Hands-on demonstration of BCS (MAXMAGN, MVISUALIZE, k-SUBGROUPMAG…)

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Three main tutorials on the programs of the BCS Magnetic Section can be directly downloaded from the webpages of the programs :

Tutorial_magnetic_section_BCS_1

Tutorial_magnetic_section_BCS_3

Tutorial_magnetic_section_BCS_2

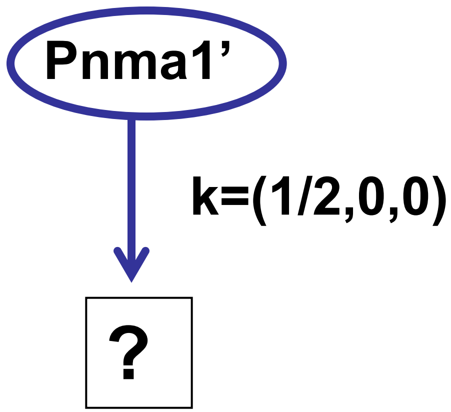
Magnetic Symmetry and Applications	
MGENPOS	General Positions of Magnetic Space Groups
MWYCKPOS	Wyckoff Positions of Magnetic Space Groups
MKVEC	The k-vector types and Brillouin zones of Magnetic Space Groups
IDENTIFY MAGNETIC GROUP	Identification of a Magnetic Space Group from a set of generators in 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

Tutorial-MAXMAGN (3 versions)

Tutorial-k-SUBGROUPSMAG (3 versions)

Symmetry based modeling of magnetic structures

Which MSGs are possible for a magnetic structure having space group Pnma in the paramagnetic phase if we know that the magnetic ordering has propagation vector (wave vector!) k=(1/2,0,0)?



$HoMnO_3$

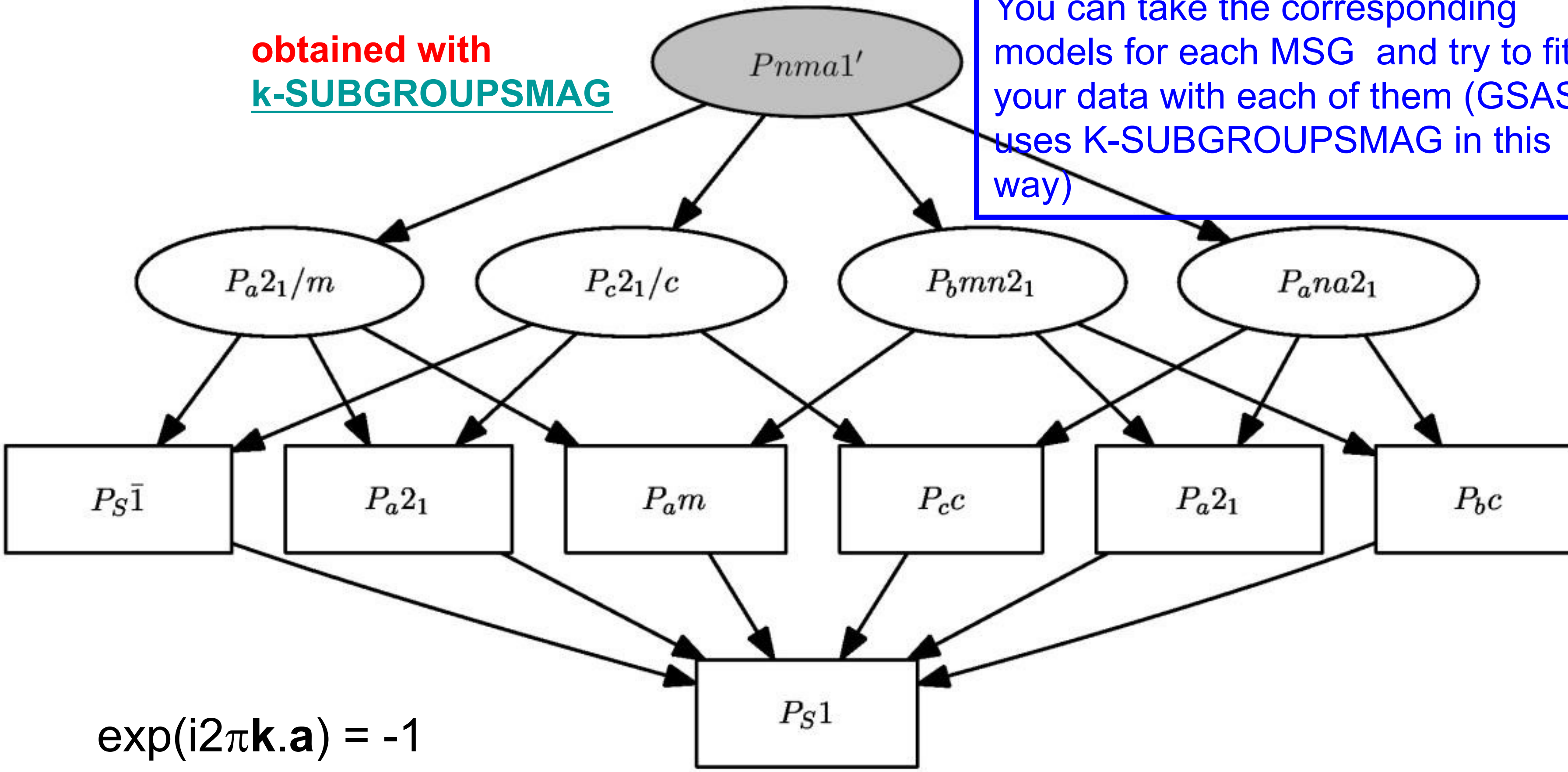
Purely mathematical problem !

Symmetry based modeling of magnetic structures

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

obtained with
k-SUBGROUPSMAG

You can take the corresponding models for each MSG and try to fit your data with each of them (GSAS-II uses K-SUBGROUPSMAG in this way)



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

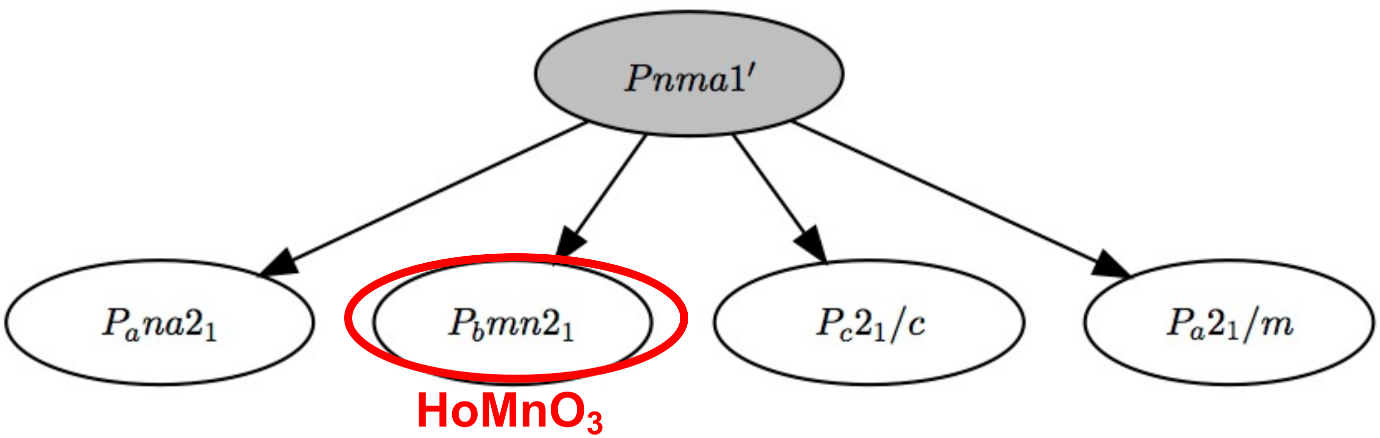
Symmetry operation {1'|1/2,0,0} is present in any case
(magnetic cell= $(2\mathbf{a}_p,\mathbf{b}_p,\mathbf{c}_p)$)

Symmetry based modeling of magnetic structures

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

ONLY MAXIMAL SUBGROUPS (k-maximal symmetries)

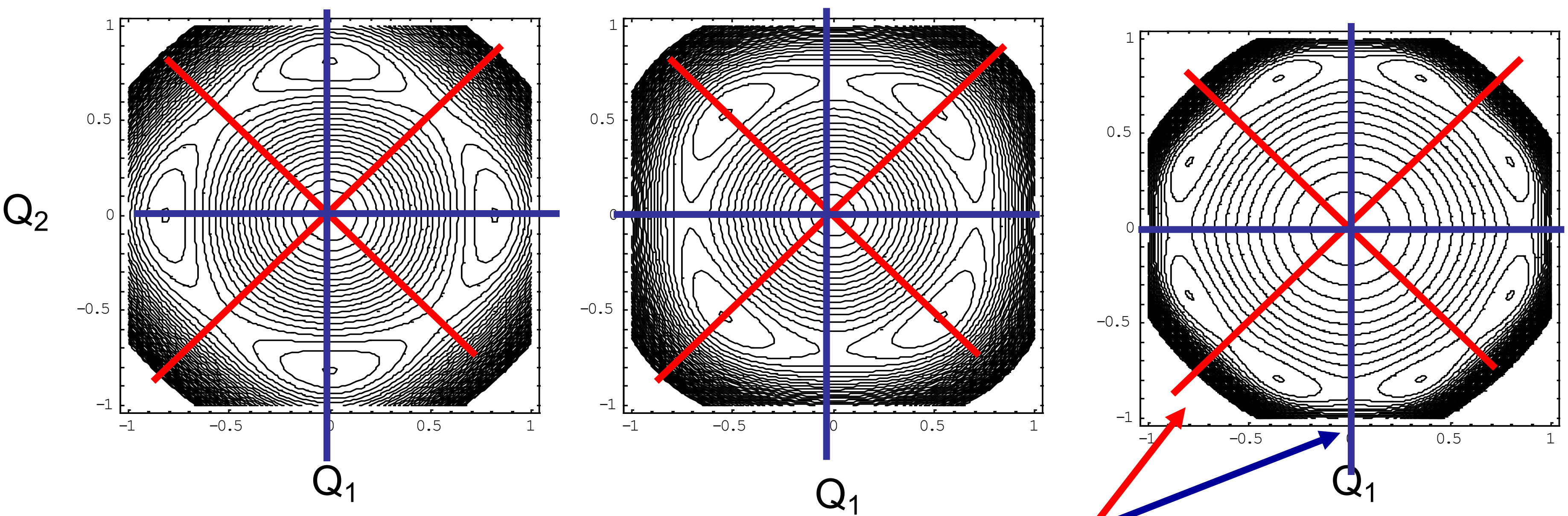
obtained with
k-SUBGROUPSMAG



About 70% of all published magnetic structures have k-maximal symmetries

Why the (magnetic) order parameter usually takes "special" directions of higher symmetry ?

Domains/variants: symmetry related configurations (energy minima) around a higher-symmetry configuration



Q_i : Symmetry-breaking coordinates

Symmetry-forced extrema

Energy in the configuration space is a SMOOTH function: Lower symmetry implies more equivalent minima, i.e. a more wavy energy function

Construction of possible models of a magnetic structure of MAXIMAL SYMMETRY compatible with its propagation vector (1k): MAXMAGN

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3 Tutorials can be downloaded from the program webpage

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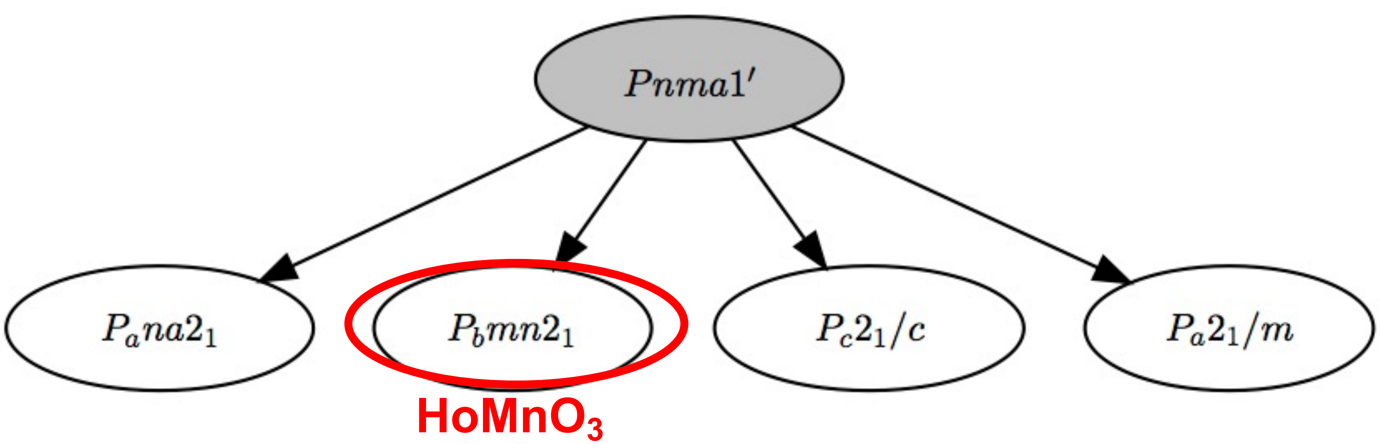
Program MAXMAGN

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	P_ana2_1 (#33.149) Go to a subgroup	$\begin{pmatrix} 2 & 0 & 0 & 1/4 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	*Systematic absences* MAGNEXT *Tensor properties* MTENSOR	Show
2	P_bmn2_1 (#31.129) Go to a subgroup	$\begin{pmatrix} 0 & -2 & 0 & 1/4 \\ 1 & 0 & 0 & 1/4 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	*Systematic absences* MAGNEXT *Tensor properties* MTENSOR	Show
3	P_c2_1/c (#14.82) Go to a subgroup	$\begin{pmatrix} 0 & 0 & 2 & 1/2 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	*Systematic absences* MAGNEXT *Tensor properties* MTENSOR	Show
4	P_a2_1/m (#11.55) Go to a subgroup	$\begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	*Systematic absences* MAGNEXT *Tensor properties* MTENSOR	Show



Unambiguous description of a MSG as subgroup of a parent gray group:

$HoMnO_3$ case

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

(P,p)

transformation to standard of the MSG

P = 3x3 matrix

p = (p_1, p_2, p_3)

Pnma1' → $\boldsymbol{P_b mn2_1}$ (**-b**, 2**a** , **c**; 1/4, 1/4, 0)

$$(\mathbf{a^s},\mathbf{b^s},\mathbf{c^s}) = (\mathbf{a_p},\mathbf{b_p},\mathbf{c_p}).\mathbf{P} \quad , \quad \mathbf{O^s} = \mathbf{O_p} + p_1\,\mathbf{a_p} + p_2\,\mathbf{b_p} + p_3\,\mathbf{c_p}$$

MSG standard unit cell — parent unit cell — origin shlft

Transformation to standard setting:

symmetry operation:

$$\left(\begin{array}{ccc|c} & R^s & & \mathbf{t}^s \\ \hline 0 & 0 & 0 & 1 \end{array}\right) = \left(\begin{array}{ccc|c} & \mathbf{P} & & \mathbf{p} \\ \hline 0 & 0 & 0 & 1 \end{array}\right)^{-1} \left(\begin{array}{ccc|c} & R & & \mathbf{t} \\ \hline 0 & 0 & 0 & 1 \end{array}\right) \left(\begin{array}{ccc|c} & \mathbf{P} & & \mathbf{p} \\ \hline 0 & 0 & 0 & 1 \end{array}\right)$$

positions:

$$\begin{pmatrix} x^s \\ y^s \\ z^s \\ 1 \end{pmatrix} = \left(\begin{array}{ccc|c} & \mathbf{P} & & \mathbf{p} \\ \hline 0 & 0 & 0 & 1 \end{array}\right)^{-1} \begin{pmatrix} x \\ y \\ z \\ 1 \end{pmatrix}$$

magnetic moment (absolute) components:

$$\begin{pmatrix} m_x^s/a^s \\ m_y^s/b^s \\ m_z^s/c^s \end{pmatrix} = \mathbf{P}^{-1} \begin{pmatrix} m_x/a \\ m_y/b \\ m_z/c \end{pmatrix}$$

One should not confuse:

When describing a subgroup of the parent group:

Parent Pnma unit cell ($\mathbf{a}_p$, $\mathbf{b}_p$, $\mathbf{c}_p$;0,0,0):

Pnma1' → $P_b mn2_1$ (**-b**, 2**a** , **c**; 1/4, 1/4, 0)

transformation to standard from the parent setting of *Pnma*

description of the subgroup by its type of MSG and a unit cell and origin with respect to the parent unit cell where it WOULD adquire its standard form

When describing a magnetic structure under this MSG using a non-standard setting:

Unit cell used (2$\mathbf{a}_p$, $\mathbf{b}_p$, $\mathbf{c}_p$;0,0,0):

$P_b mn2_1$ (**-b**, **a** , **c**; 1/8, 1/4, 0)

transformation to standard from the setting used for the MSG.

