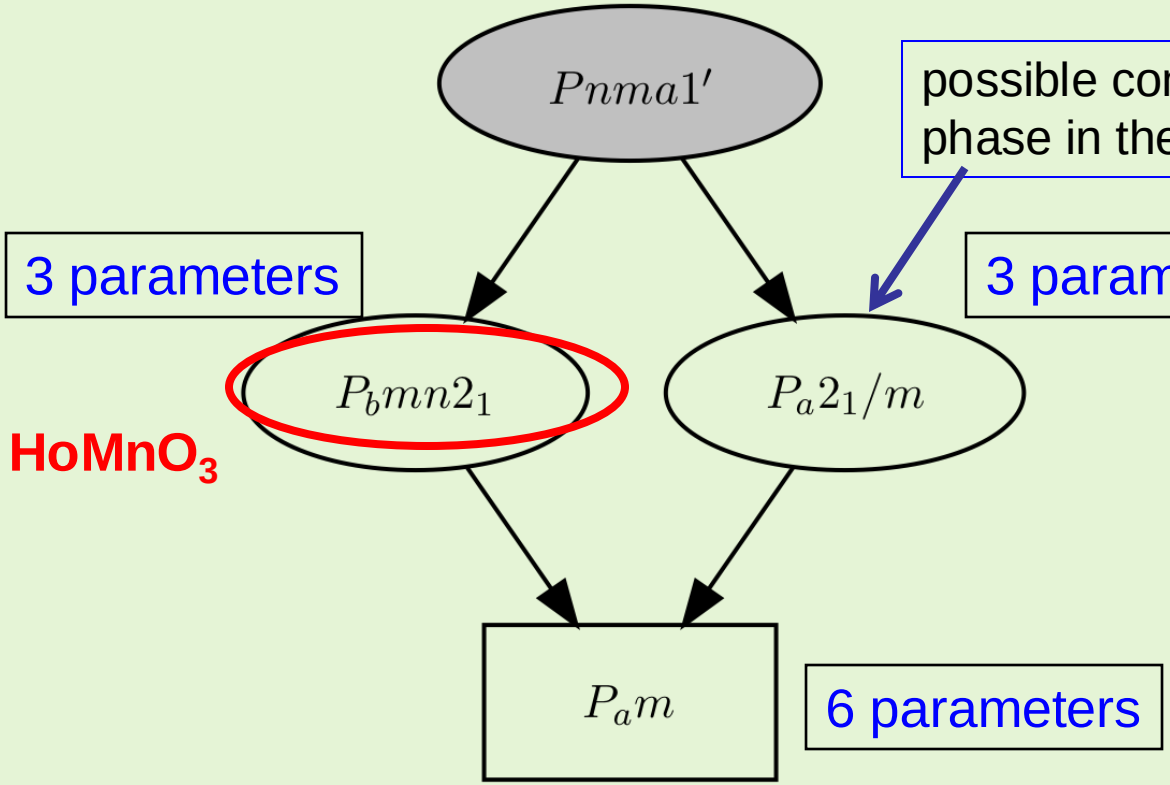
Give the Wyckoff positions Wyckoff

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

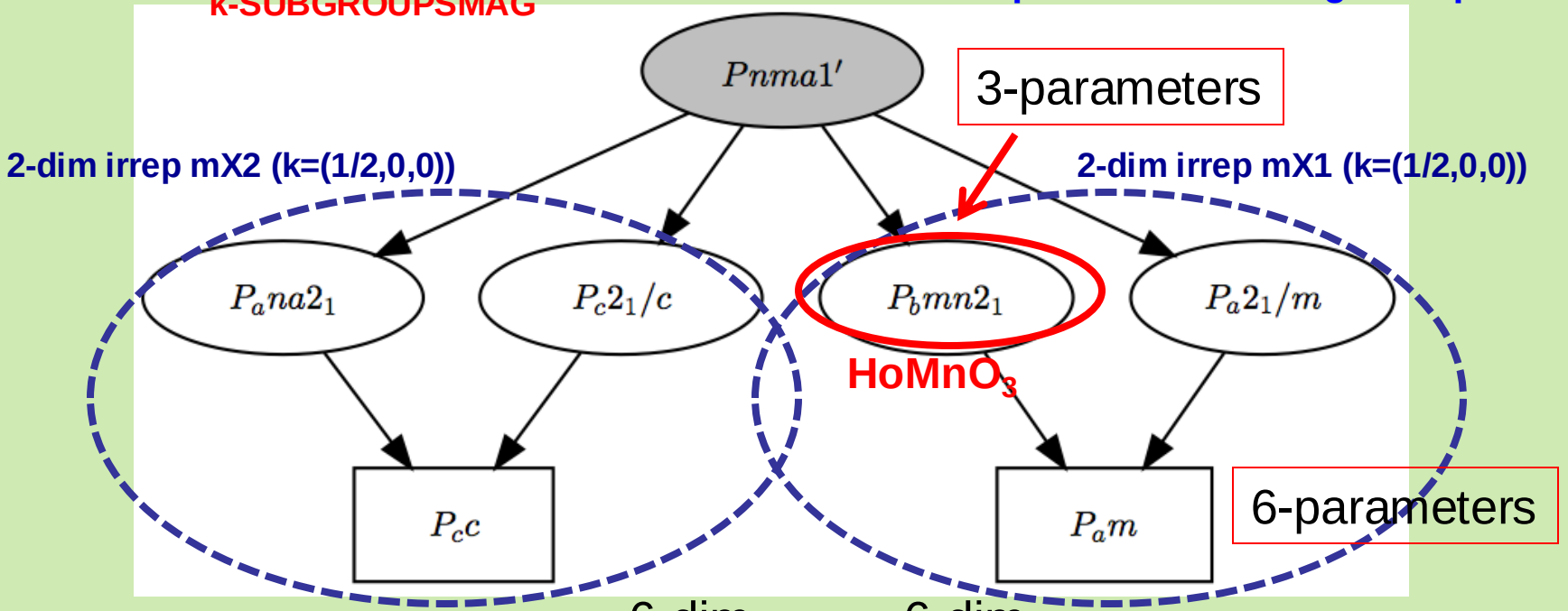
Symmetry based modeling in magnetic structures

