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Symmetry-based computational tool for magnetic crystallography in the Bilbao Crystallographic Server: Hands on tutorial

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Open access website with crystallographic databases and programs for structural and mathematical crystallography, solid state physics and structural chemistry (PHASE TRANSITIONS).

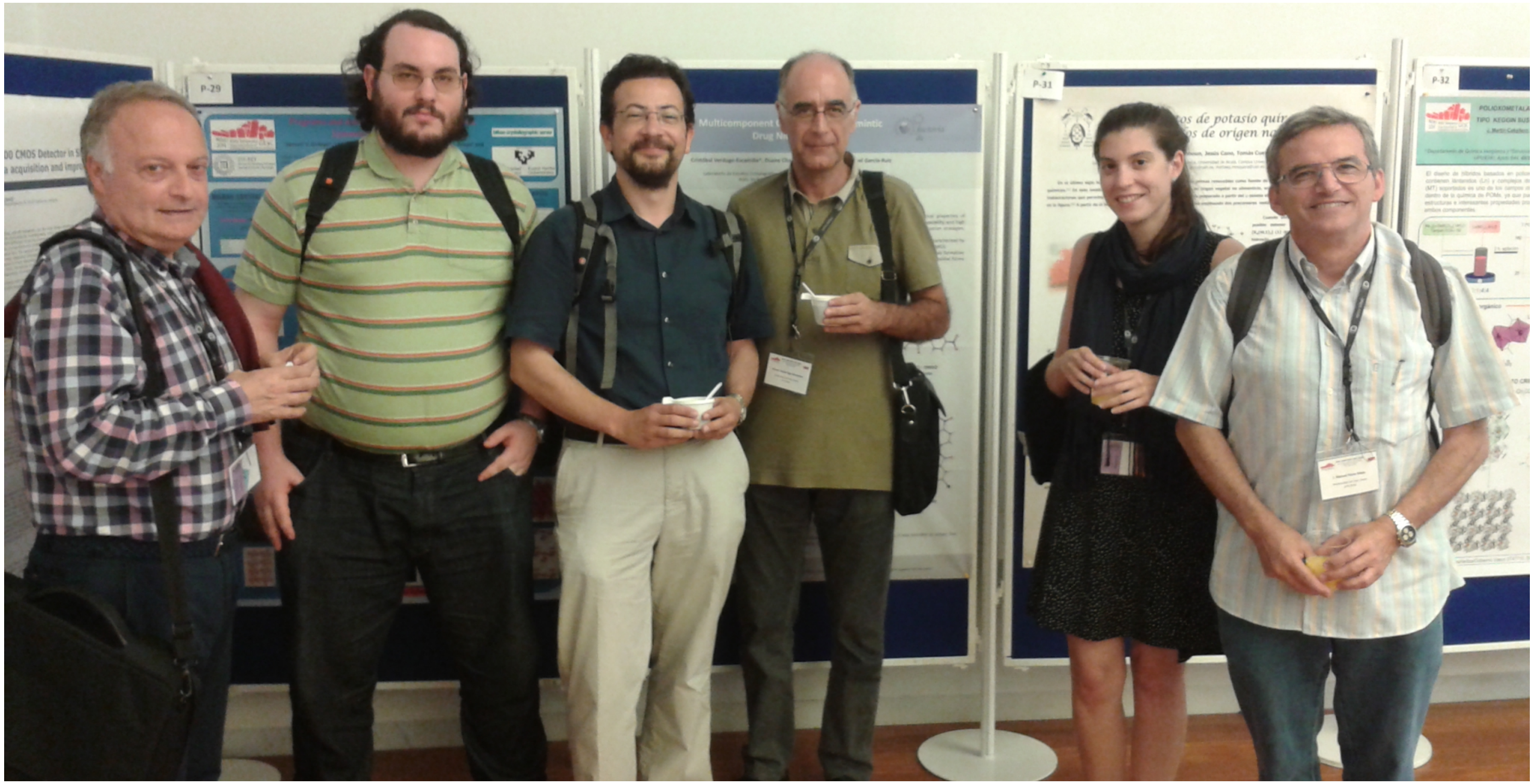
bilbao crystallographic server

[The crystallographic site at the Condensed Matter Physics Dept. of the University of the Basque Country]

started in 1997

present team:

- Emre Tasci
- Gemma de la Flor
- Samuel V. Gallego
- Luis Elcoro
- Gotzon Madariaga
- Mois I. Aroyo
- J. Manuel Perez-Mato



bilbao crystallographic server

[The crystallographic site at the Condensed Matter Physics Dept. of the University of the Basque Country]

started 1997

past members:

- D. Orobengoa
- C. Capillas
- E. Kroumova
- S. Ivantchev

external contributors:

- H. Stokes& B. Campbell (USA) - ISODISTORT
- H. Wondratchek (Germany)
- J. Rodriguez-Carvajal (France) - FULLPROF
- V. Petricek (Chequia) – JANA2006
- A. Kirov (Bulgaria)
- M. Nespolo (France)
- K. Momma (Japan) - VESTA
- R. Hanson (USA) - Jmol

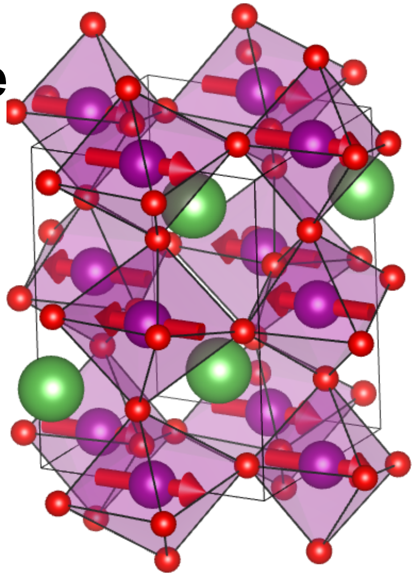
Magnetic Space Groups	
MGENPOS	General Positions of Magnetic Space Groups
MWYCKPOS	Wyckoff Positions of Magnetic Space Groups
MAGNEXT	Extinction Rules of Magnetic Space Groups
MAXMAGN	Maximal magnetic space groups for a given space group and a propagation vector

General Positions of the Group *Pn'ma'* (#62.448)

For this space group, BNS and OG settings coincide.
Its label in the OG setting is given as: Pn'ma' (#62.8.509)

