ZTF-FCT
Zientzia eta Teknologia Fakultatea
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Representation analysis vs. Magnetic Groups

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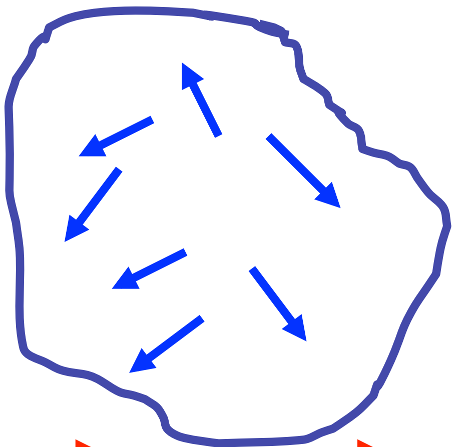
Phase Transition / Symmetry break / Order Parameter

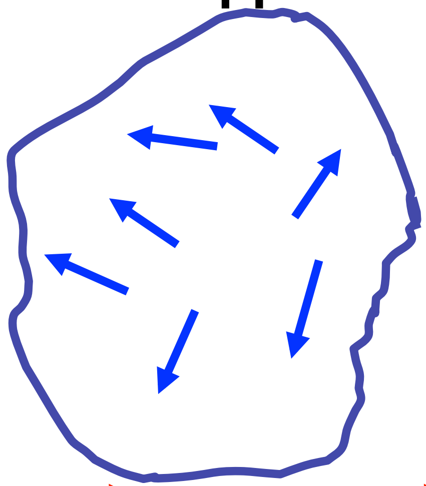
High symmetry group $G_o1' = \{g_i\}$

Key concept of a symmetry break: order parameter

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



$$\vec{Q} \xrightarrow{g_i} \vec{Q}'$$



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

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

Irreducible representation of G (irrep) (matrices)

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

distortions: Vectors in a multidimensional space

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:

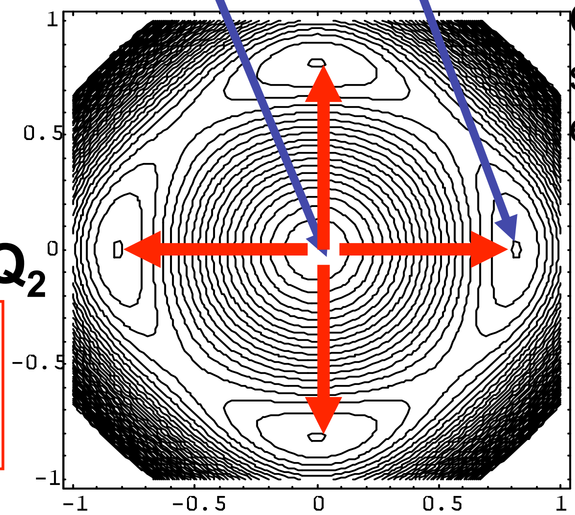
G → F | F: isotropy subgroup

High symmetry **Low symmetry**

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

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

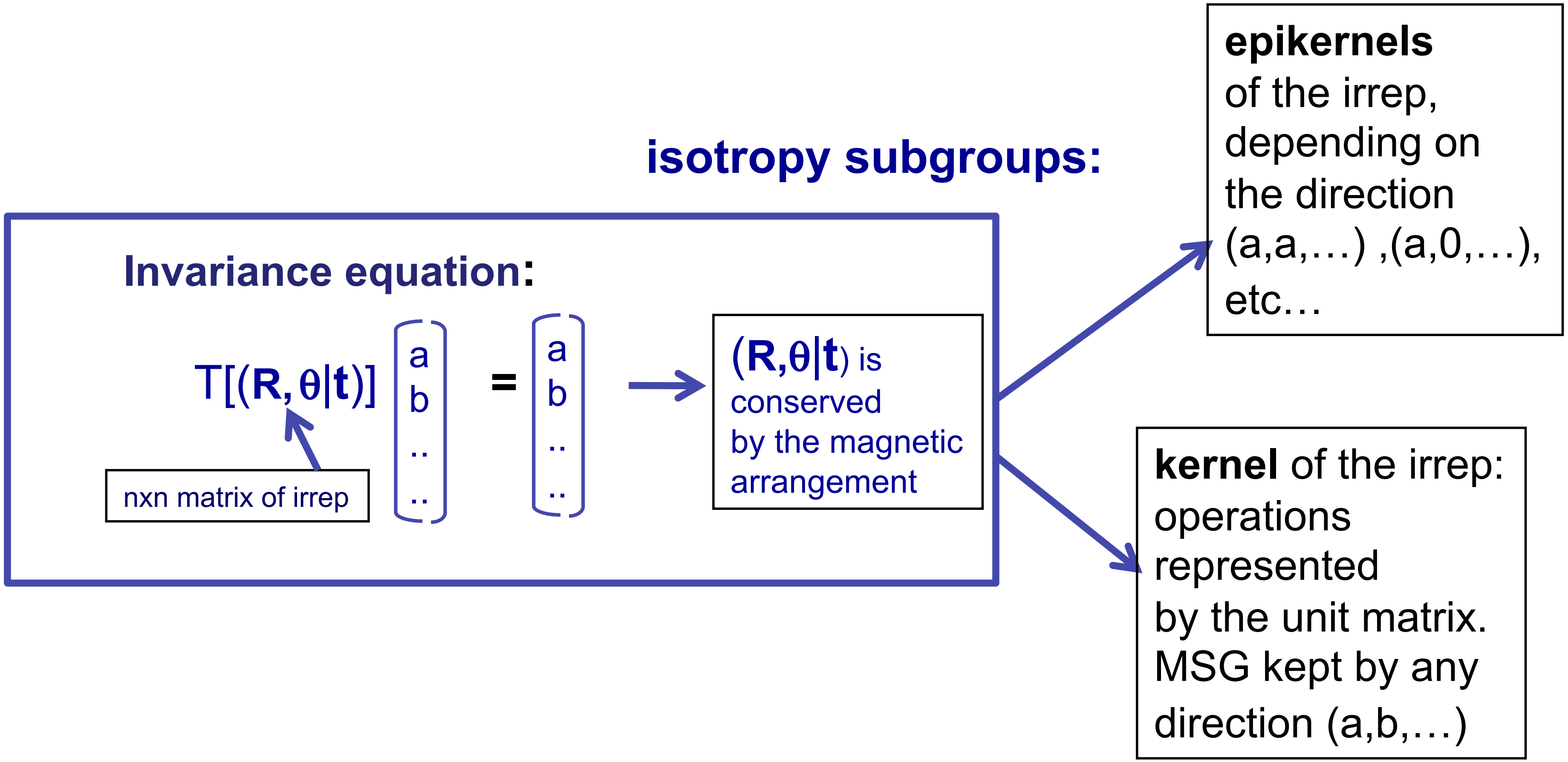
Q_2



Q_1

Key concept of a symmetry break ← Order parameter $\vec{Q} = (Q_1,Q_2) = \rho\,(a_1,a_2)$ ← **amplitude**

$a_1^2+a_2^2 = 1$


isotropy subgroups:
Invariance equation:
T[(R,θ|t)] (a, b, .., ..) = (a, b, .., ..)
nxn matrix of irrep
(R,θ|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,…)

Single irrep assignment vs. magnetic space groups (MSG) in commensurate structures. Cases

1) *1-dim. irrep: irrep and MSG assignment are equivalent for defining the constraints on the atomic magn. moments*

Description in terms of irreps

(Irrep = irreducible representation)

Pn'ma' === one irrep

Character Table

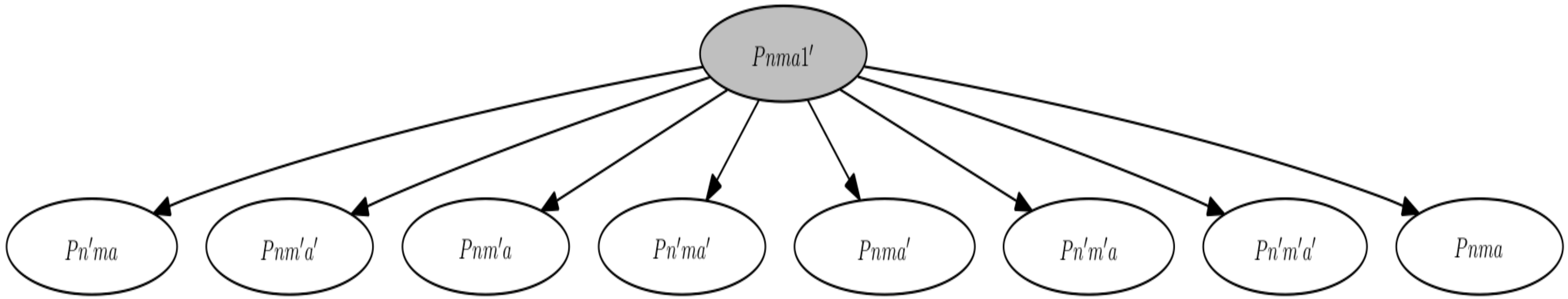
k=0

	#	1	2_z	2_y	2_x	-1	m_z	m_y	m_x	**1'**
Pnma	Γ_1^+	1	1	1	1	1	1	1	1	-1
Pn'm'a	Γ_3^+	1	1	-1	-1	1	1	-1	-1	-1
Pn'ma'	Γ_2^+	1	-1	1	-1	1	-1	1	-1	-1
Pnm'a'	Γ_4^+	1	-1	-1	1	1	-1	-1	1	-1
Pn'm'a'	Γ_1^-	1	1	1	1	-1	-1	-1	-1	-1
Pnma'	Γ_3^-	1	1	-1	-1	-1	-1	1	1	-1
Pnm'a	Γ_2^-	1	-1	1	-1	-1	1	-1	1	-1
Pn'ma	Γ_4^-	1	-1	-1	1	-1	1	1	-1	-1

$2_z'$	$2_y'$	$2_x'$	$-1'$	m_z'	m_y'	m_x'
1	-1	1	-1	1	-1	1

Example: parent space group Pnma (Pnma1')

k=0   8 possible irreps, all 1-dim



One to one correspondence between each irrep and one MSG

Maximal magnetic space groups for the parent space group 62 (*Pnma*) and the propagation vector k = (0, 0, 0)

Maximal subgroups which allow non-zero magnetic moments for at least one atom are coloured

N	Group (BNS)	Transformation matrix	General positions	Systematic absences	Magnetic structure
1	*Pn'm'a'* (#62.449) Go to a subgroup	(1 0 0 0 / 0 1 0 0 / 0 0 1 0) Alternatives (domain-related)	Show	Show	Show
2	*Pn'ma'* (#62.448) Go to a subgroup	(1 0 0 0 / 0 1 0 0 / 0 0 1 0) Alternatives (domain-related)	Show	Show	Show
3	*Pnm'a'* (#62.447) Go to a subgroup	(1 0 0 0 / 0 1 0 0 / 0 0 1 0) Alternatives (domain-related)	Show	Show	Show
4	*Pn'm'a* (#62.446) Go to a subgroup	(1 0 0 0 / 0 1 0 0 / 0 0 1 0) Alternatives (domain-related)	Show	Show	Show
5	*Pnma'* (#62.445) Go to a subgroup	(1 0 0 0 / 0 1 0 0 / 0 0 1 0) Alternatives (domain-related)	Show	Show	Show
6	*Pnm'a* (#62.444) Go to a subgroup	(1 0 0 0 / 0 1 0 0 / 0 0 1 0) Alternatives (domain-related)	Show	Show	Show
7	*Pn'ma* (#62.443) Go to a subgroup	(1 0 0 0 / 0 1 0 0 / 0 0 1 0) Alternatives (domain-related)	Show	Show	Show
8	*Pnma* (#62.441) Go to a subgroup	(1 0 0 0 / 0 1 0 0 / 0 0 1 0) Alternatives (domain-related)	Show	Show	Show

Only non-zero moments for the MSGs associated with the irreps present in the magnetic representation

mGM4+

mGM3+

mGM2+

mGM1+

Filter in k-SUBGROUPSMAG restricting to one or more irreps

Space group of the paramagnetic phase: *Pnma* (No. 62)
Choose the irreducible representation(s) for each propagation vector

If no Wyckoff position has been given, a general position will be assumed

Non bolded irreps are incompatible with the given Wyckoff positions
Bolded irreps are compatible with at least one given Wyckoff position
Red colored irreps are compatible with all the Wyckoff positions given

Possible magnetic irreducible representations

Propagation wave-vector(s)

GM:(0,0,0)

Descomposition of the magnetic representation(s) into irreps.

