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

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Universidad del País Vasco
Euskal Herriko Unibertsitatea

II. Modeling of commensurate magnetic structures and the Bilbao crystallographic server

J. Manuel Perez-Mato
Facultad de Ciencia y Tecnología
Universidad del País Vasco, UPV-EHU
BILBAO, SPAIN

Symmetry-Based Computational Tools for Magnetic Crystallography

J.M. Perez-Mato,[1] S.V. Gallego,[1] E.S. Tasci,[2] L. Elcoro,[1] G. de la Flor,[1] and M.I. Aroyo[1]

[1]Departamento de Física de la Materia Condensada, Facultad de Ciencia y Tecnología, Universidad del País Vasco, UPV/EHU, 48080 Bilbao, Spain; email: jm.perez-mato@ehu.es

[2]Department of Physics Engineering, Hacettepe University, 06800 Ankara, Turkey

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Symmetry based modeling …

- First step?:

Assume a specific MSG and check if it works ….

But which MSGs are possible for a given material????

To answer this question is the real first step…

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)?

Pnma1'

k=(1/2,0,0)

?

$HoMnO_3$

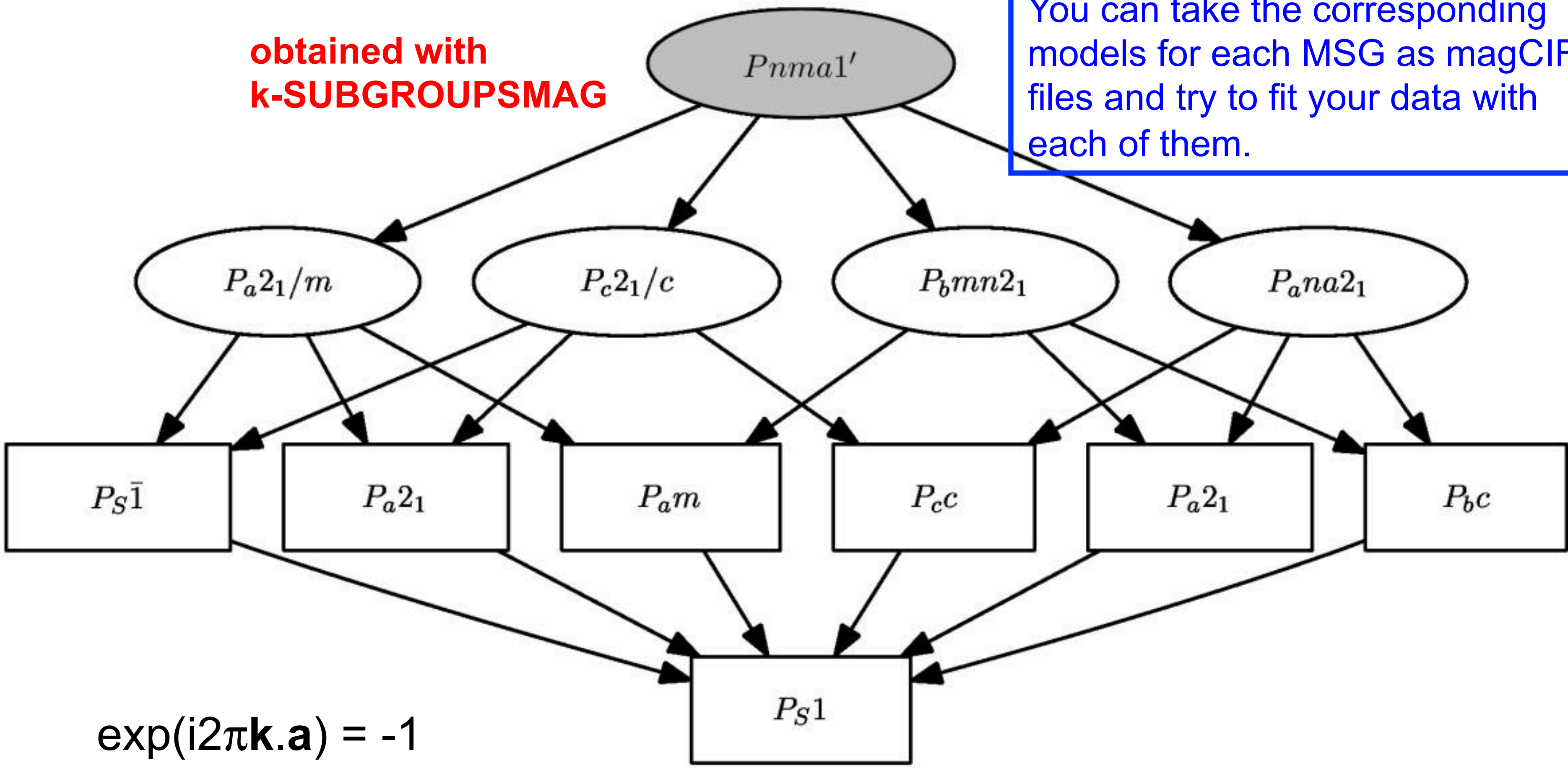
Purely mathematical problem !