N	Standard/Default Setting			
	(x,y,z) form	Matrix form	Geom. interp.	Seitz notation
1	x, y, z, +1 m_x,m_y,m_z	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	1 +1	(1|0,0,0)
2	-x, -y, -z, +1 m_x,m_y,m_z	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \end{pmatrix}$	-1 0,0,0 +1	(-1|0,0,0)
3	-x, y+1/2, -z, +1 $-m_x,m_y,-m_z$	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1/2 \\ 0 & 0 & -1 & 0 \end{pmatrix}$	2 (0,1/2,0) 0,y,0 +1	(2_y|0,1/2,0)
4	x, -y+1/2, z, +1 $-m_x,m_y,-m_z$	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 1/2 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	m x,1/4,z +1	(m_y|0,1/2,0)
5	x+1/2, -y+1/2, -z+1/2, -1 $-m_x,m_y,m_z$	$\begin{pmatrix} 1 & 0 & 0 & 1/2 \\ 0 & -1 & 0 & 1/2 \\ 0 & 0 & -1 & 1/2 \end{pmatrix}'$	2 (1/2,0,0) x,1/4,1/4 -1	(2_x'|1/2,1/2,1/2)
6	-x+1/2, -y, z+1/2, -1 $m_x,m_y,-m_z$	$\begin{pmatrix} -1 & 0 & 0 & 1/2 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 1/2 \end{pmatrix}'$	2 (0,0,1/2) 1/4,0,z -1	(2_z'|1/2,0,1/2)
7	-x+1/2, y+1/2, z+1/2, -1 $-m_x,m_y,m_z$	$\begin{pmatrix} -1 & 0 & 0 & 1/2 \\ 0 & 1 & 0 & 1/2 \\ 0 & 0 & 1 & 1/2 \end{pmatrix}'$	n (0,1/2,1/2) 1/4,y,z -1	(m_x'|1/2,1/2,1/2)
8	x+1/2, y, -z+1/2, -1 $m_x,m_y,-m_z$	$\begin{pmatrix} 1 & 0 & 0 & 1/2 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 1/2 \end{pmatrix}'$	a x,y,1/4 -1	(m_z'|1/2,0,1/2)

Example



$LaMnO_3$

Pn'ma' (62.448)

Magnetic Space Groups	
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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

Wyckoff Positions of the Group *Pn'ma'* (#62.448)

For this space group, BNS and OG settings coincide.
Its label in the OG setting is given as: Pn'ma' (#62.8.509)

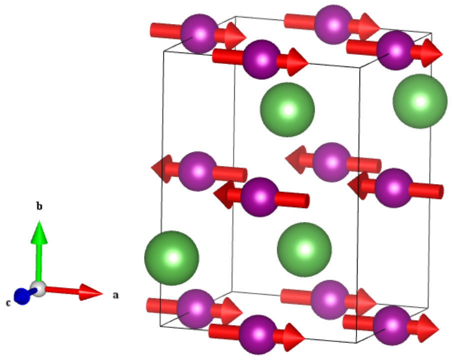
Multiplicity	Wyckoff letter	Coordinates	
8	d	$(x,y,z \mid m_x,m_y,m_z)$	$(x+1/2,-y+1/2,-z+1/2 \mid -m_x,m_y,m_z)$
		$(-x,y+1/2,-z \mid -m_x,m_y,-m_z)$	$(-x+1/2,-y,z+1/2 \mid m_x,m_y,-m_z)$
		$(-x,-y,-z \mid m_x,m_y,m_z)$	$(-x+1/2,y+1/2,z+1/2 \mid -m_x,m_y,m_z)$
		$(x,-y+1/2,z \mid -m_x,m_y,-m_z)$	$(x+1/2,y,-z+1/2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

Site Symmetries of the Wyckoff Positions

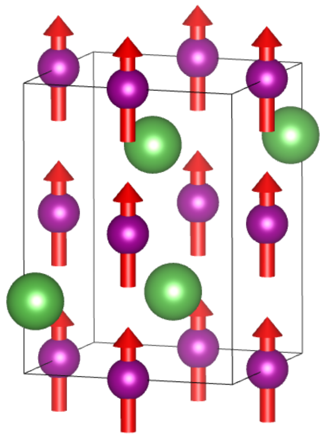
WP	Representative	Site symmetry
4a	$(0,0,0 \mid m_x,m_y,m_z)$	-1
4b	$(0,0,1/2 \mid m_x,m_y,m_z)$	-1
4c	$(x,1/4,z \mid 0,m_y,0)$	.m.
8d	$(x,y,z \mid m_x,m_y,m_z)$	1

Space Group:
Pn'ma'

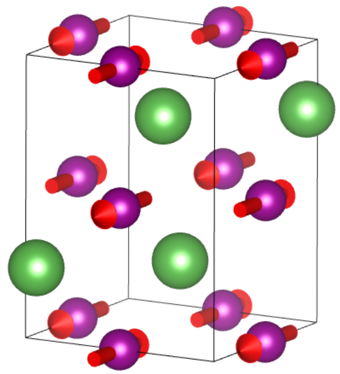
<table>
<tr><th>Multiplicity</th><th>Wyckoff letter</th><th>Coordinates</th><th></th></tr>
<tr><td>8</td><td>d</td><td>$(x,y,z \mid m_x,m_y,m_z)$ $(x+1/2,-y+1/2,-z+1/2 \mid -m_x,m_y,m_z)$
$(-x,y+1/2,-z \mid -m_x,m_y,-m_z)$ $(-x+1/2,-y,z+1/2 \mid m_x,m_y,-m_z)$
$(-x,-y,-z \mid m_x,m_y,m_z)$ $(-x+1/2,y+1/2,z+1/2 \mid -m_x,m_y,m_z)$
$(x,-y+1/2,z \mid -m_x,m_y,-m_z)$ $(x+1/2,y,-z+1/2 \mid m_x,m_y,-m_z)$</td><td></td></tr>
<tr><td>4</td><td>c</td><td>$(x,1/4,z \mid 0,m_y,0)$ $(x+1/2,1/4,-z+1/2 \mid 0,m_y,0)$
$(-x,3/4,-z \mid 0,m_y,0)$ $(-x+1/2,3/4,z+1/2 \mid 0,m_y,0)$</td><td>**La**</td></tr>
<tr><td>4</td><td>b</td><td>$(0,0,1/2 \mid \boxed{m_x,m_y,m_z})$ $(1/2,1/2,0 \mid \boxed{-m_x,m_y,m_z})$
$(0,1/2,1/2 \mid \boxed{-m_x,m_y,-m_z})$ $(1/2,0,0 \mid \boxed{m_x,m_y,-m_z})$</td><td>**Mn**</td></tr>
<tr><td>4</td><td>a</td><td>$(0,0,0 \mid m_x,m_y,m_z)$ $(1/2,1/2,1/2 \mid -m_x,m_y,m_z)$
$(0,1/2,0 \mid -m_x,m_y,-m_z)$ $(1/2,0,1/2 \mid m_x,m_y,-m_z)$</td><td></td></tr>
</table>



A_x mode along x



F_y mode along y
weak ferromagnet



G_z mode along z

Magnetic Space Groups

MGENPOS	General Positions of Magnetic Space Groups
MWYCKPOS	Wyckoff Positions of Magnetic Space Groups
MAGNEXT	Extinction Rules of Magnetic Space Groups