4b:(0,0,1/2) → 3×mGM1+(1) ⊕ 3×mGM2+(1) ⊕ 3×mGM3+(1) ⊕ 3×mGM4+(1)

Choose the representation(s)

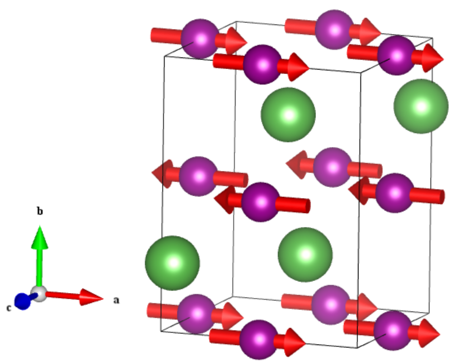
irreps:	☐ mGM1+(1)	☐ mGM2+(1)	☐ mGM3+(1)	☐ mGM4+(1)	mGM1-(1)	mGM2-(1)	mGM3-(1)	mGM4-(1)

Submit

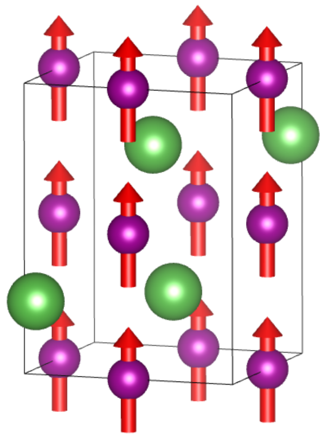
Space Group:
Pn'ma'

irrep basis spin modes equivalent to Wyckoff position constraints

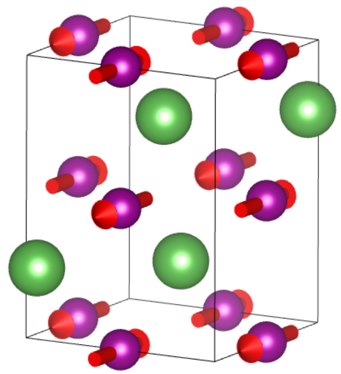
Multiplicity	Wyckoff letter	Coordinates	
8	d	$(x,y,z \mid m_x,m_y,m_z)$ $(x+1/2,-y+1/2,-z+1/2 \mid -m_x,m_y,m_z)$ $(-x,y+1/2,-z \mid -m_x,m_y,-m_z)$ $(-x+1/2,-y,z+1/2 \mid m_x,m_y,-m_z)$ $(-x,-y,-z \mid m_x,m_y,m_z)$ $(-x+1/2,y+1/2,z+1/2 \mid -m_x,m_y,m_z)$ $(x,-y+1/2,z \mid -m_x,m_y,-m_z)$ $(x+1/2,y,-z+1/2 \mid m_x,m_y,-m_z)$	
4	c	$(x,1/4,z \mid 0,m_y,0)$ $(x+1/2,1/4,-z+1/2 \mid 0,m_y,0)$ $(-x,3/4,-z \mid 0,m_y,0)$ $(-x+1/2,3/4,z+1/2 \mid 0,m_y,0)$	**La**
4	b	$(0,0,1/2 \mid m_x,m_y,m_z)$ $(1/2,1/2,0 \mid -m_x,m_y,m_z)$ $(0,1/2,1/2 \mid -m_x,m_y,-m_z)$ $(1/2,0,0 \mid m_x,m_y,-m_z)$	**Mn**
4	a	$(0,0,0 \mid m_x,m_y,m_z)$ $(1/2,1/2,1/2 \mid -m_x,m_y,m_z)$ $(0,1/2,0 \mid -m_x,m_y,-m_z)$ $(1/2,0,1/2 \mid m_x,m_y,-m_z)$	



A_x mode along x



F_y mode along y
weak ferromagnet



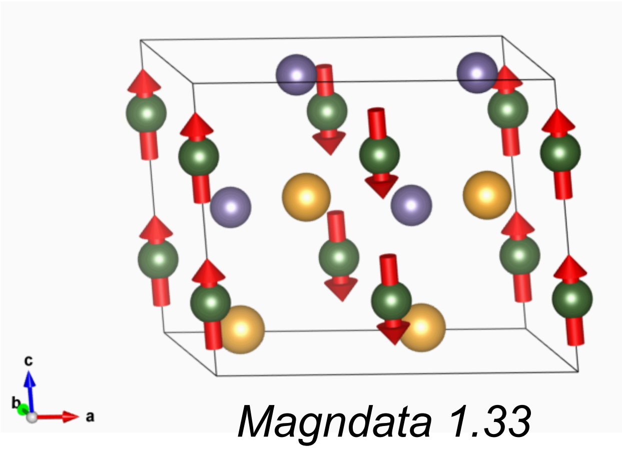
G_z mode along z

Single irrep assignment vs. magnetic space groups (MSG) in commensurate structures. Cases

1) 1-dim. irrep: irrep and MSG assignment are equivalent for spin relations.

It includes the case of 1k-structures witth k≠0 and –k **equivalent** to k, and the small irrep active being 1-dim

1k magn. structure with -k equiv. to k and small irrep 1-dim: MSG and irrep assignment equivalent for spin constraints



Magndata 1.33

ErAuGe

Paramagnetic symmetry: **$P6_3mc1'$**

k=(1/2,0,0) (point M in the BZ)

Magnetic phase symmetry: P_Cna21 (#33.154)

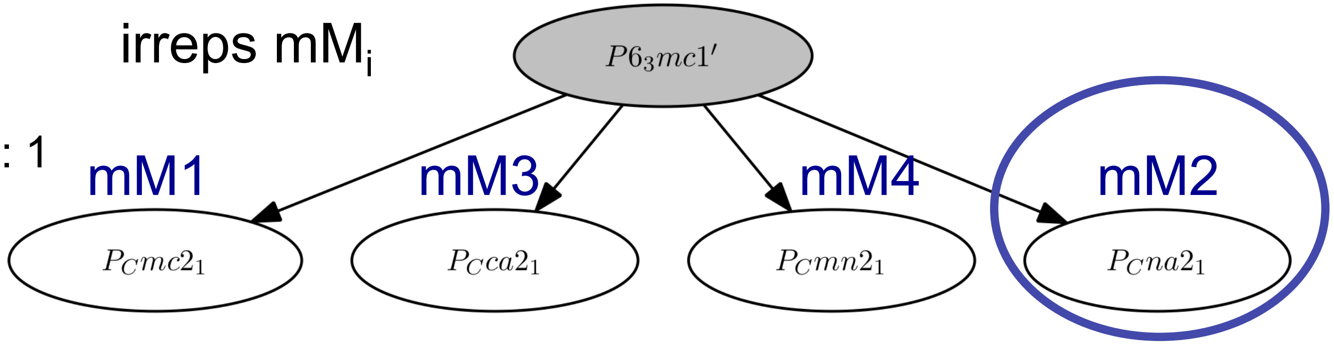
Label	Atom type	x	y	z	Symmetry constraints on M	M_x	M_y	M_z
Er1	Er	0.00000	0.00000	0.25	$2m_y,m_y,m_z$	0.0	0.0	8.8

irrep star: 3 k

dim. extended small irrep: 1

dim. full irrep: 3

irreps mM_i



One to one correspondence MSG : irrep

However it is convenient to know that the magnetic point group is **mm21'** ….

and the effective space group for atomic positions in case of magnetostructural non-negligible effects is: **$Cmc2_1$** ….

Single irrep assignment vs. magnetic space groups (MSG) in commensurate structures. Cases

1) 1-dim. irrep: irrep and MSG assignment are equivalent for spin relations**.**

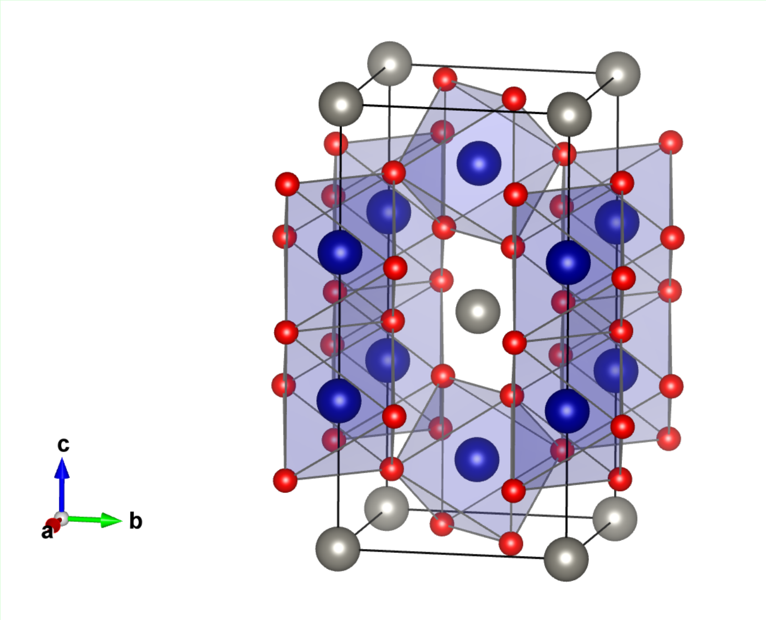
2) N dim. irrep, N>1: several MSG (epikernels or isotropy subgroups of the irrep) are possible for the same irrep. The MSG depends on the way the spin basis functions are combined. The assignment of a MSG restricts the magnetic configuration beyond the restrictions coming from the irrep.

Single irrep assignment vs. magnetic space groups (MSG) in commensurate structures. Cases

1) 1-dim. irrep: irrep and MSG assignment are equivalent for spin relations.