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 as magCIF files and try to fit your data with each of them.



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

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

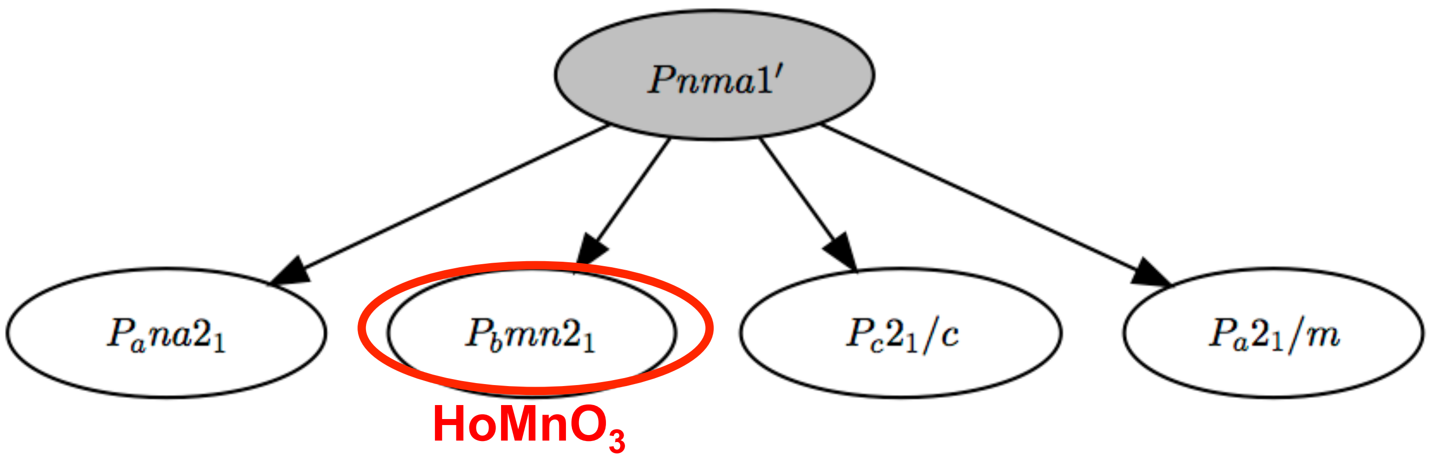
(magnetic cell= ($2\mathbf{a}_p,\mathbf{b}_p,\mathbf{c}_p$))

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)