Alternative unit cell and origin with respect to the unit cell used where the MSG WOULD adquire its standard form

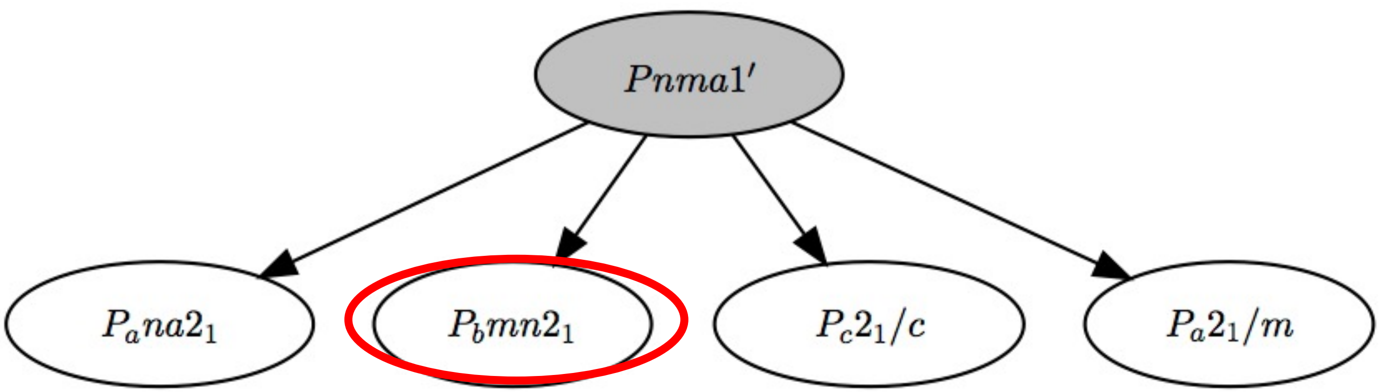
```
_parent_space_group.name_H-M_alt  'P  n  m  a'
_parent_space_group.IT_number                    62
_parent_space_group.transform_Pp_abc  'a,b,c;0,0,0'

loop_
_parent_propagation_vector.id
_parent_propagation_vector.kxkykz
k1 [1/2 0 0]

_parent_space_group.child_transform_Pp_abc  '2a,b,c;0,0,0'
_space_group_magn.transform_BNS_Pp_abc  'b,-a,c;1/8,1/4,0'


_space_group_magn.number_BNS  31.129
_space_group_magn.name_BNS  "P_b  m  n  2_1"
_cell_length_a              11.67080
_cell_length_b              7.36060
_cell_length_c              5.25720
_cell_angle_alpha           90.00
_cell_angle_beta            90.00
_cell_angle_gamma           90.00
```

```
loop_
_space_group_symop_magn_operation.id
_space_group_symop_magn_operation.xyz
1 x,y,z,+1
2 -x+1/4,-y,z+1/2,+1
3 x,-y+1/2,z,+1
4 -x+1/4,y+1/2,z+1/2,+1

loop_
_space_group_symop_magn_centering.id
_space_group_symop_magn_centering.xyz
1 x,y,z,+1
2 x+1/2,y,z,-1

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
Ho_1 Ho 0.04195 0.25000 0.98250
Ho_2 Ho  0.95805 0.75000 0.01750
Mn Mn 0.00000 0.00000 0.50000
O1_1 O 0.23110 0.25000 0.11130
O1_2 O  0.76890 0.75000 0.88870
O2_1 O 0.16405 0.05340 0.70130
O2_2 O  0.83595 0.55340 0.29870

loop_
_atom_site_moment.label
_atom_site_moment.crystalaxis_x
_atom_site_moment.crystalaxis_y
_atom_site_moment.crystalaxis_z
_atom_site_moment.symmform
Ho_1 0.00000 0.00000 0.00000 0,my,0
Ho_2 0.00000 0.00000 0.00000 0,my,0
Mn 1.00000 0.00000 0.00000 mx,my,mz
```

Program MAXMAGN

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	$P_a na2_1$ (#33.149) Go to a subgroup	$\begin{pmatrix} 2 & 0 & 0 & 1/4 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	*Systematic absences* MAGNEXT *Tensor properties* MTENSOR	Show
2	$P_b mn2_1$ (#31.129) Go to a subgroup	$\begin{pmatrix} 0 & -2 & 0 & 1/4 \\ 1 & 0 & 0 & 1/4 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	*Systematic absences* MAGNEXT *Tensor properties* MTENSOR	Show
3	$P_c 2_1/c$ (#14.82) Go to a subgroup	$\begin{pmatrix} 0 & 0 & 2 & 1/2 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	*Systematic absences* MAGNEXT *Tensor properties* MTENSOR	Show
4	$P_a 2_1/m$ (#11.55) Go to a subgroup	$\begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	*Systematic absences* MAGNEXT *Tensor properties* MTENSOR	Show



$HoMnO_3$

Selected magnetic space group: 3- P_c2_1/c (#14.82)

Setting parent-like (**2a, b, c** ; 0, 0, 0)

Parent space group *Pnma* (No. 62)

Lattice parameters: a=11.67070, b=7.36060, c=5.25720, alpha=90.00, beta=90.00, gamma=90.00

[Go to setting standard (**-c, b, 2a** ; 1/2, 0, 0)]
[Go to an alternative setting]

Export data to MCIF file/Visualize | Go to a subgroup

Atomic positions, Wyckoff positions and Magnetic Moments

N	Atom	New WP	Multiplicity	Magnetic moment	Values of M_x, M_y, M_z
1	Ho1_1 Ho 0.04195 0.25000 0.98250	(x,1/4,z | m_x,0,m_z) (-x,3/4,-z | $-m_x$,0,$-m_z$) (x+1/2,1/4,z | $-m_x$,0,$-m_z$) (-x+1/2,3/4,-z | m_x,0,m_z)	4	(M_x,0,M_z)	M_x = 0.0000 M_z = 0.0000
	Ho1_2 Ho 0.20805 0.75000 0.48250	(-x+1/4,3/4,z+1/2 | m_x,0,m_z) (x+1/4,1/4,-z+1/2 | m_x,0,m_z) (-x+3/4,3/4,z+1/2 | $-m_x$,0,$-m_z$) (x+3/4,1/4,-z+1/2 | $-m_x$,0,$-m_z$)	4	(M_x,0,M_z)	M_x = 0.0000 M_z = 0.0000
2	Mn1_1 Mn 0.00000 0.00000 0.50000	(0,0,1/2 | 0,0,0) (0,1/2,1/2 | 0,0,0) (1/2,0,1/2 | 0,0,0) (1/2,1/2,1/2 | 0,0,0)	4	(0,0,0)	-
	Mn1_2 Mn 0.25000 0.00000 0.00000	(1/4,0,0 | m_x,m_y,m_z) (1/4,1/2,0 | m_x,$-m_y$,m_z) (3/4,0,0 | $-m_x$,$-m_y$,$-m_z$) (3/4,1/2,0 | $-m_x$,m_y,$-m_z$)	4	(M_x,M_y,M_z)	M_x = 0.0000 M_y = 0.0000 M_z = 0.0000
3	O1_1 O 0.23110 0.25000 0.11130	(x,1/4,z | m_x,0,m_z) (-x,3/4,-z | $-m_x$,0,$-m_z$) (x+1/2,1/4,z | $-m_x$,0,$-m_z$) (-x+1/2,3/4,-z | m_x,0,m_z)	4	-	-
	O1_2 O 0.01890 0.75000 0.61130	(-x+1/4,3/4,z+1/2 | m_x,0,m_z) (x+1/4,1/4,-z+1/2 | m_x,0,m_z) (-x+3/4,3/4,z+1/2 | $-m_x$,0,$-m_z$) (x+3/4,1/4,-z+1/2 | $-m_x$,0,$-m_z$)	4	-	-
4	O2_1 O 0.16405 0.05340 0.70130	(x,y,z | m_x,m_y,m_z) (-x,y+1/2,-z | $-m_x$,m_y,$-m_z$) (-x,-y,-z | $-m_x$,$-m_y$,$-m_z$) (x,-y+1/2,z | m_x,$-m_y$,m_z) (x+1/2,y,z | $-m_x$,$-m_y$,$-m_z$) (-x+1/2,y+1/2,-z | m_x,$-m_y$,m_z) (-x+1/2,-y,-z | m_x,m_y,m_z) (x+1/2,-y+1/2,z | $-m_x$,m_y,$-m_z$)	8	-	-
	O2_2 O 0.08595 0.94660 0.20130	(-x+1/4,-y,z+1/2 | m_x,m_y,m_z) (x+1/4,-y+1/2,-z+1/2 | m_x,$-m_y$,m_z) (x+1/4,y,-z+1/2 | m_x,m_y,m_z) (-x+1/4,y+1/2,z+1/2 | m_x,$-m_y$,m_z) (-x+3/4,-y,z+1/2 | $-m_x$,$-m_y$,$-m_z$) (x+3/4,-y+1/2,-z+1/2 | $-m_x$,m_y,$-m_z$) (x+3/4,y,-z+1/2 | $-m_x$,$-m_y$,$-m_z$) (-x+3/4,y+1/2,z+1/2 | $-m_x$,m_y,$-m_z$)	8	-	-

half of the Mn atoms must have zero spins

Program MAXMAGN

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	$P_a na2_1$ (#33.149) Go to a subgroup	$\begin{pmatrix} 2 & 0 & 0 & 1/4 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	*Systematic absences* MAGNEXT *Tensor properties* MTENSOR	Show
2	$P_b mn2_1$ (#31.129) Go to a subgroup	$\begin{pmatrix} 0 & -2 & 0 & 1/4 \\ 1 & 0 & 0 & 1/4 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	*Systematic absences* MAGNEXT *Tensor properties* MTENSOR	Show
3	$P_c 2_1/c$ (#14.82) Go to a subgroup	$\begin{pmatrix} 0 & 0 & 2 & 1/2 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	*Systematic absences* MAGNEXT *Tensor properties* MTENSOR	Show
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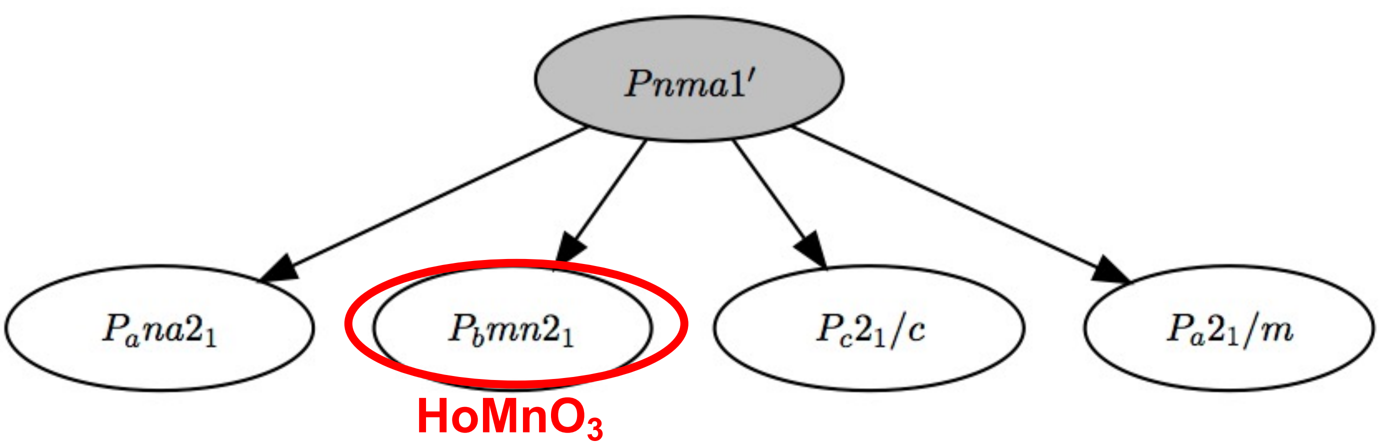

Selected magnetic space group: 2- P_bmn2_1 (#31.129)

Setting parent-like (**2a, b, c** ; 0, 0, 0)

Parent space group *Pnma* (No. 62)

Lattice parameters: a=11.67070, b=7.36060, c=5.25720, alpha=90.00, beta=90.00, gamma=90.00

[Go to setting standard (**b, -2a, c** ; 1/4, 1/4, 0)]
[Go to an alternative setting]

Export data to MCIF file/Visualize | Go to a subgroup

Atomic positions, Wyckoff positions and Magnetic Moments

N	Atom	New WP	Multiplicity	Magnetic moment	Values of M_x, M_y, M_z
1	Ho1_1 Ho 0.04195 0.25000 0.98250	$(x,1/4,z \mid 0,m_y,0)$ $(-x+1/4,3/4,z+1/2 \mid 0,-m_y,0)$ $(x+1/2,1/4,z \mid 0,-m_y,0)$ $(-x+3/4,3/4,z+1/2 \mid 0,m_y,0)$	4	**$(0,M_y,0)$**	M_y = 0.0000
	Ho1_2 Ho 0.95805 0.75000 0.01750	$(-x,3/4,-z \mid 0,m_y,0)$ $(x+1/4,1/4,-z+1/2 \mid 0,-m_y,0)$ $(-x+1/2,3/4,-z \mid 0,-m_y,0)$ $(x+3/4,1/4,-z+1/2 \mid 0,m_y,0)$	4	**$(0,M_y,0)$**	M_y = 0.0000
2	Mn1 Mn 0.00000 0.00000 0.50000	$(0,0,1/2 \mid m_x,m_y,m_z)$ $(1/4,0,0 \mid -m_x,-m_y,m_z)$ $(0,1/2,1/2 \mid -m_x,m_y,-m_z)$ $(1/4,1/2,0 \mid m_x,-m_y,-m_z)$ $(1/2,0,1/2 \mid -m_x,-m_y,-m_z)$ $(3/4,0,0 \mid m_x,m_y,-m_z)$ $(1/2,1/2,1/2 \mid m_x,-m_y,m_z)$ $(3/4,1/2,0 \mid -m_x,m_y,m_z)$	8	**(M_x,M_y,M_z)**	M_x = 1 M_y = 0.0000 M_z = 0.0000
3	O1_1 O 0.23110 0.25000 0.11130	$(x,1/4,z \mid 0,m_y,0)$ $(-x+1/4,3/4,z+1/2 \mid 0,-m_y,0)$ $(x+1/2,1/4,z \mid 0,-m_y,0)$ $(-x+3/4,3/4,z+1/2 \mid 0,m_y,0)$	4	-	-
	O1_2 O 0.76890 0.75000 0.88870	$(-x,3/4,-z \mid 0,m_y,0)$ $(x+1/4,1/4,-z+1/2 \mid 0,-m_y,0)$ $(-x+1/2,3/4,-z \mid 0,-m_y,0)$ $(x+3/4,1/4,-z+1/2 \mid 0,m_y,0)$	4	-	-
4	O2_1 O 0.16405 0.05340 0.70130	$(x,y,z \mid m_x,m_y,m_z)$ $(-x+1/4,-y,z+1/2 \mid -m_x,-m_y,m_z)$ $(x,-y+1/2,z \mid -m_x,m_y,-m_z)$ $(-x+1/4,y+1/2,z+1/2 \mid m_x,-m_y,-m_z)$ $(x+1/2,y,z \mid -m_x,-m_y,-m_z)$ $(-x+3/4,-y,z+1/2 \mid m_x,m_y,-m_z)$ $(x+1/2,-y+1/2,z \mid m_x,-m_y,m_z)$ $(-x+3/4,y+1/2,z+1/2 \mid -m_x,m_y,m_z)$	8	-	-
	O2_2 O 0.83595 0.55340 0.29870	$(-x,y+1/2,-z \mid m_x,m_y,m_z)$ $(x+1/4,-y+1/2,-z+1/2 \mid -m_x,-m_y,m_z)$ $(-x,-y,-z \mid -m_x,m_y,-m_z)$ $(x+1/4,y,-z+1/2 \mid m_x,-m_y,-m_z)$ $(-x+1/2,y+1/2,-z \mid -m_x,-m_y,-m_z)$ $(x+3/4,-y+1/2,-z+1/2 \mid m_x,m_y,-m_z)$ $(-x+1/2,-y,-z \mid m_x,-m_y,m_z)$ $(x+3/4,y,-z+1/2 \mid -m_x,m_y,m_z)$	8	-	-

mCIF file of the structure

Submit this mcif file to MVISUALIZE for 3D visualization of the estructure using Jmol: Submit to MVISUALIZE

Download mCIF file: bcs_file.mcif

[The preview text below is non-editable, only copy-allowed]

```
#\#CIF_2.0
# Created by the Bilbao Crystallographic Server
# http://www.cryst.ehu.es
# Date: 26/10/2025 17:42:49
# HoMnO3_Munoz_icsd_165196.cif

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;

_active_magnetic_irreps_details
;
k-maximal magnetic symmetry
;

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_parent_space_group.IT_number                62
```
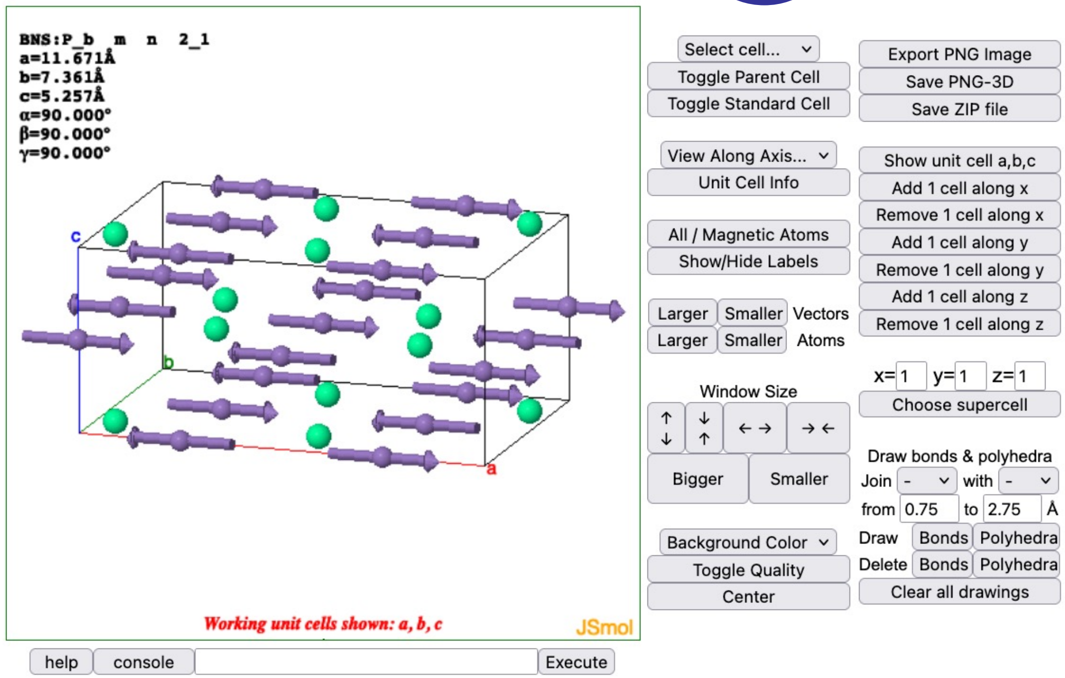