2) N dim. irrep, N>1: several MSG (epikernels or isotropy subgroups of the irrep) are possible for the same irrep. The assignment of a MSG restricts the magnetic configuration beyond the restrictions coming from the irrep.

case 2.1: The MSG is a k-maximal subgroup: it only allows a spin ordering according to a single irrep (further restricted to fulfill the MSG constraints). No other irrep arrangements are compatible with the MSG.



Parent space group:

***$P4_2/mnm$* (N. 136)**

Propagation vector:

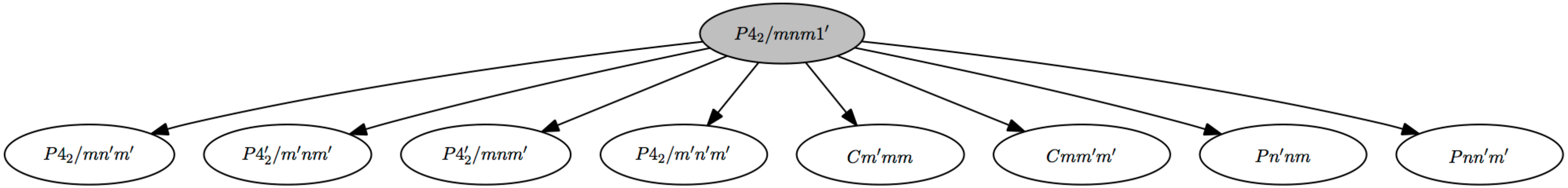
k= (0,0,0)

Magnetic site:

Cr 4e (0,0,z)

File: 6.Cr2WO6_parent.cif

K-SUBGROUPSMAG: maximal subgroups



Maximal magnetic space groups for the parent space group 136 ($P4_2/mnm$) and the propagation vector k = (0, 0, 0)

Maximal subgroups which allow non-zero magnetic moments for at least one atom are coloured

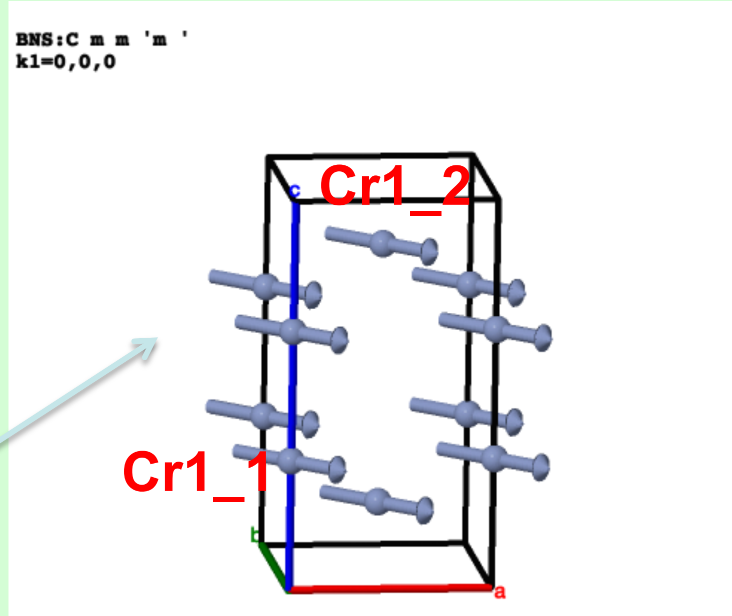
N	Group (BNS)	Transformation matrix	General positions	Properties	Magnetic structure
1	$P4_2/m'n'm'$ (#136.503) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	*Systematic absences* MAGNEXT *Tensor properties* MTENSOR	Show
2	$P4_2'/m'nm'$ (#136.502) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	*Systematic absences* MAGNEXT *Tensor properties* MTENSOR	Show
3	$P4_2/mn'm'$ (#136.501) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	*Systematic absences* MAGNEXT *Tensor properties* MTENSOR	Show
4	$P4_2'/m'n'm$ (#136.500) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	*Systematic absences* MAGNEXT *Tensor properties* MTENSOR	Show
5	$P4_2'/mnm'$ (#136.499) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	*Systematic absences* MAGNEXT *Tensor properties* MTENSOR	Show
6	$P4_2'/mn'm$ (#136.498) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	*Systematic absences* MAGNEXT *Tensor properties* MTENSOR	Show
7	$P4_2/m'nm$ (#136.497) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	*Systematic absences* MAGNEXT *Tensor properties* MTENSOR	Show
8	$P4_2/mnm$ (#136.495) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	*Systematic absences* MAGNEXT *Tensor properties* MTENSOR	Show
9	$Cmm'm'$ (#65.486) Go to a subgroup	$\begin{pmatrix} 1 & 1 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	*Systematic absences* MAGNEXT *Tensor properties* MTENSOR	Show
10	$Cm'mm$ (#65.483) Go to a subgroup	$\begin{pmatrix} 1 & 1 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	*Systematic absences* MAGNEXT *Tensor properties* MTENSOR	Show
11	$Pnn'm'$ (#58.398) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	*Systematic absences* MAGNEXT *Tensor properties* MTENSOR	Show

MAXMAGN

or

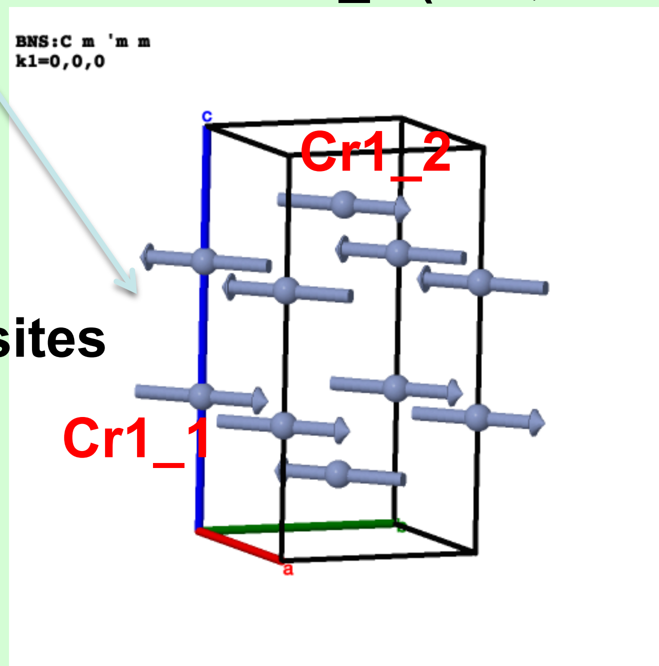
MAGMODELIZE

8	$P4_2/mnm$ (#136.495) Go to a subgroup	(1 0 0 0 / 0 1 0 0 / 0 0 1 0) Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
9	Cmm'm' (#65.486) Go to a subgroup	(1 1 0 0 / −1 1 0 0 / 0 0 1 0) Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
10	Cm'mm (#65.483) Go to a subgroup	(1 1 0 0 / −1 1 0 0 / 0 0 1 0) Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
11	Pnn'm' (#58.398) Go to a subgroup	(1 0 0 0 / 0 1 0 0 / 0 0 1 0) Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
12	Pn'nm (#58.395) Go to a subgroup	(1 0 0 0 / 0 1 0 0 / 0 0 1 0) Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show



Cr1_1 (mx,-mx,0)

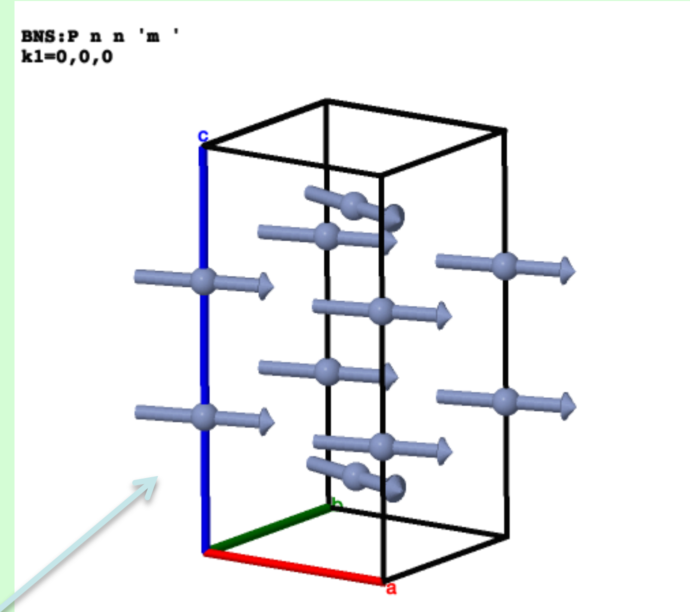
Cr1_2 (mx',-mx',0)



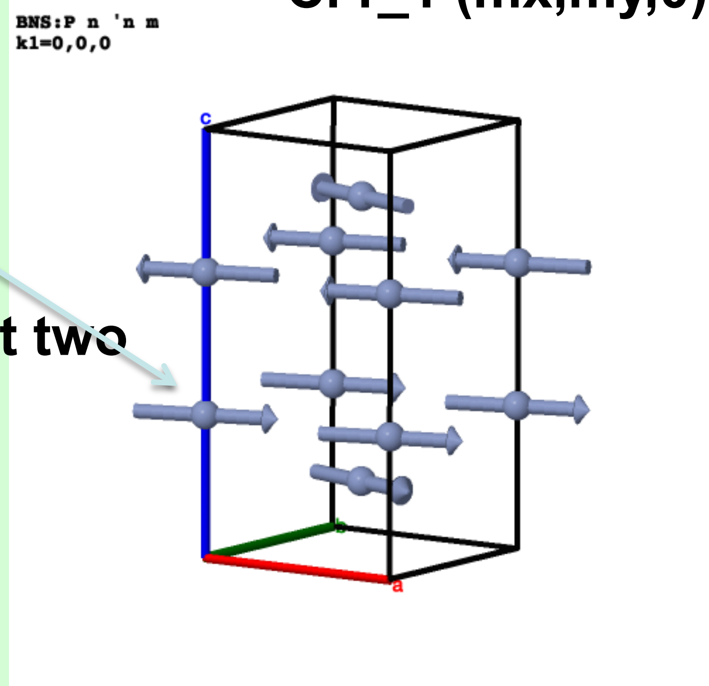
Magnetic site splits into two independent sites

Two spin parameters to be fit

8	*P4$_2$/mnm* (#136.495) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT *Tensor properties* MTENSOR	Show
9	*Cmm'm'* (#65.486) Go to a subgroup	$\begin{pmatrix} 1 & 1 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	*Systematic absences* MAGNEXT *Tensor properties* MTENSOR	Show
10	*Cm'mm* (#65.483) Go to a subgroup	$\begin{pmatrix} 1 & 1 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	*Systematic absences* MAGNEXT *Tensor properties* MTENSOR	Show
11	*Pnn'm'* (#58.398) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	*Systematic absences* MAGNEXT *Tensor properties* MTENSOR	Show
12	*Pn'nm* (#58.395) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	*Systematic absences* MAGNEXT *Tensor properties* MTENSOR	Show



Cr1_1 (mx,my,0)



