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

eman ta zabal zazu
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Hand-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
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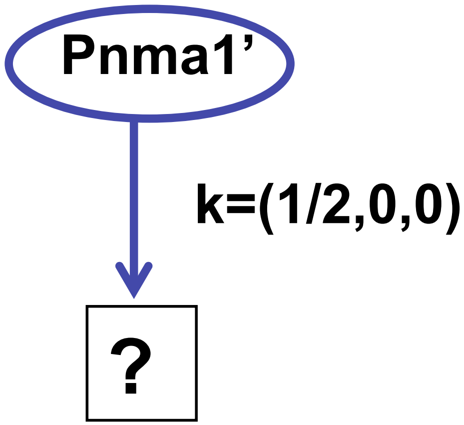
Get_mirreps	Irreps and order parameters in a paramagnetic space group- magnetic subgroup phase transition

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)?



$HoMnO_3$

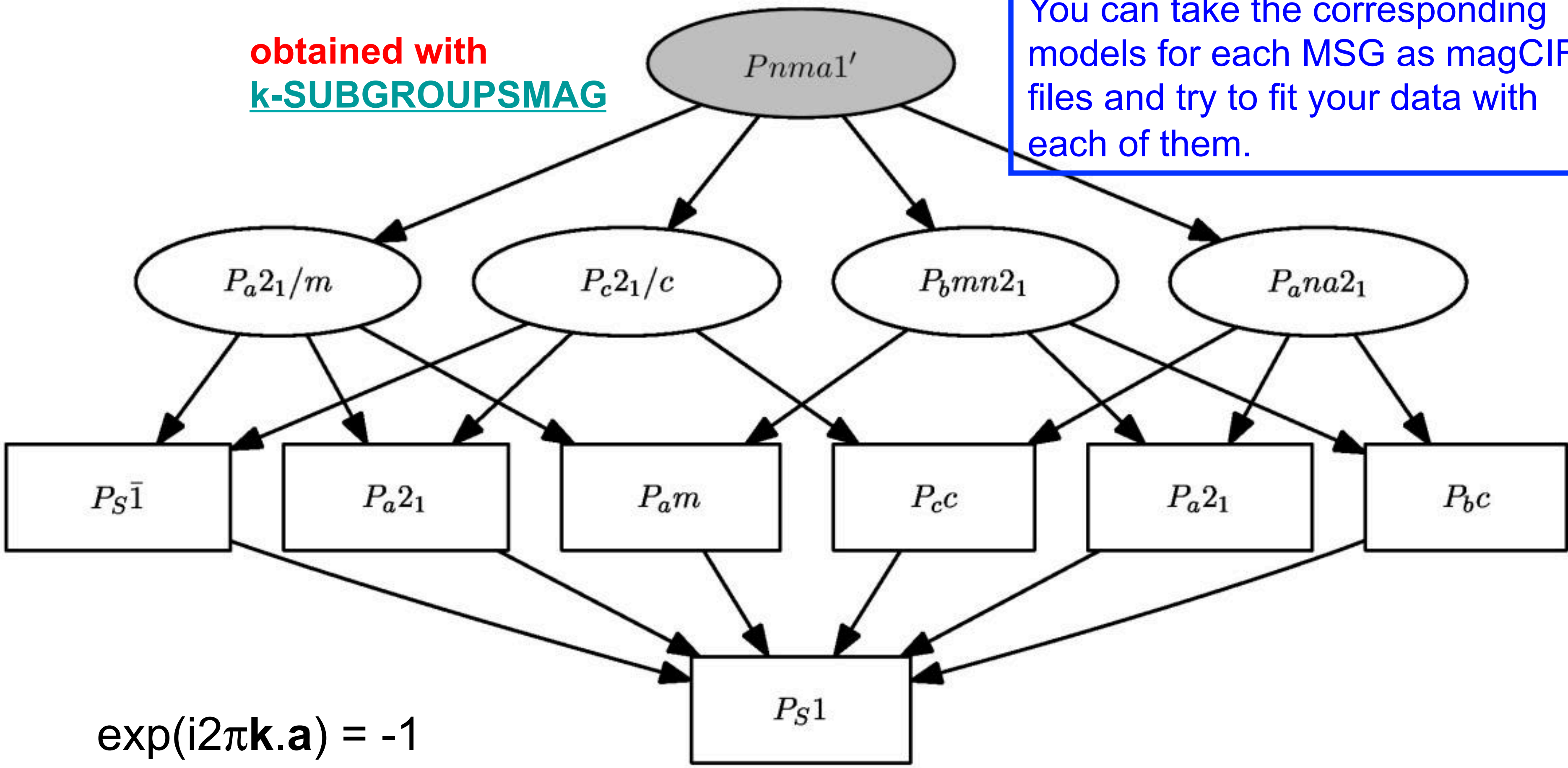
Purely mathematical problem !