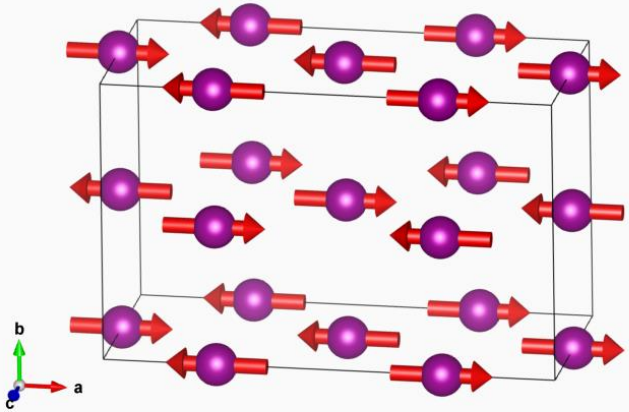
Possible magnetic symmetries for a magnetic phase with propagation vector (1/2,0,0) and parent space group Pnma

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

obtained with k-SUBGROUPSMAG

case : 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_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**

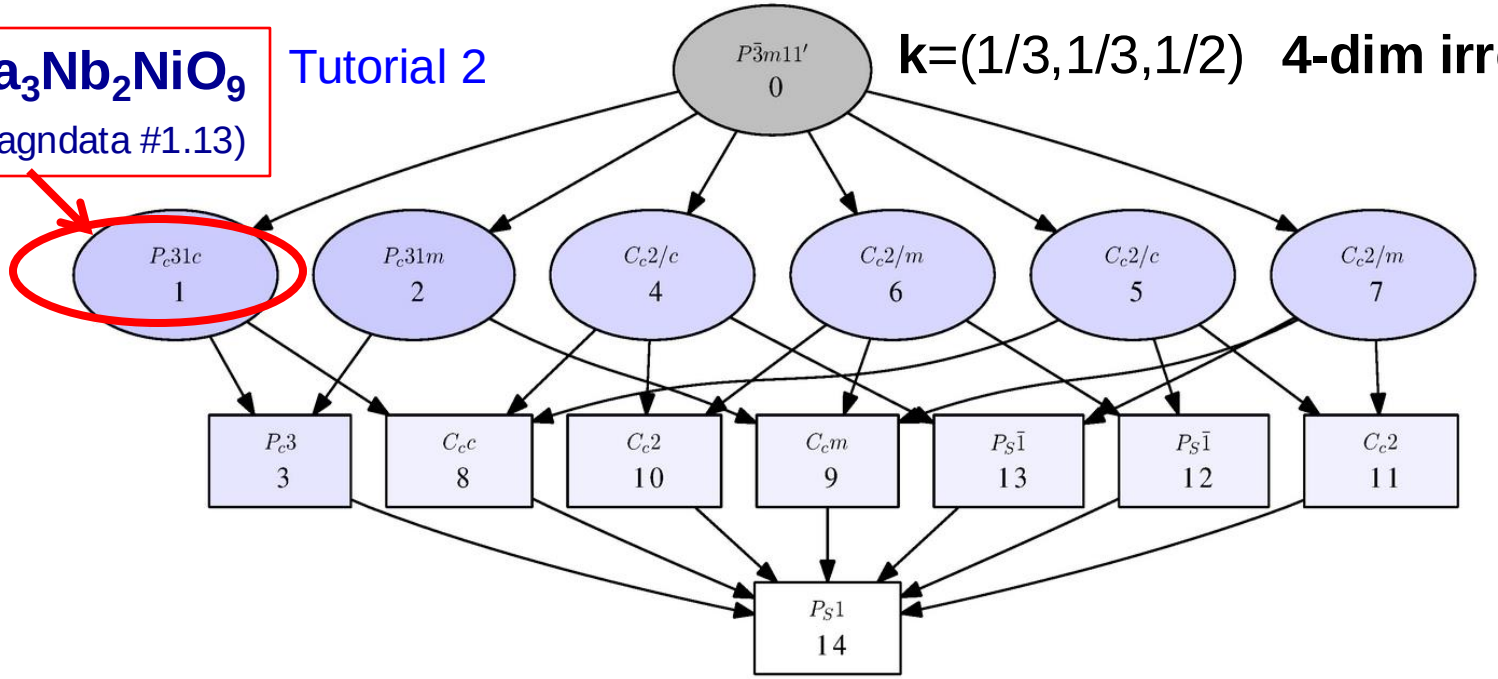
Does the identification of the irrep bring some additional knowledge or constraint? …NO

