Modeling of commensurate magnetic structures with the Bilbao crystallographic server

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Symmetry-Based Computational Tools for Magnetic Crystallography

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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).
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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

Symmetry based modeling of magnetic structures

Which MSGs are possible for a magnetic structure having space group Pnma in the paramagnetic phase and a magnetic ordering with propagation vector k=(1/2,0,0)?

$$\text{Pnma.1'} \xrightarrow{k=(1/2,0,0)} \boxed{?}$$

$HoMnO_3$

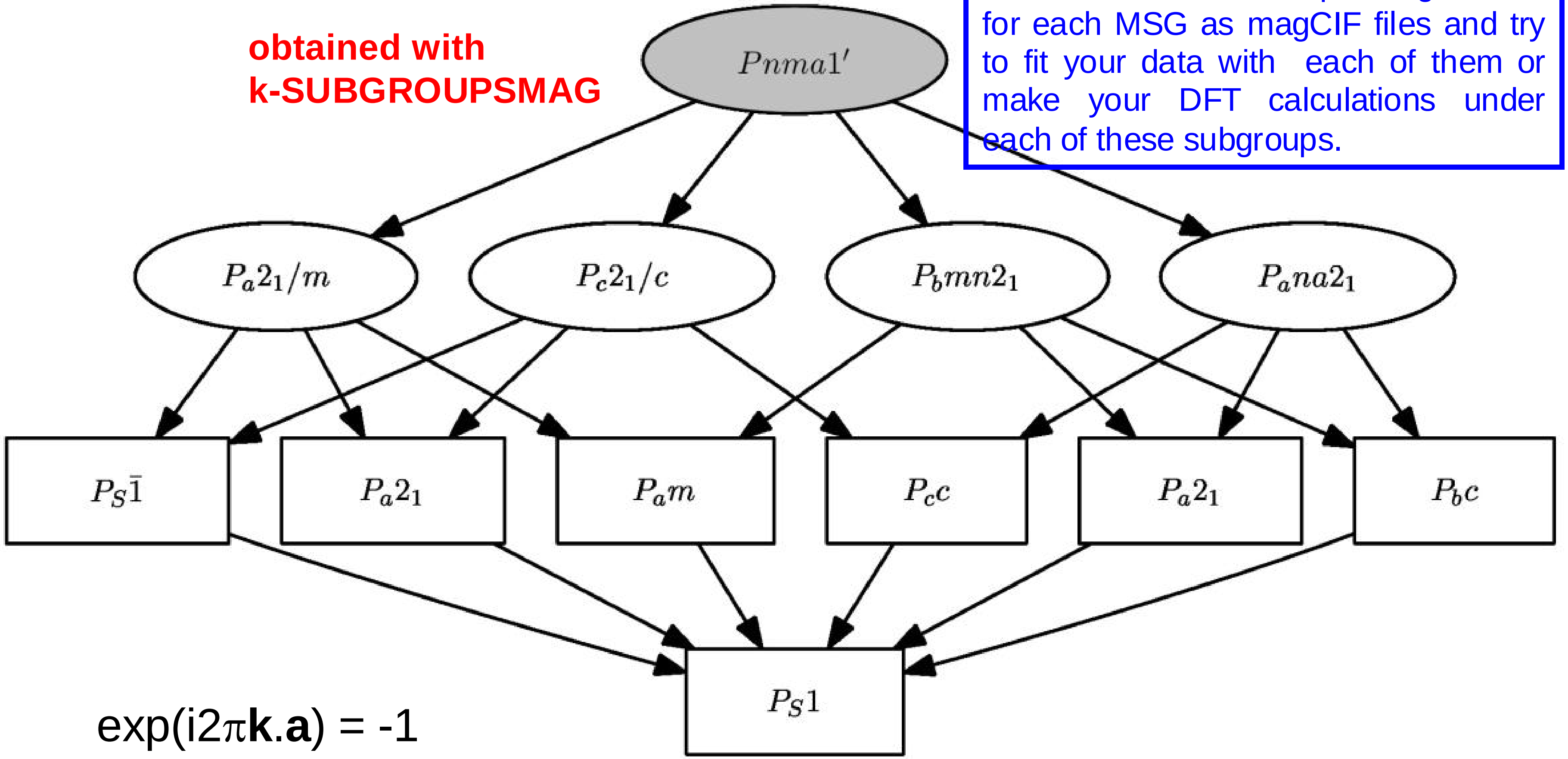
Purely mathematical problem !

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

You can take the corresponding models for each MSG as magCIF files and try to fit your data with each of them or make your DFT calculations under each of these subgroups.

obtained with k-SUBGROUPSMAG



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

Symmetry operation {1'|1/2,0,0} is present in any case

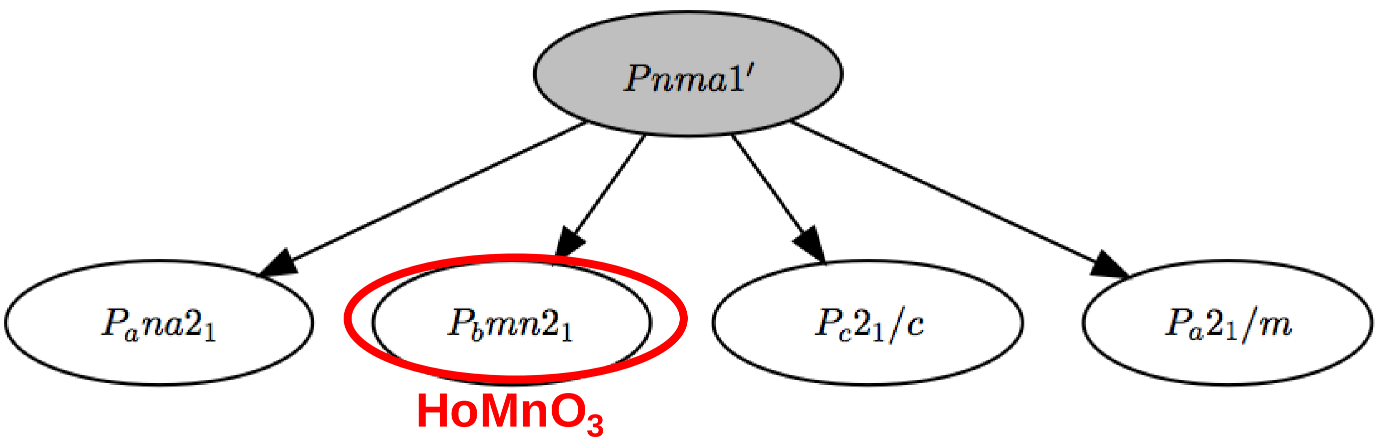
(magnetic cell= $(2\mathbf{a}_p,\mathbf{b}_p,\mathbf{c}_p)$)