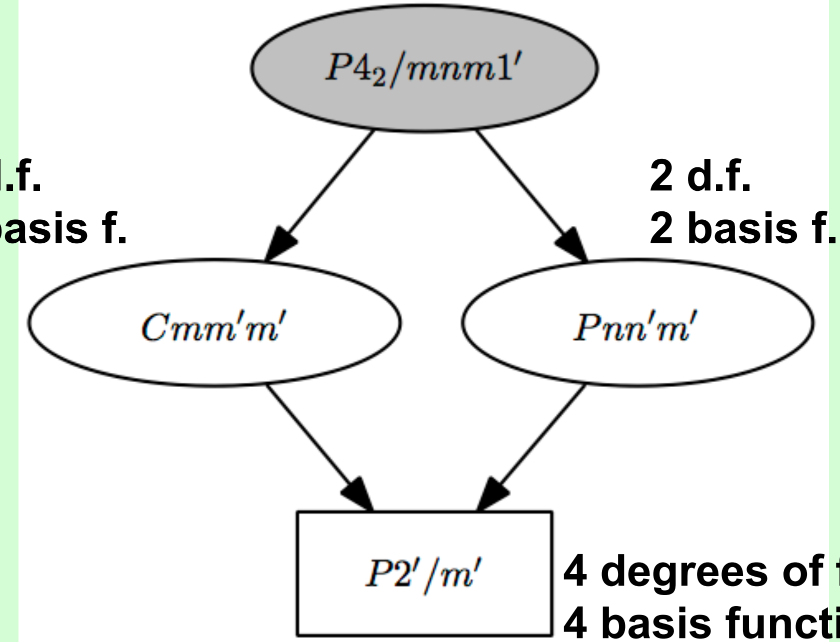
Only ONE independent magnetic site. But two independent spin components.

Spin canting symmetry allowed

Two spin parameters to be fit

k-SUBGROUPSMAG: filter by irreps

Irrep mGM5+ :

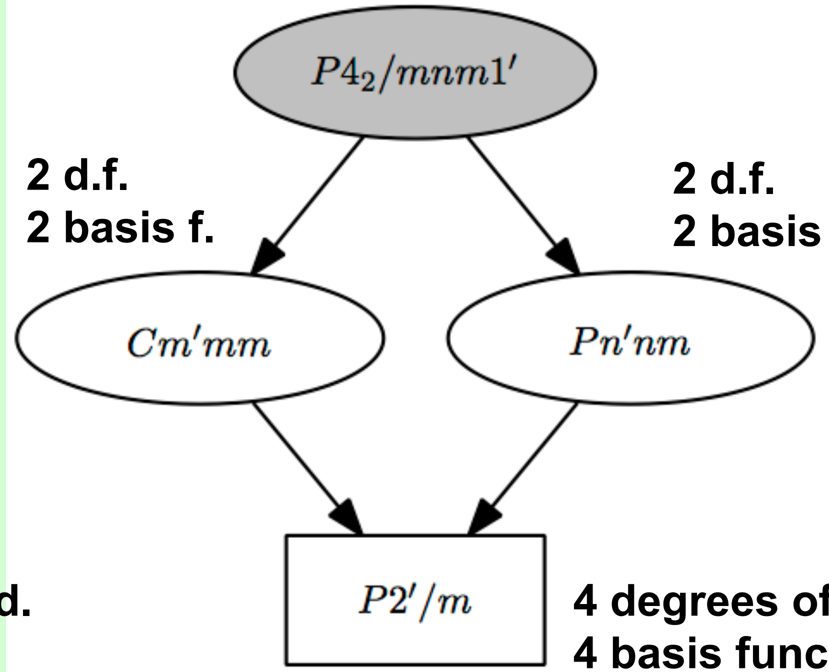


2 d.f.
2 basis f.

2 d.f.
2 basis f.

4 degrees of freed.
4 basis functions

Irrep mGM5-:



2 d.f.
2 basis f.

2 d.f.
2 basis f.

4 degrees of freed.
4 basis functions

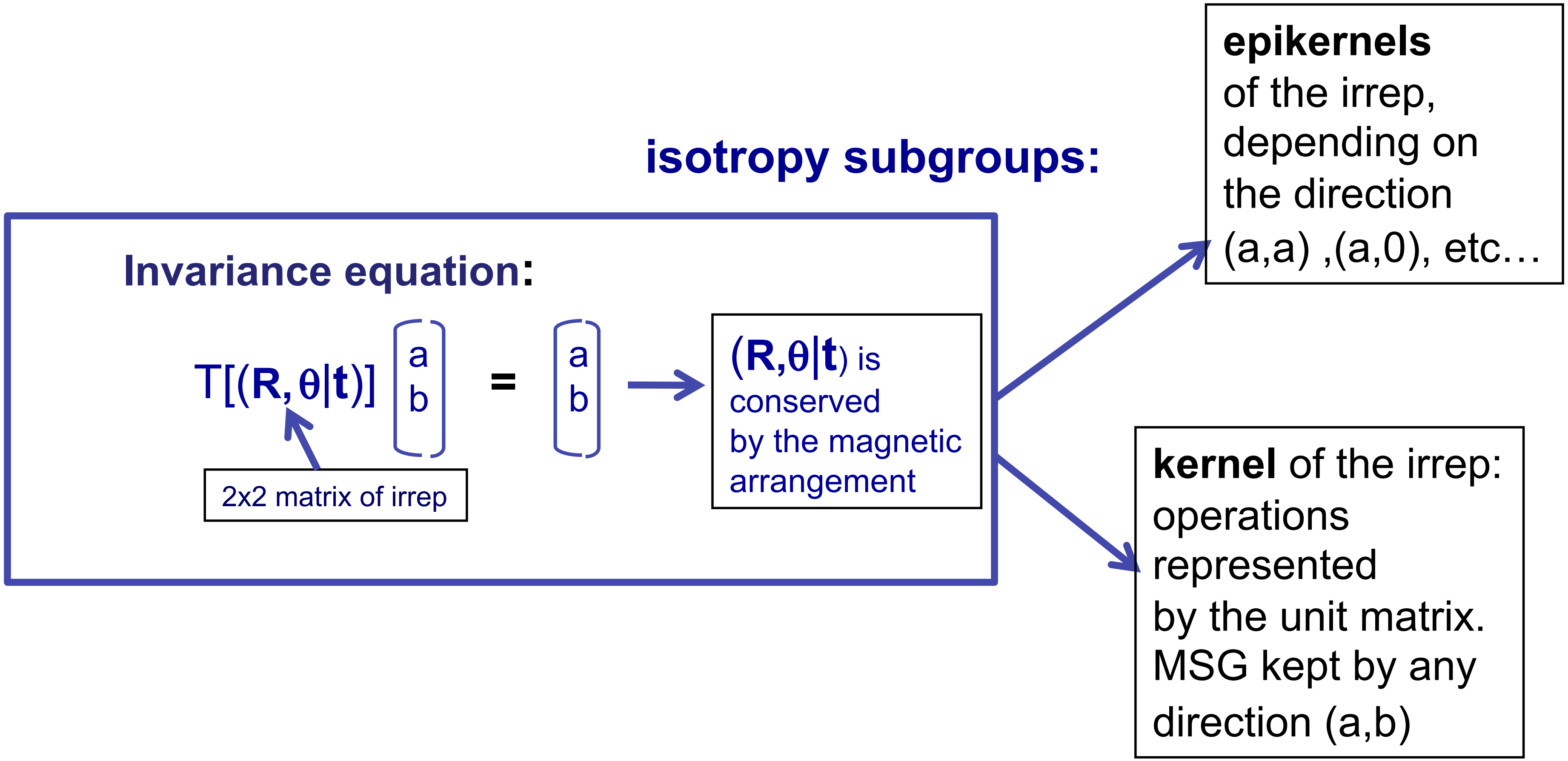
Invariance equation:

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

2x2 matrix of irrep

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

possible MSGs depending on the direction of the order parameter (a,b)


isotropy subgroups:
Invariance equation:
T[(R,θ|t)] (a, b) = (a, b)
2x2 matrix of irrep
(R,θ|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)

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:

http://jana.fzu.cz/ V. Petricek, Prague

JANA

Institute of Physics
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

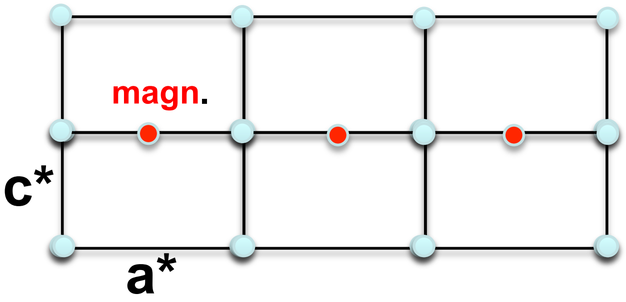
Vaclav Petricek, Michal Dusek & Lukas Palatinus

News

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

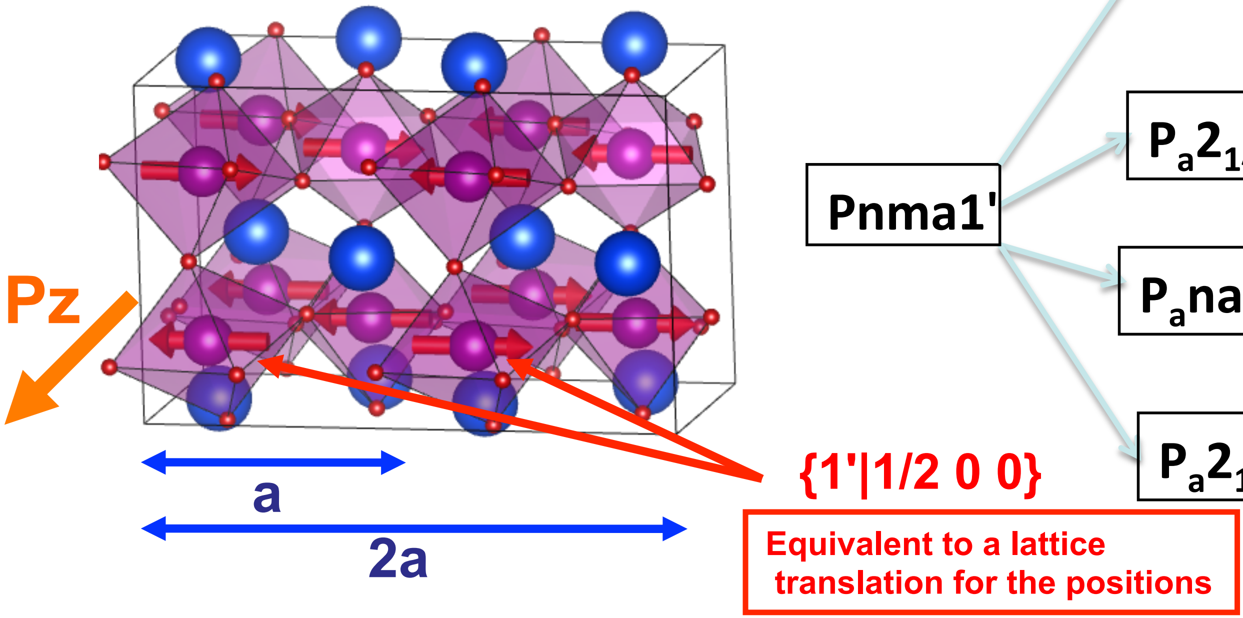
$HoMnO_3$ (Muñoz et al. Inorg. Chem. 2001)