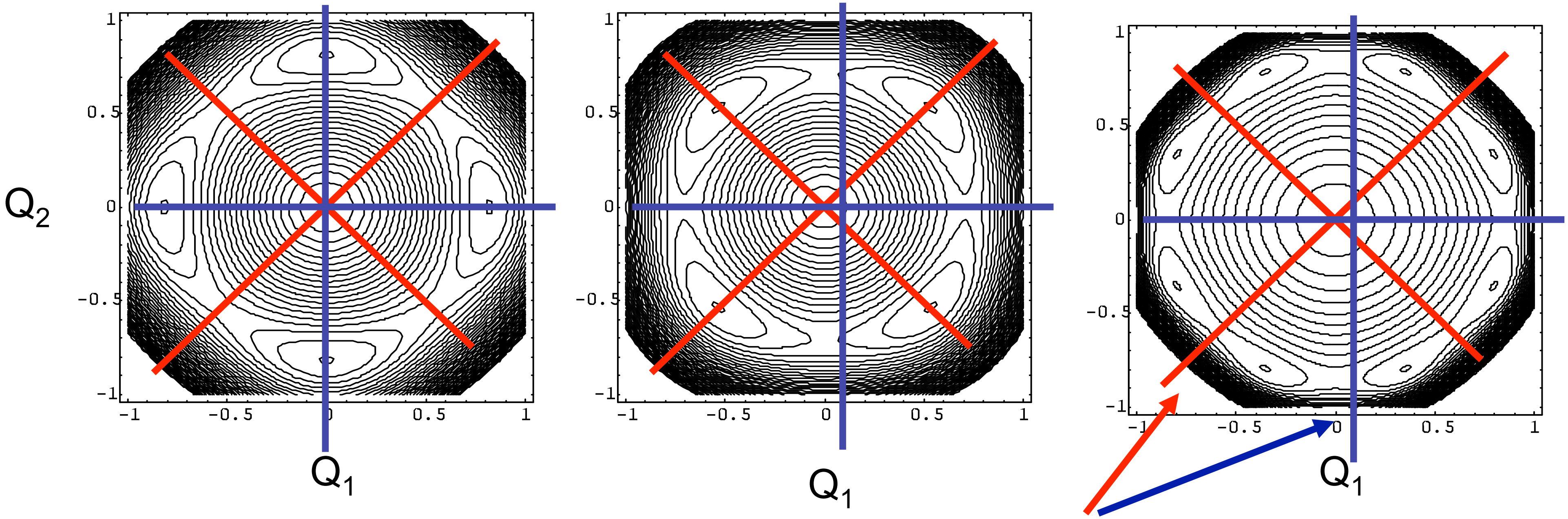
obtained with
k-SUBGROUPSMAG



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

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

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
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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

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')   *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
$Pnma1'$ (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)

$$Pnma1' \rightarrow P_bmn2_1\ (\mathbf{-b}, 2\mathbf{a}, \mathbf{c}; 1/4, 1/4, 0)$$