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



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

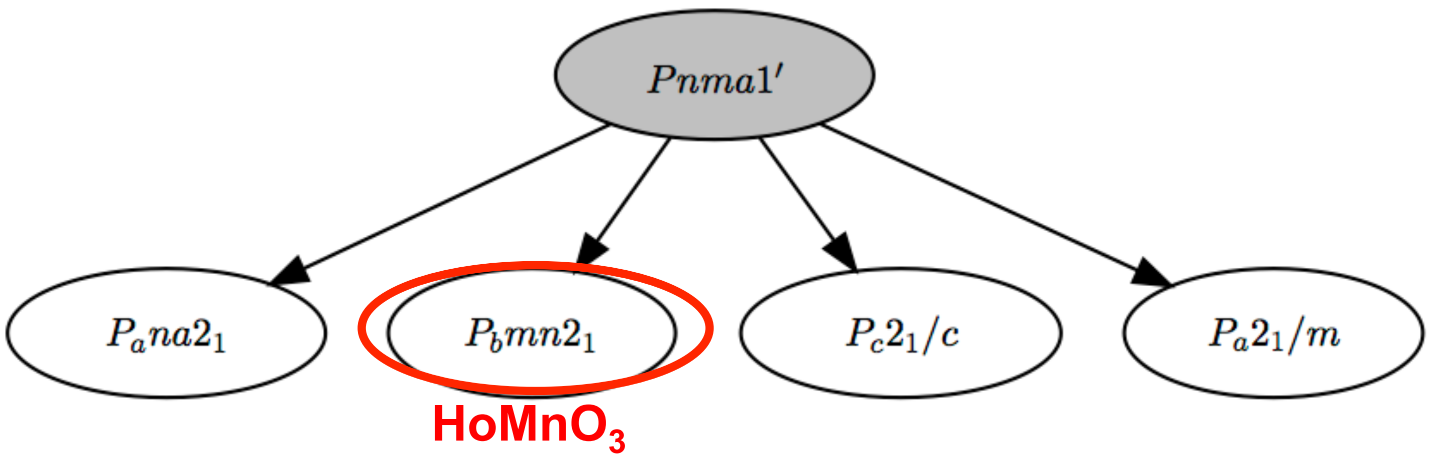
Symmetry operation {1'|1/2,0,0} is present in any case
(magnetic cell= $(2\mathbf{a}_p,\mathbf{b}_p,\mathbf{c}_p)$)

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)