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

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

$Ba_3Nb_2NiO_9$
(magndata #1.13)

Tutorial 2



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)

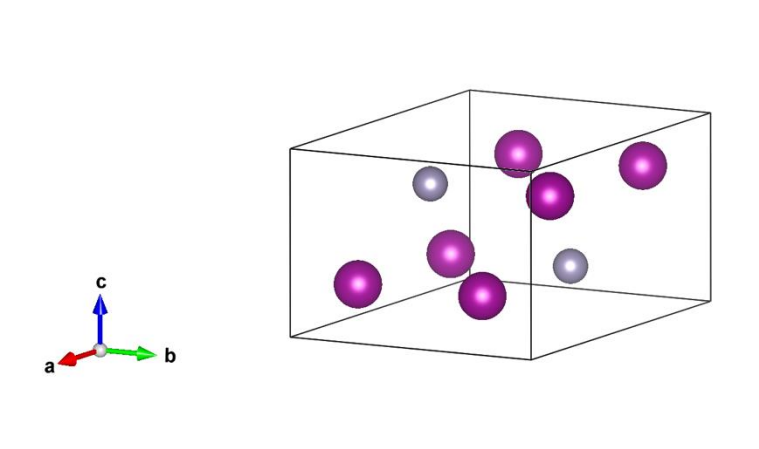
Another example irreps vs MSG with some more complications:

Mn_3Sn

k=(0,0,0)

$P6_3/mmc.1'$ ⟶ *??*

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

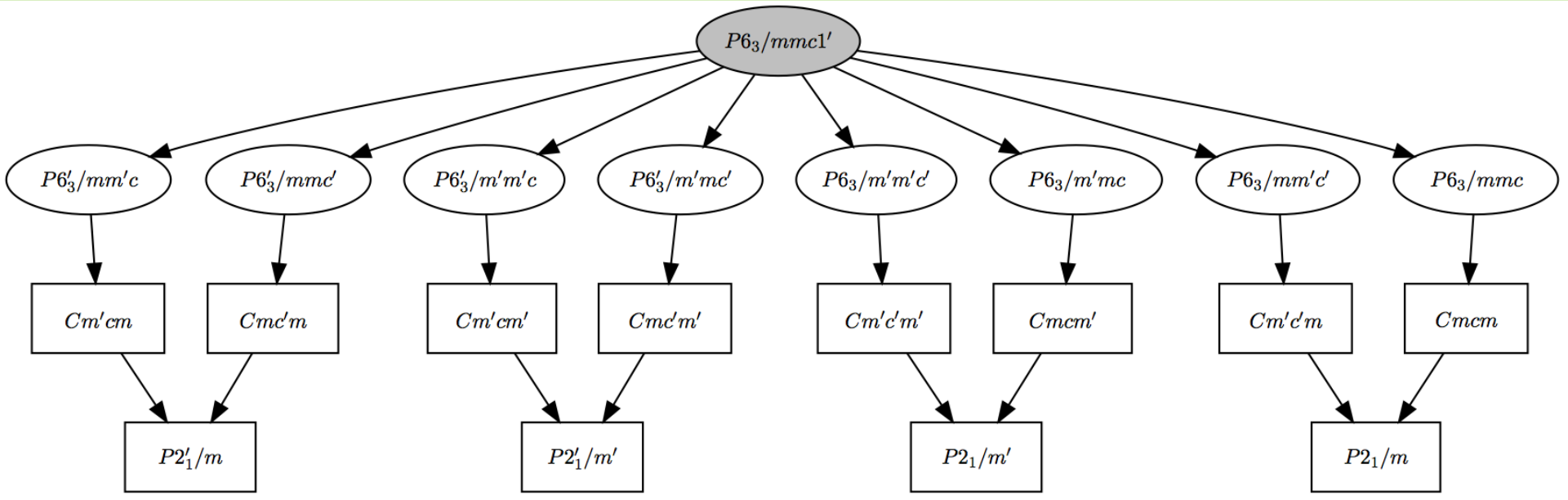
Mn_3Sn

k=(0,0,0)

$P6_3/mmc1'$ ⟶ ??