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

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_bmn2_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_bmn2_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
```

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
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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 | 0,m_y,m_z) (0,1/2,1/2 | 0,-m_y,m_z) (1/2,1/2,0 | 0,-m_y,-m_z) (1/2,0,1/2 | 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 | 0,m_y,m_z) (0,-y+1/2,1/2 | 0,-m_y,m_z) (0,1/2,-z+1/2 | 0,-m_y,m_z) (0,-y,-z | 0,m_y,m_z) (1/2,1/2,0 | 0,-m_y,-m_z) (1/2,-y,1/2 | 0,m_y,-m_z) (1/2,0,-z+1/2 | 0,m_y,-m_z) (1/2,-y+1/2,-z | 0,-m_y,-m_z)	8	-	-
3	O1 O 0.25000 -0.00510 0.25000	(1/4,y,1/4 | 0,m_y,0) (3/4,-y+1/2,3/4 | 0,-m_y,0) (3/4,-y,3/4 | 0,m_y,0) (1/4,1/2,1/4 | 0,-m_y,0) (3/4,1/2,1/4 | 0,-m_y,0) (1/4,-y,3/4 | 0,m_y,0) (1/4,-y+1/2,3/4 | 0,-m_y,0) (3/4,0,1/4 | 0,m_y,0)	8	-	-