MVISUALIZE: 3D Visualization of magnetic structures with Jmol

MVISUALIZE Main Page

Show/Hide File



Note: *If the application stops working right or any malfunction is observed, it is probably a temporal problem due to the cache memory of your browser. Clear your web browser cache to solve it. If you still observe any malfunction, write an e-mail to cryst@wm.lc.ehu.es explaining the problem in detail.*

Maximal magnetic space groups for the space group 64 (*Cmce*) and the propagation vector k = (1, 0, 0)

Group (BNS)	Transformation matrix	General positions	Systematic absences	Magnetic structure
P_Cnma (#62.455)	$\begin{pmatrix} 0 & 1 & 0 & 1/4 \\ -1 & 0 & 0 & 1/4 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (twin-related)	Show	Show	Show
P_Cbca (#61.439)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (twin-related)	Show	Show	Show
P_Abcn (#60.429)	$\begin{pmatrix} 0 & 1 & 0 & 1/4 \\ 0 & 0 & 1 & 1/4 \\ 1 & 0 & 0 & 0 \end{pmatrix}$ Alternatives (twin-related)	Show	Show	Show
P_Bbcm (#57.390)	$\begin{pmatrix} 0 & 0 & 1 & 1/4 \\ 1 & 0 & 0 & 1/4 \\ 0 & 1 & 0 & 0 \end{pmatrix}$ Alternatives (twin-related)	Show	Show	Show
P_Accn (#56.374)	$\begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}$ Alternatives (twin-related)	Show	Show	Show
P_Abam (#55.362)	$\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}$ Alternatives (twin-related)	Show	Show	Show
P_Acca (#54.349)	$\begin{pmatrix} 0 & 1 & 0 & 1/4 \\ 0 & 0 & 1 & 1/4 \\ 1 & 0 & 0 & 0 \end{pmatrix}$ Alternatives (twin-related)	Show	Show	Show
P_Cmna (#53.335)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (twin-related)	Show	Show	Show

La_2CuO_4

Parent symmetry group:

Cmce (Cmca.1′) Cu at WP 4a

propagation vector: k=(1,0,0)

(it is NOT equivalent to k=0 !)

MAXMAGN:
Possible alternative maximal magnetic symmetries and corresponding models of the magnetic structure

Selected magnetic space group: 5- $P_A ccn$ (#56.374)

Setting of the parent group

Lattice parameters: a=5.35700, b=13.14800, c=5.40600, alpha=90., beta=90., gamma=90.

Magnetic Moments associated to magnetic atoms

N	Atom	New WP	Multiplicity	Magnetic moment	Values of M_x, M_y, M_z
1	Cu1 Cu 0.00000 0.00000 0.00000	$(0,0,0 \mid 0,m_y,m_z)$ $(0,1/2,1/2 \mid 0,-m_y,m_z)$ $(1/2,1/2,0 \mid 0,-m_y,-m_z)$ $(1/2,0,1/2 \mid 0,m_y,-m_z)$	4	$(0,M_y,M_z)$	M_y = 0.0000 M_z = 0.0000
2	La1 La 0.00000 0.36110 0.00460	$(0,y,z \mid 0,m_y,m_z)$ $(0,-y+1/2,1/2 \mid 0,-m_y,m_z)$ $(0,1/2,-z+1/2 \mid 0,-m_y,m_z)$ $(0,-y,-z \mid 0,m_y,m_z)$ $(1/2,1/2,0 \mid 0,-m_y,-m_z)$ $(1/2,-y,1/2 \mid 0,m_y,-m_z)$ $(1/2,0,-z+1/2 \mid 0,m_y,-m_z)$ $(1/2,-y+1/2,-z \mid 0,-m_y,-m_z)$	8	-	-
3	O1 O 0.25000 -0.00510 0.25000	$(1/4,y,1/4 \mid 0,m_y,0)$ $(3/4,-y+1/2,3/4 \mid 0,-m_y,0)$ $(3/4,-y,3/4 \mid 0,m_y,0)$ $(1/4,1/2,1/4 \mid 0,-m_y,0)$ $(3/4,1/2,1/4 \mid 0,-m_y,0)$ $(1/4,-y,3/4 \mid 0,m_y,0)$ $(1/4,-y+1/2,3/4 \mid 0,-m_y,0)$ $(3/4,0,1/4 \mid 0,m_y,0)$	8	-	-
4	O2 O 0.00000 0.18300 -0.02430	$(0,y,z \mid 0,m_y,m_z)$ $(0,-y+1/2,1/2 \mid 0,-m_y,m_z)$ $(0,1/2,-z+1/2 \mid 0,-m_y,m_z)$ $(0,-y,-z \mid 0,m_y,m_z)$ $(1/2,1/2,0 \mid 0,-m_y,-m_z)$ $(1/2,-y,1/2 \mid 0,m_y,-m_z)$ $(1/2,0,-z+1/2 \mid 0,m_y,-m_z)$ $(1/2,-y+1/2,-z \mid 0,-m_y,-m_z)$	8	-	-

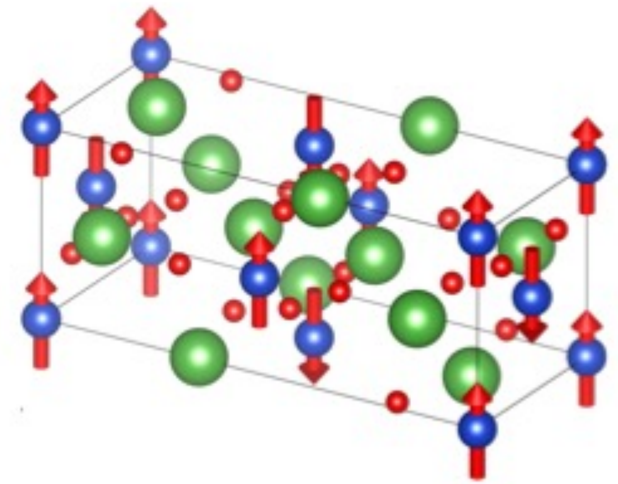
[Go to setting standard (**c**, **a**, **b** ; 0, 0, 0)]

Export data to MCIF file | Go to a subgroup

Maximal magnetic space groups for the space group 64 (*Cmce*) and the propagation vector k = (1, 0, 0)

Group (BNS)	Transformation matrix	General positions	Systematic absences	Magnetic structure
P_Cnma (#62.455)	(0 1 0 1/4; −1 0 0 1/4; 0 0 1 0) Alternatives (twin-related)	Show	Show	Show
P_Cbca (#61.439)	(1 0 0 0; 0 1 0 0; 0 0 1 0) Alternatives (twin-related)	Show	Show	Show
P_Abcn (#60.429)	(0 1 0 1/4; 0 0 1 1/4; 1 0 0 0) Alternatives (twin-related)	Show	Show	Show
P_Bbcm (#57.390)	(0 0 1 1/4; 1 0 0 1/4; 0 1 0 0) Alternatives (twin-related)	Show	Show	Show
P_Accn (#56.374)	(0 1 0 0; 0 0 1 0; 1 0 0 0) Alternatives (twin-related)	Show	Show	Show
P_Abam (#55.362)	(0 0 1 0; 0 −1 0 0; 1 0 0 0) Alternatives (twin-related)	Show	Show	Show
P_Acca (#54.349)	(0 1 0 1/4; 0 0 1 1/4; 1 0 0 0) Alternatives (twin-related)	Show	Show	Show
P_Cmna (#53.335)	(1 0 0 0; 0 1 0 0; 0 0 1 0) Alternatives (twin-related)	Show	Show	Show

La_2CuO_4



P_Accn (56.374)

Cu1 (0,0,0)

M_{Cu1} = (0, my, m_z)

Refinement result (Magndata #1.23):

M_{Cu1} = (0, 0, 0.17)

symmetry forced

approximate value

Construction of possible models of a magnetic structure from the knowledge of its propagation vector(s):

k-SUBGROUPSMAG & MAGMODELIZE

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

For non-maximal symmetries and/or more than one propagation vector

k-SUBGROUPSMAG & MAGMODELIZE

Tutorial_magnetic_section_BCS_3

Tutorial_magnetic_section_BCS_2

Tutorial-k-SUBGROUPSMAG (3 versions)

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
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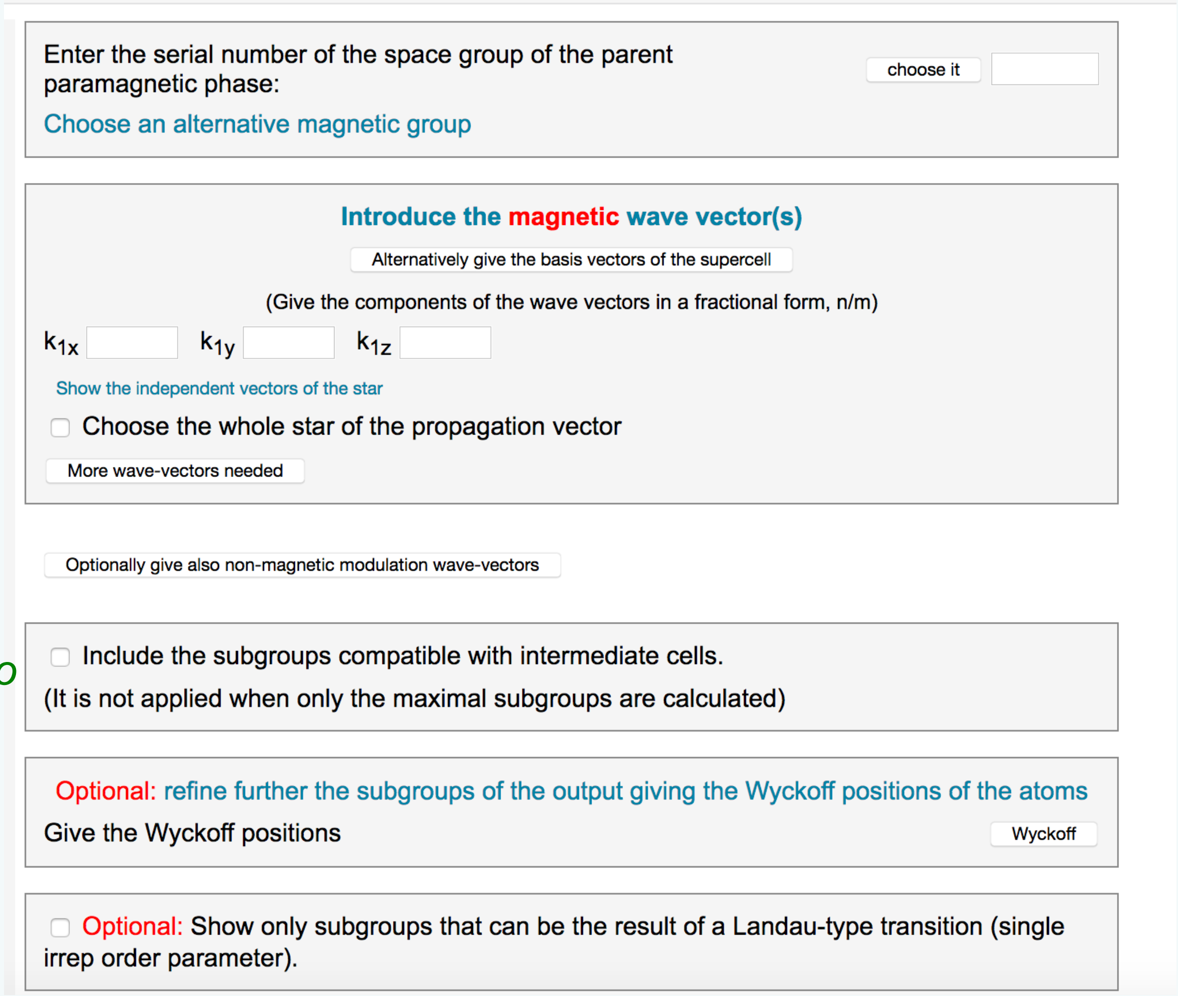
MVISUALIZE	3D Visualization of magnetic structures with Jmol
MTENSOR	Symmetry-adapted form of crystal tensors in magnetic phases
MAGNETIC REP.	Decomposition of the magnetic representation into irreps
Get_mirreps	Irreps and order parameters in a paramagnetic space group- magnetic subgroup phase transition

k-SUBGROUPSMAG & MAGMODELIZE

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



***k-SUBGROUPSMAG** is called by the refinement program **GSAS-II** through an internal link in order to obtain all possible alternative symmetries for a given set of propagation vectors.*

k-SUBGROUPSMAG

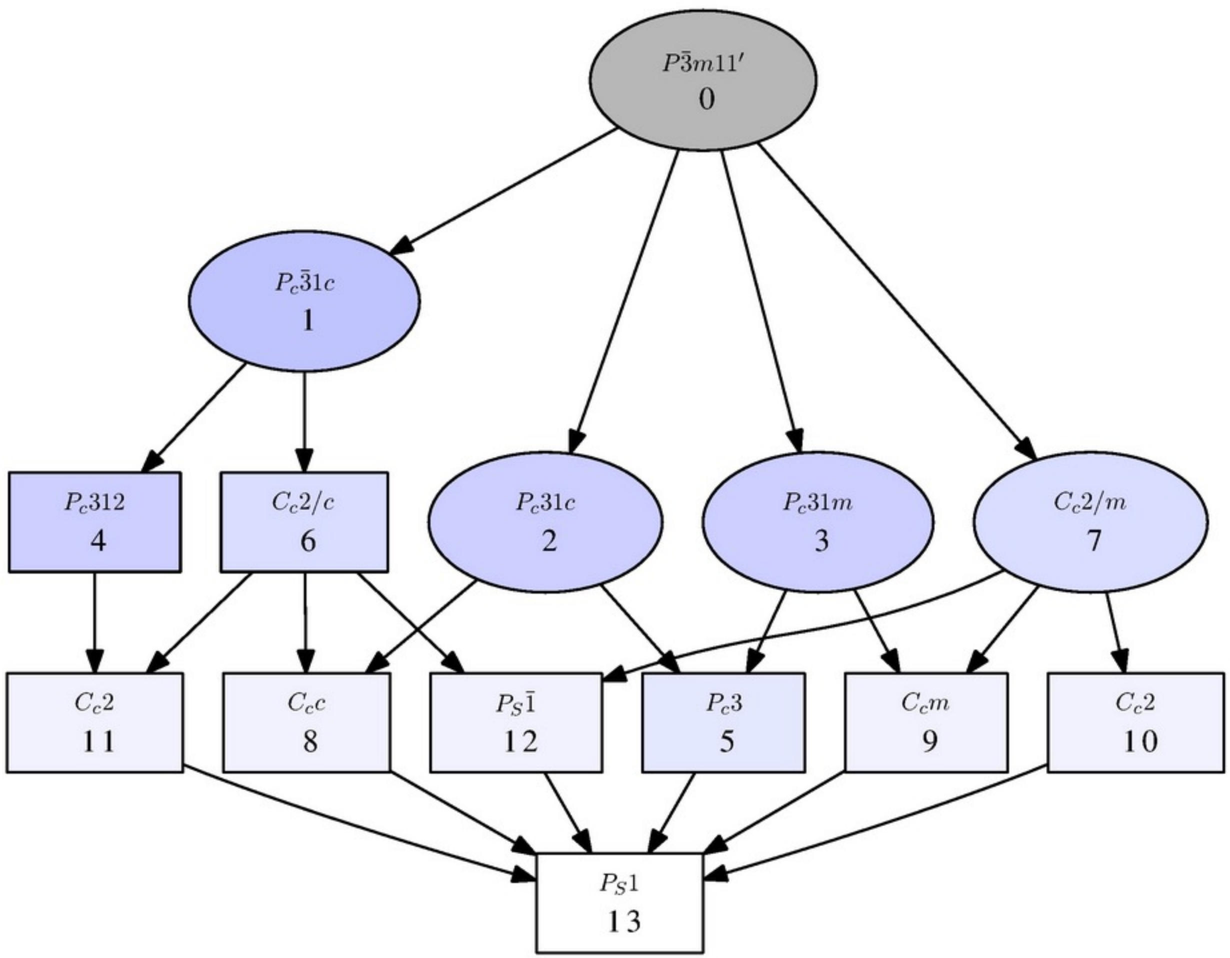
Example: Ba3Nb2NiO9
MAGNDATA #1.13

Possible magnetic symmetries for a magnetic phase with parent space group P-3m1 (N. 164), propagation vector (1/3,1/3,1/2) and magnetic atom at 1b (0,0,1/2) allowing zon-zero momento on all sites