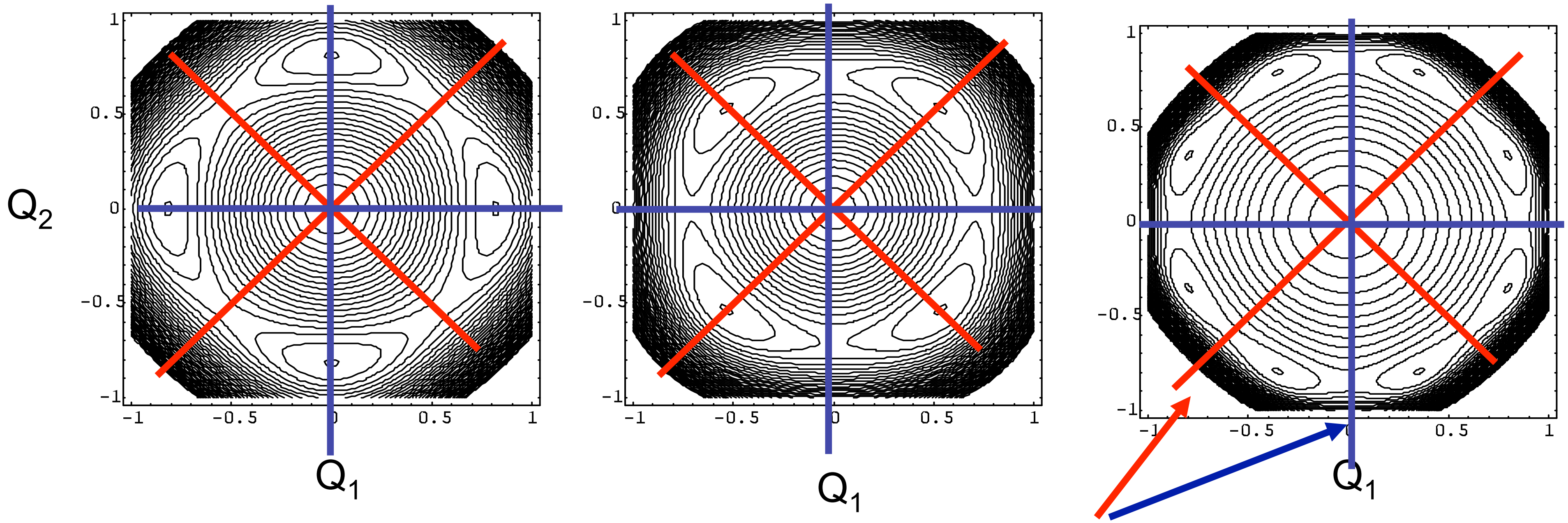
obtained with
k-SUBGROUPSMAG



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

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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 (Cmca1') *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

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

HoMnO$_3$ case

Group→subgroup	Transformation matrix
*Pnma*1' (N. 62.442)→$P_b mn2_1$ (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' → ***$P_b mn2_1$*** (**-b**, 2**a** , **c**; 1/4, 1/4, 0)

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

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, 2a , 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):

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

transformation to standard from the setting used for the MSG.

Alternative unit cell and origin 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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$P_{A}bcn$ (#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 (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

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

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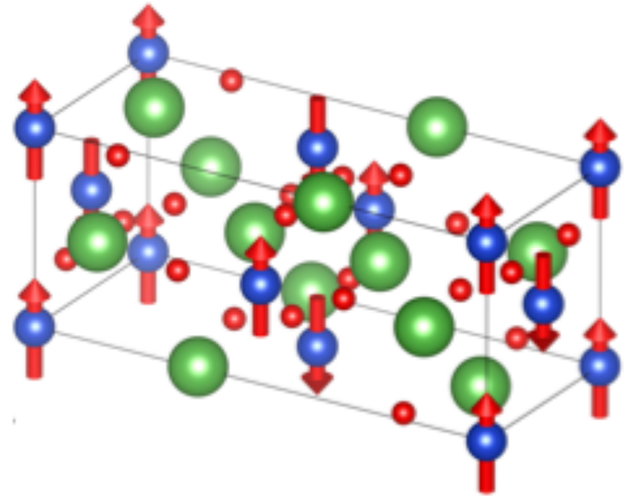
La_2CuO_4