MAGNEXT

MAGNEXT: Magnetic Systematic Absences

tinction rules for
any Shubnikov magnetic

pe obtained introducing the
d 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

Diffraction symmetry (non-polarized) and systematic absences

Non-polarized magnetic diffraction at diffraction vector $\boldsymbol{H}$ is proportional to the component of $\boldsymbol{F}_M(\boldsymbol{H})$ perpendicular to $\boldsymbol{H}$

$$\boldsymbol{H} = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^* = (h,k,l)$$

Consequences of a symmetry operation $\{\boldsymbol{R},\theta|\boldsymbol{t}\}$:

non-magnetic: $F(\boldsymbol{H}) = e^{i2\pi \boldsymbol{H}.\boldsymbol{t}}\, F(\boldsymbol{H}.\boldsymbol{R})$ Intensity($\boldsymbol{H}.\boldsymbol{R}$)=Intensity($\boldsymbol{H}$)

magnetic: $\boldsymbol{F}_M(\boldsymbol{H}) = \theta\, det(\boldsymbol{R})\, e^{i2\pi \boldsymbol{H}.\boldsymbol{t}}\, \boldsymbol{R}.\, \boldsymbol{F}_M(\boldsymbol{H}.\boldsymbol{R})$ Intensity($\boldsymbol{H}.\boldsymbol{R}$)=Intensity($\boldsymbol{H}$)

$$\boldsymbol{H}.\boldsymbol{t} = ht_1+kt_2+lt_3$$

$$\boldsymbol{H}.\boldsymbol{R} = (h,k,l).\boldsymbol{R}$$

Diffraction symmetry (non-polarized) and systematic absences

$$\boldsymbol{H} = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^* = (h,k,l)$$

Extinction rules: ("trivial" cases)

{1'| 0 0 0 }

(non-magnetic structures)

$$F(\boldsymbol{H}) = e^{i2\pi \boldsymbol{H.t}} F(\boldsymbol{H.R}) \rightarrow F(\boldsymbol{H}) = F(\boldsymbol{H})$$

no condition

$$\boldsymbol{F}_M(\boldsymbol{H}) = \theta\, det(\boldsymbol{R})\, e^{i2\pi \boldsymbol{H.t}}\, \boldsymbol{R}.\, \boldsymbol{F}_M(\boldsymbol{H.R}) \rightarrow \boldsymbol{F}_M(\boldsymbol{H}) = -\boldsymbol{F}_M(\boldsymbol{H})$$

zero!

{1'| 0 0 1/2 }

(type IV MSG)

$$F(\boldsymbol{H}) = e^{i\pi l} F(\boldsymbol{H})$$

Nuclear diffraction: absent l = odd

$$\boldsymbol{F}_M(\boldsymbol{H}) = -\, e^{i\pi l}\, \boldsymbol{F}_M(\boldsymbol{H})$$

Magnetic diffraction: absent l= even

Diffraction symmetry (non-polarized) and systematic absences

$$\boldsymbol{H} = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^* \quad = \quad (h,k,l)$$

Extinction rules:

$\{2_z | \, 0\ 0\ 0\ \}$

$\boldsymbol{H}=(0,0,l)$

$\boldsymbol{H}.2_z = \boldsymbol{H}$

$F(\boldsymbol{H}) = e^{i2\pi \boldsymbol{H}.\boldsymbol{t}} F(\boldsymbol{H}) \rightarrow F(\boldsymbol{H}) = F(\boldsymbol{H}) \rightarrow$ no condition

$\boldsymbol{F}_M(\boldsymbol{H}) = \theta\, det(\boldsymbol{2_z})\, e^{i2\pi \boldsymbol{H}.\boldsymbol{t}}\, \boldsymbol{2_z}.\, \boldsymbol{F}_M(\boldsymbol{H}) \rightarrow \boldsymbol{F}_M(\boldsymbol{H}) = \boldsymbol{2_z}.\, \boldsymbol{F}_M(\boldsymbol{H})$

$e^{i2\pi \boldsymbol{H}.\boldsymbol{t}}$

$\boldsymbol{F}_M=(0,0,Fz)$ // $\boldsymbol{H}$ **absence for all (0,0,*l*)**

$\{2_z | \, 0\ 0\ ½\ \}$

$\boldsymbol{H}=(0,0,l)$

$\boldsymbol{H}.2_z = \boldsymbol{H}$

$F(\boldsymbol{H}) = e^{i2\pi \boldsymbol{H}.\boldsymbol{t}} F(\boldsymbol{H}) \rightarrow F(\boldsymbol{H}) = e^{i\pi l} F(\boldsymbol{H}) \rightarrow$ absence for *l*=odd

$\boldsymbol{F}_M(\boldsymbol{H}) = \theta\, det(\boldsymbol{2_z})\, e^{i2\pi \boldsymbol{H}.\boldsymbol{t}}\, \boldsymbol{2_z}.\, \boldsymbol{F}_M(\boldsymbol{H}) \rightarrow$

$\boldsymbol{F}_M(\boldsymbol{H}) = e^{i\pi l}\, \boldsymbol{2_z}.\, \boldsymbol{F}_M(\boldsymbol{H})$

l =even: $\boldsymbol{F}_M=(0,0,Fz)$ // $\boldsymbol{H}$ **absence**

l =odd $\boldsymbol{F}_M=(Fx,Fy,0)$ not parallel to $\boldsymbol{H}$ **presence**

Systematic absences for $\{2'_z | \, 0\ 0\ ½\ \}$?

Using MAGNEXT in its option B, re-obtain the systematic absences for the symmetry operations $\{2_z \mid 0\ 0\ 0\}$; and for $\{2_z \mid 0\ 0\ ½\}$, and obtain those for the corresponding primed operations.
(exercise 5)

Using MAGNEXT obtain the systematic absences that should fulfill the magnetic diffraction of LaMnO3
(space group Pn'ma', moments along x)
(exercise 6)

Magnetic diffraction Systematic Absences for the group *Pn'ma'* (#62.448)

For this space group, BNS and OG settings coincide.
Its label in the OG setting is given as: Pn'ma' (#62.8.509)

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

Systematic absences for special reflections:

Diffraction vector type: **(0 k 0)** -> Systematic absence: **k = 2n**

```
For k = 1:    I /= 0    F = (Fx,0,0)
For k = 2:    I = 0     F = (0,Fy,0)
```

Diffraction vector type: **(h 0 0)** -> Systematic absence: **h = 2n + 1**

```
For h = 1:    I = 0     F = (0,0,0)
For h = 2:    I /= 0    F = (0,Fy,0)
```

Diffraction vector type: **(0 0 l)** -> Systematic absence: **l = 2n + 1**

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

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

Go to the list of the General Positions of the Group *Pn'ma'* (#62.448) [OG:*Pn'ma'* (#62.8.509)]
Go to the list of the Wyckoff Positions of the Group *Pn'ma'* (#62.448) [OG:*Pn'ma'* (#62.8.509)]