N	Group Symbol	Transformation matrix	Group-Subgroup index	Other members of the Conjugacy Class	irreps	Magnetic structure models (MAGMODELIZE)
1	$P_c\bar{3}1c$ (No. 163.84)	$\begin{pmatrix} 1 & 1 & 0 & 0 \\ -1 & 2 & 0 & 1 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	6=6x1	Conjugacy Class	Get irreps	
2	P_c31c (No. 159.64)	$\begin{pmatrix} 1 & 1 & 0 & -2/3 \\ -1 & 2 & 0 & -1/3 \\ 0 & 0 & 2 & 0 \end{pmatrix}$	12=6x2	Conjugacy Class	Get irreps	
3	P_c31m (No. 157.56)	$\begin{pmatrix} 1 & 1 & 0 & -2/3 \\ -1 & 2 & 0 & -1/3 \\ 0 & 0 & 2 & 0 \end{pmatrix}$	12=6x2	Conjugacy Class	Get irreps	
4	P_c312 (No. 149.24)	$\begin{pmatrix} 1 & 1 & 0 & 0 \\ -1 & 2 & 0 & 0 \\ 0 & 0 & 2 & 0 \end{pmatrix}$	12=6x2	Conjugacy Class	Get irreps	
5	P_c3 (No. 143.3)	$\begin{pmatrix} 2 & -1 & 0 & 1/3 \\ 1 & 1 & 0 & -1/3 \\ 0 & 0 & 2 & 0 \end{pmatrix}$	24=6x4	Conjugacy Class	Get irreps	
6	C_c2/c (No. 15.90)	$\begin{pmatrix} 2 & 0 & 0 & 0 \\ 1 & 3 & 0 & -1/2 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	18=6x3	Conjugacy Class	Get irreps	
7	C_c2/m (No. 12.63)	$\begin{pmatrix} 2 & 0 & 0 & 0 \\ 1 & 3 & 0 & -1/2 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	18=6x3	Conjugacy Class	Get irreps	
8	C_cc (No. 9.40)	$\begin{pmatrix} 2 & 0 & 0 & 1/5 \\ 1 & 3 & 0 & -2/5 \\ 0 & 0 & 2 & 0 \end{pmatrix}$	36=6x6	Conjugacy Class	Get irreps	

k-SUBGROUPSMAG (Example $Ba_3Nb_2NiO_9$ Ni at WP 1b)

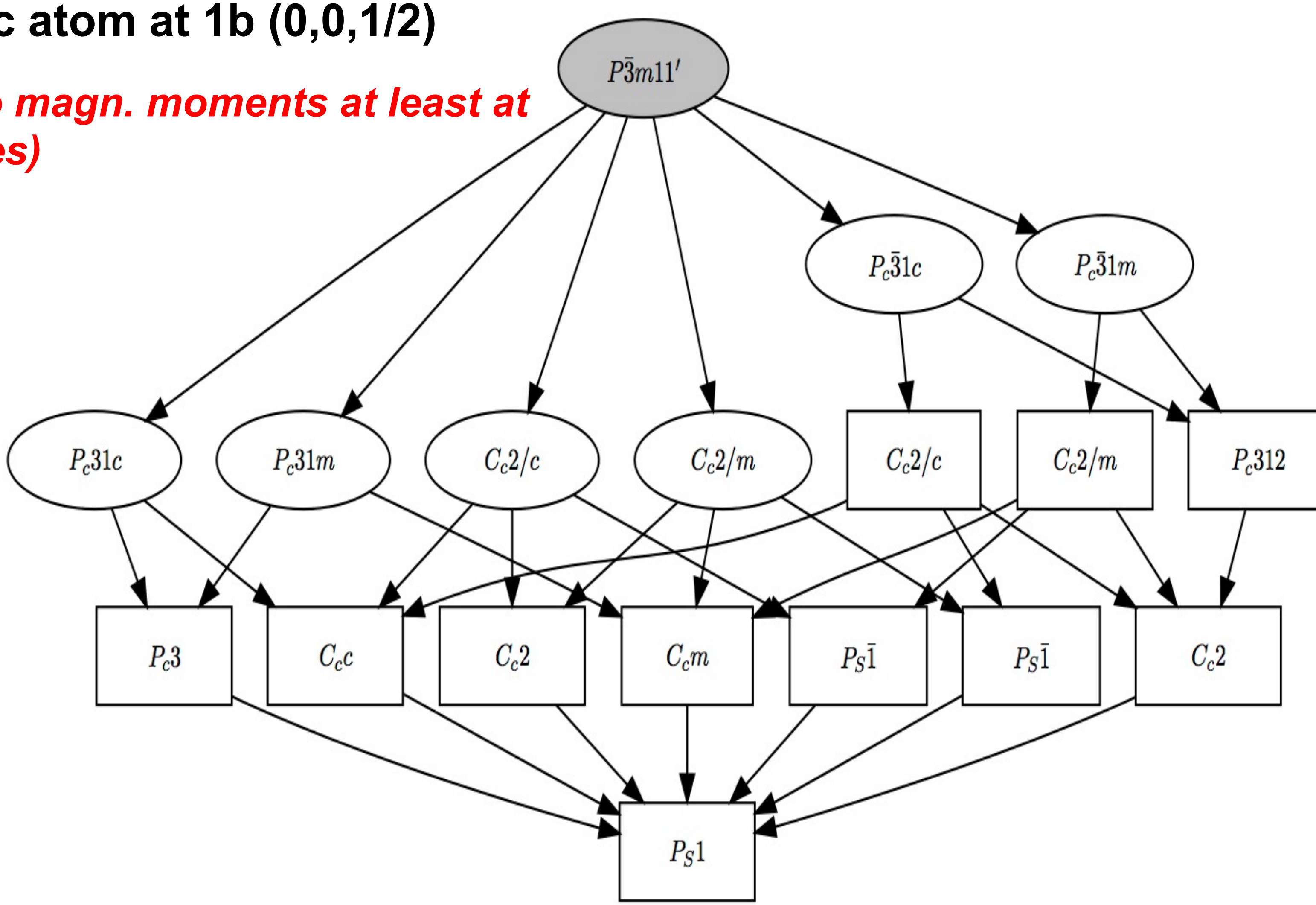
Possible magnetic symmetries for a magnetic phase with parent space group P-3m1, propagation vector (1/3,1/3,1/2) and magnetic atom at 1b (0,0,1/2) ***(non-zero magn. moments at all sites!)***



k-SUBGROUPSMAG (Example $Ba_3Nb_2NiO_9$ Ni at WP 1b)

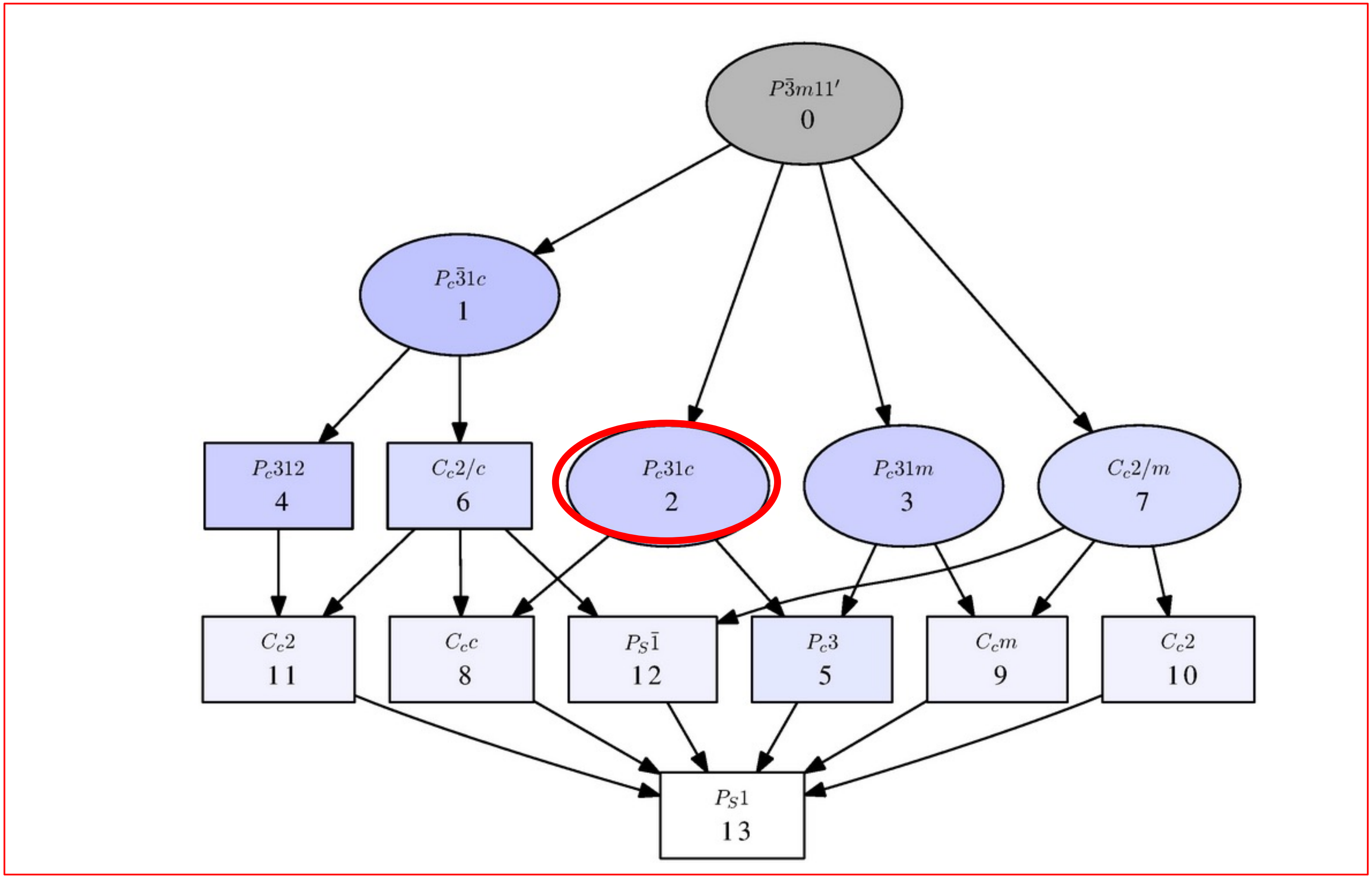
Possible magnetic symmetries for a magnetic phase with parent space group P-3m1, propagation vector (1/3,1/3,1/2) and magnetic atom at 1b (0,0,1/2)

(non-zero magn. moments at least at some sites)



k-SUBGROUPSMAG (Example $Ba_3Nb_2NiO_9$ Ni at WP 1b)

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) *(non-zero magn. moments at all sites!)*



k-SUBGROUPSMAG

Example: $Ba_3Nb_2NiO_9$
MAGNDATA #1.13

Possible MAXIMAL 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) allowing zon-zero moments on all 1b sites

N	Group (BNS)	Transformation matrix	General positions	Properties	Magnetic structure
1	P_c-31c (#163.84) Go to a subgroup	$\begin{pmatrix} 2 & -1 & 0 & 1 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$ Alternatives (domain-related)	Show	*Systematic absences* MAGNEXT *Tensor properties* MTENSOR	Show
2	P_c31c (#159.64) Go to a subgroup	$\begin{pmatrix} 2 & -1 & 0 & 7/3 \\ 1 & 1 & 0 & 8/3 \\ 0 & 0 & 2 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	*Systematic absences* MAGNEXT *Tensor properties* MTENSOR	Show
3	P_c31m (#157.56) Go to a subgroup	$\begin{pmatrix} 2 & -1 & 0 & 7/3 \\ 1 & 1 & 0 & 8/3 \\ 0 & 0 & 2 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	*Systematic absences* MAGNEXT *Tensor properties* MTENSOR	Show
4	C_c2/m (#12.63) Go to a subgroup	$\begin{pmatrix} 2 & 0 & 0 & 0 \\ 1 & 3 & 0 & 5/2 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$ Alternatives (domain-related)	Show	*Systematic absences* MAGNEXT *Tensor properties* MTENSOR	Show

mCIFs of the transformed structure in the selected subgroups ('ksubgroupsmag_mCIFs_1473394.zip')

k-SUBGROUPSMAG

Example: Ba3Nb2NiO9
MAGNDATA #1.13

Selected magnetic space group: 2- P_c31c (#159.64)

Setting parent-like (**3a, 3b, 2c** ; 0, 0, 0)

Parent space group P-3m1 (No. 164)

Lattice parameters: a=17.26500, b=17.26500, c=14.13120, alpha=90.00, beta=90.00, gamma=120.00

[Go to setting standard (**2a+b, -a+b, 2c** ; 7/3, 8/3, 0)]
[Go to an alternative setting]

Export data to MCIF file/Visualize | Go to a subgroup

Atomic positions, Wyckoff positions and Magnetic Moments

2	Ba2 Ba 0.00000 0.00000 0.00000	(0,0,0 | $2m_y,m_y,m_z$) (0,0,1/2 | $-2m_y,-m_y,-m_z$) (0,1/3,0 | $-m_y,-2m_y,m_z$) (0,1/3,1/2 | $m_y,2m_y,-m_z$) (0,2/3,0 | $-m_y,m_y,m_z$) (0,2/3,1/2 | $m_y,-m_y,-m_z$) (1/3,0,0 | $-m_y,-2m_y,m_z$) (1/3,0,1/2 | $m_y,2m_y,-m_z$) (1/3,1/3,0 | $-m_y,m_y,m_z$) (1/3,1/3,1/2 | $m_y,-m_y,-m_z$) (1/3,2/3,0 | $2m_y,m_y,m_z$) (1/3,2/3,1/2 | $-2m_y,-m_y,-m_z$) (2/3,0,0 | $-m_y,m_y,m_z$) (2/3,0,1/2 | $m_y,-m_y,-m_z$) (2/3,1/3,0 | $2m_y,m_y,m_z$) (2/3,1/3,1/2 | $-2m_y,-m_y,-m_z$) (2/3,2/3,0 | $-m_y,-2m_y,m_z$) (2/3,2/3,1/2 | $m_y,2m_y,-m_z$)	18	-	-
3	Ni1 Ni 0.00000 0.00000 0.25000	(0,0,1/4 | $2m_y,m_y,m_z$) (0,0,3/4 | $-2m_y,-m_y,-m_z$) (0,1/3,1/4 | $-m_y,-2m_y,m_z$) (0,1/3,3/4 | $m_y,2m_y,-m_z$) (0,2/3,1/4 | $-m_y,m_y,m_z$) (0,2/3,3/4 | $m_y,-m_y,-m_z$) (1/3,0,1/4 | $-m_y,-2m_y,m_z$) (1/3,0,3/4 | $m_y,2m_y,-m_z$) (1/3,1/3,1/4 | $-m_y,m_y,m_z$) (1/3,1/3,3/4 | $m_y,-m_y,-m_z$) (1/3,2/3,1/4 | $2m_y,m_y,m_z$) (1/3,2/3,3/4 | $-2m_y,-m_y,-m_z$) (2/3,0,1/4 | $-m_y,m_y,m_z$) (2/3,0,3/4 | $m_y,-m_y,-m_z$) (2/3,1/3,1/4 | $2m_y,m_y,m_z$) (2/3,1/3,3/4 | $-2m_y,-m_y,-m_z$) (2/3,2/3,1/4 | $-m_y,-2m_y,m_z$) (2/3,2/3,3/4 | $m_y,2m_y,-m_z$)	18	**($2M_y,M_y,M_z$)**	M_y = 0.00000 M_z = 0.00000

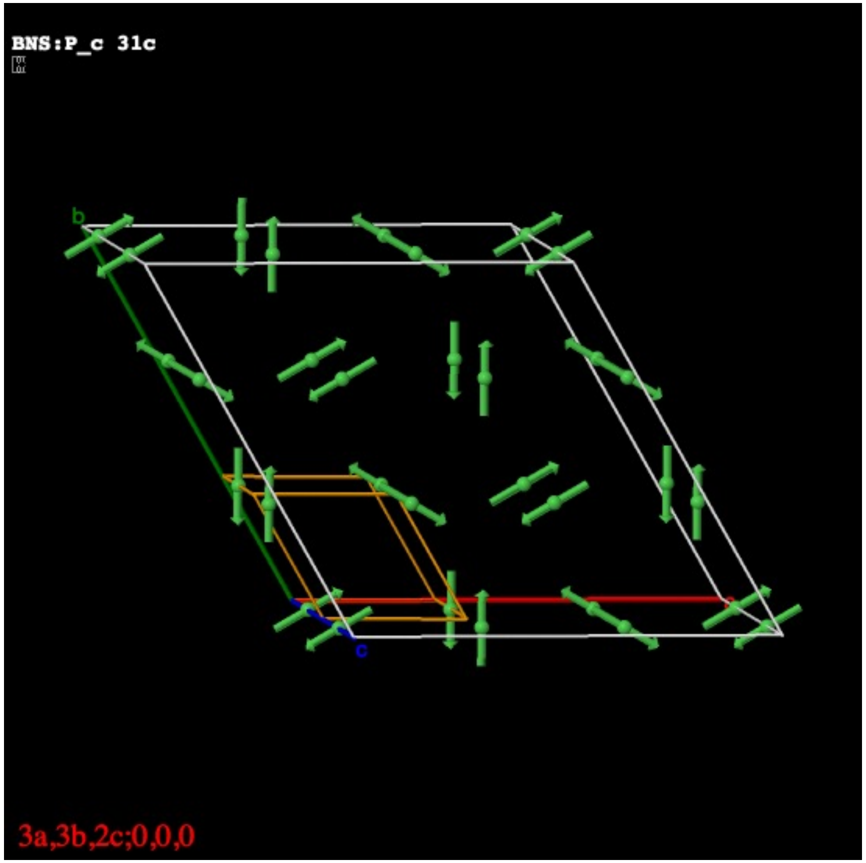
k-SUBGROUPSMAG

Example: Ba3Nb2NiO9 **Parent space group P-3m1**

MAGNDATA #1.13

k= (1/3,1/3,1/2)

site:1b(001/2)