Symmetry based modeling in 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

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

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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
$P_{C}nma$ (#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
$P_{C}bca$ (#61.439)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (twin-related)	Show	Show	Show
$P_{A}bcn$ (#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
$P_{B}bcm$ (#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
$P_{A}ccn$ (#56.374)	$\begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}$ Alternatives (twin-related)	Show	Show	Show
$P_{A}bam$ (#55.362)	$\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}$ Alternatives (twin-related)	Show	Show	Show
$P_{A}cca$ (#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
$P_{C}mna$ (#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)

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

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' **→** P_bmn2_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' **→** $\boldsymbol{P_b mn2_1}$ (**-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 <u>with respect to the parent unit cell</u> 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):

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

transformation to standard from the setting used for the MSG.

Alternative unit cell and origin <u>with respect to the unit cell used</u> 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
```

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 (Cmca1')

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

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)

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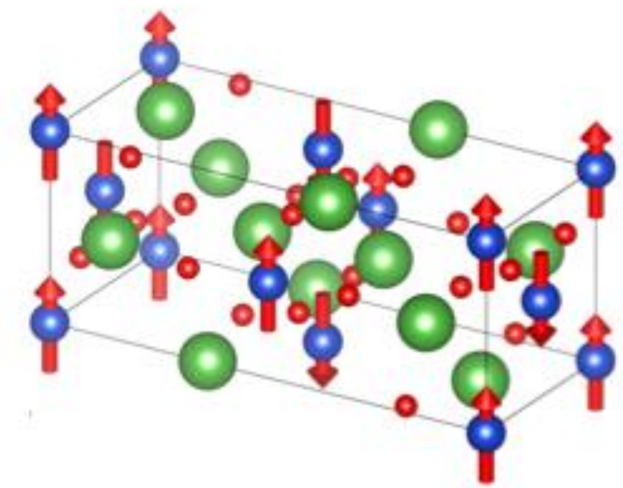