4	O2 O 0.00000 0.18300 -0.02430	(0,y,z | 0,m_y,m_z) (0,-y+1/2,1/2 | 0,-m_y,m_z) (0,1/2,-z+1/2 | 0,-m_y,m_z) (0,-y,-z | 0,m_y,m_z) (1/2,1/2,0 | 0,-m_y,-m_z) (1/2,-y,1/2 | 0,m_y,-m_z) (1/2,0,-z+1/2 | 0,m_y,-m_z) (1/2,-y+1/2,-z | 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

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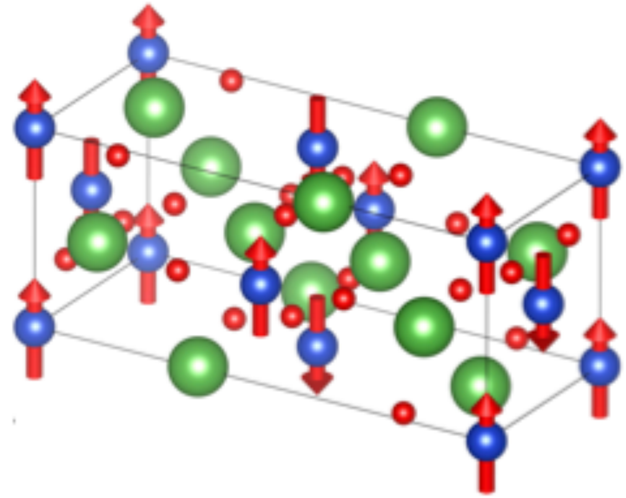
La_2CuO_4



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

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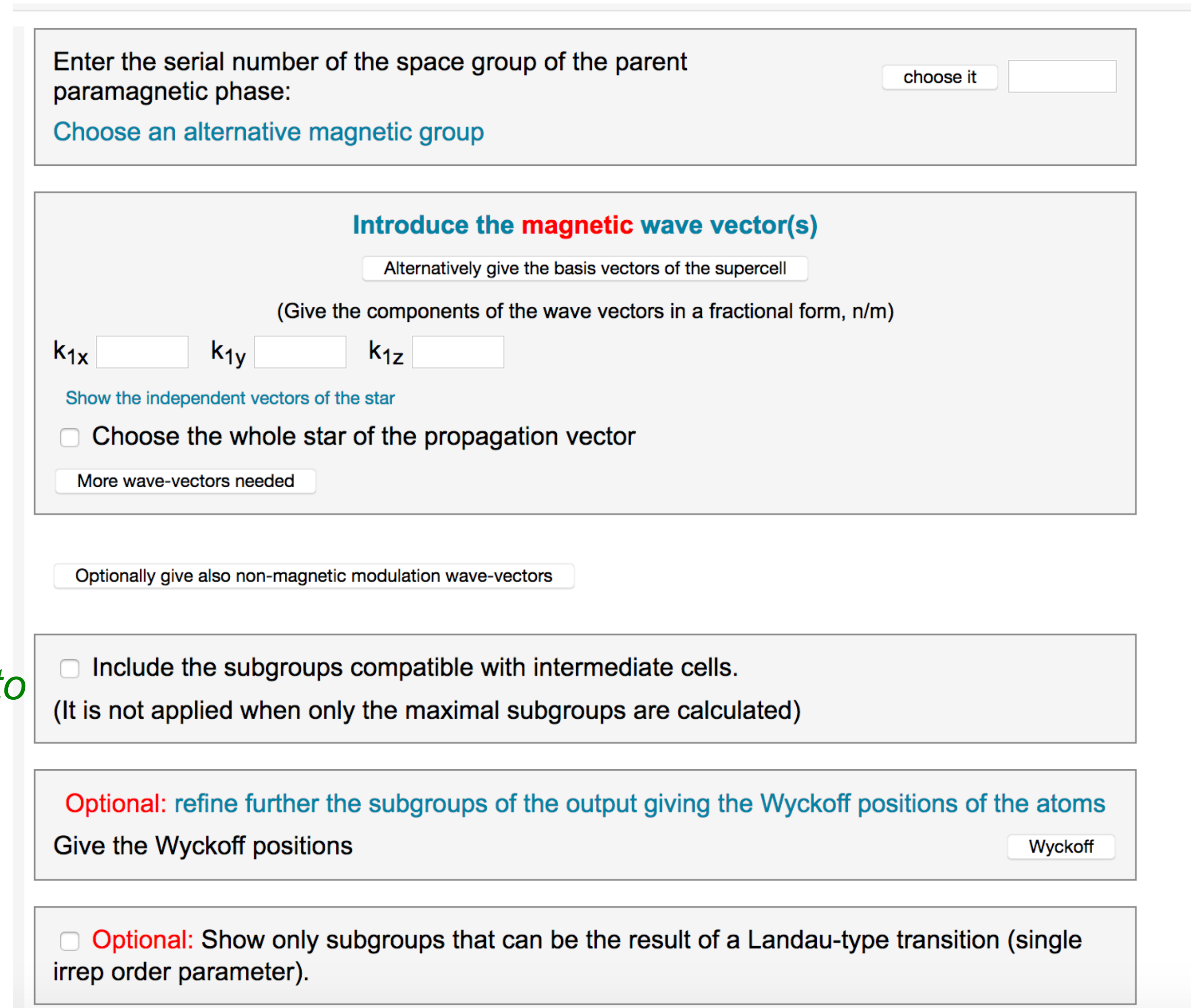
Get_mirreps	Irreps and order parameters in a paramagnetic space group- magnetic subgroup phase transition

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

k-SUBGROUPSMAG & MAGMODELIZE

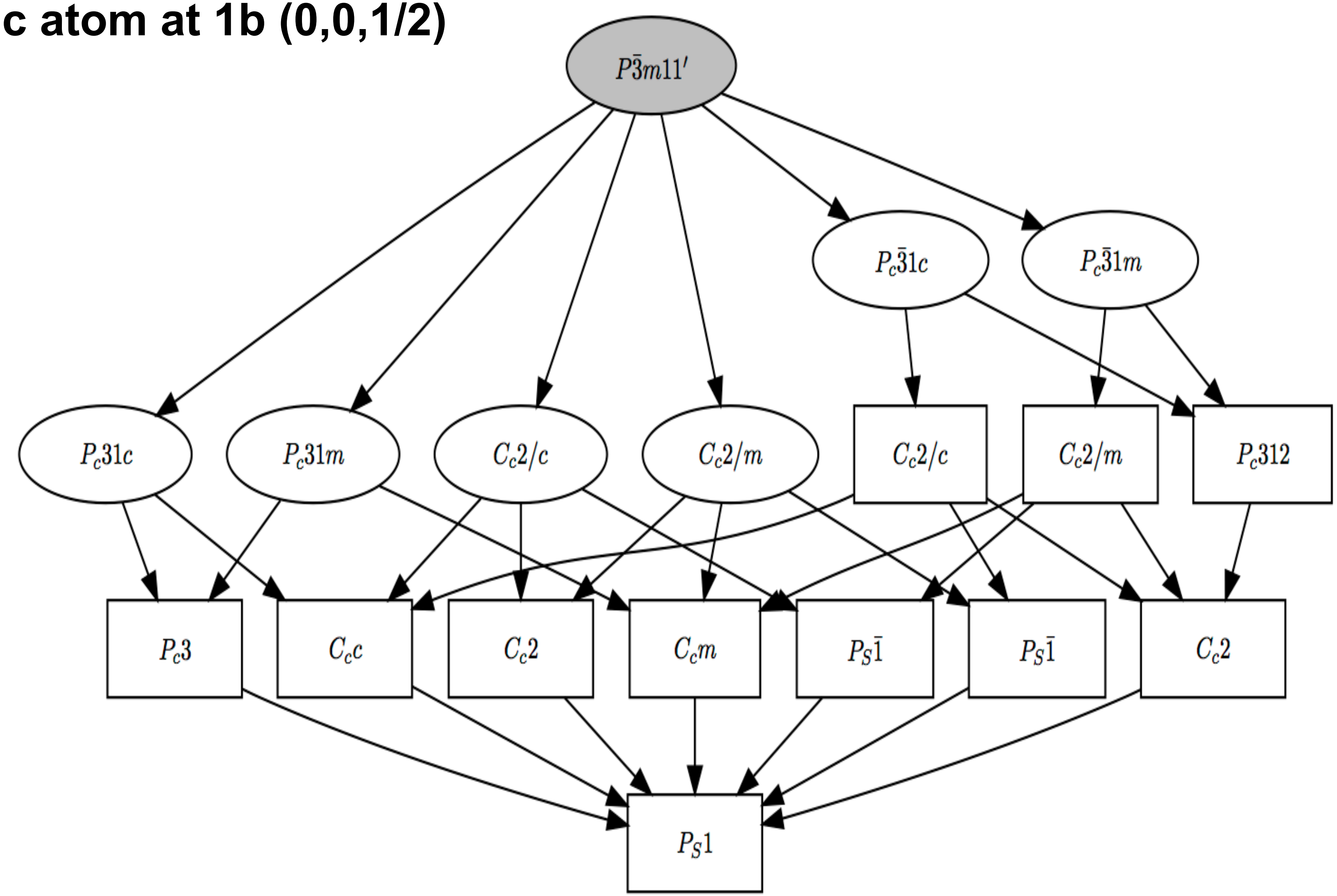
k-Subgroupsmag: Magnetic subgroups compatible with some given propagation vector(s) or a supercell.



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

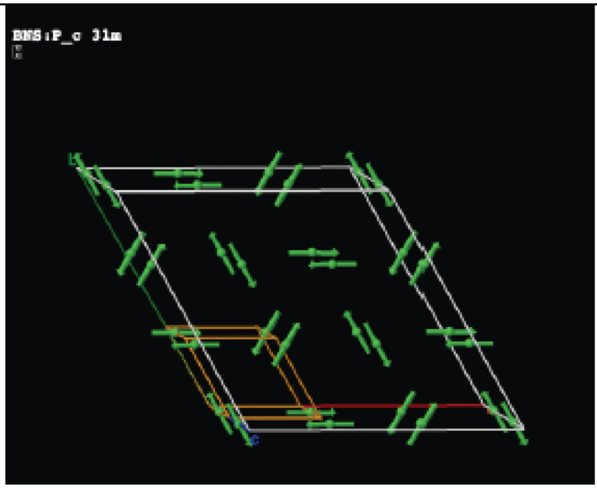
Possible magnetic symmetries for a magnetic phase with parent space group P-3m1, propagation vector (1/3,1/3,1/2) and magnetic atom at 1b (0,0,1/2)



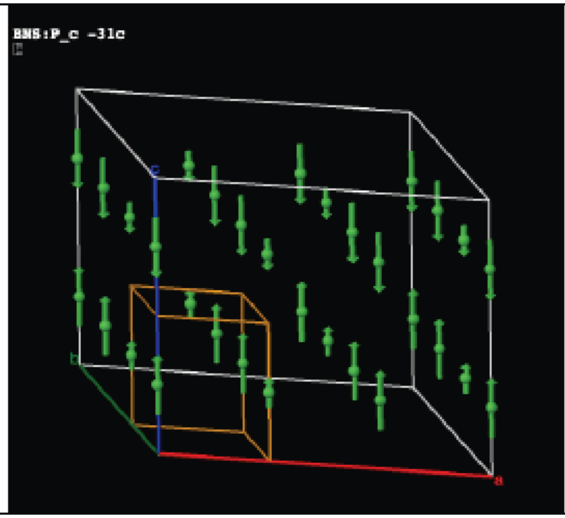