[Show systematic absences in a different setting]

Symmetry-adapted form of the Structure Factors

Magnetic Space Group: *Pn'ma'* (#62.448) [OG: *Pn'ma'* (#62.8.509)]

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

Structure factors for general reflections (produced by centrings):

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

For any h,k,l:	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,k,0**

For k = 1:	I /= 0	F = (Fx,0,0)
For k = 2:	I = 0	F = (0,Fy,0)

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

For h = 1, l = 1:	I /= 0	F = (0,Fy,0)
For h = 1, l = 2:	I /= 0	F = (0,Fy,0)
For h = 2, l = 1:	I /= 0	F = (0,Fy,0)
For h = 2, l = 2:	I /= 0	F = (0,Fy,0)

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

For h = 1:	I = 0	F = (0,0,0)
For h = 2:	I /= 0	F = (0,Fy,0)

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

For l = 1:	I = 0	F = (0,0,0)
For l = 2:	I /= 0	F = (0,Fy,0)

For more subtle systematic absences in LaMnO3 (due to the special position of the magnetic atoms), see:

research papers

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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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Magnetic Space Groups	
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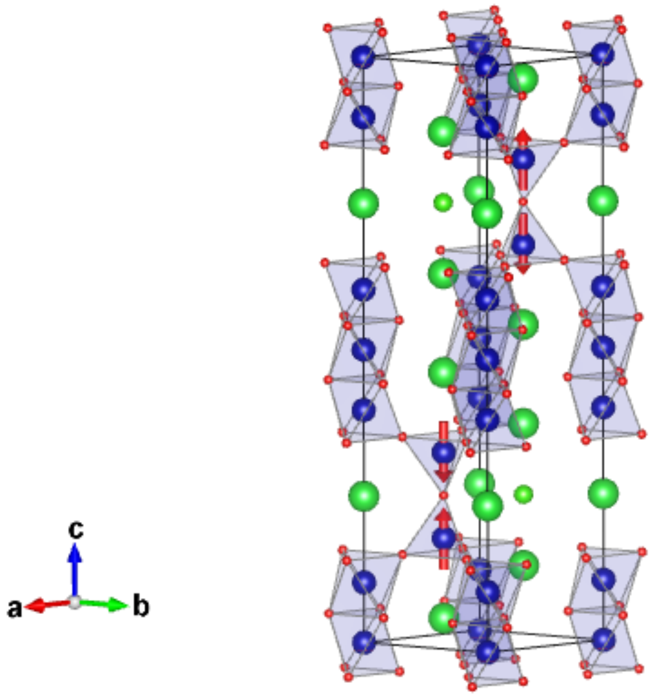
$Ba_5Co_5ClO_{13}$



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**
present l odd

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

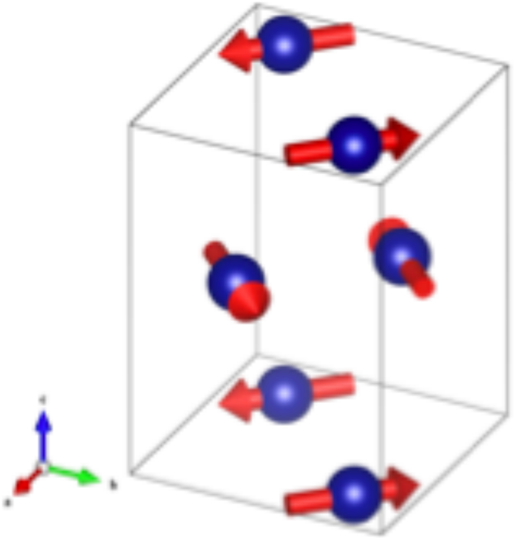
(spins are symmetry restricted to be along c in both groups)

Paraelectric phase **$P4_2/mnm$**

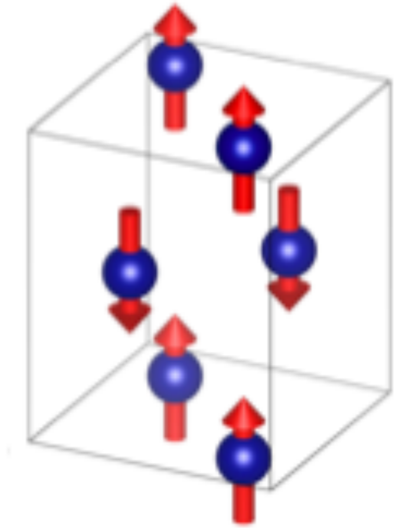
Site 4f

magnetic absences
(*common for the two MSGs*)

(h,0,0) h even
(0,k,0) k even
(0,0,l) l any



(a) $P4_2'/m'n'm$ (136.499)



(b) $P4_2'/mnm'$ (136.500)

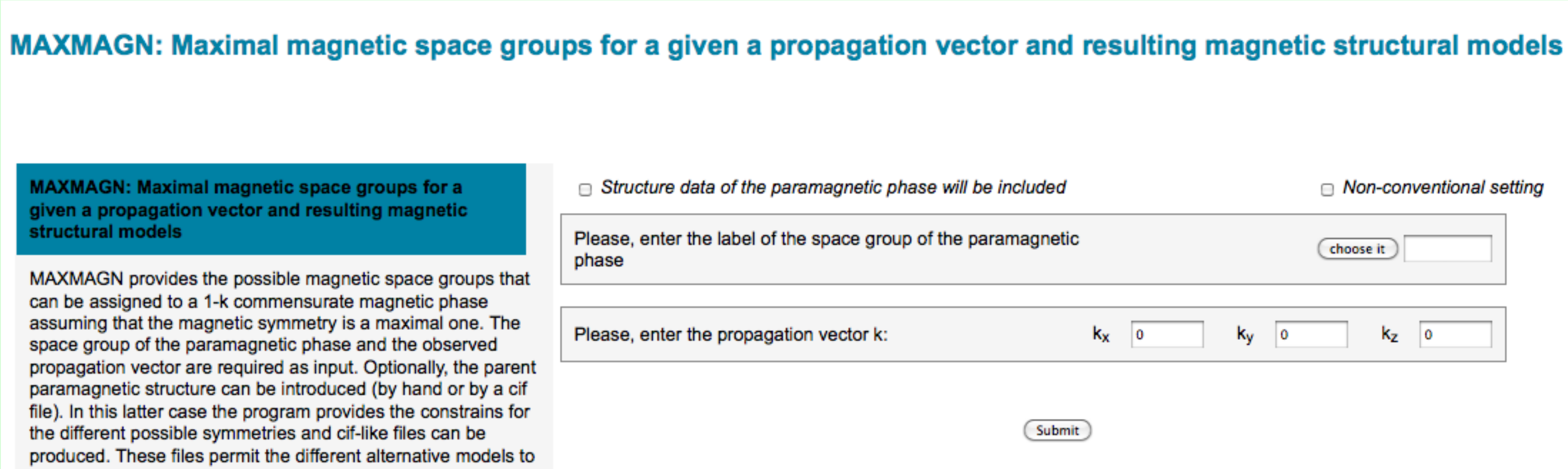
structure factor is necessarily of the form:

(0,0,Fz)

(0,k,l) k+l odd (Fx,0,0)
(h,0,l) h+l odd (0,Fy,0)

absences that permit to distinguish the two MSGs

Magnetic Symmetry and Applications	
MGENPOS	General Positions of Magnetic Space Groups
MWYCKPOS	Wyckoff Positions of Magnetic Space Groups
MAGNEXT	Extinction Rules of Magnetic Space Groups
IDENTIFY MAGNETIC GROUP	Identification of a Magnetic Space Group from a set of generators in an arbitrary setting
MPOINT ⚠	Magnetic Point Group Tables
MAXMAGN	Maximal magnetic space groups for a given a propagation vector and resulting magnetic structural models
MAGMODELIZE	Magnetic structure models for any given magnetic symmetry
k-SUBGROUPSMAG	Magnetic subgroups consistent with some given propagation vector(s) or a supercell
MAGNDATA ⚠	A collection of magnetic structures with transportable cif-type files
MVISUALIZE ⚠	3D Visualization of magnetic structures with Jmol
MTENSOR ⚠	Symmetry-adapted form of magnetic crystal tensors



MAXMAGN

The program provides ALL possible MAXIMAL magnetic symmetries for single-k magnetic structures compatible with a known propagation vector.

For each possible symmetry, a starting magnetic structure model is provided, with the symmetry constraints and the parameters to be fitted.

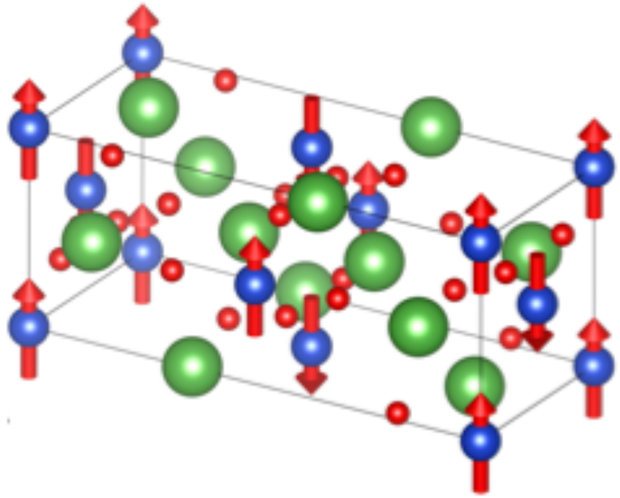
Usually magnetic phases comply with one of these MAXIMAL symmetries. But if necessary, one can descend to lower symmetries, liberating some of the constraints on the magnetic moments (and atomic positions).

For simple propagation vectors: A very efficient and simpler alternative method to representation method

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



$P_A ccn$ (56.374)

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

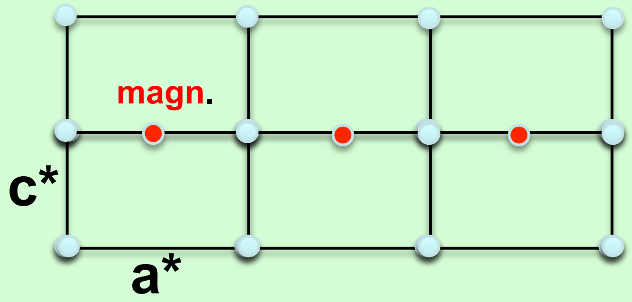
Use MAXMAGN to explore the four possible alternative models of maximal symmetry for $HoMnO_3$ (exercise 7)

7. Obtain with MAXMAGN the four possible alternative models of maximal symmetry for the magnetic structure of $HoMnO_3$, which are compatible with its propagation vector k= (1/2,0,0) (upload as starting data the cif file of its parent Pnma structure). Obtain the symmetry constraints for the moments of the Ho atoms, in each case. Check that the two possible orthorhombic symmetries can be distinguished by the systematic absence of all reflections of type (h, 0,l)+k, which will happen for one of the groups and not the other, if the spins are aligned along a. See tutorial of MAXMAGN, example 2, for a more detailed tutorial exercise. (file required: *3.HoMnO3_parent.cif*).

Tutorial MAXMAGN, example 2

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

diffraction peaks:



Gp= Pnma

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

Maximal magnetic space groups for the space group 62 (*Pnma*) and the propagation vector k = (1/2, 0, 0)

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

N	Group (BNS)	Transformation matrix	General positions	Systematic absences	Magnetic structure
1	$P_a na2_1$ (#33.149)	$\begin{pmatrix} -2 & 0 & 0 & 1/4 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (twin-related)	Show	Show	Show
2	$P_b mn2_1$ (#31.129)	$\begin{pmatrix} 0 & 2 & 0 & 1/4 \\ -1 & 0 & 0 & 1/4 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (twin-related)	Show	Show	Show
3	$P_c 2_1/c$ (#14.82)	$\begin{pmatrix} -2 & 0 & 2 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}$ Alternatives (twin-related)	Show	Show	Show
4	$P_a 2_1/m$ (#11.55)	$\begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (twin-related)	Show	Show	Show