P_Bbcm (#57.390)	$\begin{pmatrix} 0 & 0 & 1 & 1/4 \\ 1 & 0 & 0 & 1/4 \\ 0 & 1 & 0 & 0 \end{pmatrix}$ Alternatives (twin-related)	Show	Show	Show
P_Accn (#56.374)	$\begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}$ Alternatives (twin-related)	Show	Show	Show
P_Abam (#55.362)	$\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}$ 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



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

Tutorial to follow :

Tutorial_MAXMAGN_ HoMnO3

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

k-SUBGROUPSMAG & MAGMODELIZE

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

Tutorial to follow:

Tutorial_magnetic_section_BCS_2

Only section 2.1 (without irreps)

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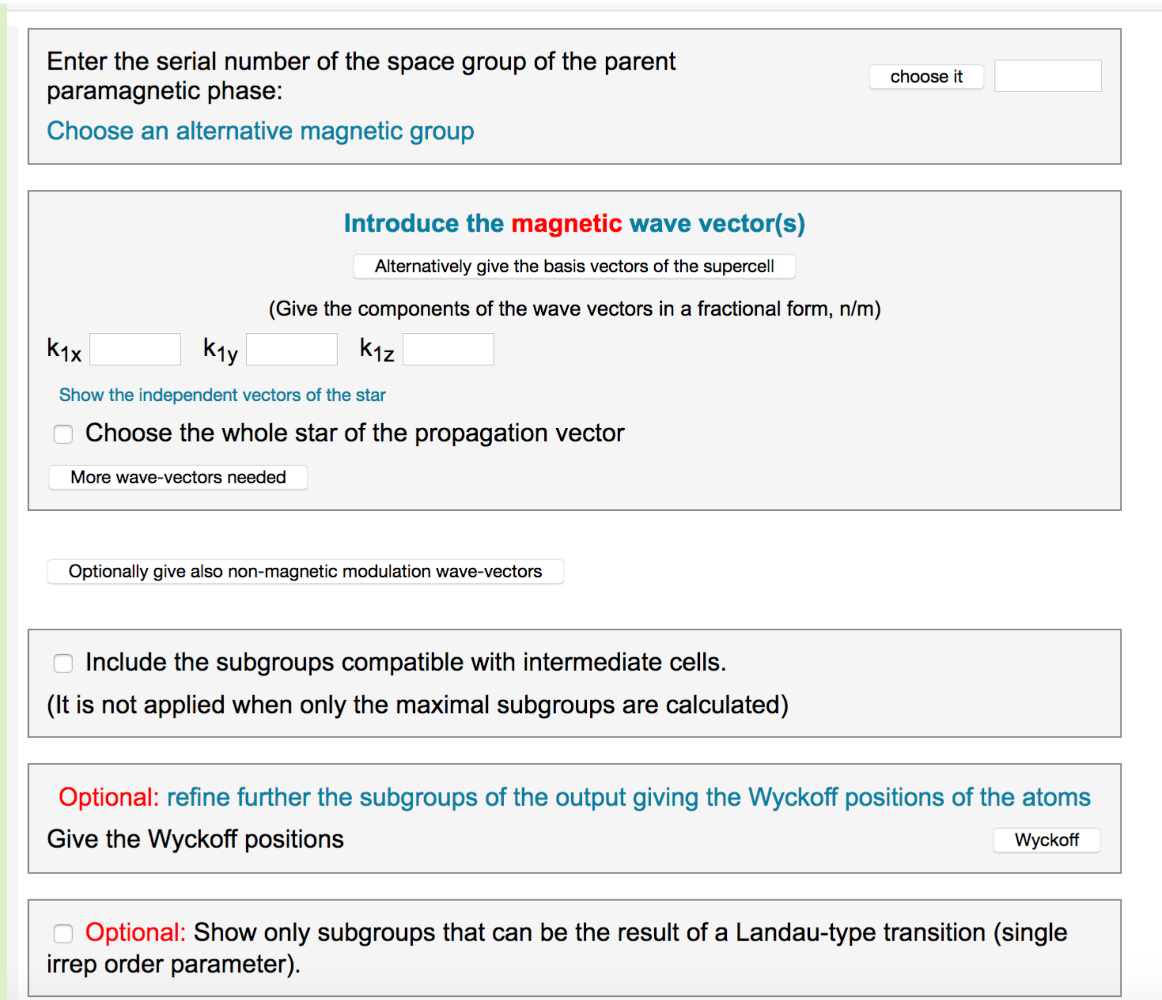
k-SUBGROUPSMAG & MAGMODELIZE

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

***k-SUBGROUPSMAG** is also used by refinement program **GSAS-II** to obtain all possible alternative symmetries for a given set of propagation vectors.*


Enter the serial number of the space group of the parent paramagnetic phase:
choose it
Choose an alternative magnetic group

Introduce the magnetic wave vector(s)
Alternatively give the basis vectors of the supercell
(Give the components of the wave vectors in a fractional form, n/m)
k_{1x} k_{1y} k_{1z}
Show the independent vectors of the star
Choose the whole star of the propagation vector
More wave-vectors needed

Optionally give also non-magnetic modulation wave-vectors

Include the subgroups compatible with intermediate cells.
(It is not applied when only the maximal subgroups are calculated)

Optional: refine further the subgroups of the output giving the Wyckoff positions of the atoms
Give the Wyckoff positions
Wyckoff

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