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

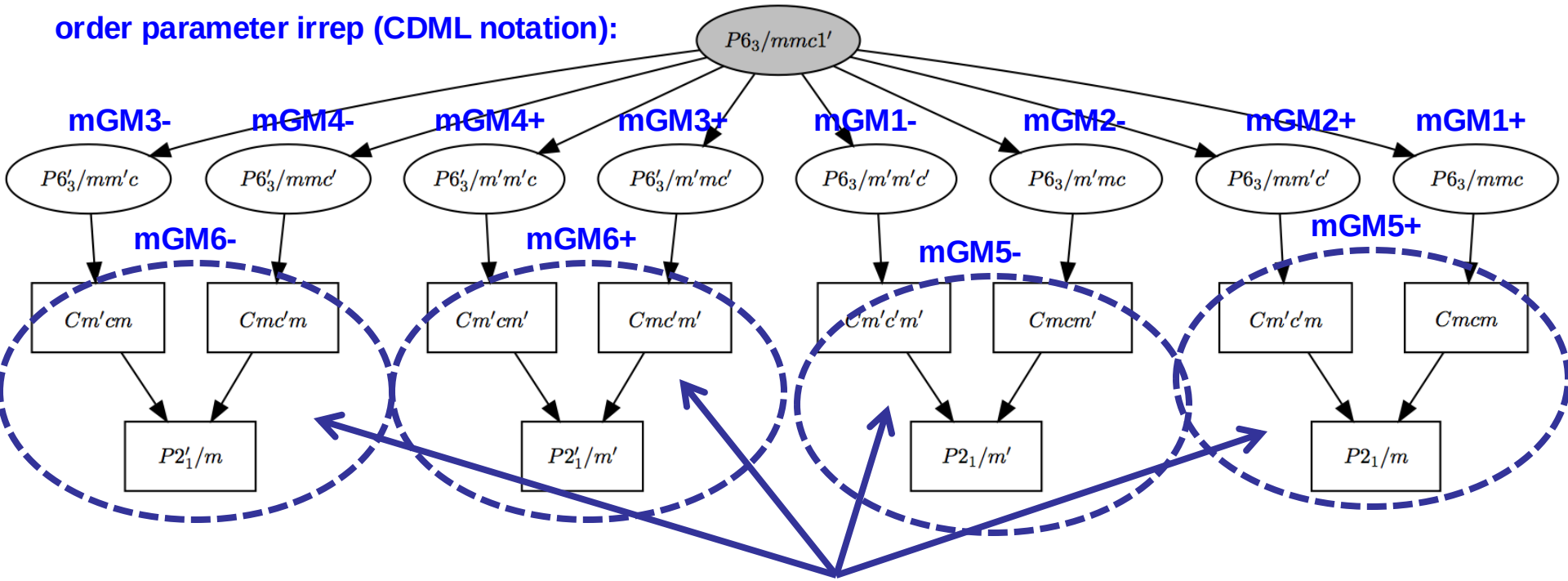
k=(0,0,0)

$P6_3/mmc1'$ ⟶ ??

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):



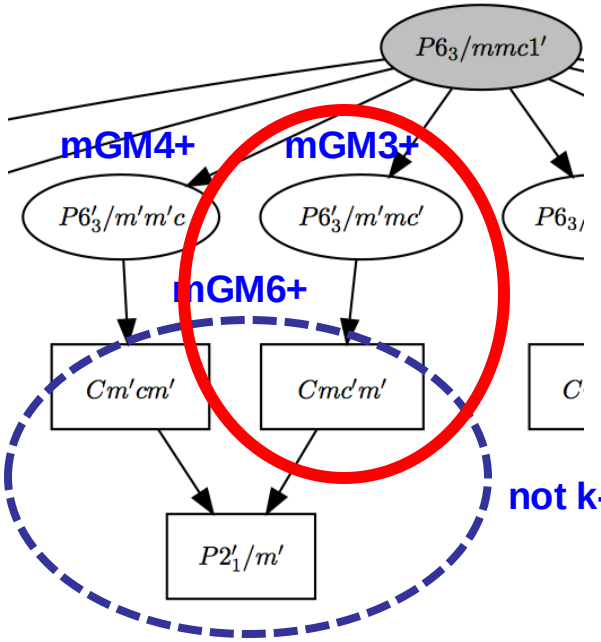
not k-maximal but possible as the result of a single active irrep

Mn_3Sn

k=(0,0,0)

$P6_3/mmc1' \longrightarrow$??