$P_a na2_1$

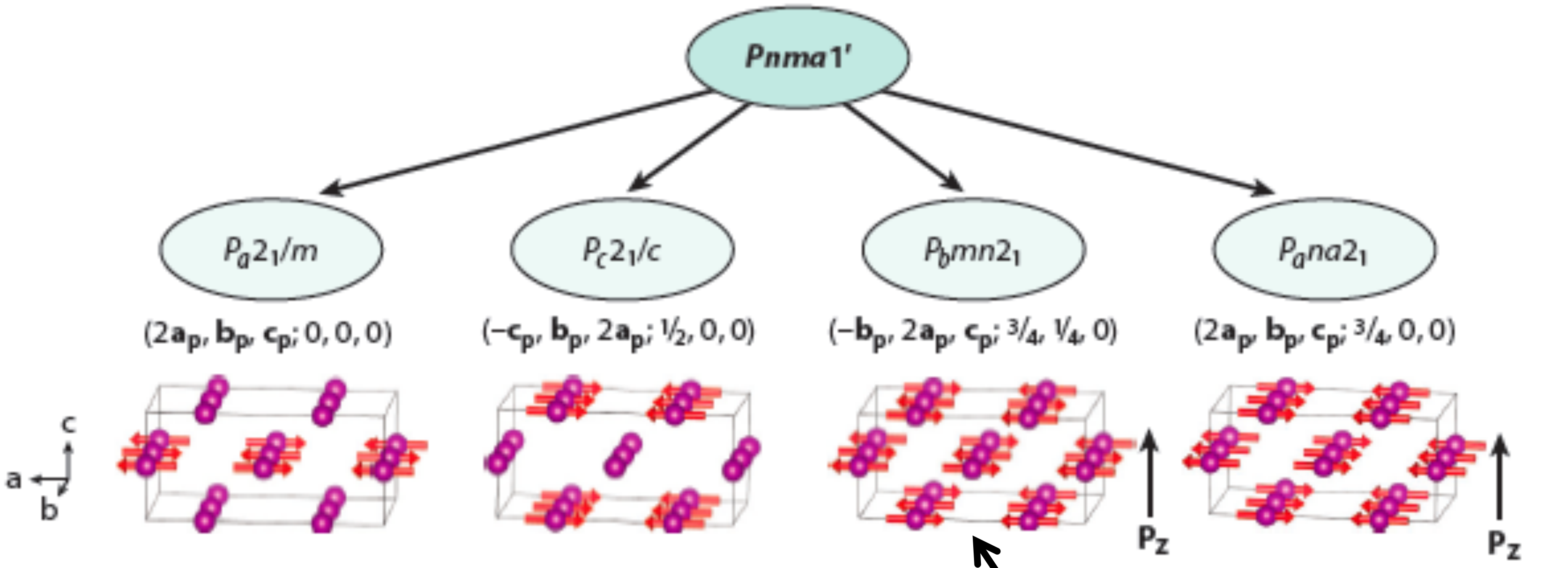
$P_a nm2_1$

$P_a 2_1/a$

$P_a 2_1/m$

$HoMnO_3$ An Inevitable Multiferroic...

parent space group: Pnma, k=(1/2,0,0)

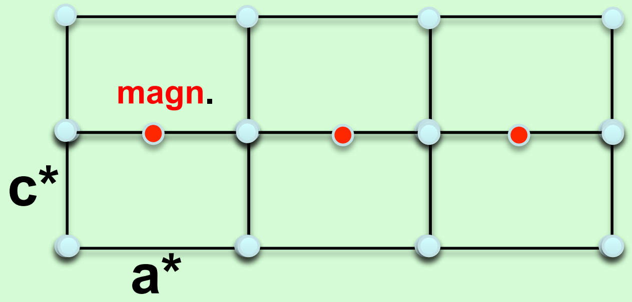


graphic models are depicted
assuming collinearity along x
(my and mz are symmetry allowed)

Structure reported in 2001, but authors unaware of its multiferroic character

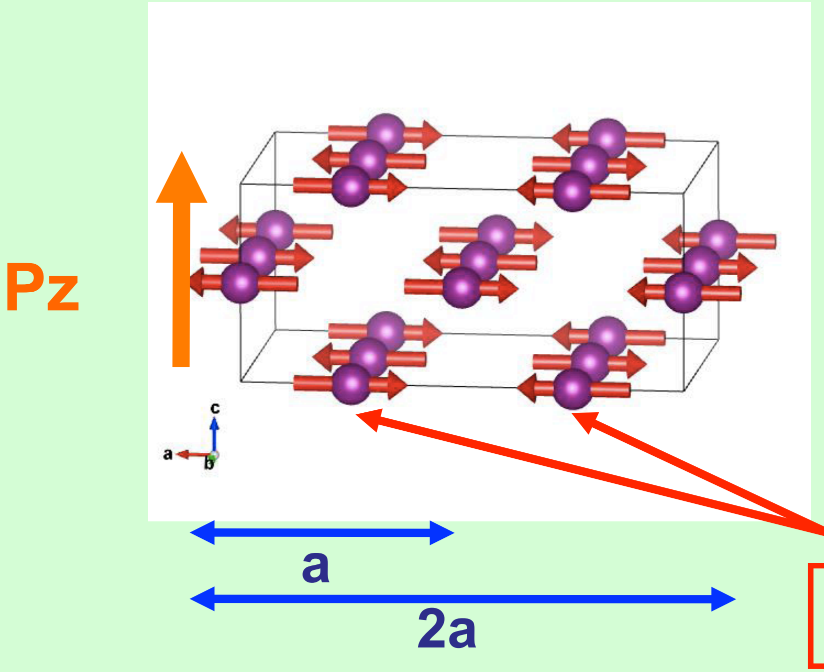
A more complex example : $HoMnO_3$ (Muñoz et al. Inorg. Chem. 2001)

diffraction peaks:



Gp= Pnma

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



{1'|1/2 0 0}

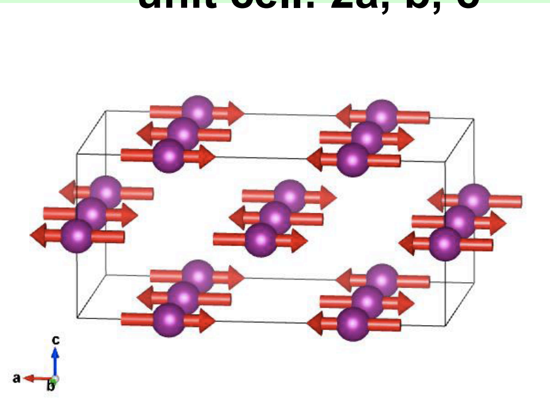
Equivalent to a lattice translation for the positions

Magnetic group		point group
Pnma1' → P_anm2_1	P_z Induced polarization: multiferroic	mm2 1’
Pnma1' → P_a2_1/m		2/m 1’
Pnma1' → P_ana2_1		mm2 1’
Pnma1' → P_a2_1/a		2/m 1’

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

$HoMnO_3$

unit cell: 2a, b, c



Magnetic space group: $P_a nm2_1$ (31.129)

(non-conventional setting)

WP	+ (1'|1/2 0 0)
8b	$(x, y, z \mid m_x, m_y, m_z)$, $(-x+1/4, -y, z+1/2 \mid -m_x, -m_y, m_z)$, $(x, -y+1/2, z \mid -m_x, m_y, -m_z)$, $(-x+1/4, y+1/2, z+1/2 \mid m_x, -m_y, -m_z)$
4a	$(x, 1/4, z \mid 0, m_y, 0)$, $(-x+1/4, 3/4, z+1/2 \mid 0, -m_y, 0)$

Equivalent to the use of space group **$Pnm2_1$(31)** with **half cell along a**:

Atomic positions of asymmetric unit:

Ho1 4a 0.04195 0.25000 0.98250
Ho2 4a 0.95805 0.75000 0.01750
Mn1 8b 0.00000 0.00000 0.50000
O1 4a 0.23110 0.25000 0.11130
O12 4a 0.76890 0.75000 0.88870
O2 8b 0.16405 0.05340 0.70130
O22 8b 0.83595 0.55340 0.29870

Split independent positions in the lower symmetry

General position:
x, y, z not restricted by symmetry!