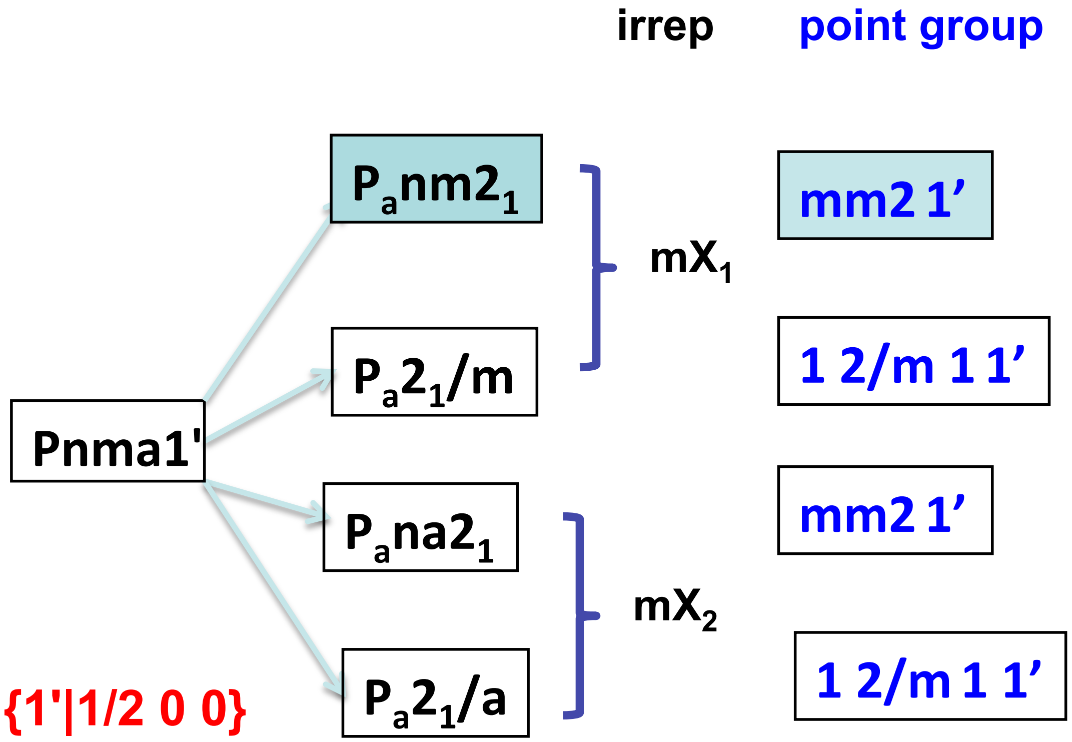
diffraction peaks:



Gp= Pnma

propagation vector k=(1/2 0 0) : point X

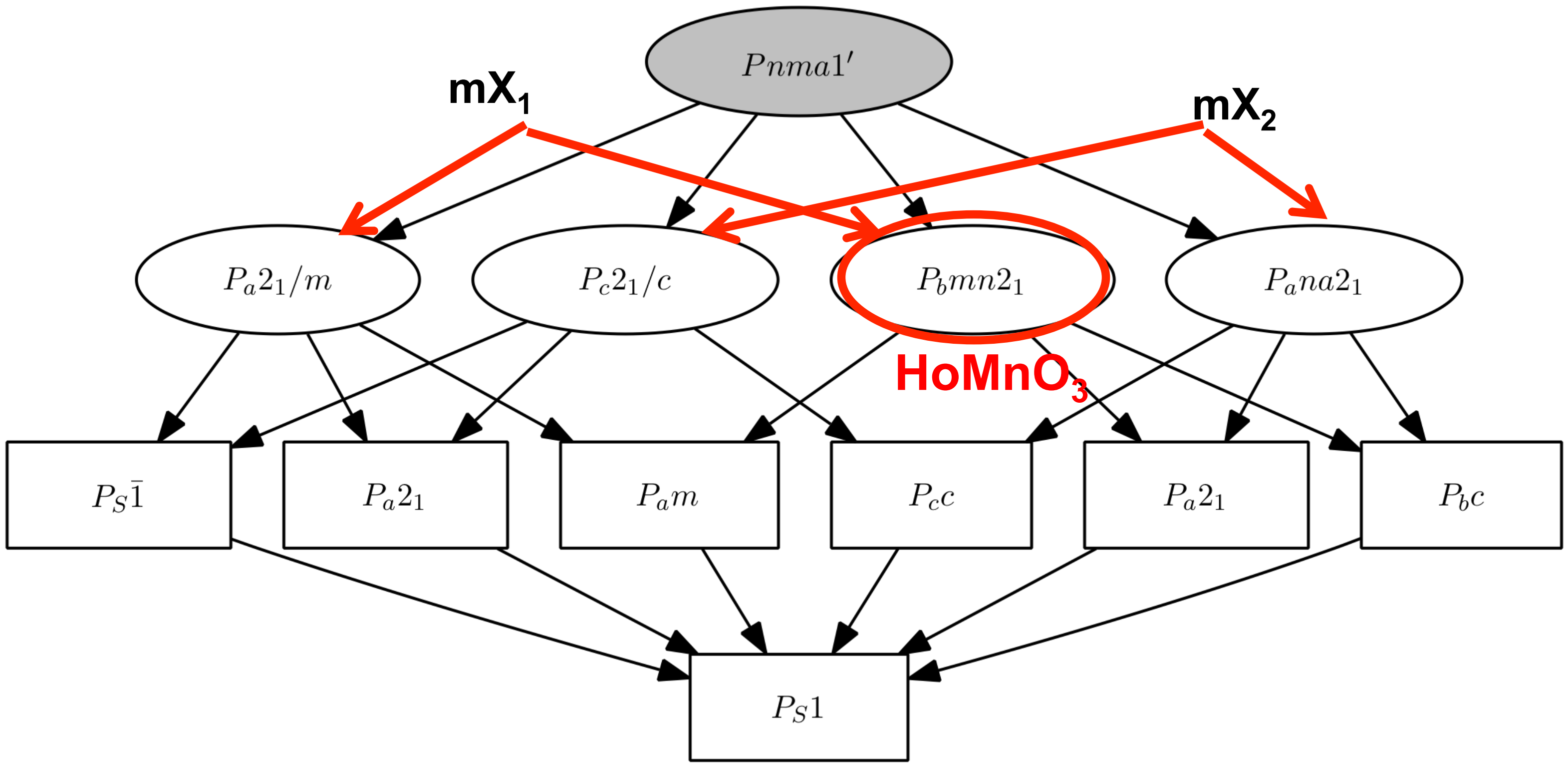




symmetry operation kept: **{1'|1/2 0 0}** → **1' belongs to the point group of the magnetic phase**

Space group: Pnma

propagation vector k=(1/2 0 0) (point X)



Single irrep assignment vs. magnetic space groups (MSG) in commensurate structures. Cases

1) 1-dim. irrep: irrep and MSG assignment are equivalent for spin relations.

2) N dim. irrep, N>1: several MSG (epikernels or isotropy subgroups) are possible for the same irrep. The assignment of a MSG restricts the magnetic configuration beyond the restrictions coming from the irrep.

case 2.1: The MSG is a k-maximal subgroup: it only allows a spin ordering according to a single irrep (further restricted to fulfill the MSG constraints). No other irrep arrangements are compatible with the MSG**.**

case 2.2: The MSG is **NOT** a k-maximal subgroup: it allows the presence of other irreps (secondary). Other irreps are compatible with the MSG. (for simple propagation vectors (2k=reciprocal lattice) not frequent)

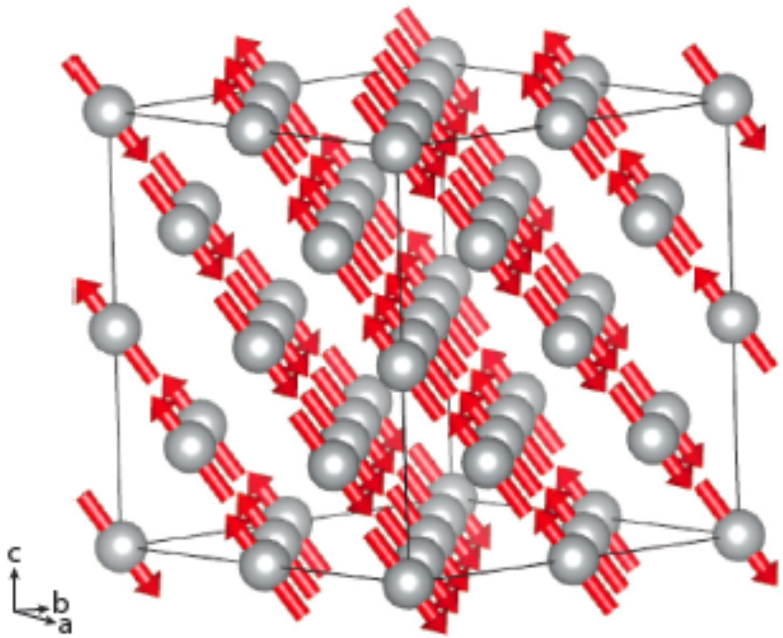
NiO

Parent space group: **Fm-3m**

k= (1/2,1/2,1/2) – point L in the BZ

MSG: **$C_c 2/c$**

M_{Ni}=m(1,1,-2)



$C_c 2/c$

(**a**/4 + **b**/4 − **c**/2, **a**/4 − **b**/4, −**a**/2 − **b**/2; 0, 0, 0)