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



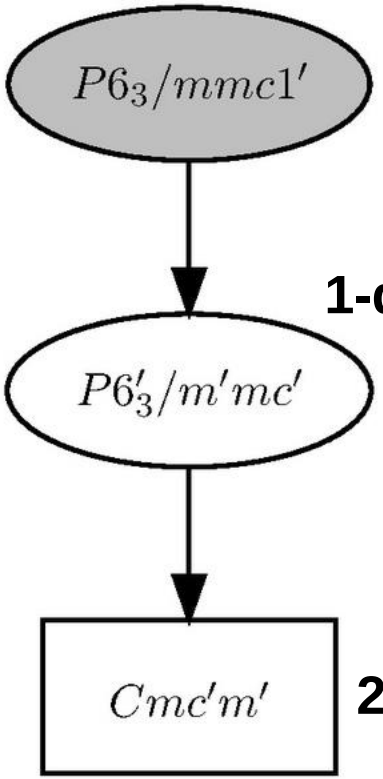
not k-maximal symmetry

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)

In this case, the MSG of the structure is compatible with more than one irrep



1-dim irrep mGM3+

2-dim irrep mGM6+

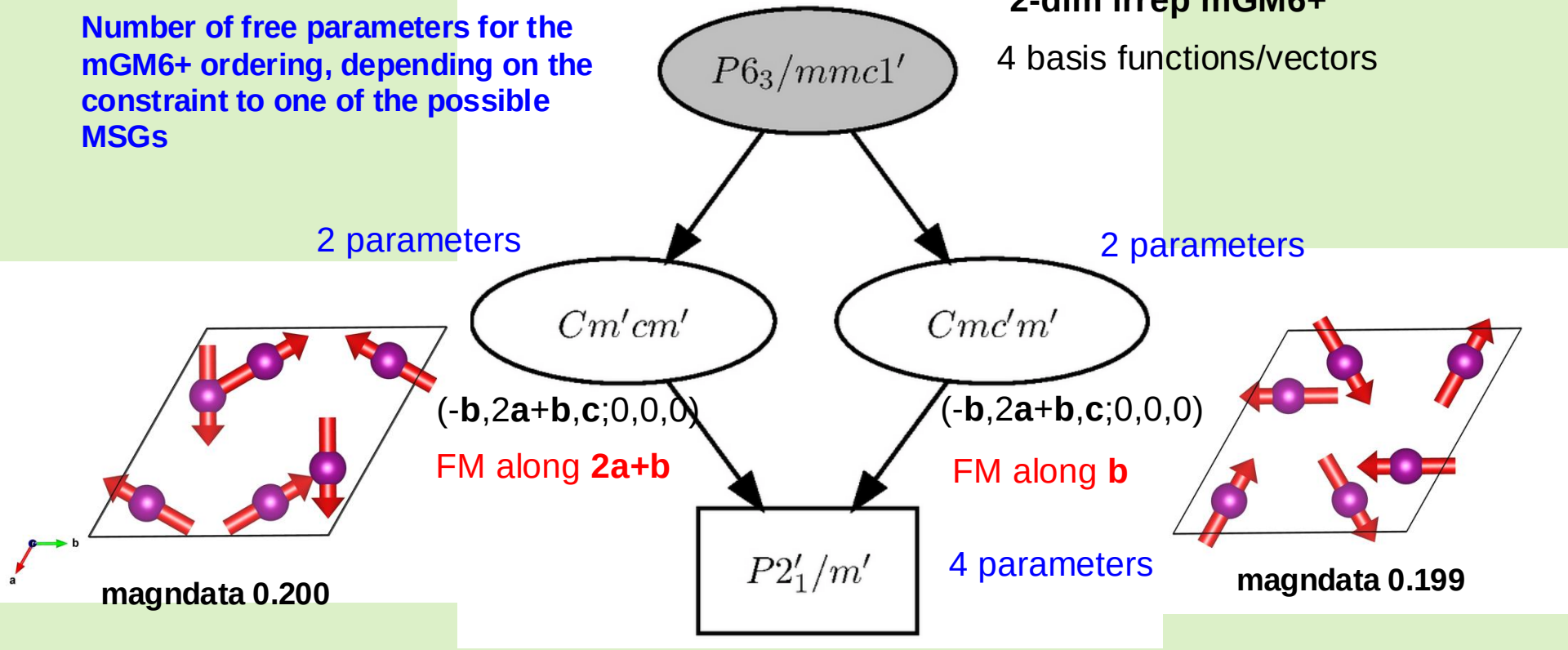
Von Neumann principle:
Everything that keeps the symmetry Cmc'm' is allowed and can happen…
Anything that keeps the symmetry P6'$_3$/m'mc' keeps the symmetry of its subgroup Cmc'm'
THEREFORE…. a spin arrangement according to the irrep mGM3+ is also allowed in the structure with MSG Cmc'm'

Mn_3Sn 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 (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