Magnetic moments of the asymmetric unit (μB):

Mn1 3.87 ≈0.0 ≈0.0

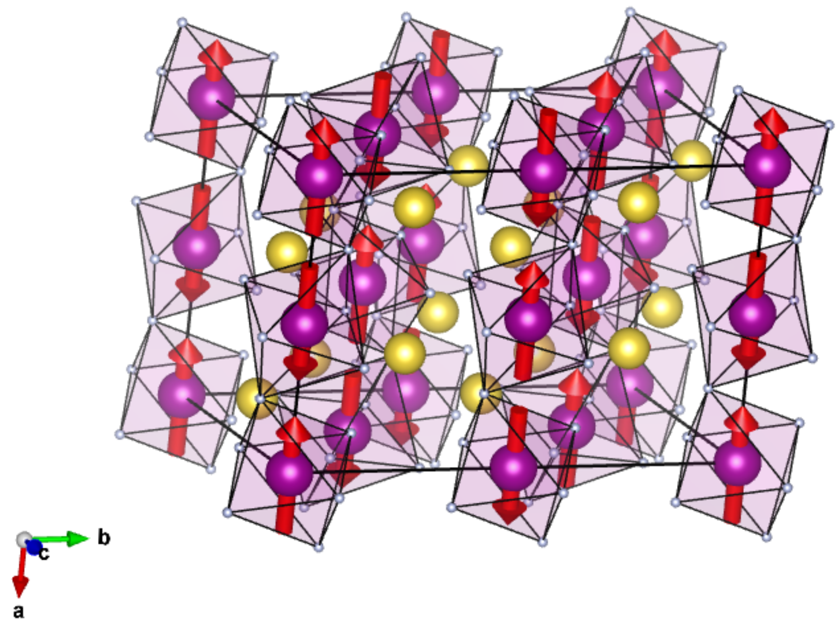
a CIF-type file can be produced:

These files permit the different alternative models to be analyzed, refined, shown graphically, transported to ab-initio codes etc., with programs as ISODISTORT, JANA2006, STRCONVERT, etc. A controlled descent to lower symmetries is also possible.

```
_space_group.magn_number_BNS   31.129
_space_group.magn_name_BNS     "P_b m n 2_1"
_space_group.magn_point_group "mm21'"
_space_group.magn_point_group_number "7.2.21"
_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_id
_space_group_symop.magn_operation_xyz
_space_group_symop.magn_operation_mxmymz
1 x,y,z,+1 mx,my,mz
2 -x+3/4,-y,z+1/2,+1 -mx,-my,mz
3 x,-y+1/2,z,+1 -mx,my,-mz
4 -x+3/4,y+1/2,z+1/2,+1 mx,-my,-mz

loop_
_space_group_symop.magn_centering_id
_space_group_symop.magn_centering_xyz
_space_group_symop.magn_centering_mxmymz
1 x,y,z,+1 mx,my,mz
2 x+1/2,y,z,-1 -mx,-my,-mz

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Ho Ho 0.04195 0.25000 0.98250 1
Ho_1 Ho 0.95805 0.75000 0.01750 1
Mn Mn 0.00000 0.00000 0.50000 1
O1 O 0.23110 0.25000 0.11130 1
O1_1 O 0.7689 0.75000 0.88870 1
O2 O 0.16405 0.05340 0.70130 1
O2_1 O 0.83595 0.55340 0.29870 1

loop_
_atom_site_moment_label
_atom_site_moment_crystalaxis_x
_atom_site_moment_crystalaxis_y
_atom_site_moment_crystalaxis_z
Mn 3.87 0.0 0.0
```

Derive the symmetry constraints on some crystal tensor properties of a magnetic phase using MTENSOR (exercise 10)

8. Use MTENSOR to obtain some of the crystal tensor properties of the magnetic phase of $HoMnO_3$ (electric polarization, magnetization, linear magnetoelectric tensor, cuadratic magnetoelectricity,...). The same for the magnetic phase of $LaMnO_3$. (Upload the corresponding mcif files in STRCONVERT, copy the list of symmetry operations in the output of STRCONVERT and paste in the option B of MTENSOR, but deleting the translational parts, so that the point-group operations are left). *(files required: 2.HoMnO3.mcif and 4.LaMnO3.mcif)*



Na_2MnF_5 Parent: $P2_1/c$

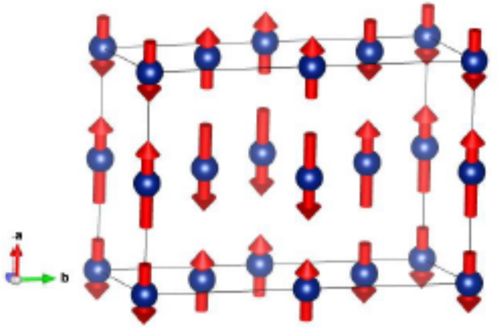
k= (0, 1/2, 0)

Derive the possible orderings of maximal symmetry

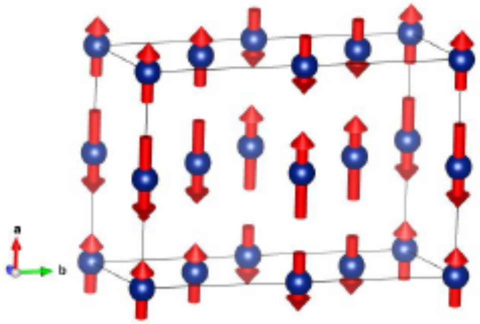
(exercise 9)

Tutorial MAXMAGN, example 2

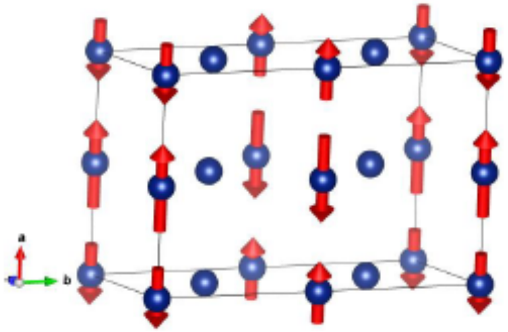
9. From the knowledge of its parent space group and its propagation vector (P21/c and k=(0,1/2,0)), use k-SUBGROUPSMAG to explore all possible symmetries of the magnetic structure of Na_2MnF_5 and check that the system is probably a multiferroic of type II, with the magnetic ordering breaking the symmetry into a polar phase. Assuming that the Fe spins are aligned along a, obtain with MAXMAGN the two possible alternative models of maximal symmetry. See tutorial of MAXMAGN, example 4. (file required: 5.Na2MnF5_parent.cif)