k-SUBGROUPSMAG

Example: Ba3Nb2NiO9
MAGNDATA #1.13

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) allowing zon-zero momento on all sites

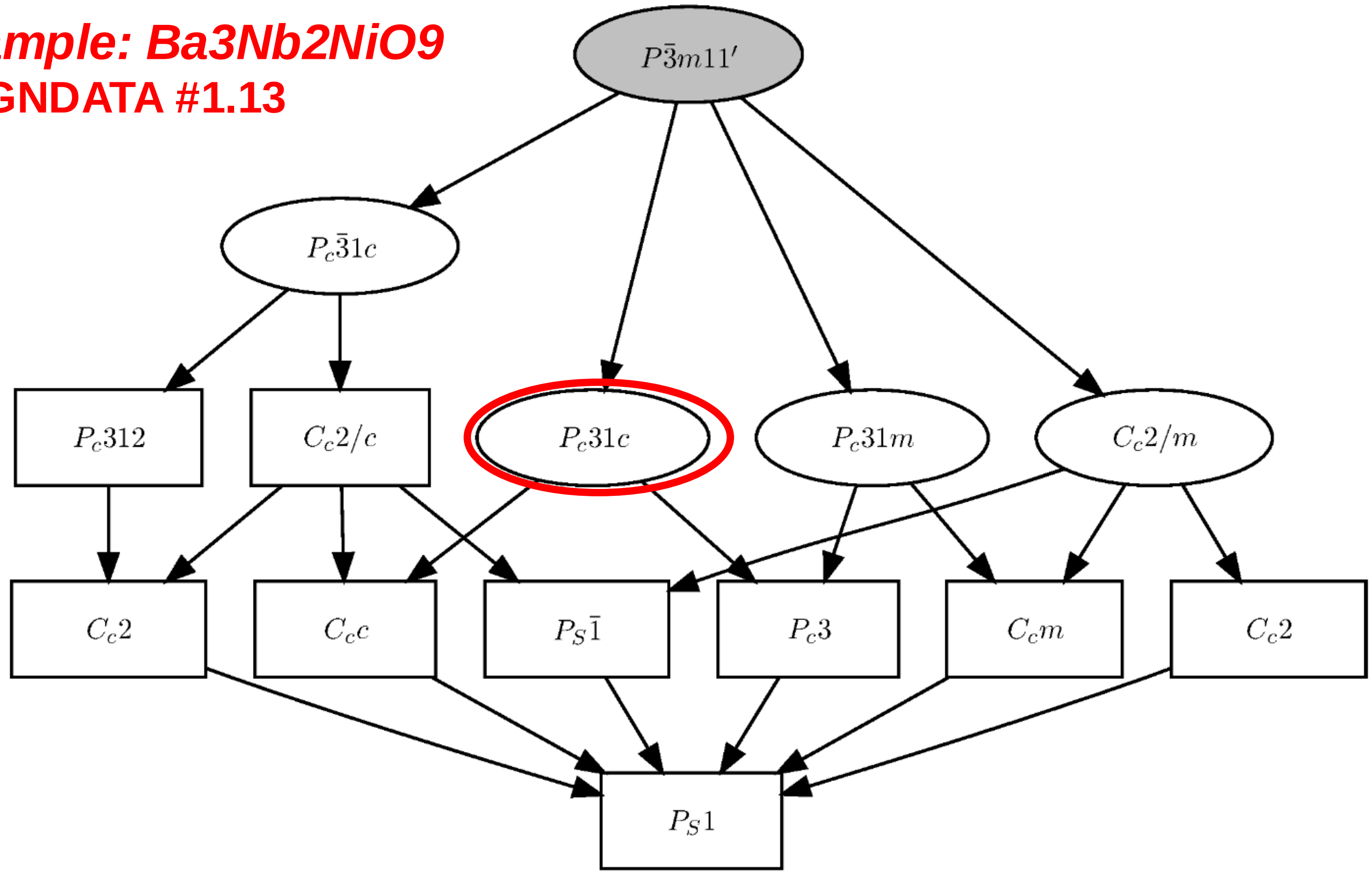
N	Group Symbol	Transformation matrix	Group-Subgroup index	Other members of the Conjugacy Class	irreps	Magnetic structure models (MAGMODELIZE)
1	$P_c\bar{3}1c$ (No. 163.84)	$\begin{pmatrix} 1 & 1 & 0 & 0 \\ -1 & 2 & 0 & 1 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	6=6x1	Conjugacy Class	Get irreps	☐
2	P_c31c (No. 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

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) allowing zon-zero momento on all sites

Example: Ba3Nb2NiO9

MAGNDATA #1.13



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	$\begin{pmatrix} 1 & 1 & 0 & 0 \\ -1 & 2 & 0 & 1 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
2	P_c31c (#159.64) Go to a subgroup	$\begin{pmatrix} 1 & 1 & 0 & 7/3 \\ -1 & 2 & 0 & 8/3 \\ 0 & 0 & 2 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
3	P_c31m (#157.56) Go to a subgroup	$\begin{pmatrix} 1 & 1 & 0 & 7/3 \\ -1 & 2 & 0 & 8/3 \\ 0 & 0 & 2 & 0 \end{pmatrix}$ 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

k-SUBGROUPSMAG

Example: Ba3Nb2NiO9
MAGNDATA #1.13

Magnetic Structure

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

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

Parent space group 164 (*P*-3*m*1)

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

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

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

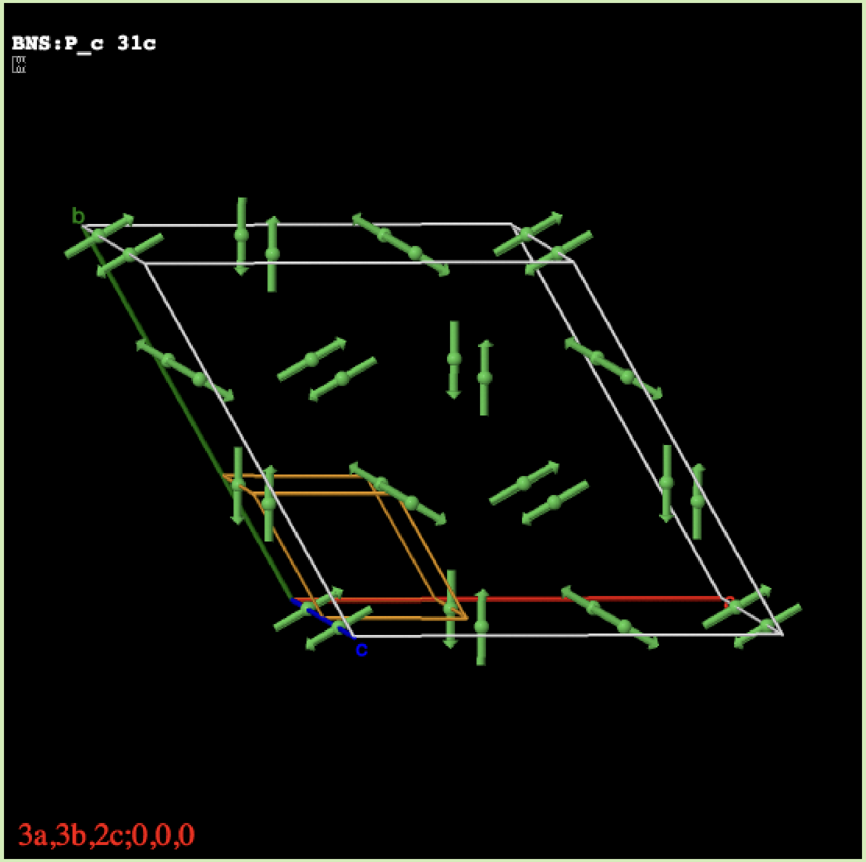
Atomic positions, Wyckoff positions and Magnetic Moments

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
MAGNDATA #1.13

Parent space group P-3m1
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'
```