NiO **parent space group: Fm-3m**

k= (1/2,1/2,1/2) – point L in the BZ **Ni site 4a (0,0,0)**

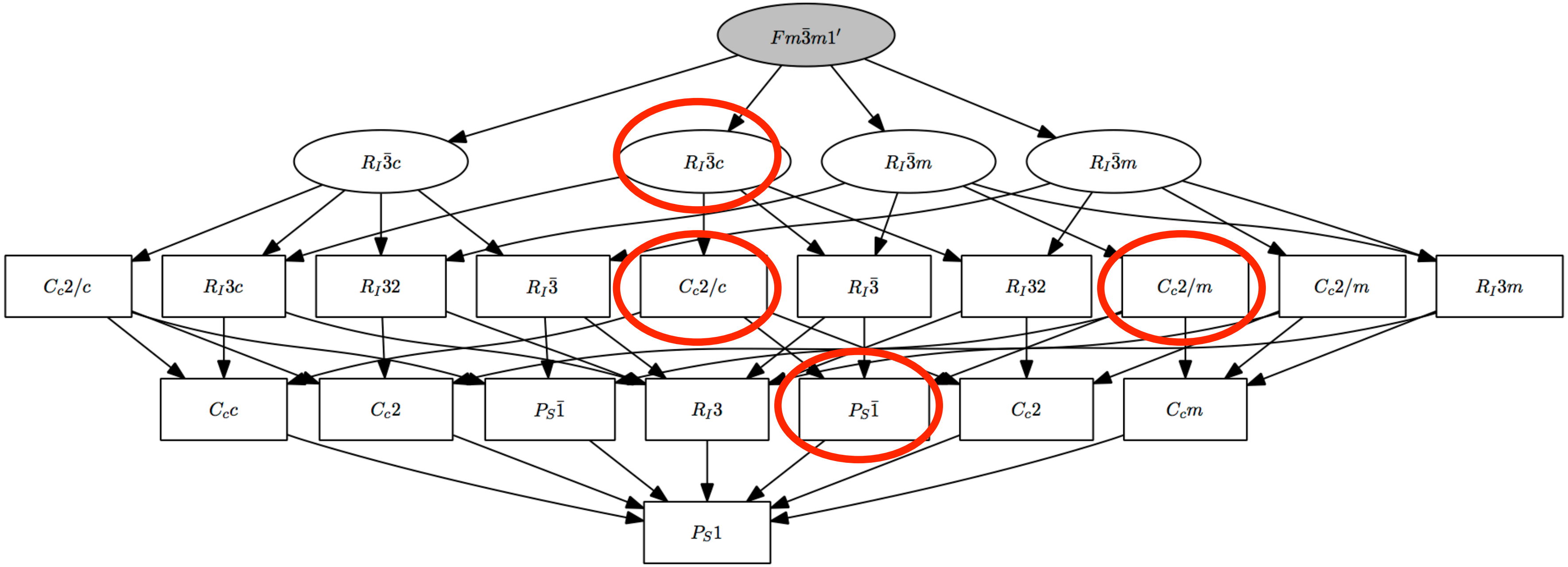
little group of **k: R-3m**

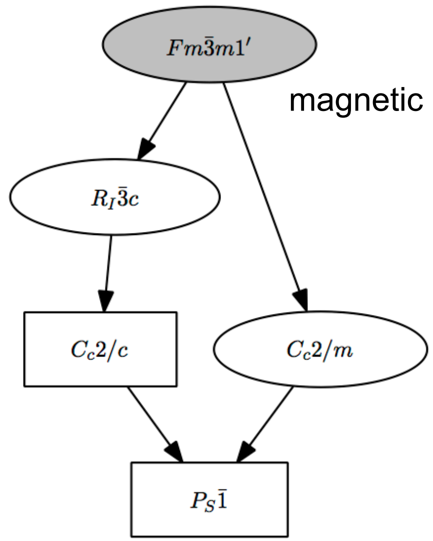
M_{rep}= **mL2+ + mL3+**

1-dim 2-dim

Relation between the irrep description and the one using a MSG in the case NiO (exercise 13)

Use k-SUBGROUPSMAG to obtain for the possible active irreps the possible resulting magnetic symmetries.

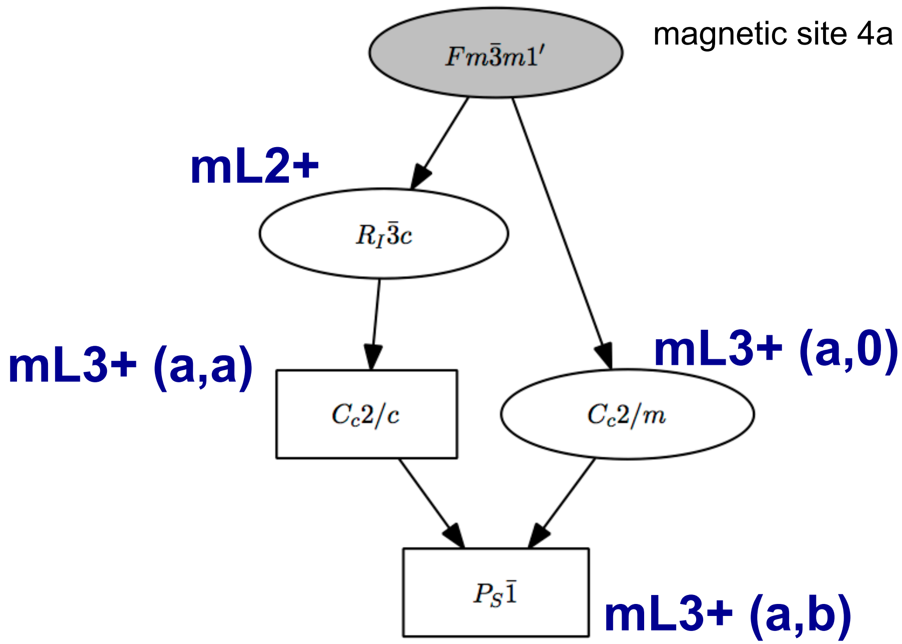


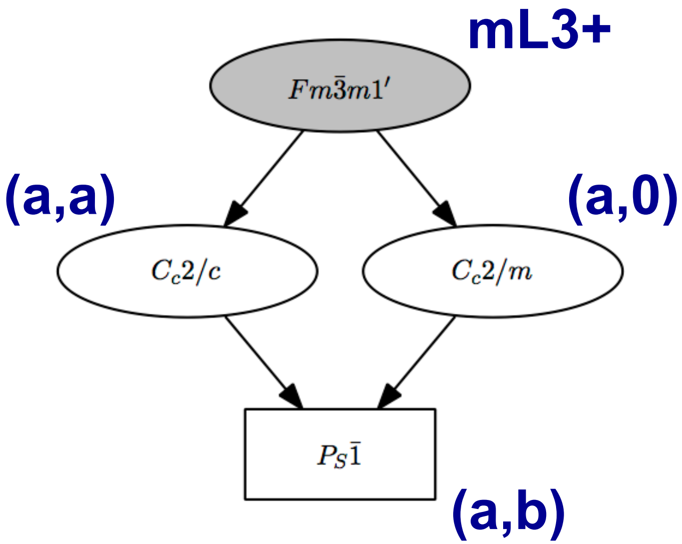


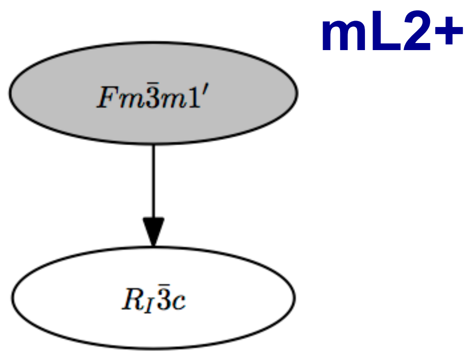
magnetic site 4a

M_{rep} (site 4a)= mL2+ + mL3+

1-dim 2-dim







NiO parent space group: Fm-3m

k= (1/2,1/2,1/2) – point L in the BZ

little group of **k: R-3m**

M_{rep}= mL2+ + mL3+

1-dim 2-dim

(obtained with k-SUBGROUPSMAG)

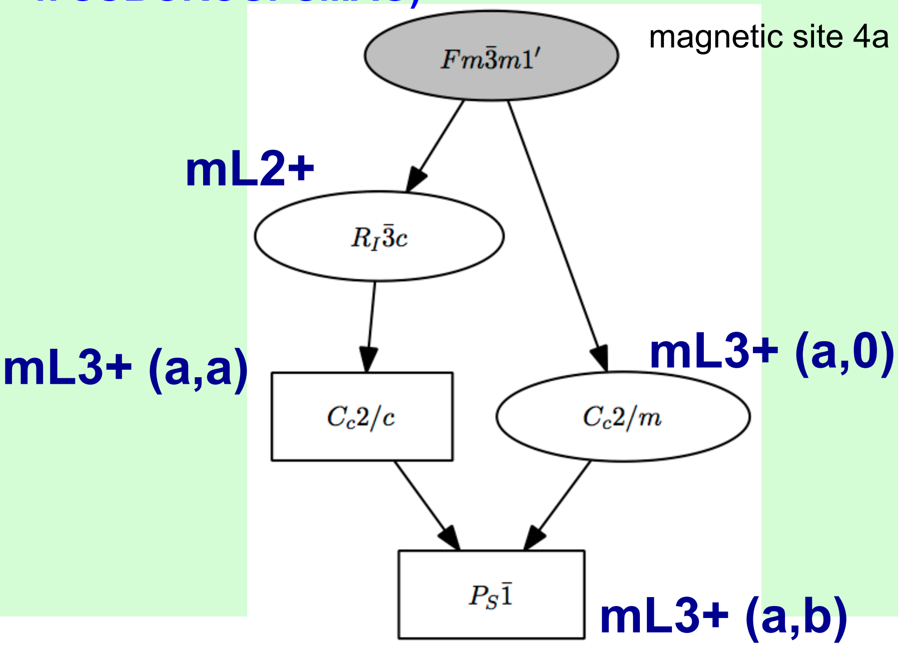
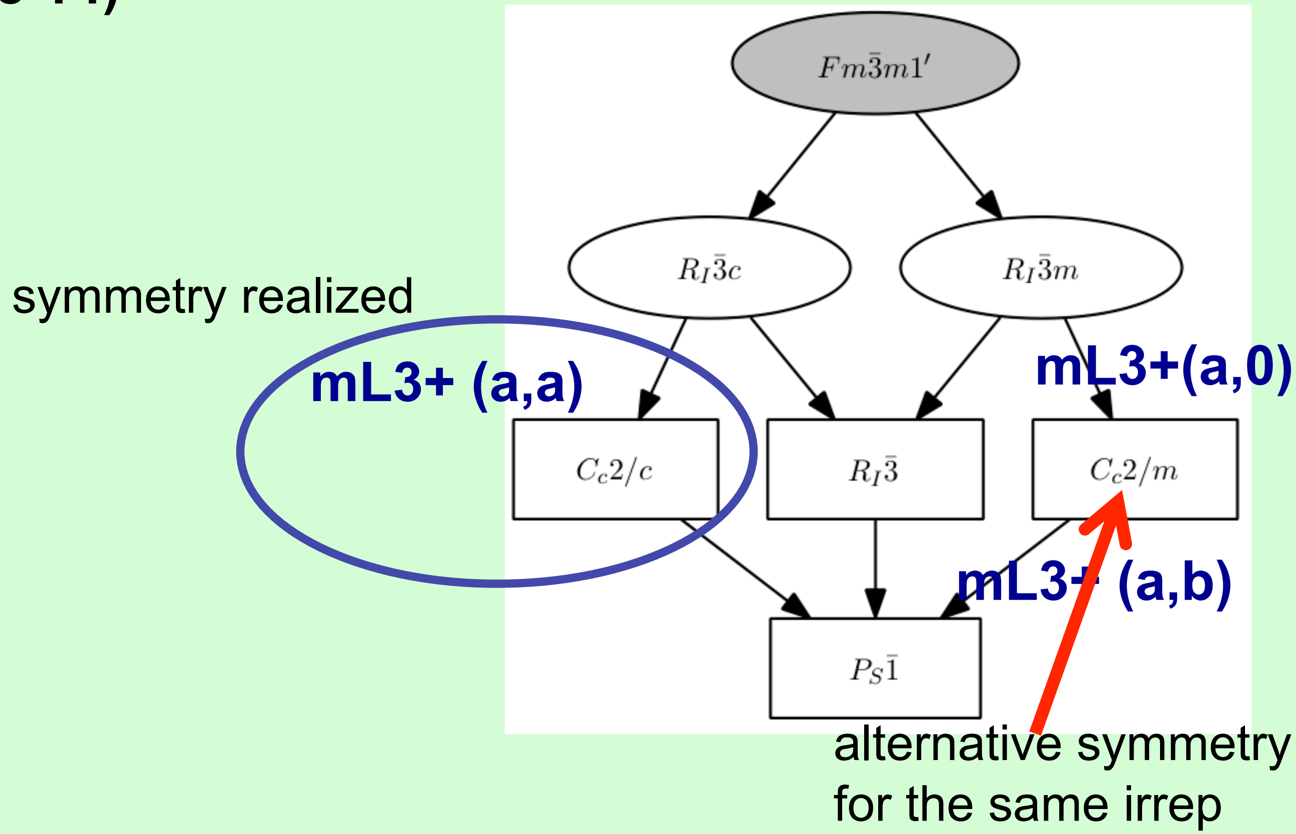