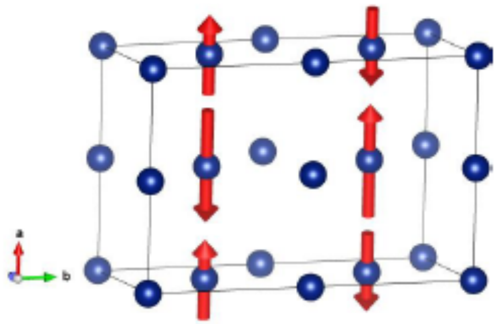
P_bc (a,2b,c;0 1/4 0)



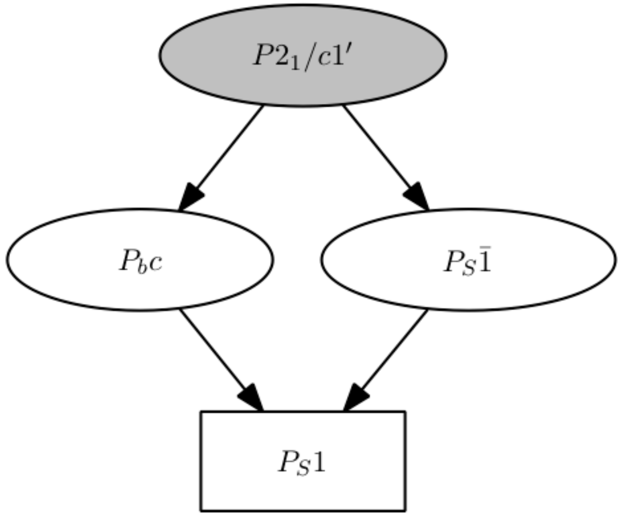
P_bc (a,2b,c;0 3/4 0)



P_s-1 (a,-c,2b;0 0 0)



P_s-1 (a,-c,2b;0 1/2 0)



Why a k=(0,1/2,0) magnetic ordering in a structure with parent space group $P2_1/c$ breaks necessarily its point group symmetry of the structure?

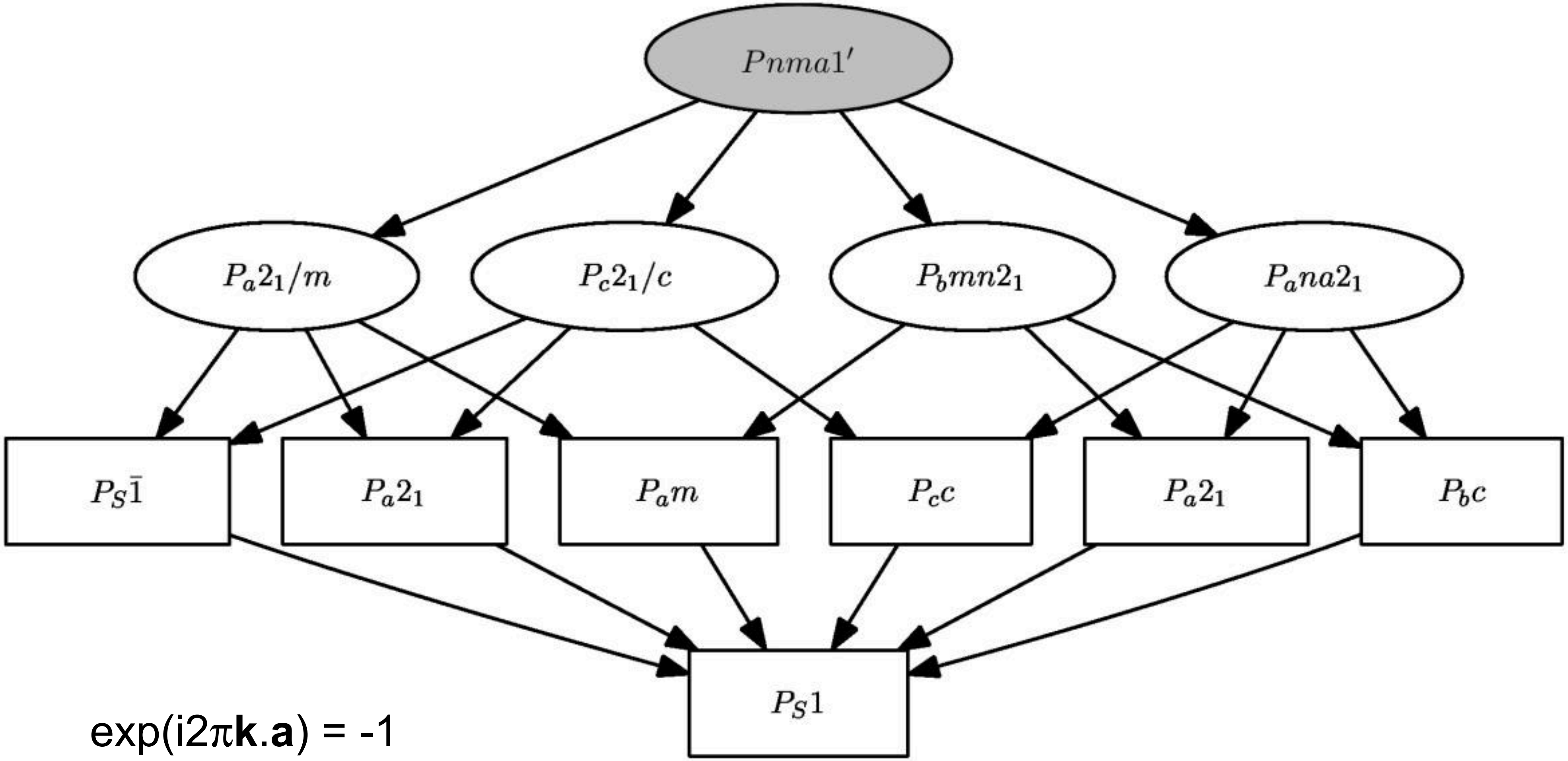
Because the lattice (and "antilattice") resulting from this k-vector is incompatible with the screw operation $\{2_y|0\ ½\ 0\}$ …

10. Using k-SUBGROUPSMAG obtain the k-maximal subgroups for the parent space group P2/c for a propagation vector k=(0,1/2,0), and compare with those obtained for $P2_1/c$. Check that in the case of a parent P2/c symmetry the inversion symmetry is not lost in any of the possible maximal MSGs. This happens fin the case of $P2_1/c$ symmetry because the binary rotation includes a non-trivial translation.

Use k-SUBGROUPSMAG to explore all possible symmetries for $HoMnO_3$ (exercise 8)

11. Using k-SUBGROUPSMAG explore all possible symmetries for the magnetic structure of $HoMnO_3$, which are compatible with its propagation vector. Check that there are two different possible MSGs of the same type, namely of type P_a2_1. From the output of the program for the two groups, determine what makes them different.

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



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

Symmetry operation {1'|1/2,0,0} is present in any case: all MSGs are type IV

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