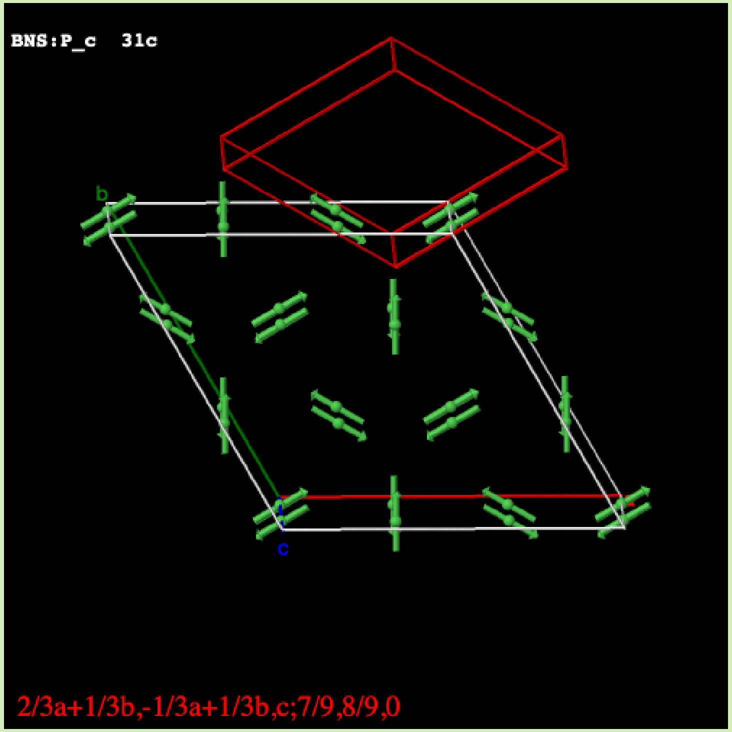
transformation to standard

k-SUBGROUPSMAG

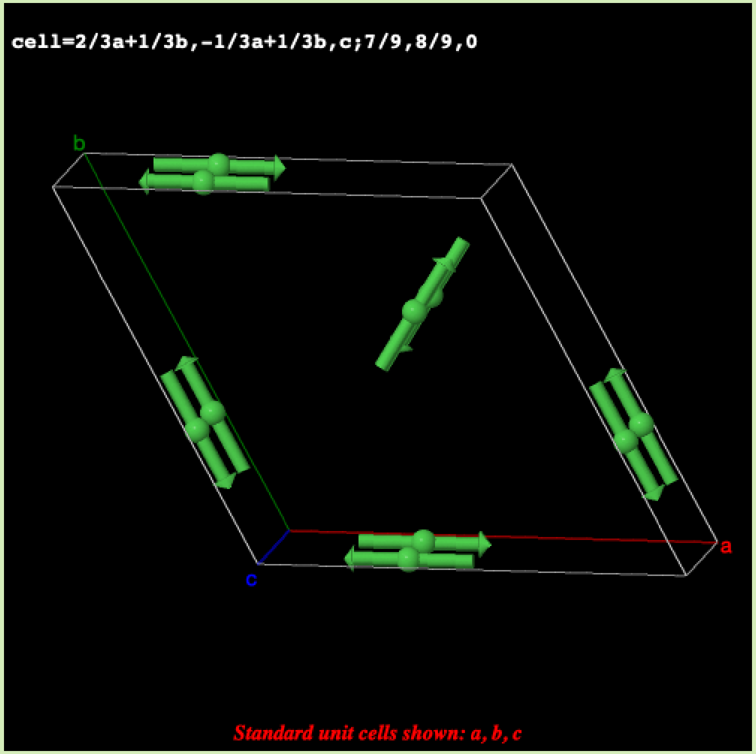
Example: Ba3Nb2NiO9
MAGNDATA #1.13

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



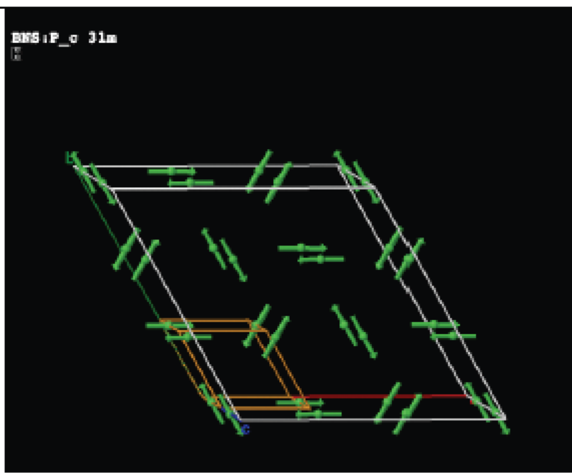
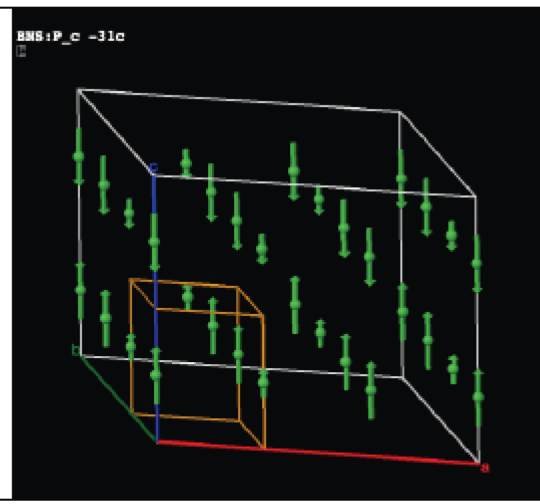
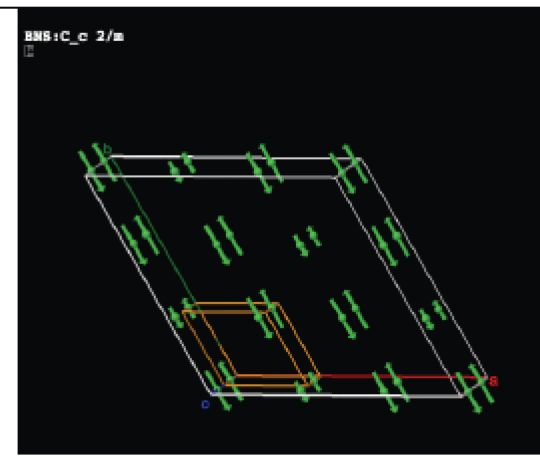
in the new mCIF file with the MSG in standard setting:

```
_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))

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

pe 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]

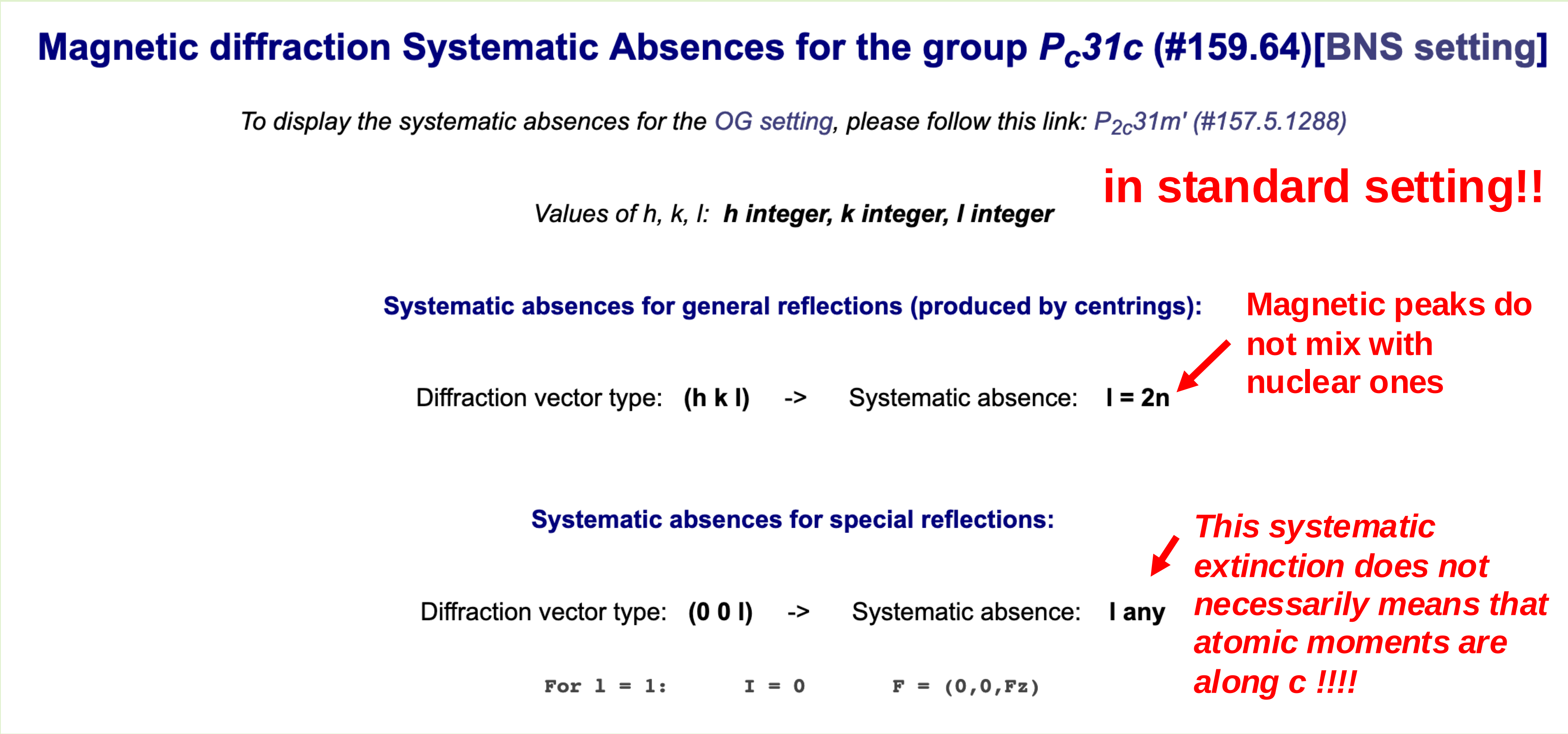
[Standard/Default Setting]