k-SUBGROUPSMAG & MAGMODELIZE

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

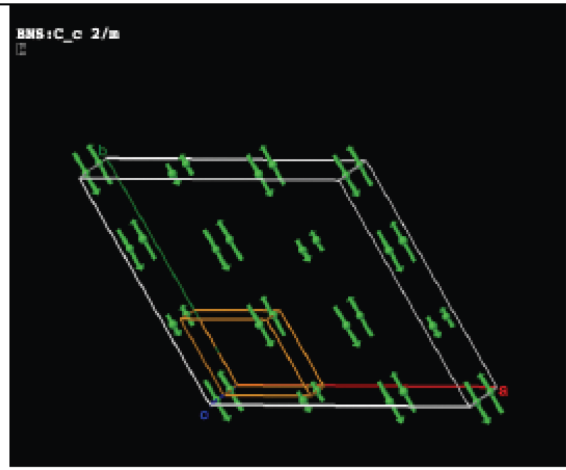
Some of the possible magnetic structures for parent space group P-3m1 propagation vector (1/3,1/3,1/2) and magnetic atom at 1b (0,0,1/2):



P_c31m



$P_c\text{-}31c$



C_c2/m

(obtained with MVISUALIZE (Jmol))

MAGNEXT: Magnetic diffraction systematic absences

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MAGNEXT: Magnetic Systematic Absences

tinction rules for
any Shubnikov magnetic

be obtained introducing the
d for this purpose at the
pted form of the structure

y 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

Magnetic diffraction Systematic Absences for the group $P6_3'/m'$ (#176.147)

For this space group, BNS and OG settings coincide.
Its label in the OG setting is given as: $P6_3'/m'$ (#176.5.1378)

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

Systematic absences for special reflections:

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

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