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

3 Tutorials can be downloaded from the program webpage

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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

k-SUBGROUPSMAG & MAGMODELIZE

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

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

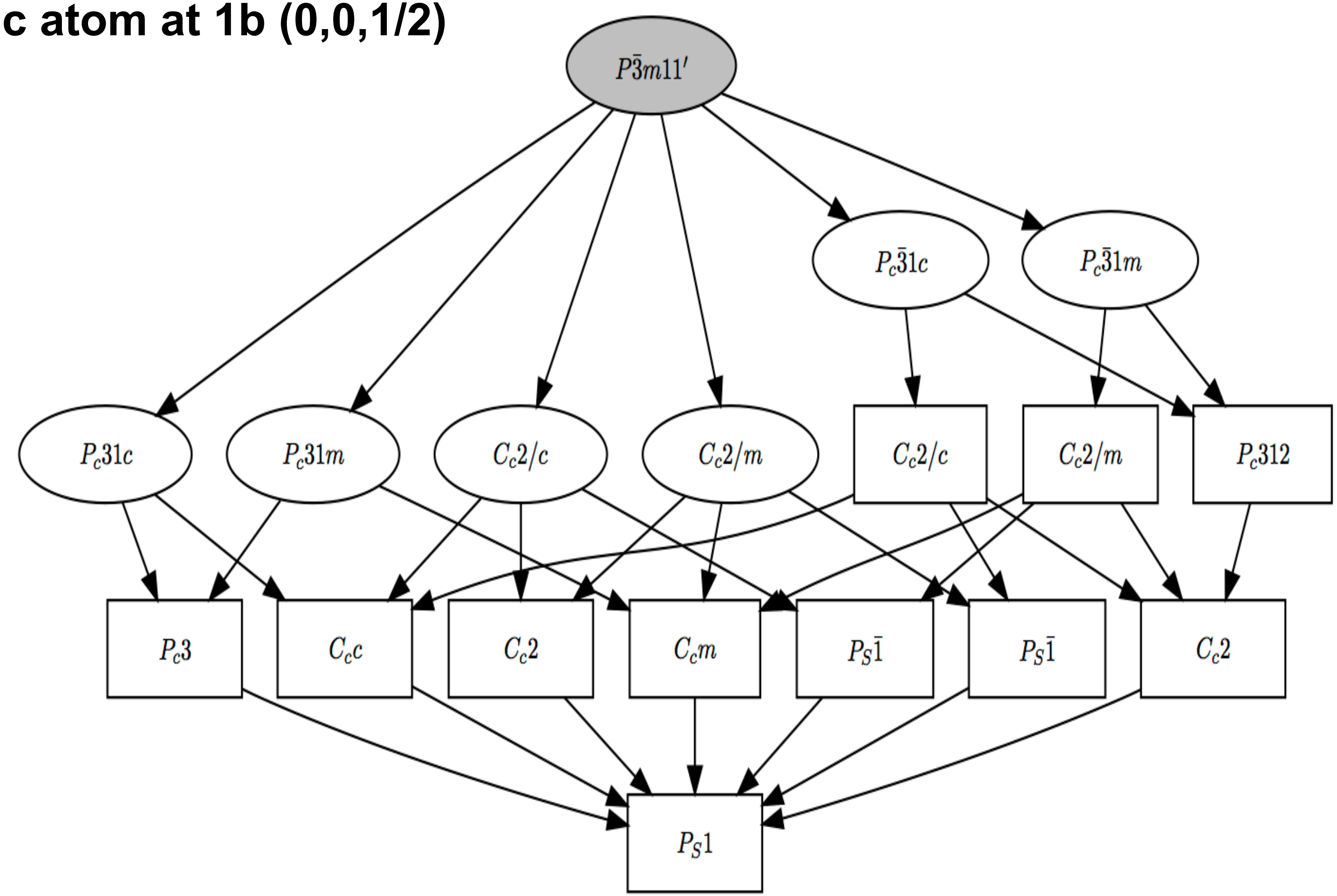
Give the Wyckoff positions Wyckoff

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

***k-SUBGROUPSMAG** 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

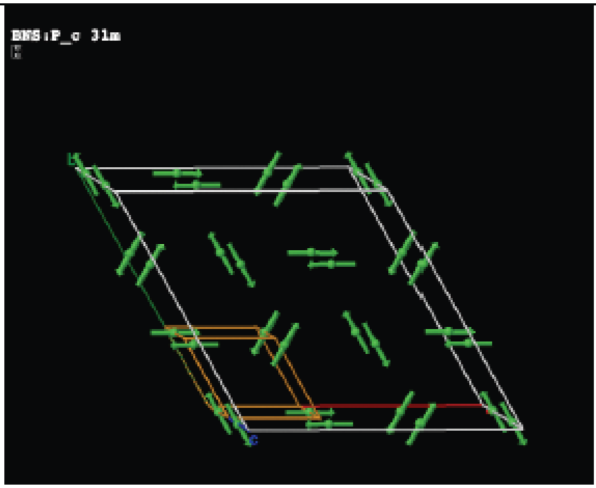
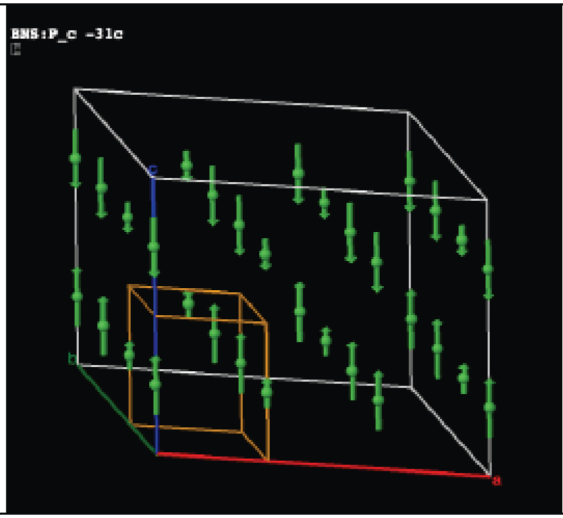
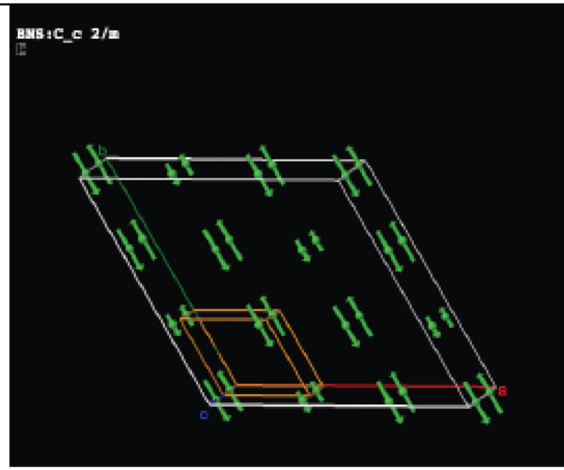
Possible magnetic symmetries for a magnetic phase with parent space group P-3m1, propagation vector (1/3,1/3,1/2) and magnetic atom at 1b (0,0,1/2)



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-31c	C_c2/m

(obtained with MVISUALIZE (Jmol))

MAGNEXT: Magnetic diffraction systematic absences

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MAGNDATA	A collection of magnetic structures with portable cif-type files
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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

MAGNEXT: example (partial output(

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***

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

Systematic absences for special reflections:

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:

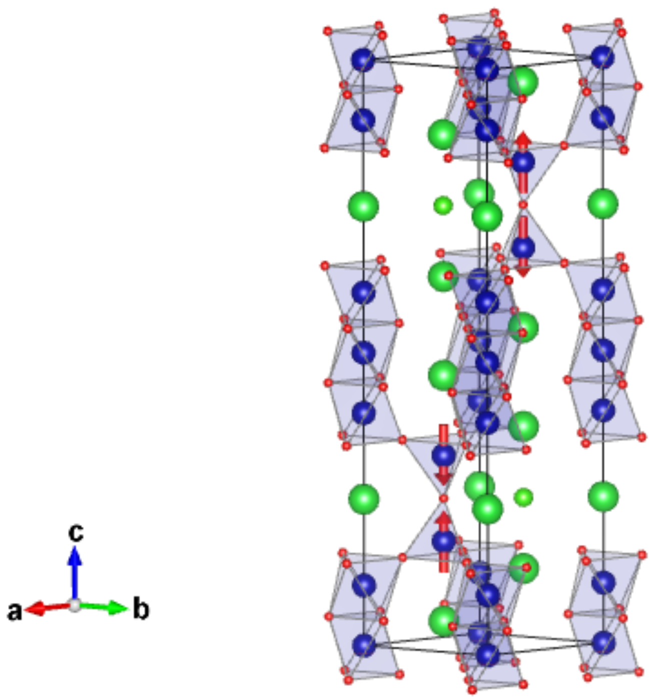
(0,0,l) absent for all l

Atoms can have moment components on the xy plane

Site Symmetries of the Wyckoff Positions

MAGNEXT can be used to discriminate between 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_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
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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_3

Magnetic Symmetry and Applications	
MGENPOS	General Positions of Magnetic Space Groups
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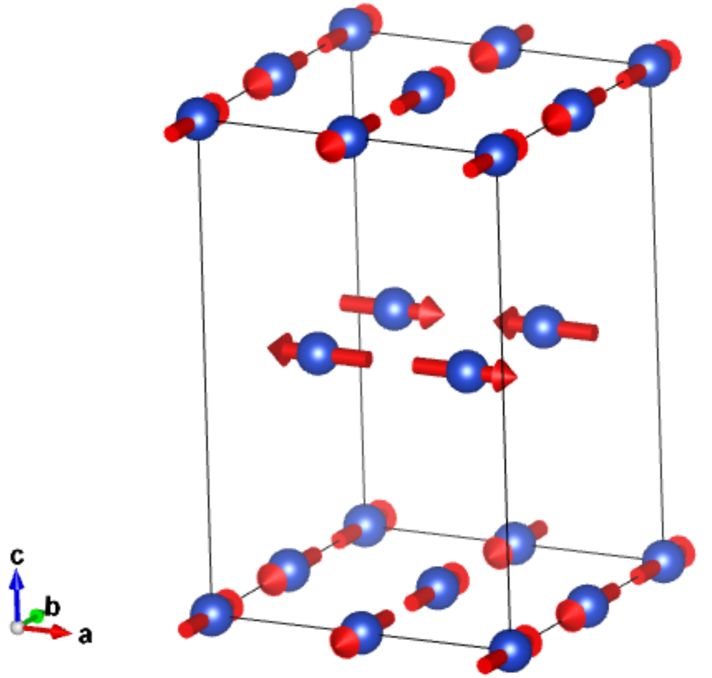
Modelling multi-k structures with KSUBGROUPSMAG & MAGMODELIZE