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

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     } mode 1 mGM3+
  1 Mn1_2  mGM3+      0.0000   0.0721   0.0000   1.00
  2 Mn1_1  mGM6+      0.0510   0.1019   0.0000   1.00     } mode 2 mGM6+
  2 Mn1_2  mGM6+      0.0000   0.0000   0.0000   1.00
  3 Mn1_1  mGM6+      0.0510   0.0000   0.0000   1.00     } mode 3 mGM6+
  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   } mode amplitudes to refine
    A3_mGM6+         0.00000    1.00   }
!
```

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

Description of the irrep basis vectors involved

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)**

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

A1_mGM3+ = 0 **A2_mGM6+ = A_3mGM6+ = some equal value**

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: C_1= 3.00(1) Mn1_1 (1, 1 , 0) 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: C_3=0.0 Mn1_1 (1, 0, 0) Mn1_2 (0, 1, 0)

What about magnetic incommensurate structures?

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

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TOPICAL REVIEW

Magnetic superspace groups and symmetry constraints in incommensurate magnetic phases

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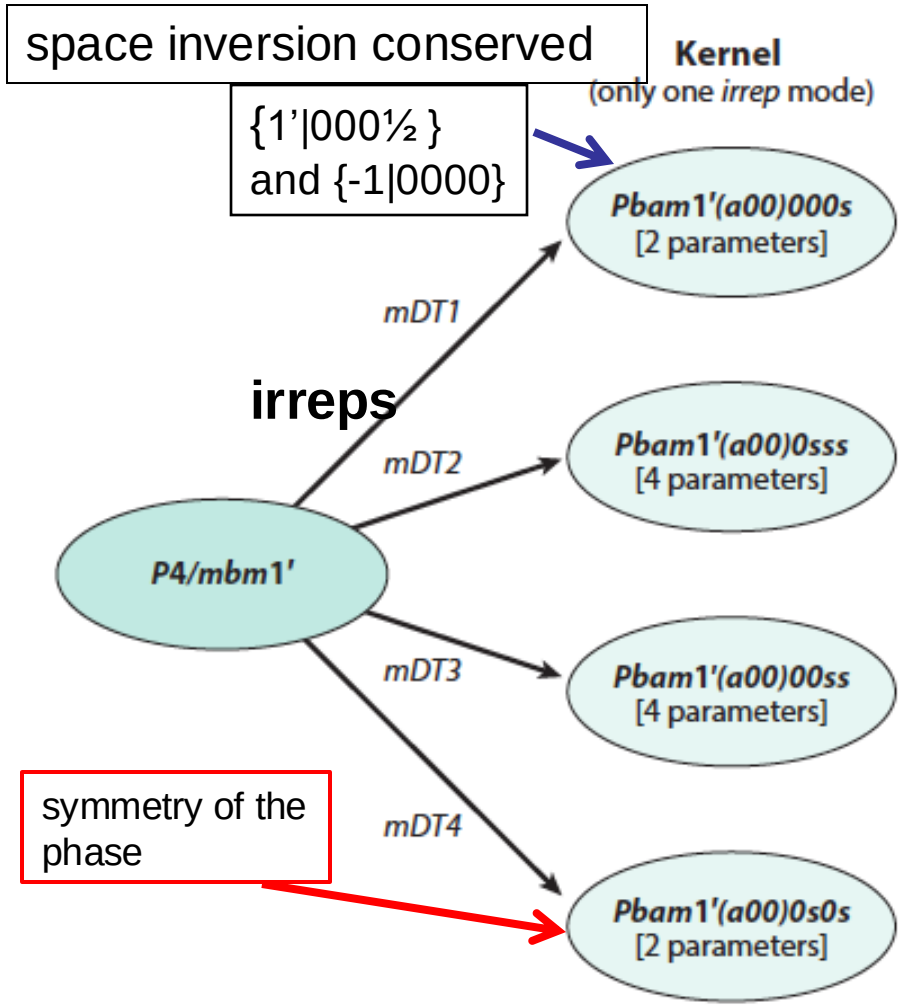
Abstract

Superspace symmetry has been for many years the standard approach for the analysis of non-magnetic modulated crystals because of its robust and efficient treatment of the structural constraints present in incommensurate phases. For incommensurate magnetic phases, this generalized symmetry formalism can play a similar role. In this context we review from a practical viewpoint the superspace formalism particularized to magnetic incommensurate phases. We analyse in detail the relation between the description using superspace symmetry

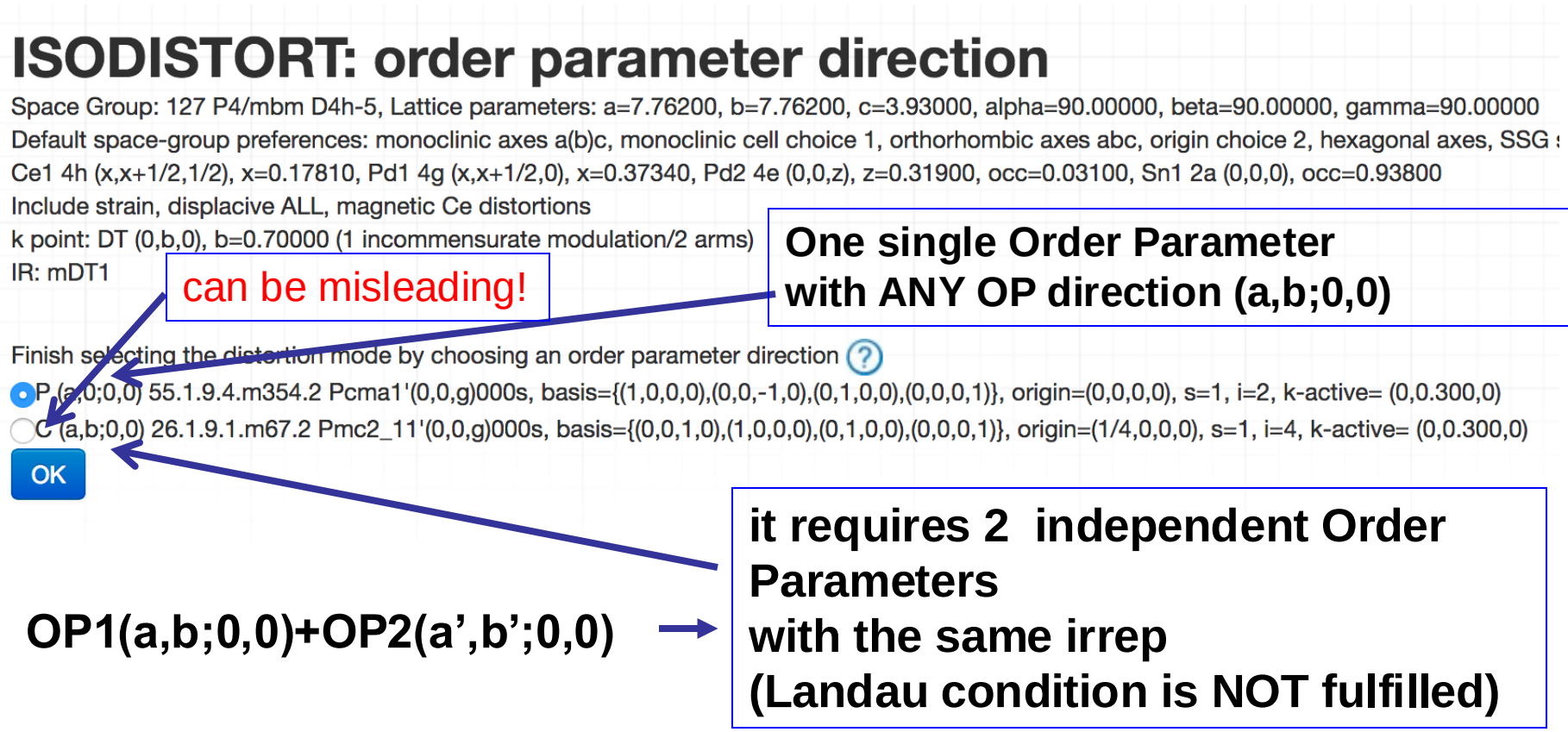