Generates an mCIF with all the information to be used in your refinement program:

it contains for instance:

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

loop_
_space_group_symop_magn_centering.id
_space_group_symop_magn_centering.xyz
1 x,y,z,+1
2 x+1/3,y+2/3,z,+1
3 x+2/3,y+1/3,z,+1
4 x,y,z+1/2,-1
5 x+1/3,y+2/3,z+1/2,-1
6 x+2/3,y+1/3,z+1/2,-1
```

```
_parent_space_group.child_transform_Pp_abc  '3a,3b,2c;0,0,0'
_space_group_magn.transform_BNS_Pp_abc  '2/3a+1/3b,-1/3a+1/3b,c;7/9,8/9,0'
```

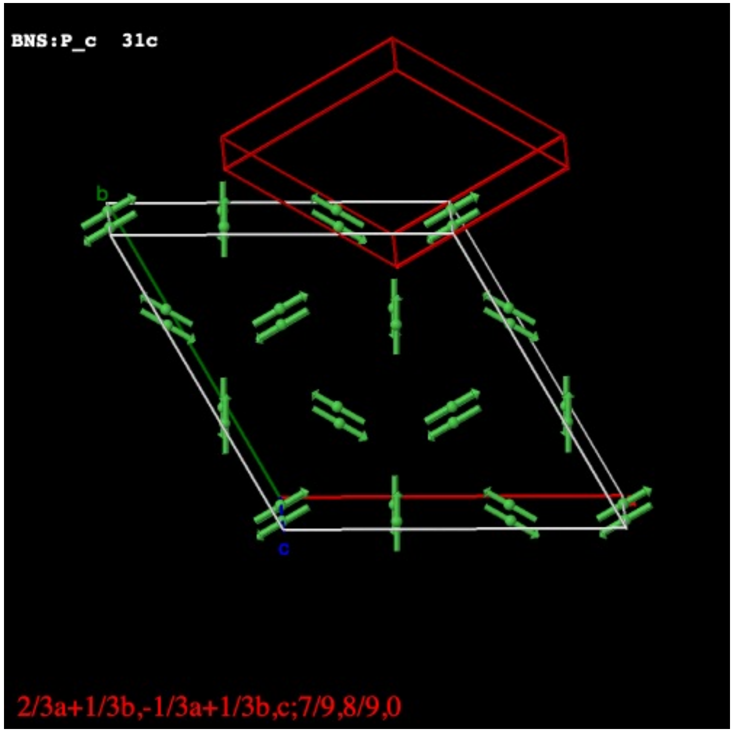
transformation to standard

k-SUBGROUPSMAG

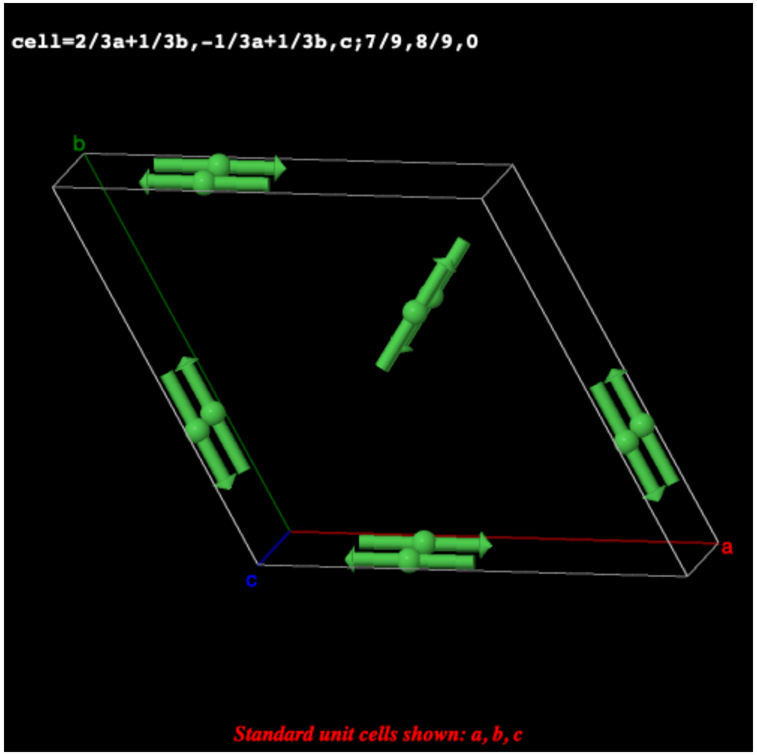
Example: Ba3Nb2NiO9
MAGNDATA #1.13

MSG: P_c31c

```
_parent_space_group.child_transform_Pp_abc  '3a,3b,2c;0,0,0'
_space_group_magn.transform_BNS_Pp_abc  '2/3a+1/3b,-1/3a+1/3b,c;7/9,8/9,0'
```



transformation to standard setting of MSG



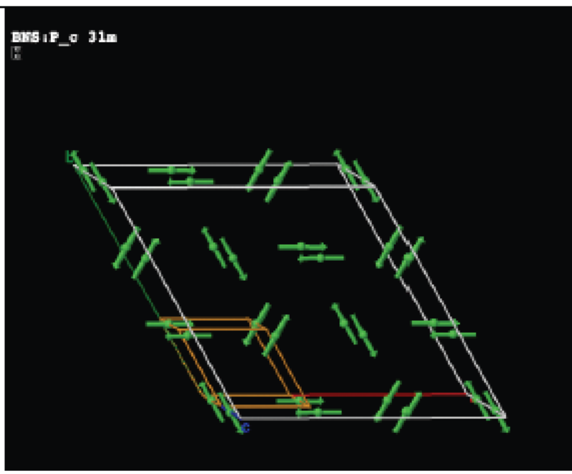
in the new mCIF file with the MSG in standard setting:

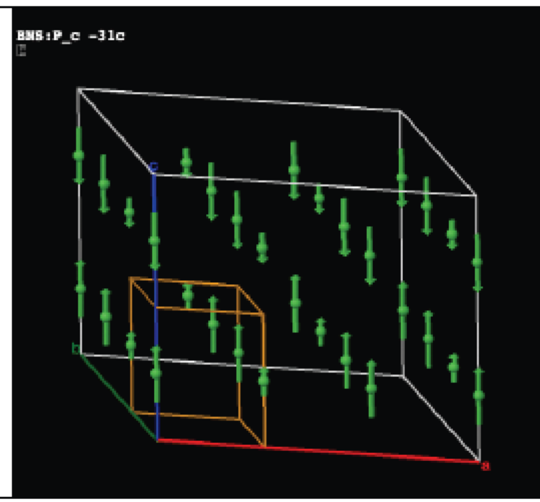
```
_parent_space_group.child_transform_Pp_abc  '2a+b,-a+b,2c;7/3,8/3,0'
_space_group_magn.transform_BNS_Pp_abc  'a,b,c;0,0,0'
```

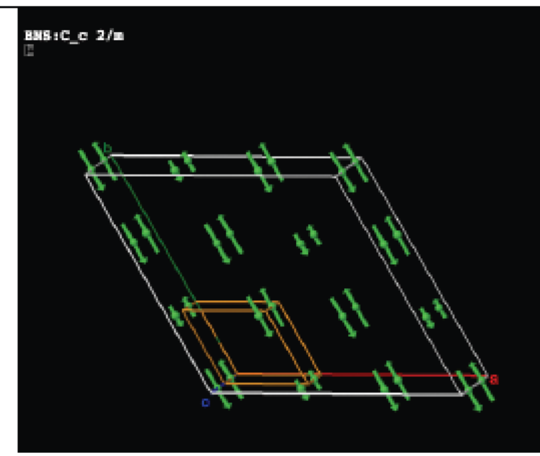
k-SUBGROUPSMAG & MAGMODELIZE

Models for each possible MSG can be constructed and magCIF files can be downloaded to use in other programs (refinement, visualization, etc.)

Some of the possible magnetic structures for parent space group P-3m1 propagation vector (1/3,1/3,1/2) and magnetic atom at 1b (0,0,1/2):







P_c31m	P_c-31c	C_c2/m

(obtained with MVISUALIZE (Jmol))

k-SUBGROUPSMAG

Example: Ba3Nb2NiO9
MAGNDATA #1.13

Possible MAXIMAL 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) allowing zon-zero momento on all 1b sites

N	Group (BNS)	Transformation matrix	General positions	Properties	Magnetic structure
1	P_c-31c (#163.84) Go to a subgroup	$\begin{pmatrix} 2 & -1 & 0 & 1 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$ Alternatives (domain-related)	Show	*Systematic absences* MAGNEXT *Tensor properties* MTENSOR	Show
2	P_c31c (#159.64) Go to a subgroup	$\begin{pmatrix} 2 & -1 & 0 & 7/3 \\ 1 & 1 & 0 & 8/3 \\ 0 & 0 & 2 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	*Systematic absences* MAGNEXT *Tensor properties* MTENSOR	Show
3	P_c31m (#157.56) Go to a subgroup	$\begin{pmatrix} 2 & -1 & 0 & 7/3 \\ 1 & 1 & 0 & 8/3 \\ 0 & 0 & 2 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	*Systematic absences* MAGNEXT *Tensor properties* MTENSOR	Show
4	C_c2/m (#12.63) Go to a subgroup	$\begin{pmatrix} 2 & 0 & 0 & 0 \\ 1 & 3 & 0 & 5/2 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$ Alternatives (domain-related)	Show	*Systematic absences* MAGNEXT *Tensor properties* MTENSOR	Show

mCIFs of the transformed structure in the selected subgroups ('ksubgroupsmag_mCIFs_1473394.zip')

MAGNEXT: Magnetic diffraction systematic absences

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

MAGNEXT: Systematic absences of msgs

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Magnetic symmetry in the Bilbao Crystallographic Server: a computer program to provide systematic absences of magnetic neutron diffraction

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MAGNEXT is a new computer program available from the Bilbao Crystallographic Server (http://www.cryst.ehu.es) that provides symmetry-forced systematic absences or extinction rules of magnetic nonpolarized neutron diffraction. For any chosen Shubnikov magnetic space group, the program lists all systematic absences, and it can also be used to obtain the list of the magnetic space groups compatible with a particular set of observed systematic absences.

MAGNEXT: Magnetic Systematic Absences

tinction rules for
any Shubnikov magnetic

)e obtained introducing the
l for this purpose at the
pted form of the structure

/ a set of generators in any

patible with a set of

or a superspace group

Option A: Systematic absences for a magnetic space group in standard settings

Magnetic Space Group number: Please, enter the label of group or [choose it]

[Standard/Default Setting]

Other interfaces for alternative uses MAGNEXT are:

- **Option B:** For systematic absences for a magnetic space group **in any setting**, click here
- **Option C:** For a list of magnetic space groups **compatible with a given set of systematic absences**, click here
- For systematic absences for ***magnetic superspace groups*** click here

also for incommensurate magnetic structures from the input of its superspace group operations

Systematic Absences of the magnetic space group P_c31c (#159.64) in the setting (3a, 3b, 2c; 0, 0, 0) parent space group *P*-3*m*1 (No. 164)

This systematic extinction does not necessarily means that atomic moments are along c !!!!

Values of h, k, l: **h integer, k integer, l integer**

Warning: h, k, l are referred to the parent-like setting

Systematic absences for general reflections (produced by centrings):

Diffraction vector type: **(h k l)** -> Systematic absence: **l = 2n or h + 2k /= 3n**

Systematic absences for special reflections:

Diffraction vector type: **(0 0 l)** -> Systematic absence: **l any**

`For l = 1 : I = 0 F = (0,0,Fz)`

[Show form of structure factor for every type of reflection]

Symmetry-adapted form of the Structure Factors

Values of h, k, l: **h integer, k integer, l integer**

<u>Warning</u>: h, k, l are referred to the parent-like setting

Structure factors for general reflections (produced by centrings):

Diffraction vector type: **h,k,l**

```
For l = 2n or h + 2k ≠ 3n:      I = 0       F = (0,0,0)
Elsewhere:      I /= 0       F = (Fx,Fy,Fz)
```

Structure factors for special reflections:

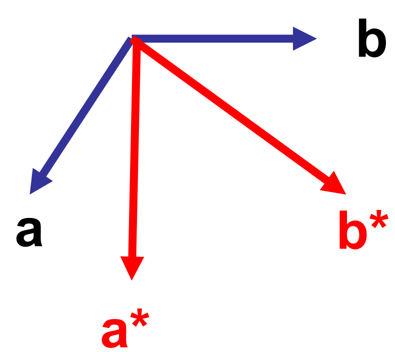
Those diffraction vector types which are fully absent due to the general rule are not listed

Diffraction vector type: **0,0,l**

```
For l = 1:      I = 0       F = (0,0,Fz)
```

Diffraction vector type: **0,k,l**

```
For k = 3, l = 1:      I /= 0       F = (Fx,2*Fx,Fz)
```



Diffraction vector type: **h,-h,l**

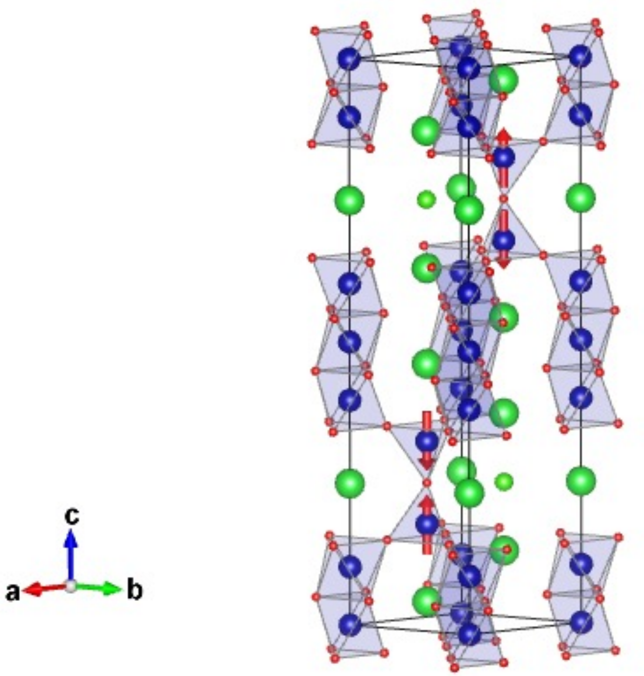
```
For h = 3, l = 1:      I /= 0       F = (Fx,-Fx,Fz)
```

Diffraction vector type: **h,0,l**