Nd_2CuO_4

Parent SG: *I4/mmm*

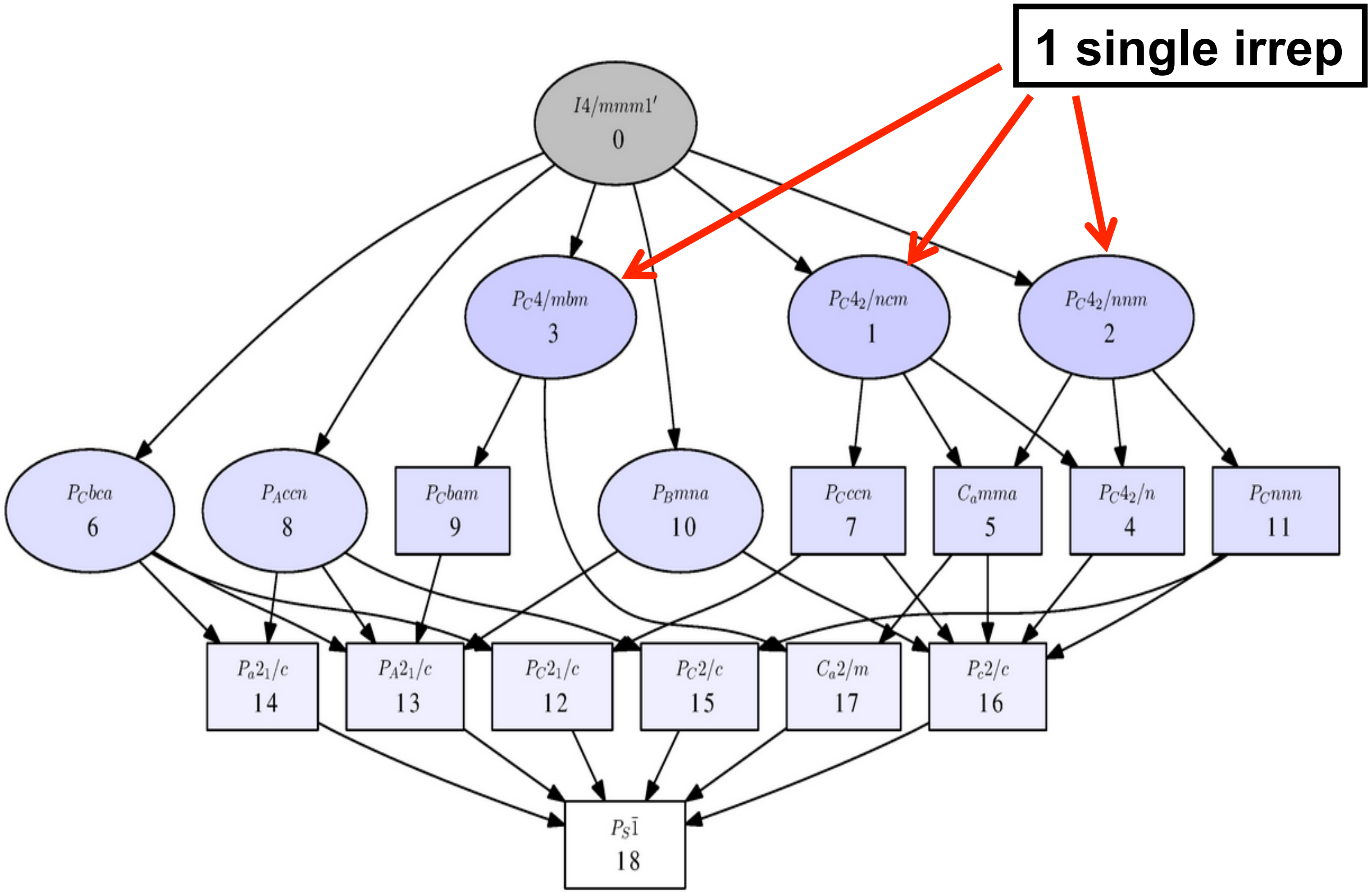
k1= (1/2,1/2,0)
k2=(-1/2,1/2,0)