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

MAGNEXT: partial ouput example



in standard setting!!

Magnetic peaks do not mix with nuclear ones

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

Wyckoff Positions of the Group P_c31c (#159.64) [BNS setting]

159.64 *P31c.1'$_c$[P31m]* (UNI symbol)

To display the Wyckoff positions in the OG setting, please follow this link: $P_{2c}31m'$ (#157.5.1288)

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

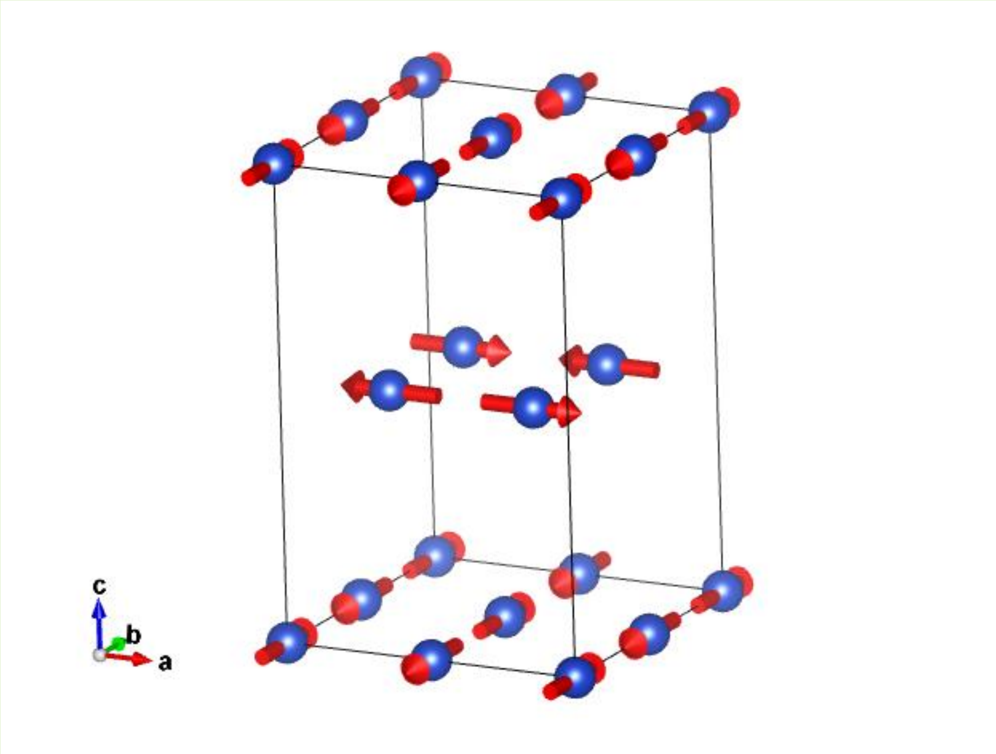
Absence:

(0,0,l) absent for all l

In our case atoms have moment components on the xy plane