```
For h = 3, l = 1:      I /= 0       F = (2*Fy,Fy,Fz)
```

MAGNEXT can be used to discriminate between possible models:

$Ba_5Co_5ClO_{13}$



nuclear/positional reflection condition:

(2h,-h,l) l=2n

(magnetic sites: 2a, 4e, 4f. all $(0,0,m_z)$)

Magnetic diffraction:

Reflection (2, -1, 3) **pure magnetic**

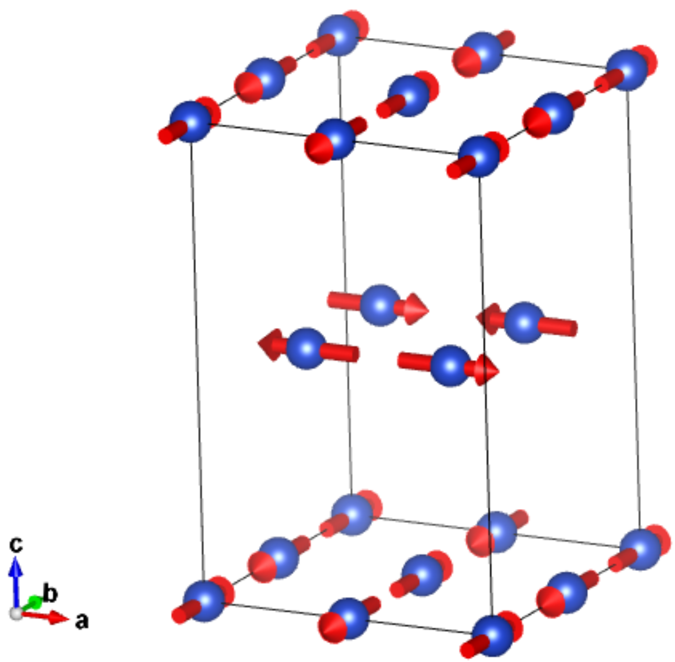
(2h,-h,l)

$P6_3'/m'm'c$ (194.268): absent l even

$P6_3/m'm'c$ (194.270): absent l odd

(spins are symmetry restricted to be along c in both groups)

Modelling multi-k structures with KSUBGROUPSMAG & MAGMODELIZE



Nd_2CuO_4

Parent SG: *I4/mmm*

k1= (1/2,1/2,0)
k2=(-1/2,1/2,0)

Cu Site: *2a (0,0,0)*

(MAGNDATA 2.6)

Tutorial_magnetic_section_BCS_3

Parent SG: *I4/mmm* **k**1= (1/2,1/2,0) Cu Site: *2a (0,0,0)*

k2=(-1/2,1/2,0)

not necessarily all moments non-zero

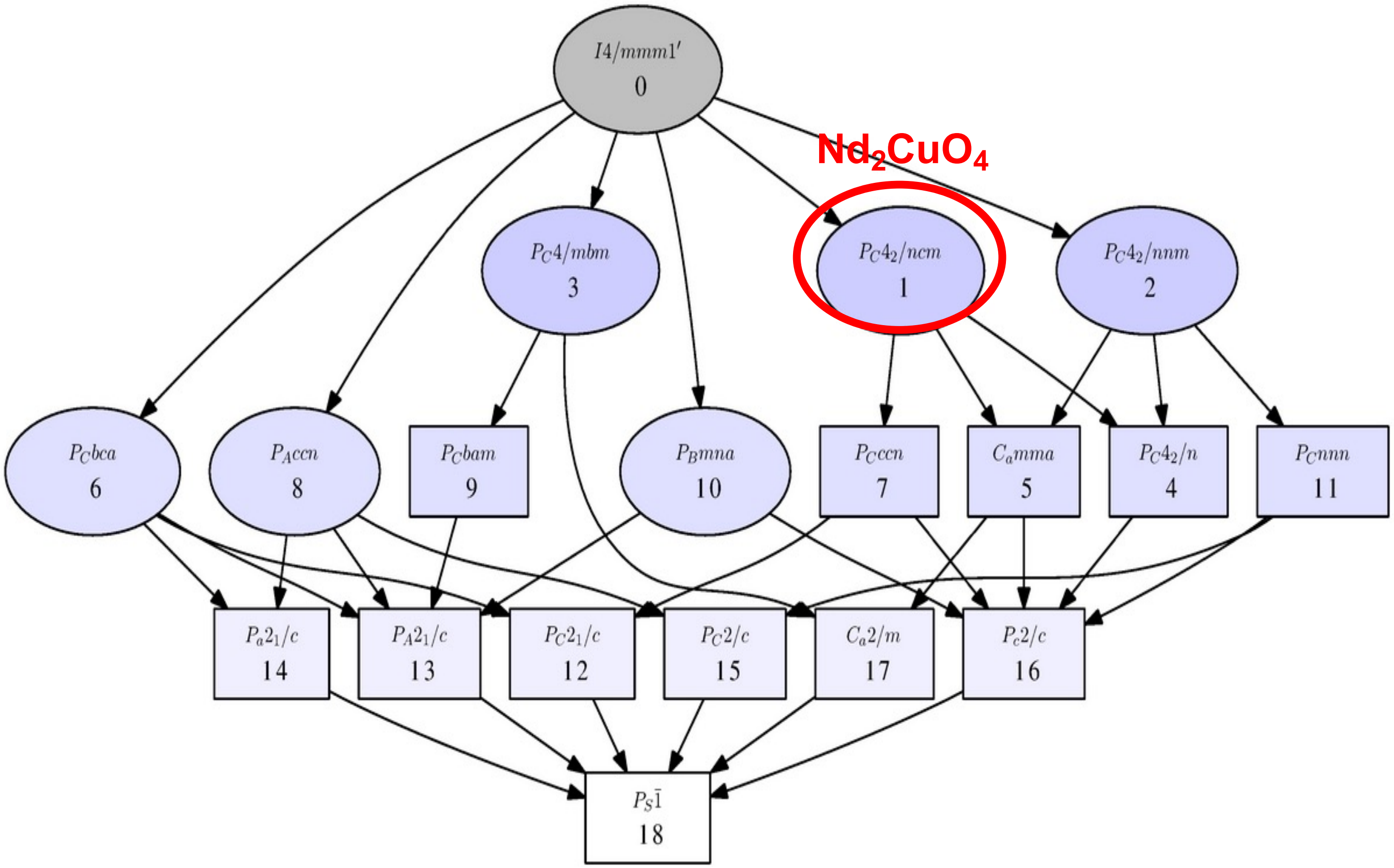
Subgroups of the paramagnetic space group :	*I4/mmm*1' (N. 139)
Lowest magnetic space group to consider:	*P*1 (N. 1.1)
Wyckoff positions occupied by the magnetic atoms	2a:(0,0,0)

List of subgroups which allow a non zero magnetic moment in some sites

Get the subgroup-graph More options

N	Group Symbol	Transformation matrix	Group-Subgroup index	Other members of the Conjugacy Class	irreps	Magnetic structure models (MAGMODELIZE)
1	P_C4_2/ncm (No. 138.529)	$\begin{pmatrix} 1 & -1 & 0 & 1/2 \\ 1 & 1 & 0 & 1/2 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	4=4x1	Conjugacy Class	Get irreps	☐
2	P_C4_2/nnm (No. 134.481)	$\begin{pmatrix} 1 & -1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	4=4x1	Conjugacy Class	Get irreps	☐
3	P_C4/mbm (No. 127.397)	$\begin{pmatrix} 1 & -1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	4=4x1	Conjugacy Class	Get irreps	☐
4	P_C4_2/n (No. 86.73)	$\begin{pmatrix} 1 & -1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	8=4x2	Conjugacy Class	Get irreps	☐
5	C_amma (No. 67.509)	$\begin{pmatrix} 2 & 0 & 0 & 1/2 \\ 0 & 2 & 0 & 1/2 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	8=4x2	Conjugacy Class	Get irreps	☐
6	P_Cbca (No. 61.439)	$\begin{pmatrix} 1 & 1 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	8=4x2	Conjugacy Class	Get irreps	☐
7	P_Cccn (No. 56.375)	$\begin{pmatrix} 1 & -1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	8=4x2	Conjugacy Class	Get irreps	☐
8	P_Accn (No. 56.374)	$\begin{pmatrix} 0 & 1 & -1 & 0 \\ 0 & 1 & 1 & 0 \\ [illegible] \end{pmatrix}$	8=4x2	Conjugacy Class	Get irreps	☐

Possible magnetic symmetries for a magnetic phase with two propagation vectors (1/2,1/2,0) and (-1/2,1/2,0), parent space group I4/mmm and magnetic atom at site 2a.



Parent SG: *I4/mmm* **k**1= (1/2,1/2,0) **k**2=(-1/2,1/2,0) Cu Site: *2a (0,0,0)*

not necessarily all moments non-zero

Subgroups of the paramagnetic space group : *I4/mmm*1' (N. 139)
Lowest magnetic space group to consider: *P*1 (N. 1.1)
Wyckoff positions occupied by the magnetic atoms 2a:(0,0,0)

List of subgroups which allow a non zero magnetic moment in some sites

Get the subgroup-graph More options

N	Group Symbol	Transformation matrix	Group-Subgroup index	Other members of the Conjugacy Class	irreps	Magnetic structure models (MAGMODELIZE)
1	P_C4_2/ncm (No. 138.529)	$\begin{pmatrix} 1 & -1 & 0 & 1/2 \\ 1 & 1 & 0 & 1/2 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	4=4x1	Conjugacy Class	Get irreps	☐
2	P_C4_2/nnm (No. 134.481)	$\begin{pmatrix} 1 & -1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	4=4x1	Conjugacy Class	Get irreps	☐
3	P_C4/mbm (No. 127.397)	$\begin{pmatrix} 1 & -1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	4=4x1	Conjugacy Class	Get irreps	☐
4	P_C4_2/n (No. 86.73)	$\begin{pmatrix} 1 & -1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	8=4x2	Conjugacy Class	Get irreps	☐
5	C_amma (No. 67.509)	$\begin{pmatrix} 2 & 0 & 0 & 1/2 \\ 0 & 2 & 0 & 1/2 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	8=4x2	Conjugacy Class	Get irreps	☐
6	P_Cbca (No. 61.439)	$\begin{pmatrix} 1 & 1 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	8=4x2	Conjugacy Class	Get irreps	☐
7	P_Cccn (No. 56.375)	$\begin{pmatrix} 1 & -1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	8=4x2	Conjugacy Class	Get irreps	☐
8	P_Accn (No. 56.374)	$\begin{pmatrix} 0 & 1 & -1 & 0 \\ 0 & 1 & 1 & 0 \end{pmatrix}$	8=4x2	Conjugacy Class	Get irreps	☐

The MSG symmetry is the result of a magnetic ordering according to a single irrep of the gray parent group
Landau condition fulfilled.

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

Input data

Group→subgroup	Transformation matrix
*I*4/*mmm*1' (N. 139.532)→P_C4_2/ncm (N. 138.529)	$\begin{pmatrix} 1 & -1 & 0 & 1/2 \\ 1 & 1 & 0 & 1/2 \\ 0 & 0 & 1 & 0 \end{pmatrix}$

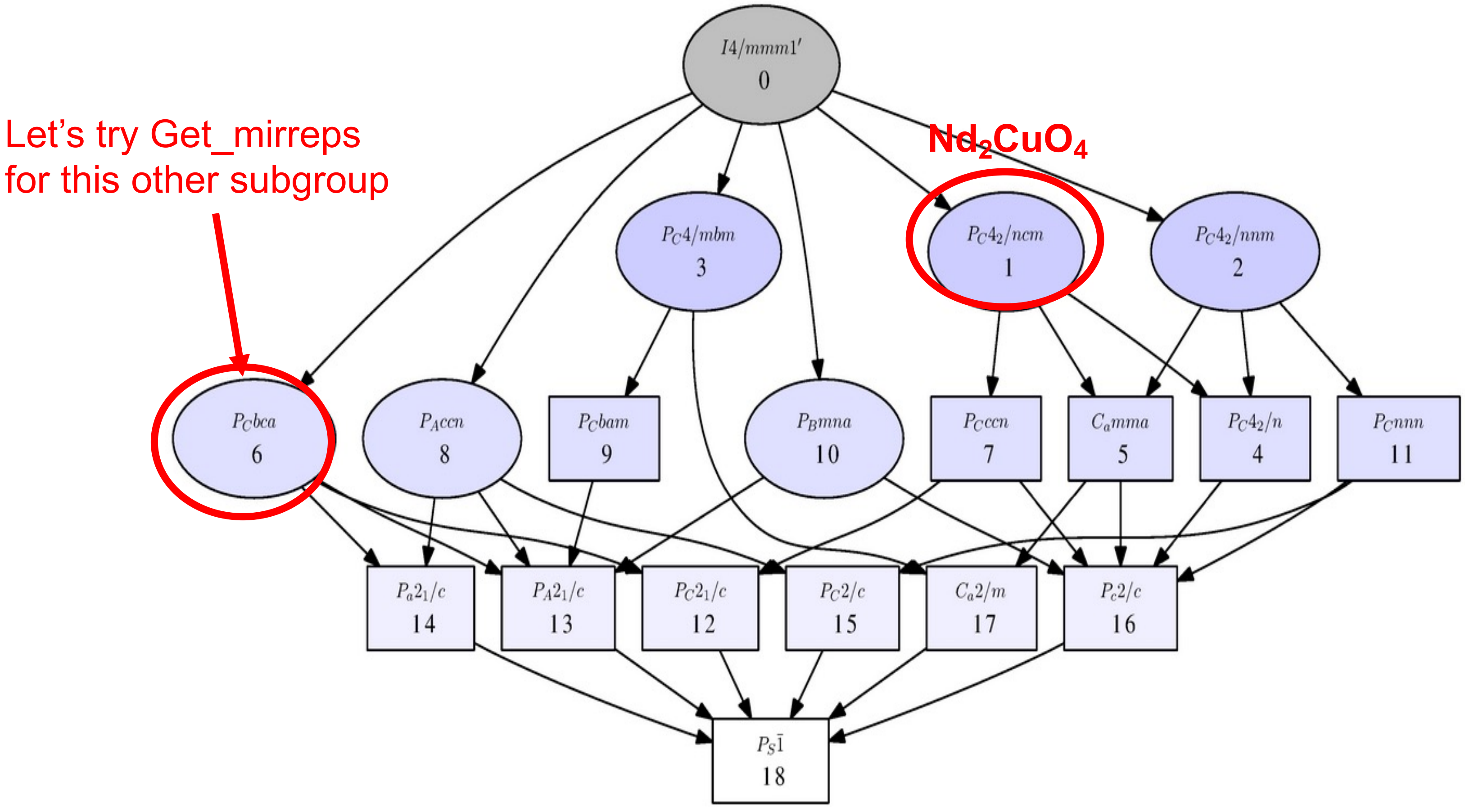
Output of Get_mirrreps for this subgroup

Representations and order parameters

Show the graph of isotropy subgroups

k-vectors	irreps and order parameters	isotropy subgroup transformation matrix	link to the irreps
GM: **(0,0,0)**	GM_1^+: (a)	*I*4/*mmm*1' (No. 139.532) a,b,c;0,0,0	matrices of the irreps
X: **(1/2,1/2,0)(1/2,1/2,1)**	mX_3^+: (a,-a)	P_C4_2/ncm (No. 138.529) a+b,-a+b,c;1/2,1/2,0	matrices of the irreps
M: **(1,1,1)**	M_2^+: (a)	$P4_2/mmc1'$ (No. 131.436) a,b,c;0,1/2,0	matrices of the irreps

Possible magnetic symmetries for a magnetic phase with two propagation vectors (1/2,1/2,0) and (-1/2,1/2,0), parent space group I4/mmm and magnetic atom at site 2a.



The MSG symmetry is NOT the result of a magnetic ordering according to a single irrep of the gray parent group

Landau condition NOT fulfilled.

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

Input data

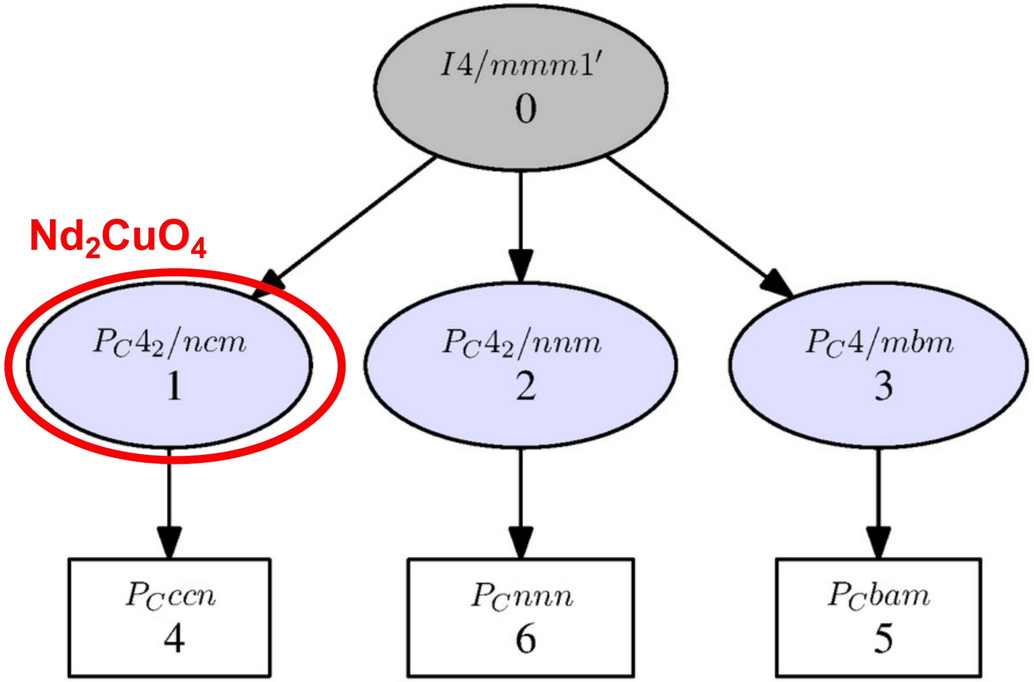
Group→subgroup	Transformation matrix
*I4/mmm*1' (N. 139.532)→$P_C bca$ (N. 61.439)	$\begin{pmatrix} 1 & 1 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$

Representations and order parameters

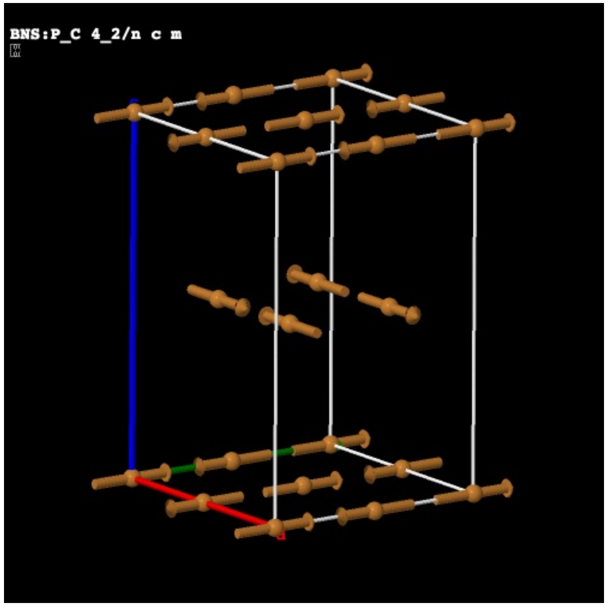
Show the graph of isotropy subgroups

k-vectors	irreps and order parameters	isotropy subgroup transformation matrix	link to the irreps
GM: **(0,0,0)**	GM_1^+: (a)	*I4/mmm*1' (No. 139.532) a,b,c;0,0,0	matrices of the irreps
	GM_4^+: (a)	*Fmmm*1' (No. 69.522) a+b,-a+b,c;0,0,0	
X: **(1/2,1/2,0)(1/2,1/2,1)**	mX_2^+: (a,0)	$C_A mca$ (No. 64.480) c,-a+b,-a-b;0,0,0	matrices of the irreps
	mX_3^+: (0,a)	$C_A mca$ (No. 64.480) a+b,-c,-a+b;0,0,0	
M: **(1,1,1)**	M_5^+: (0,a)	*Cmca*1' (No. 64.470) a-b,a+b,c;0,0,0	matrices of the irreps

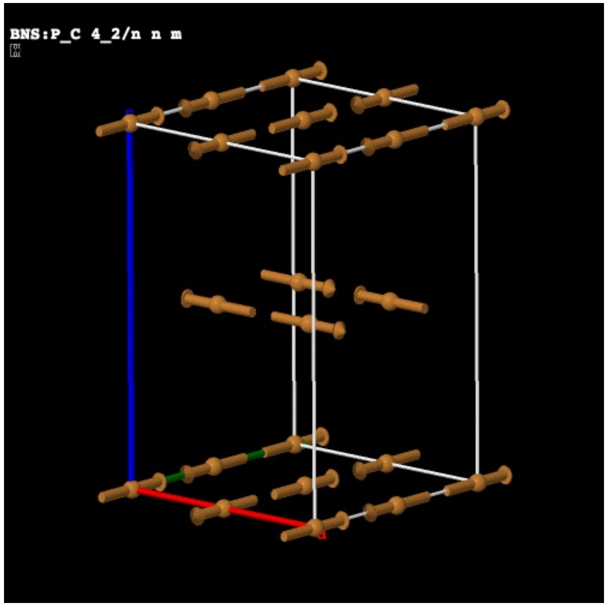
Possible magnetic symmetries for a magnetic phase with two propagation vectors (1/2,1/2,0) and (-1/2,1/2,0), parent space group I4/mmm and magnetic atom at site 2[a], and a single primary irrep active (Landau condition)



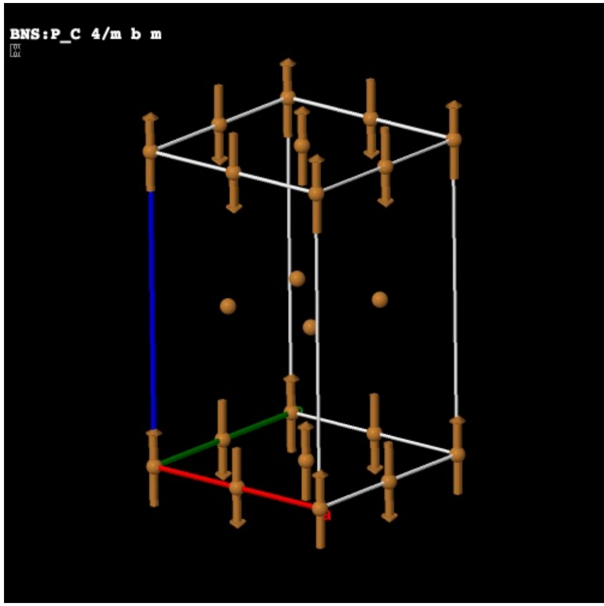