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

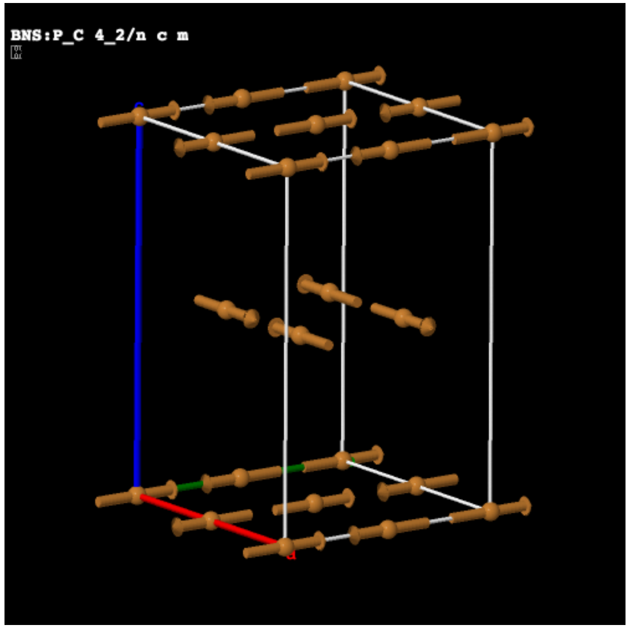
(MAGNDATA 2.6)

Tutorial_magnetic_section_BCS_3

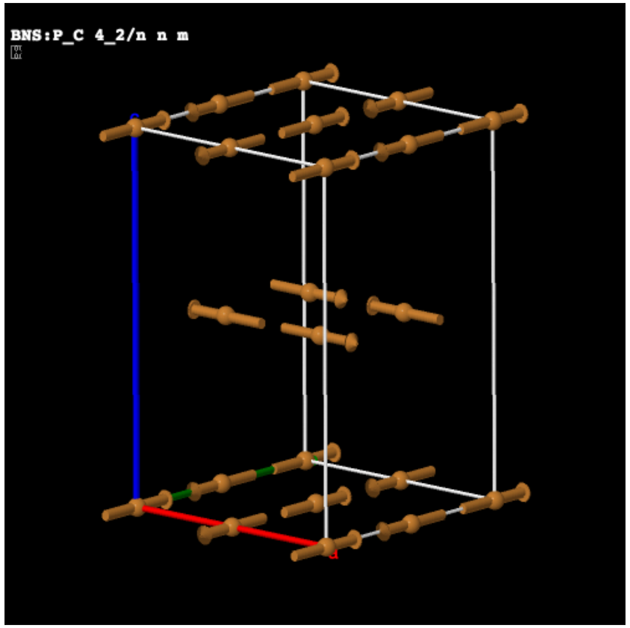
Possible magnetic symmetries for a magnetic phase with two propagation vectors (1/2,1/2,0) and (-1/2,1/2,0), parent space group I4/mmm and magnetic atom at site 2a.



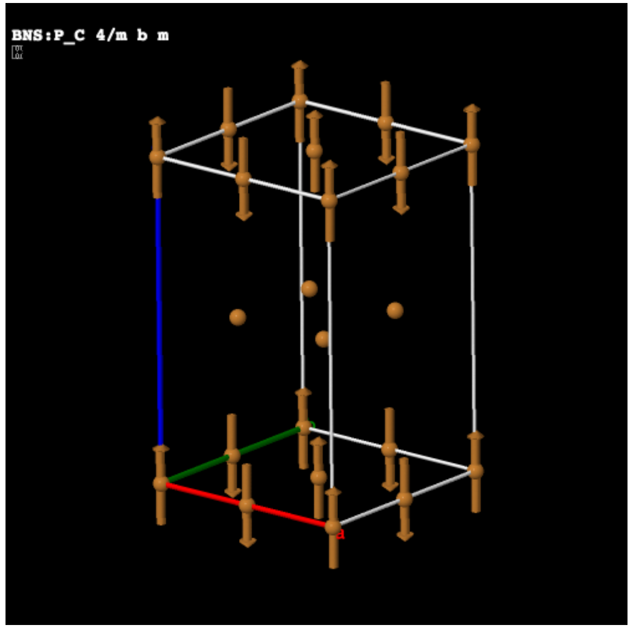
Scheme of the three possible 2k magnetic structures of maximal symmetry with propagation vectors (1/2,1/2,0) and (-1/2,1/2,0), parent space group /4/mmm, magnetic atom at site 2a, and a single primary irrep active.



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)