The systematic absence is general due to the MSG symmetry

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- section 2

Tutorial to follow:

Tutorial_magnetic_section _BCS_3 – section 2

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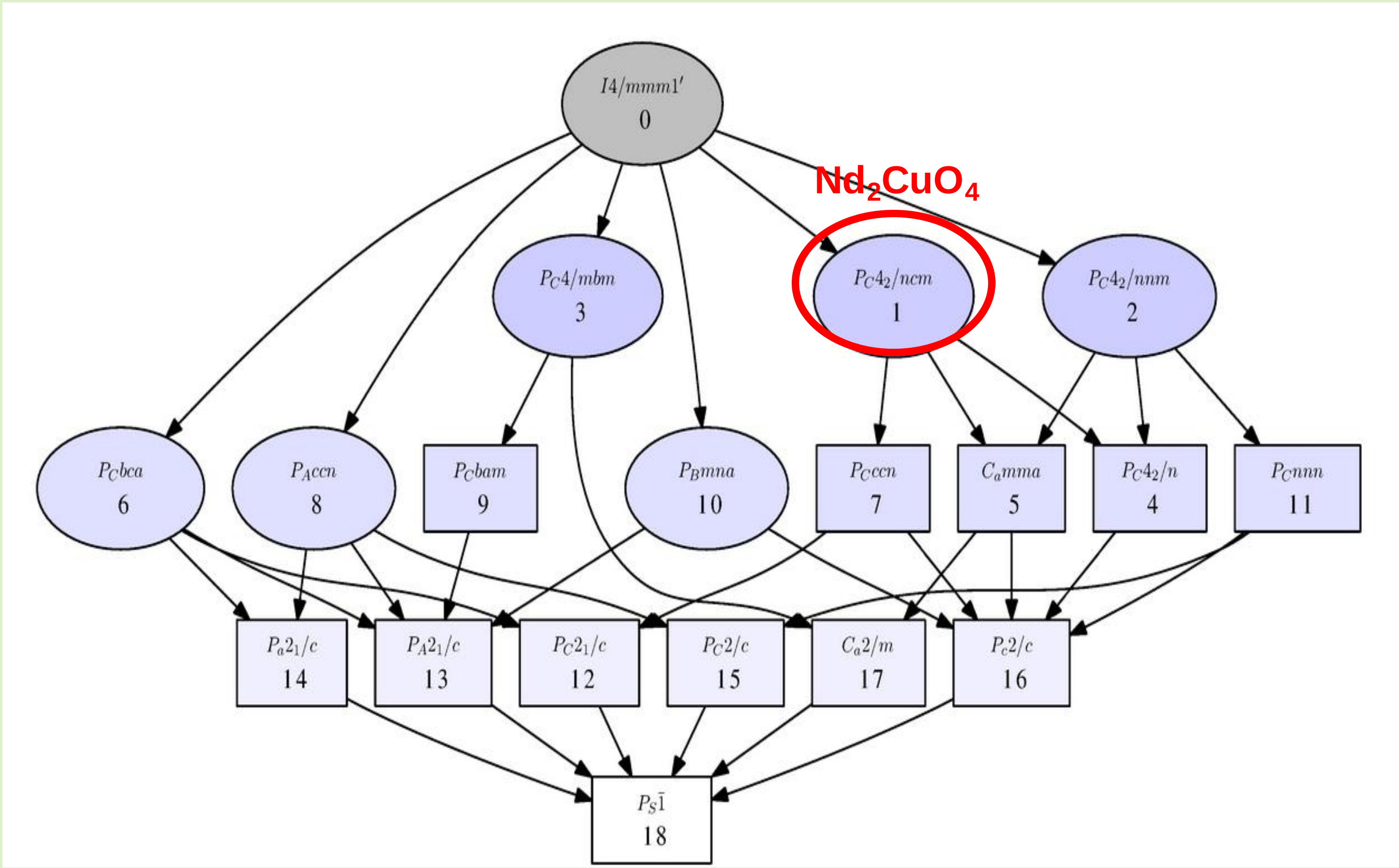
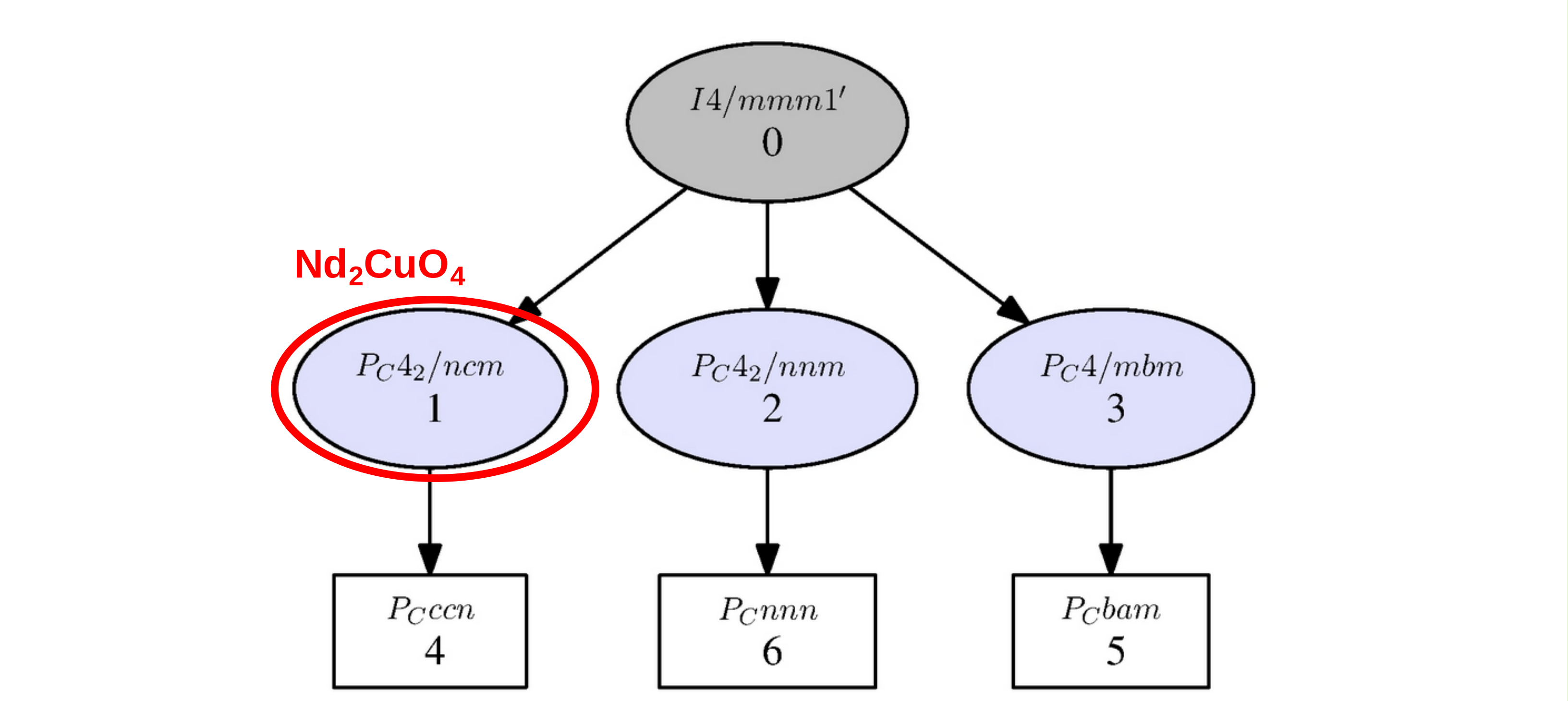
MAGNETIC REP.	Decomposition of the magnetic representation into irreps
Get_mirreps	Irreps and order parameters in a paramagnetic space group- magnetic subgroup phase transition

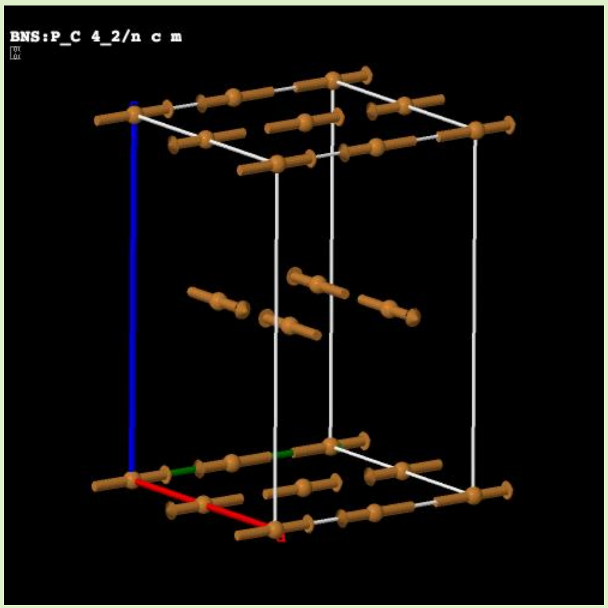
Possible magnetic symmetries for a magnetic phase with two propagation vectors (1/2,1/2,0) and (-1/2,1/2,0), parent space group I4/mmm and magnetic atom at site 2a.