Scheme of the three possible 2k magnetic structures of maximal symmetry with propagation vectors (1/2,1/2,0) and (-1/2,1/2,0), parent space Igroup I4/mmm, magnetic atom at site 2a, and a single primary irrep active.



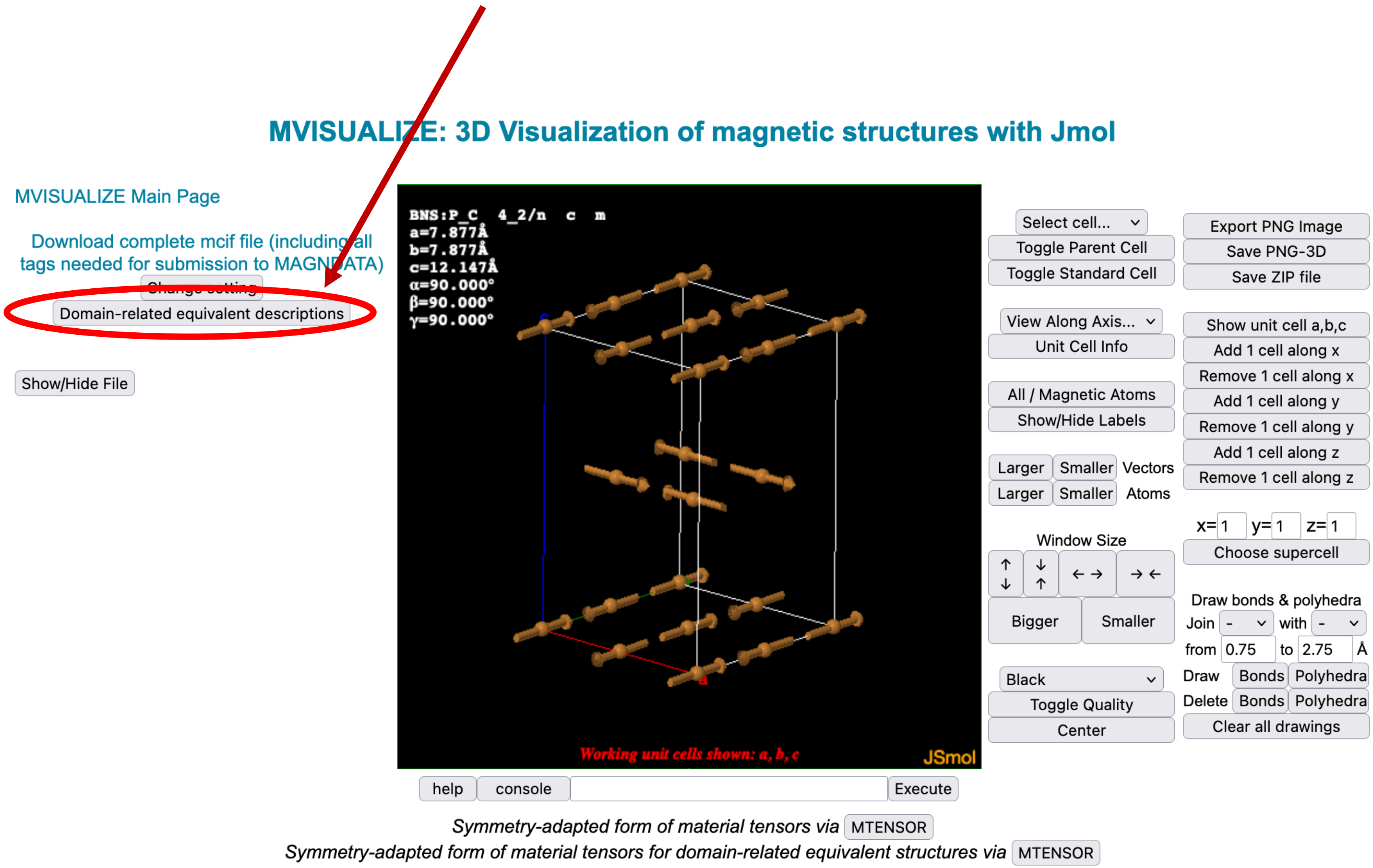
P_C4_2/ncm
(a+b,-a+b,c; ½, ½, 0)



P_C4_2/nnm
(a+b,-a+b,c; 0, 0, 0)

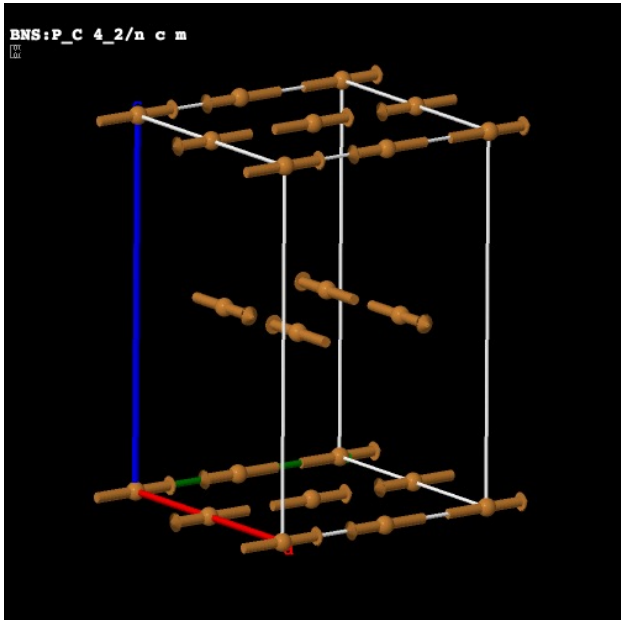


P_C4_2/mbm
(a+b,-a+b,c; 0, 0, 0)


MVISUALIZE: 3D Visualization of magnetic structures with Jmol
MVISUALIZE Main Page
Download complete mcif file (including all tags needed for submission to MAGNDATA)
Change setting
Domain-related equivalent descriptions
Show/Hide File
BNS:P_C 4_2/n c m
a=7.877Å
b=7.877Å
c=12.147Å
α=90.000°
β=90.000°
γ=90.000°
Working unit cells shown: a, b, c
JSmol
help
console
Execute
Select cell...
Toggle Parent Cell
Toggle Standard Cell
View Along Axis...
Unit Cell Info
All / Magnetic Atoms
Show/Hide Labels
Larger Smaller Vectors
Larger Smaller Atoms
Window Size
Bigger
Smaller
Black
Toggle Quality
Center
Export PNG Image
Save PNG-3D
Save ZIP file
Show unit cell a,b,c
Add 1 cell along x
Remove 1 cell along x
Add 1 cell along y
Remove 1 cell along y
Add 1 cell along z
Remove 1 cell along z
x=1 y=1 z=1
Choose supercell
Draw bonds & polyhedra
Join - with -
from 0.75 to 2.75 Å
Draw Bonds Polyhedra
Delete Bonds Polyhedra
Clear all drawings
Symmetry-adapted form of material tensors via MTENSOR
Symmetry-adapted form of material tensors for domain-related equivalent structures via MTENSOR

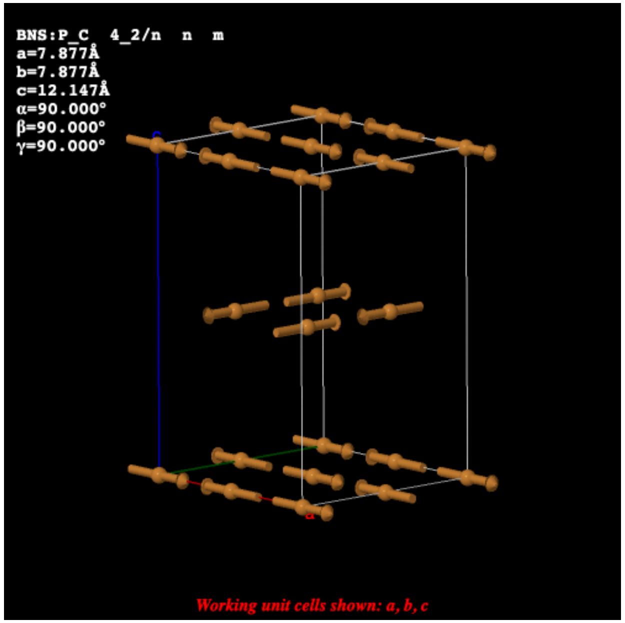
Domain-related equivalent structures

N	Coset representatives (x,y,z) form	Coset representatives Seitz notation	Transformation matrix	Magnetic Structure
1	x,y,z,+1	{ 1 | 0 }	$\begin{pmatrix} 1 & -1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	Show
2	x+3/2,y+1/2,z+1/2,+1	{ 1 | 3/2 1/2 1/2 }	$\begin{pmatrix} 1 & -1 & 0 & 3/2 \\ 1 & 1 & 0 & 1/2 \\ 0 & 0 & 1 & 1/2 \end{pmatrix}$	Show



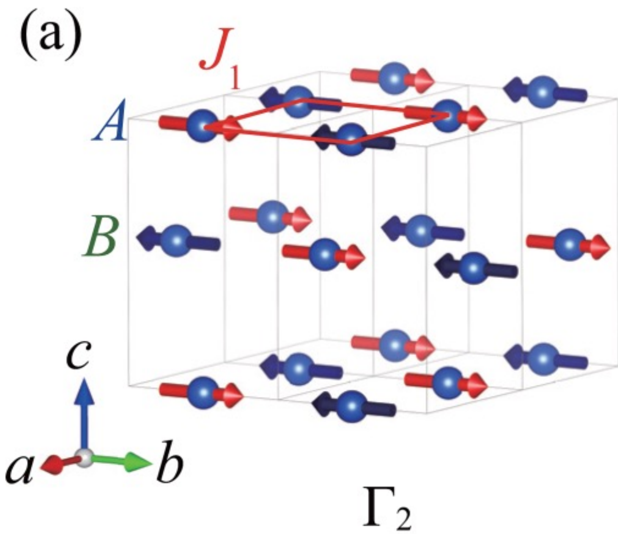
P_C4_2/ncm
(a+b,-a+b,c; ½, ½, 0)

{1| ½ ½ ½ }



P_C4_2/ncm
(a+b,-a+b,c; ½, ½, ½)

The confusion between EQUIVALENT (domain-related) magnetic structures and DIFFERENT models fitting equally the diffraction data

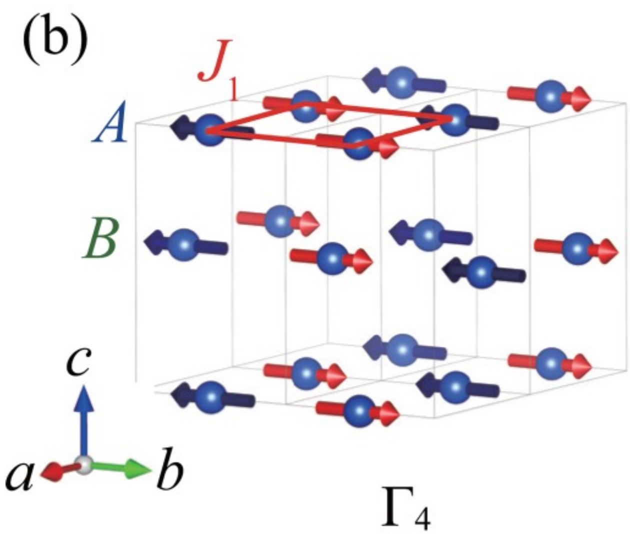


$SrLaCuSbO_6$ (MAGNDATA #1.674)

Phys. Rev. B (2022) **k**=(½ ½ 0)

These two arrangements are reported to fit equally well the data....They are claimed to correspond to two different irreps and represent two different alternative models…

BUT in fact: … they are the SAME magnetic structure!



They are related by some of the lost symmetry operations. They represent the two forms that the same magnetic ordering can be realized in the parent structure, forming twin domains

The two irreps are complex conjugate: they cannot yield different REAL magnetic arrangements! They form a SINGLE PHYSICALLY irreducible representation

Consequences of symmetry

From Neumann's principle:

- all variables/parameters/degrees of freedom compatible with the symmetry will be present (their magnitude may be small or large, but they are not forced to be zero).

- Tensor crystal properties are constrained by the (magnetic) point group symmetry of the crystal.

- Reversely: any tensor property allowed by the (magnetic) point group symmetry can exist (large or small, but it is not forced to be zero)

Magnetic point group symmetry assumes a non-zero SOC, and therefore it necessarily includes all possible SOC effects, independently of their magnitude.

MPGs do NOT introduce constraints that can be broken by spin-orbit (SOC) effects

MTENSOR: Symmetry-adapted form of crystal tensors properties of magnetic crystals

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

MTENSOR: Tensor calculation for Magnetic Point Groups

For the symmetry-adapted form of non-magnetic crystal tensors see TENSOR

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Magnetic Point or Space Group number: [choose it]

Please, choose a tensor by one of these ways:

◉ **Choose a tensor from the lists**

☐ Show symmetry-adapted tensors for all the magnetic point groups in standard setting
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○ **Build your own tensor**

- Introduce Jahn's symbol without superscripts. Examples: (1) [[V2][V2]], (2) a{V2}*, (3) (V2[V2])*

Detailed information in. Gallego et al., Acta Cryst. A (2019) 75, 438-447.
and tutorial: Tutorial_magnetic_section_BCS_1.pdf

MTENSOR: Symmetry-adapted form of crystal tensors properties of magnetic crystals

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
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122 Magnetic Point Groups

from MPOINT

Magnetic Point Group Tables

(Labels are presented in UNI notation - to see them in the Hermann-Mauguin notation click here)

ll et al.

Choose a magnetic point group from the next table

1.1.1	1.1	1.2.2	1.1'	2.1.3	-1.1	2.2.4	-1.1'	2.3.5	-1'	3.1.6	2.1	3.2.7	2.1'	3.3.8	2'
4.1.9	m.1	4.2.10	m.1'	4.3.11	m'	5.1.12	2/m.1	5.2.13	2/m.1'	5.3.14	2'/m	5.4.15	2/m'	5.5.16	2'/m'
6.1.17	222.1	6.2.18	222.1'	6.3.19	2'2'2	7.1.20	mm2.1	7.2.21	mm2.1'	7.3.22	m'm2'	7.4.23	m'm'2	8.1.24	mmm.1
8.2.25	mmm.1'	8.3.26	m'mm	8.4.27	m'm'm	8.5.28	m'm'm'	9.1.29	4.1	9.2.30	4.1'	9.3.31	4'	10.1.32	-4.1
10.2.33	-4.1'	10.3.34	-4'	11.1.35	4/m.1	11.2.36	4/m.1'	11.3.37	4'/m	11.4.38	4/m'	11.5.39	4'/m'	12.1.40	422.1
12.2.41	422.1'	12.3.42	4'22'	12.4.43	42'2'	13.1.44	4mm.1	13.2.45	4mm.1'	13.3.46	4'm'm	13.4.47	4m'm'	14.1.48	-42m.1
14.2.49	-42m.1'	14.3.50	-4'2'm	14.4.51	-4'2m'	14.5.52	-42'm'	15.1.53	4/mmm.1	15.2.54	4/mmm.1'	15.3.55	4/m'mm	15.4.56	4'/mm'm
15.5.57	4'/m'm'm	15.6.58	4/mm'm'	15.7.59	4/m'm'm'	16.1.60	3.1	16.2.61	3.1'	17.1.62	-3.1	17.2.63	-3.1'	17.3.64	-3'
18.1.65	32.1	18.2.66	32.1'	18.3.67	32'	19.1.68	3m.1	19.2.69	3m.1'	19.3.70	3m'	20.1.71	-3m.1	20.2.72	-3m.1'
20.3.73	-3'm	20.4.74	-3'm'	20.5.75	-3m'	21.1.76	6.1	21.2.77	6.1'	21.3.78	6'	22.1.79	-6.1	22.2.80	-6.1'
22.3.81	-6'	23.1.82	6/m.1	23.2.83	6/m.1'	23.3.84	6'/m	23.4.85	6/m'	23.5.86	6'/m'	24.1.87	622.1	24.2.88	622.1'
24.3.89	6'22'	24.4.90	62'2'	25.1.91	6mm.1	25.2.92	6mm.1'	25.3.93	6'mm'	25.4.94	6m'm'	26.1.95	-6m2.1	26.2.96	-6m2.1'
26.3.97	-6'm'2	26.4.98	-6'm2'	26.5.99	-6m'2'	27.1.100	6/mmm.1	27.2.101	6/mmm.1'	27.3.102	6/m'mm	27.4.103	6'/mmm'	27.5.104	6'/m'mm'
27.6.105	6/mm'm'	27.7.106	6/m'm'm'	28.1.107	23.1	28.2.108	23.1'	29.1.109	m-3.1	29.2.110	m-3.1'	29.3.111	m'-3'	30.1.112	432.1
30.2.113	432.1'	30.3.114	4'32'	31.1.115	-43m.1	31.2.116	-43m.1'	31.3.117	-4'3m'	32.1.118	m-3m.1	32.2.119	m-3m.1'	32.3.120	m'-3'm
32.4.121	m-3m'	32.5.122	m'-3'm'												

Magnetic Point Group Tables of 42'2' (#12.4.43)

from MPOINT

N	(x,y,z) form	matrix form	Seitz symbol
1	x,y,z, +1 m_x,m_y,m_z	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	{ 1 | 0 }
2	-x,-y,z, +1 $-m_x,-m_y,m_z$	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	{ 2_{001} | 0 }