Table 5 Epikernels and kernels of some magnetic *irreps* of $Fm\bar{3}m1'$ at the *L* point[a] of the Brillouin zone

Irrepg	Order parameter direction	Magnetic space group	Transformation to standard	Spin degrees of freedom[b]	Ni spin basis modes
mL2+	(*a*)	$R_I\bar{3}c$ (#167.108)	$(-\mathbf{a}_p/2+\mathbf{c}_p/2, \mathbf{b}_p/2-\mathbf{c}_p/2, -2\mathbf{a}_p-2\mathbf{b}_p-2\mathbf{c}_p; 0, 0, 0)$	1	(1, 1, 1)
mL3+	(*a*, 0)	C_c2/m (#12.63)	$(\mathbf{a}_p/2+\mathbf{b}_p/2-\mathbf{c}, \mathbf{a}_p/2-\mathbf{b}_p/2, -\mathbf{a}_p-\mathbf{b}_p; 0, 0, 0)$	1	(1, −1, 0)
	(*a*, *a*)	C_c2/c (#15.90)	$(\mathbf{a}_p/2+\mathbf{b}_p/2-\mathbf{c}, \mathbf{a}_p/2-\mathbf{b}_p/2, -\mathbf{a}_p-\mathbf{b}_p; 0, 0, 0)$	1	(1, 1, −2)
	(*a*, *b*)	$P_S\bar{1}$ (#7.28)	$(-\mathbf{b}_p/2+\mathbf{c}_p/2, \mathbf{a}_p/2-\mathbf{b}_p/2, \mathbf{a}_p+\mathbf{c}_p; 0, 0, 0)$	2	(1, −1, 0) (1, 1, −2)

(obtained with ISODISTORT)

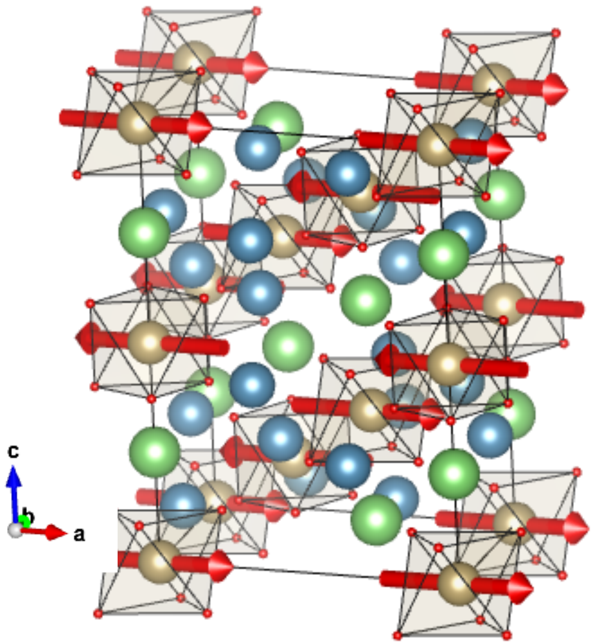
Possible alternative model for NiO of maximal symmetry for the same irrep mL3+ (exercise 14)



Using k-SUBGROUPSMAG and MAGMODELIZE obtain an mcif file of the alternative model for NiO with symmetry C_c2/m, which can result if the irrep mL3+ is the active one and visualize it. (file required: 6.NiO_parent.cif).

Ca_3LiOsO_6

(Calder et al PRB 2012)



Magndata 0.3

Paramagnetic symmetry: R-3c1 1'

Magnetic space group of magnetic phase:

C2'/c' (monoclinic axis along x)

Label	Atom type	x	y	z	Symmetry constraints on M	Mx	My	Mz
Os	Os	0.00000	0.00000	0.00000	m_x,m_y,m_z	2.20000	0.000000	0.00000

They **can** be non-zero. They are symmetry-forced to be equal for all atoms.

Predicted to be weak ferromagnet along z and along $(1,2,0)_H$ (perp. to the monoclinic axes)

Atom	x	y	z	Symmetry constraints on M	Mx	My	Mz
1	0.66667	0.33333	0.33333	m_x,m_y,m_z	2.20000	0.00000	0.00000
2	0.33333	0.66667	0.66667	m_x,m_y,m_z	2.20000	0.00000	0.00000
3	0.00000	0.00000	0.00000	m_x,m_y,m_z	2.20000	0.00000	0.00000
4	0.00000	0.00000	0.50000	$-m_x+m_y,m_y,m_z$	-2.20000	0.00000	0.00000
5	0.33333	0.66667	0.16667	$-m_x+m_y,m_y,m_z$	-2.20000	0.00000	0.00000
6	0.66667	0.33333	0.83333	$-m_x+m_y,m_y,m_z$	-2.20000	0.00000	0.00000

Our example: Ca_3LiOsO_6

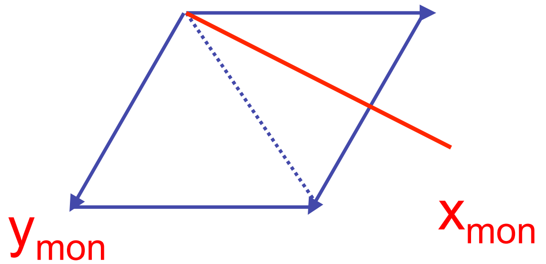
Isotropy subgroups (kernel and epikernels) of mGM3+:

> Specific combinations of the irrep basis modes (from Basirreps, for instance)

R-3c1' → **irrep mGM3+** (2-dim irrep)

- Especial directions 1: **C2/c** → **P-1**
- Especial directions 2: **C2'/c'** → **P-1**

P-1 — kernel: common to any mGM3+ ordering



Invariance equation:

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

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

2x2 matrix of irrep mGM3+

Isotropy subgroups (kernel and epikernels) are derived by programs as: ISODISTORT or JANA2006

R-3c1'

Possible different magnetic space groups for the same irrep

irrep mGM3+

$w=e^{i2\pi/3}$

K=0

All lattice translations:

{1|T}
1 0 0 1

{1|000} {-1|000}	{3+|000} {-3+|000}	{3-|000} {-3-|000}	{2_x|001/2{m_x|001/2}	{2_y|001/2} {m_y|001/2}	{2_{xy}|001/2} {m_{xy}|001/2}
1 0 0 1	w 0 0 w*	w* 0 0 w	0 w* w 0	0 w w* 0	0 1 1 0
{1'|000} {-1'|000}	{3'+|000} {-3'+|000}	{3'-|000} {-3'-|000}	{$2'_x$|001/2} {m'_x|001/2}	{$2'_y$|001/2} {m'_y|001/2}	{$2'_{xy}$|001/2} {m'_{xy}|001/2}
-1 0 0 -1	-w 0 0 -w*	-w* 0 0 -w	0 -w* -w 0	0 -w -w* 0	0 -1 -1 0

Q=(S,S*) Q= $\rho e^{i\alpha}$

For any phase α of the order parameter Q. symmetry operations {1|000} and {-1|000} plus the lattice are coserved

If $\alpha=0,\pi$ {2_{xy}|000} and {m_{xy}|000}

If $\alpha=2\pi/3,-2\pi/6$ {2_x|000} and {m_x|000}

If α=-$2\pi/3, 2\pi/6$ {2_y|000} and {m_y|000}

C2/c

If $\alpha=\pi/2,-\pi/2$ {$2'_{xy}$|000} and {m'_{xy}|000}

If α=-$5\pi/6,\pi/6$ {$2'_x$|000} and {m'_x|000}

If α=-$\pi/6, 5\pi/6$ {$2'_y$|000} and {m'_y|000}

C2'/c'

Basirreps output

Magnetic representation: mGM1$^+$ + mGM2$^+$ + 2mGM3$^+$

```
 ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
=> Basis functions of Representation IRrep( 6) of dimension  2 contained 2 times in GAMMA
 ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

            SYMM  x,y,z   y,x,-z+1/2
            Atoms:      Os_1              Os_2
BsV( 1, 1: 2):Re (    1    0    0) (    0    0    0)
             Im (-0.58-1.15 0.00) ( 0.00 0.00 0.00)
BsV( 2, 1: 2):Re (    0    0    0) (    0    1    0)
             Im ( 0.00 0.00 0.00) ( 1.15 0.58 0.00)
BsV( 3, 1: 2):Re (    0    0    0) (    0    1    0)
             Im ( 0.00 0.00 0.00) (-1.15-0.58 0.00)
BsV( 4, 1: 2):Re (    1    0    0) (    0    0    0)
             Im ( 0.58 1.15 0.00) ( 0.00 0.00 0.00)
```

mGM3$^+$

4 basis functions: 4 parameters

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

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

      SYMM x,y,z                                                   Atom: Os_1     0.0000  0.0000  0.0000
      Sk(1): (u+p,0,0)+i.(-r0.u+r0.p,-r1.u+r1.p,0)

      SYMM y,x,-z+1/2                                              Atom: Os_2     0.0000  0.0000  0.5000
      Sk(2): (0,v+w,0)+i.(r1.v-r1.w,r0.v-r0.w,0)


       Values of real constants r0,r1,...
             r0 =   0.577350     r1 =   1.154700
```

Sarah output **Transformation to basis functions**

mGM3$^+$ irrep

```
IR # 6, BASIS VECTOR: #   1 (ABSOLUTE NUMBER:# 3)
ATOM  1:   (     6     0     0)  +  i(     0     0     0)
ATOM  2:   (     0     0     0)  +  i(     0     0     0)

IR # 6, BASIS VECTOR: #   2 (ABSOLUTE NUMBER:# 4)
ATOM  1:   (     0     0     0)  +  i(     0     0     0)
ATOM  2:   (     0     6     0)  +  i(     0     0     0)

IR # 6, BASIS VECTOR: #   3 (ABSOLUTE NUMBER:# 5)
ATOM  1:   (     0     0     0)  +  i(     0     0     0)
ATOM  2:   ( 6.928 3.464     0)  +  i(     0     0     0)