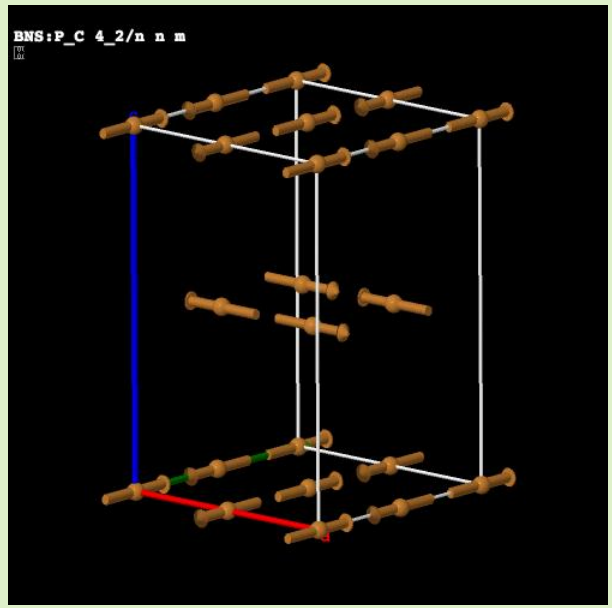
Possible magnetic symmetries for a magnetic phase with two propagation vectors (1/2,1/2,0) and (-1/2,1/2,0), parent space group I4/mmm and magnetic atom at site 2[a], and a single primary irrep active (Landau condition)



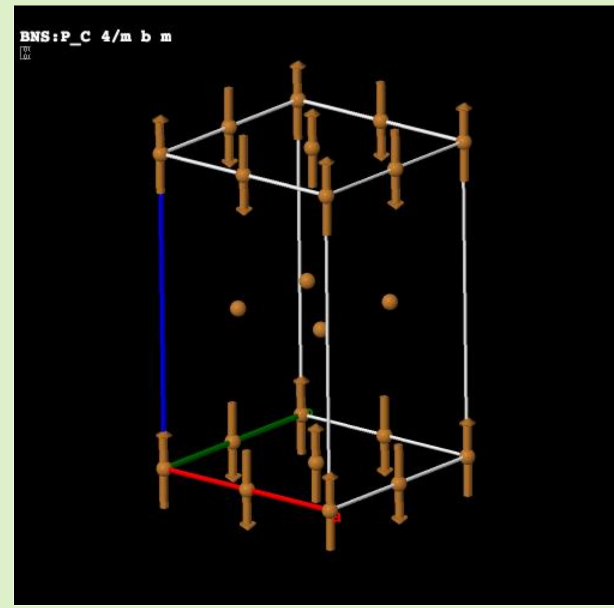
Scheme of the three possible 2k magnetic structures of maximal symmetry with propagation vectors (1/2,1/2,0) and (-1/2,1/2,0), parent space group /4/mmm, magnetic atom at site 2a, and a single primary irrep active.



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)