Ce_2Pd_2Sn magndata 1.1.9 space inversion is maintained !

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

k= (α,0,0)



Beware when interpreting ISODISTORT output:



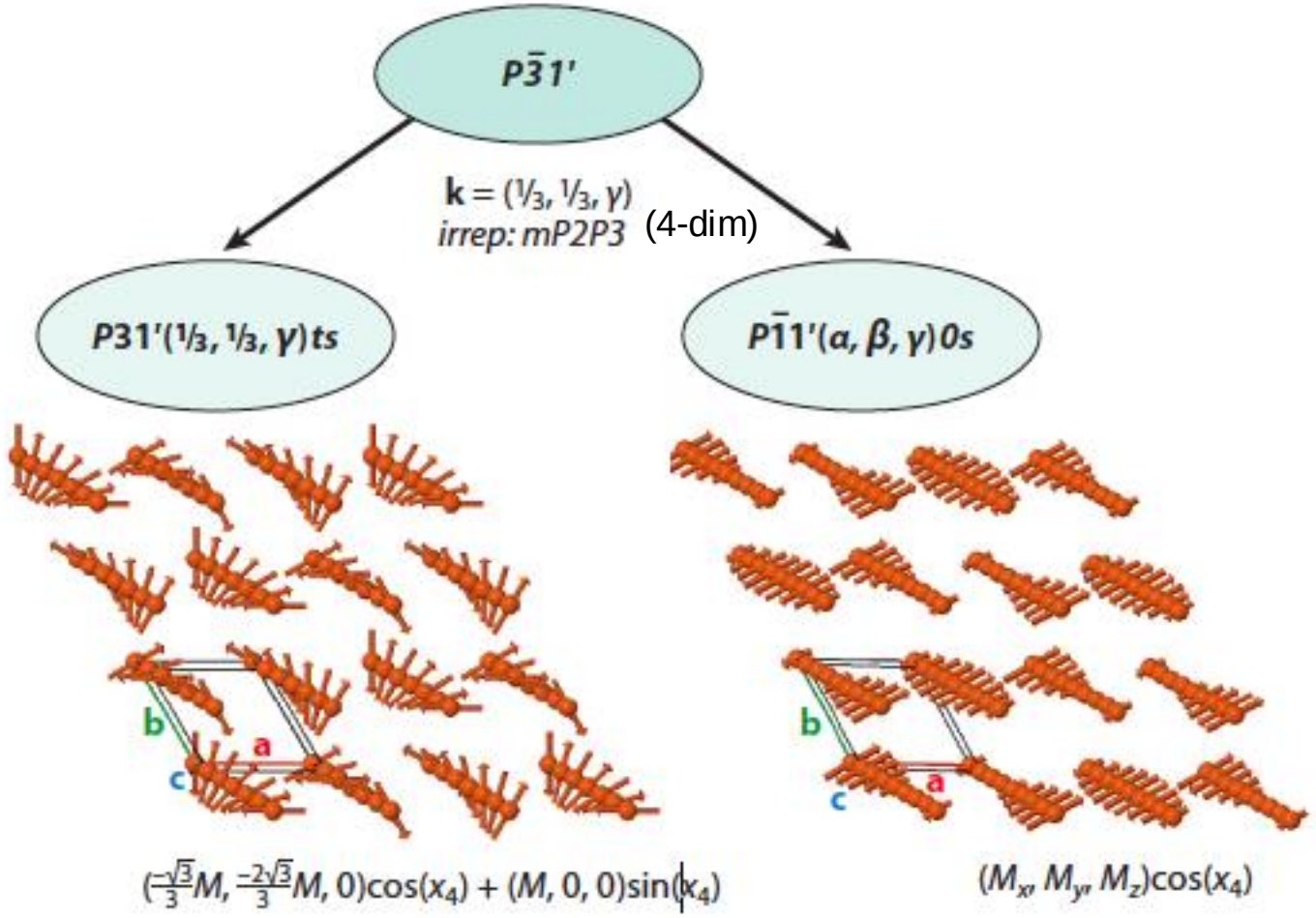
can be misleading!

One single Order Parameter with ANY OP direction (a,b;0,0)

OP1(a,b;0,0)+OP2(a’,b’;0,0) →

it requires 2 independent Order Parameters with the same irrep (Landau condition is NOT fulfilled)

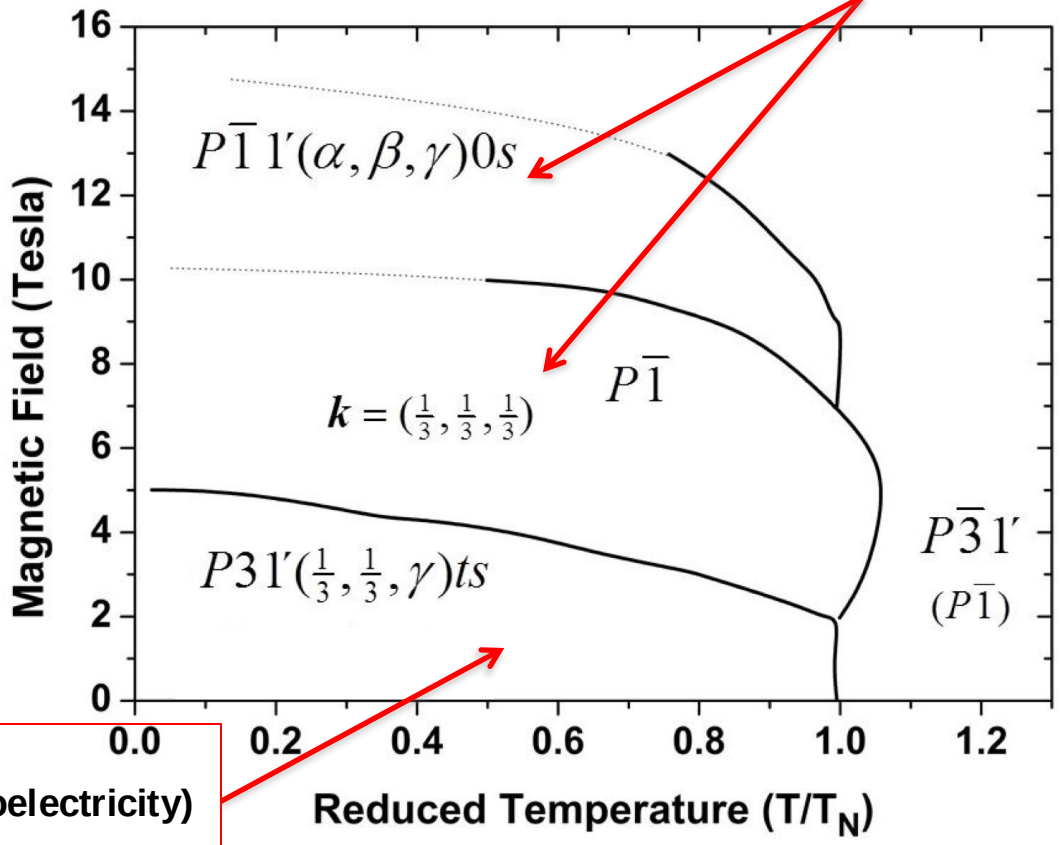
Two possible higher alternative superspace symmetries for the same irrep.



$RbFe(MoO_4)_2$: A phase diagram with phases and symmetries caused by a single active 4-dim magnetic irrep

Non-polar symmetry: No polarization

Magnetic field along [1,-1,0]



Phase diagram after Kenzelmann et al.

PRL 2007

Polar symmetry: induced (improper ferroelectricity) Multiferroic phase

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 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).