3	-y,x,z, +1 $-m_y,m_x,m_z$	$\begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	{ 4^+_{001} | 0 }
4	y,-x,z, +1 $m_y,-m_x,m_z$	$\begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	{ 4^-_{001} | 0 }
5	x,-y,-z, -1 $-m_x, m_y, m_z$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}'$	{ $2'_{100}$ | 0 }
6	-x,y,-z, -1 $m_x, -m_y, m_z$	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}'$	{ $2'_{010}$ | 0 }
7	-y,-x,-z, -1 m_y, m_x, m_z	$\begin{pmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}'$	{ $2'_{1-10}$ | 0 }
8	y,x,-z, -1 $-m_y, -m_x, m_z$	$\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}'$	{ $2'_{110}$ | 0 }

Subgroups Table

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Choose a tensor from the lists

Show symmetry-adapted tensors for all the magnetic point groups in standard setting
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OPTICAL TENSORS

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TRANSPORT TENSORS

Build your own tensor

- Introduce Jahn's symbol without superscripts. Examples: (1) [[V2][V2]], (2) a{V2}*, (3) (V2[V2])*

Detailed information in. Gallego et al., Acta Cryst. A (2019) 75, 438-447.
and tutorial: Tutorial_magnetic_section_BCS_1.pdf

	Λ_{ij}		
aeV^2	Isothermal magnetoelectric effect tensor (inverse effect) A^T_{ij}	$M_i=A^T_{ij}D_j$	
	Magnetoelectric tensor (direct effect) α_{ij}	$P_i=\alpha_{ij}H_j$	
	Magnetoelectric tensor (inverse effect) α^T_{ij}	$M_i=\alpha^T_{ij}E_j$	
$[V^2]V$	Acoustoelectricity tensor ρ_{ijk}	$\sigma_{ij}=\rho_{ijk}J_k$	
	Isothermal piezoelectric tensor (inverse effect) e^T_{ijk}	$\sigma_{ij}=-e^T_{ijk}E_k$	
	Piezoelectric tensor (inverse effect) d^T_{ijk}	$\varepsilon_{ij}=d^T_{ijk}E_k$	
$V[V^2]$	Isothermal piezoelectric tensor (direct effect) e_{ijk}	$D_i=e_{ijk}\varepsilon_{jk}$	
	Piezoelectric tensor (direct effect) d_{ijk}	$P_i=d_{ijk}\sigma_{jk}$	
	Second order magnetoelectric tensor (direct effect) α_{ijk}	$P_i=\alpha_{ijk}H_jH_k$	
$a[V^2]V$	Piezotoroidic tensor (inverse effect) γ^T_{ijk}	$\varepsilon_{ij}=\gamma^T_{ijk}S_k$	
$aV[V^2]$	Piezotoroidic tensor (direct effect) γ_{ijk}	$T_i=\gamma_{ijk}\sigma_{jk}$	
$ae[V^2]V$	Isothermal piezomagnetic tensor (inverse effect) e^{mT}_{ijk}	$\sigma_{ij}=-e^{mT}_{ijk}H_k$	
	Piezomagnetic tensor (inverse effect) Λ^T_{ijk}	$\varepsilon_{ij}=\Lambda^T_{ijk}H_k$	
$aeV[V^2]$	Isothermal piezomagnetic tensor (direct effect) e^m_{ijk}	$M_i=e^m_{ijk}\varepsilon_{jk}$	
	Piezomagnetic tensor (direct effect) Λ_{ijk}	$M_i=\Lambda_{ijk}\sigma_{jk}$	
	Second order magnetoelectric tensor (inverse effect) α^T_{ijk}	$M_i=\alpha^T_{ijk}E_jE_k$	
$[[V^2][V^2]]$	Elastic compliance tensor S_{ijkl}	$\varepsilon_{ij}=S_{ijkl}\sigma_{kl}$	
	Elastic stiffness tensor C_{ijkl}	$\sigma_{ij}=C_{ijkl}\varepsilon_{kl}$	
	Viscosity tensor η_{ijkl}	$\sigma_{ij}=\eta_{ijkl}\partial\varepsilon_{kl}/\partial t$	

Jahn Symbols: rank 1 tensors

	V	eV	aV	aeV
R	**R**.T	det(**R**)**R**.T	**R**.T	det(**R**)**R**.T
R'	**R**.T	det(**R**)**R**.T	-**R**.T	-det(**R**)**R**.T

Intrinsic symmetry	Tensor description	Defining equation
V	Electric polarization vector P_i	-
	Electrocaloric effect tensor $p^T{}_i$	$\Delta S=p^T{}_i E_i$
	Electrothermal effect tensor t_i	$E_i=-t_i\Delta T$
	Heat of polarization tensor $t^T{}_i$	$\Delta S=t^T{}_i\Delta P_i$
	Piezoelectric polarization tensor under hydrostatic pressure d_{ijj}	$P_i=-d_{ijj}p$
	Pyroelectric tensor p_i	$\Delta P_i=p_i\Delta T$
eV	Axial toroidal moment A_i	-
aV	Polar Toroidal moment T_i	-
	Pyrotoroidic tensor r_i	$T_i=r_i\Delta T$
	Toroidalcaloric tensor $r^T{}_i$	$\Delta S=r^T{}_i S_i$
aeV	Heat of Magnetization tensor $t^T{}_i$	$\Delta S=t^T{}_i M_i$
	Magnetization vector M_i	-
	Magnetocaloric tensor $q^T{}_i$	$\Delta S=q^T{}_i H_i$
	Magnetothermal effect tensor t_i	$H_i=-t_i\Delta T$
	Pyromagnetic tensor (direct effect) q_i	$M_i=q_i\Delta T$

MTENSOR

Magnetoelectric tensor:

Group 6/m' (#23.4.85)

α^T_{ij}	j=1	j=2	j=3
i=1	α^T_{11}	α^T_{12}	0
i=2	$-\alpha^T_{12}$	α^T_{11}	0
i=3	0	0	α^T_{33}

Number of independent coefficients: 3

Group 622 (#24.1.87)

α^T_{ij}	j=1	j=2	j=3
i=1	α^T_{11}	0	0
i=2	0	α^T_{11}	0
i=3	0	0	α^T_{33}

Number of independent coefficients: 2

Group 62'2' (#24.4.90)

α^T_{ij}	j=1	j=2	j=3
i=1	0	α^T_{12}	0
i=2	$-\alpha^T_{12}$	0	0
i=3	0	0	0

Number of independent coefficients: 1

Group 6mm (#25.1.91)

α^T_{ij}	j=1	j=2	j=3
i=1	0	α^T_{12}	0
i=2	$-\alpha^T_{12}$	0	0
i=3	0	0	0

Number of independent coefficients: 1

Group 6m'm' (#25.4.94)

α^T_{ij}	j=1	j=2	j=3
i=1	α^T_{11}	0	0
i=2	0	α^T_{11}	0
i=3	0	0	α^T_{33}

Number of independent coefficients: 2

Group -6'm'2 (#26.3.97)

α^T_{ij}	j=1	j=2	j=3
i=1	α^T_{11}	0	0
i=2	0	α^T_{11}	0
i=3	0	0	α^T_{33}

Number of independent coefficients: 2

Group -6'm2' (#26.4.98)

α^T_{ij}	j=1	j=2	j=3
i=1	0	α^T_{12}	0
i=2	$-\alpha^T_{12}$	0	0
i=3	0	0	0

Number of independent coefficients: 1

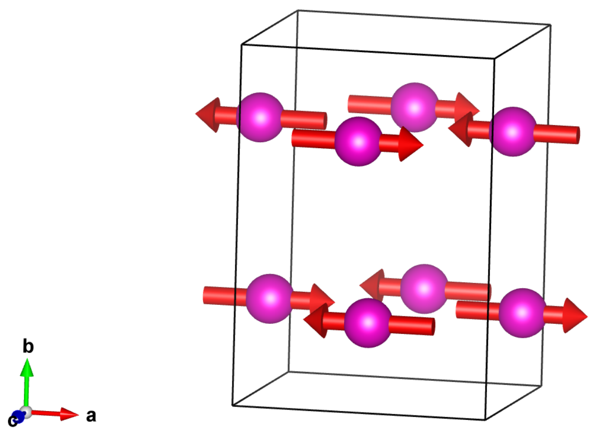
Group 6/m'mm (#27.3.102)

α^T_{ij}	j=1	j=2	j=3
i=1	0	α^T_{12}	0
i=2	$-\alpha^T_{12}$	0	0
i=3	0	0	0

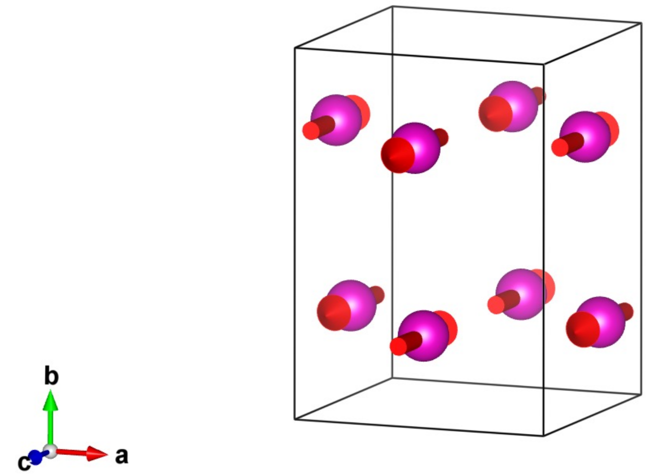
Number of independent coefficients: 1

Consequences of symmetry

$EuZrO_3$: magndata #0.146 & 0.147



Pnm'a



Pn'm'a'

Table of tensor components

α^T_{ij}		j		
		1	2	3
i	1	0	0	α^T_{13}
	2	0	0	0
	3	α^T_{31}	0	0

Number of independent coefficients: 2

Information about the selected tensor

- 2 nd rank Magnetoelectric tensor α^T_{ij} (inverse effect)
- Axial tensor which inverts under time-reversal symmetry operation
- Defining equation: $\mathbf{P_i=\alpha^T_{ij}H_j}$
- Relates Magnetic field **H** with Polarization **P**
- Intrinsic symmetry symbol: **aeV^2**

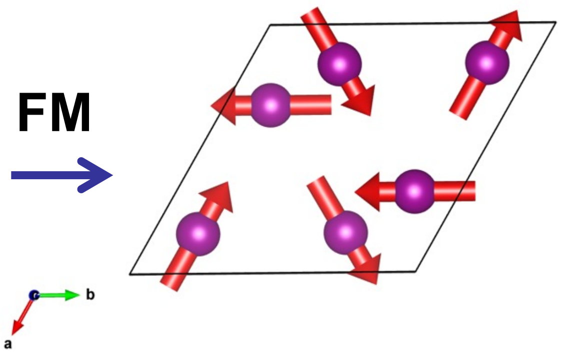
Output of MTENSOR

Table of tensor components

$^T_{ij}$		j		
		1	2	3
	1	α^T_{11}	0	0
	2	0	α^T_{22}	0
	3	0	0	α^T_{33}

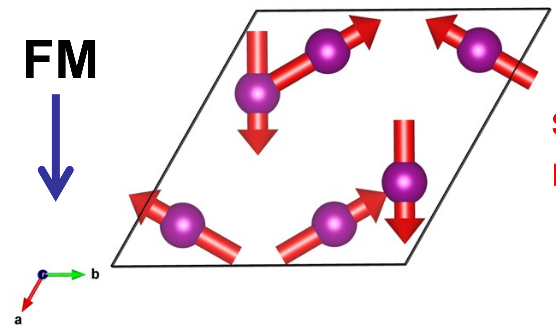
lumber of independent coefficients: 3

Mn_3Sn



MSG: Cmc′m′ **(-b,** 2**a**+**b**,**c;**0,0,0**)**

Magndata #0.199



spins are all rotated 90 degrees

MSG: Cm′cm′ **(-b,** 2**a**+**b**,**c;**0,0,0**)**

Magndata #0.200

Magnetization:

Table of tensor components

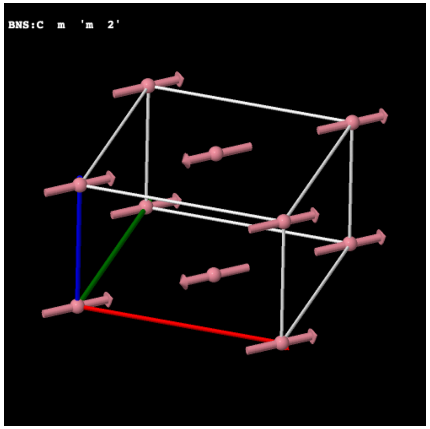
M_i		
i	*1*	M_1
	2	0
	3	0

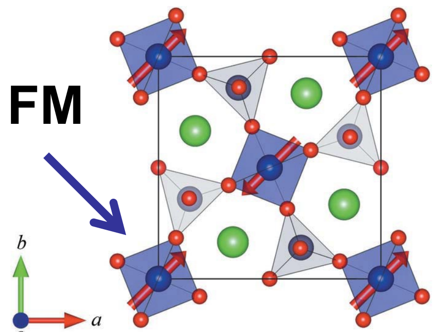
Number of independent coefficients: 1

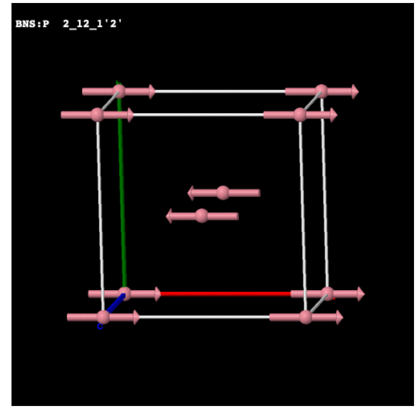
Table of tensor components

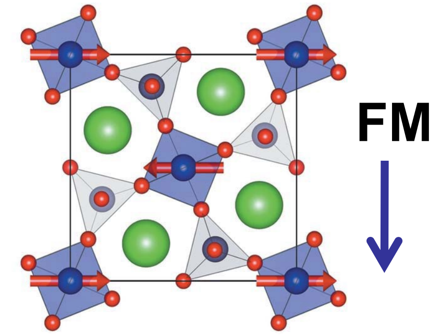
M_i		
i	*1*	0
	2	M_2
	3	0

Number of independent coefficients: 1









Cm'm2' (**a**+**b**,-**a**+**b**,**c**;1/2,0,0)

P2₁2₁'2' (-**b**,**a**,**c**;0,0,0)

Table of tensor components

P_i		
i	*1*	0
	2	0
	3	P_3

Number of independent coefficients: 1

Information about the selected tensor

- 1 st rank Electric polarization vector P_i
- Polar tensor invariant under time-reversal symmetry operation
- Intrinsic symmetry symbol: **V**

non-polar group

P=0

Murakawa et al. PRL (2010):