```
For l = 1:     I = 0     F = (0,0,Fz)
For l = 2:     I = 0     F = (0,0,0)
```

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

Go to the list of the General Positions of the Group $P6_3'/m'$ (#176.147) [OG:$P6_3'/m'$ (#176.5.1378)]
Go to the list of the Wyckoff Positions of the Group $P6_3'/m'$ (#176.147) [OG:$P6_3'/m'$ (#176.5.1378)]

[Show systematic absences in a different setting]

Wyckoff Positions of the Group $P6_3'/m'$ (#176.147)

For this space group, BNS and OG settings coincide.
Its label in the OG setting is given as: $P6_3'/m'$ (#176.5.1378)

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

Absence:

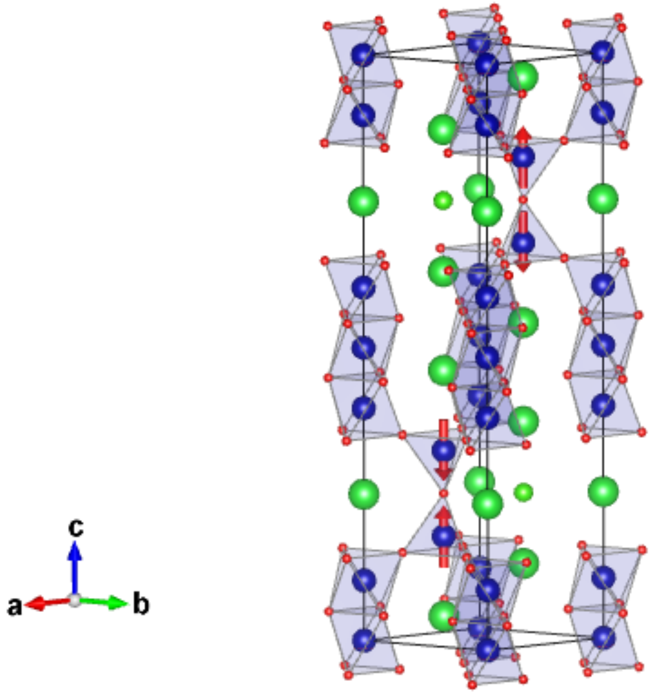
(0,0,l) absent for all l

Atoms can have moment components on the xy plane

Site Symmetries of the Wyckoff Positions

MAGNEXT can be used to discriminate between two 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)

Tutorial to follow :

Tutorial_MAXMAGN_ HoMnO3

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 to follow:

Tutorial_magnetic_section_BCS_2
Only section 2.1

Magnetic Symmetry and Applications	
MGENPOS	General Positions of Magnetic Space Groups
MWYCKPOS	Wyckoff Positions of Magnetic Space Groups
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