IR # 6, BASIS VECTOR: #   4 (ABSOLUTE NUMBER:# 6)
ATOM  1:   (-3.464-6.928     0)  +  i(     0     0     0)
ATOM  2:   (     0     0     0)  +  i(     0     0     0)
```

4 basis functions: 4 parameters

<u>For multidimensiona irreps</u>, assigning an irrep is NOT equivalent to the assigning of a magnetic space group:

Our example: Ca_3LiOsO_6

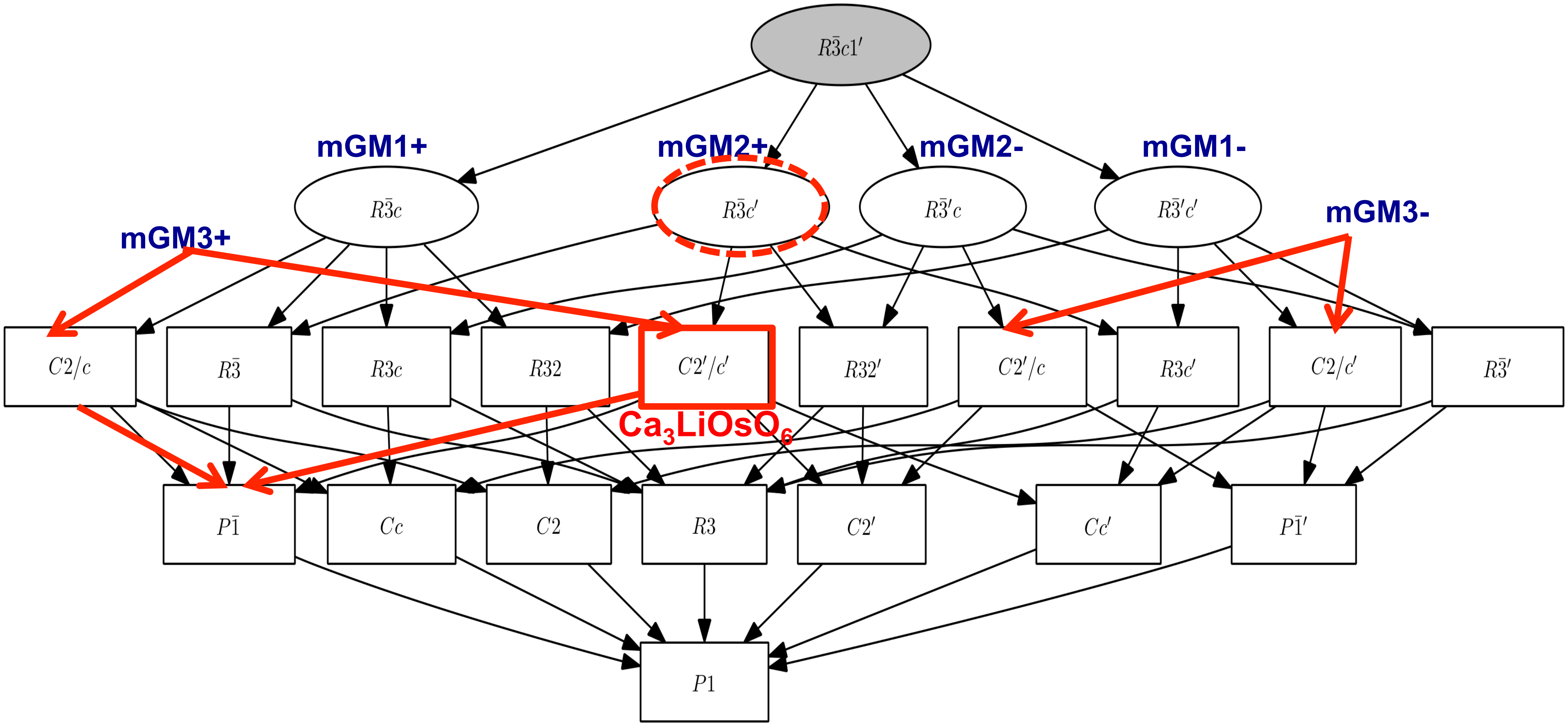
Magnetic symmetry is MORE restrictive than assigning an irrep…

Label	Atom type	x	y	z	Symmetry constraints on M
Os	Os	0.00000	0.00000	0.00000	m_x,m_y,m_z

3 parameters

Space group: R-3c

propagation vector k=(0 0 0) (GM point)

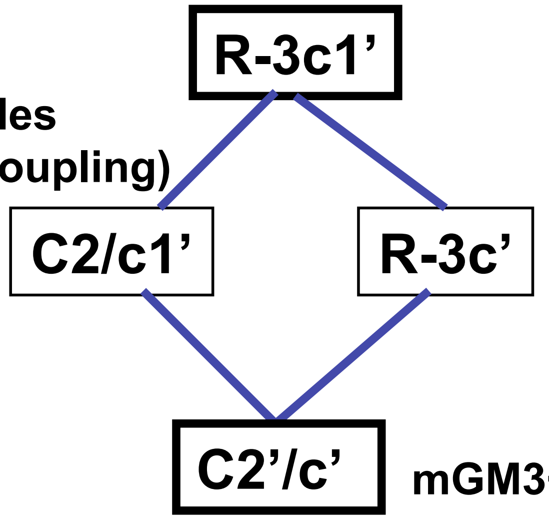


Magnetic symmetry is MORE restrictive than assigning an irrep…

BUT also LESS restrictive than assigning an irrep !:

Irrep mGM3+ restricts the spins to the xy plane (R-setting), but the magnetic group C2'/c' allows a FM component along z.

GM3+, displacive modes (magneto-structural coupling) (strain)



mGM2+, FM spins along z

1 parameter (mz)

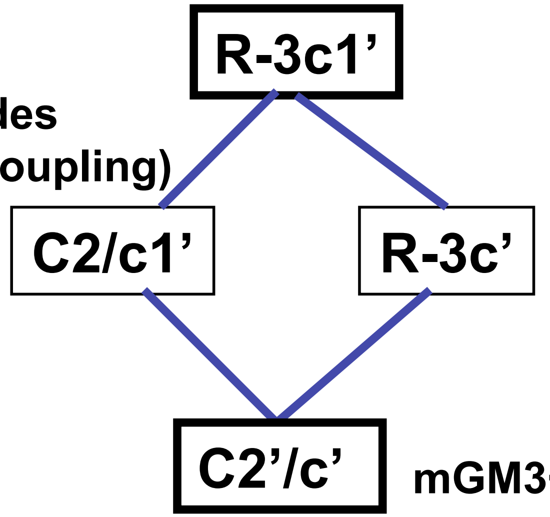
mGM3+, special combination of irrep basis modes)

(special direction of the OP)

2 parameters (mx,my)

The same symmetry change as in classical weak ferromagnets $NiCO_3$, $CoCO_3$, $MnCO_3$

GM3+, displacive modes (magneto-structural coupling)



mGM2+, FM spins along z

mGM3+, special combination of irrep basis modes)

(special direction of the OP)

mGM3+ distortion restricted to C2'/c' symmetry:
(2 parameters)

atom	x,y,z	moment restrictions
Os	0,0,0	mx,my,0

FM canting

mGM2+ distortion (R-3c' symmetry):
(1 parameter)

atom	x,y,z	moment restrictions
Os	0,0,0	0,0,mz

FM canting

C2'/c' symmetry (all compatible irreps allowed) →

Label	Atom type	x	y	z	Symmetry constraints on M
Os	Os	0.00000	0.00000	0.00000	m_x,m_y,m_z

Mx	My	Mz
2.20000	0.000000	0.00000

Why an MSG may allow the presence of secondary irreps?

….because the symmetry of the primary magnetic ordering allows adequate couplings which can induce their appearance without any additional symmetry break.

No need to make a book keeping of these possible couplings… The MSG does it for us!:

All irrep modes compatible with the MSG have adequate couplings with the primary order parameter to allow their non-zero value.

One can always find a symmetry-consistent microscopic mechanism explaining its existence as an induced effect (Dzyaloshinski-Moriya…)

Symmetry-allowed coupling inducing weak FM along z (mGM2+)

Q=(S,S*)

S= $\rho e^{i\alpha}$

	{1|000} {-1|000}	{3+|000} {-3+|000}	{3-|000} {-3-|000}	{2_x| 001/2{m_x| 001/2}	{2_y|001/2} {m_y|001/2}	{2_{xy}|001/2} {m_{xy}|001/2}	
	1 0 0 1	w 0 0 w*	w* 0 0 w	0 w* w 0	0 w w* 0	0 1 1 0	**mGM3+**
(S^3+S^{*3})	1	1	1	1	1	1	**mGM1+**
(S^3-S^{*3})	1	1	1	-1	-1	-1	**mGM2+**

	{1'|000} {-1'|000}	{3'+|000} {-3'+|000}	{3'-|000} {-3'-|000}	{2'$_x$|001/2} {m'$_x$|001/2}	{2'$_y$|001/2} {m'$_y$|001/2}	{2'$_{xy}$|001/2} {m'$_{xy}$|001/2}	
	-1 0 0 -1	-w 0 0 -w*	-w* 0 0 -w	0 -w* -w 0	0 -w -w* 0	0 -1 -1 0	**mGM3+**
(S^3+S^{*3})	-1	-1	-1	-1	-1	-1	**mGM1+**
(S^3-S^{*3})	-1	-1	-1	1	1	1	**mGM2+**

Allowed energetical coupling terms:

S_1: mGM1+ **(S^3+S^{*3})S_1≈** $\rho^3 \cos(3\alpha)\, S_1$ → $S_1 \approx \rho^3 \cos(3\alpha)$

S_2: mGM2+ **(S^3- S^{*3})S_2≈** $\rho^3 \sin(3\alpha)\, S_2$ → $S_2 \approx \rho^3 \sin(3\alpha)$

C2'/c': $S_1 = 0$, $S_2\ \alpha\ \rho^3$

$\alpha = n\pi/3 + \pi/2$

mGM2+

S_2 = FM component along z

C2/c: $S_1\ \alpha\ \rho^3$, $S_2 = 0$

$\alpha = n\pi/3$

mGM1+

Single irrep assignment vs. magnetic space groups (MSG) in commensurate structures. Cases

1) 1-dim. irrep: irrep and MSG assignment are equivalent for spin relations.

2) N dim. irrep, N>1: several MSG (epikernels or isotropy subgroups) are possible for the same irrep. The assignment of a MSG restricts the magnetic configuration beyond the restrictions coming from the irrep.

case 2.1: The MSG is a k-maximal subgroup: it only allows a spin ordering according to a single irrep (further restricted to fulfill the MSG relations). No other irrep arrangements are compatible with the MSG.

case 2.2: The symmetry allows the presence of other secondary irreps. Other irrep arrangements are compatible with the MSG.

Exceptionally: two different irreps may have the same MSG as epikernel….

Conclusions:

- ***Properties of magnetic phases are constrained by their magnetic symmetry: a magnetic space group (if commensurate) or superspace group (if incommensurate)***

- ***Whatever method one has employed to determine a magnetic structure, the final model should include its magnetic symmetry.***

- ***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)***

- ***The best approach: to combine both representation analysis and magnetic symmetry***

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The past and present team in Bilbao of the…

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