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).
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started in 1997

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started 1997
### 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)

#### Magnetic Space Groups

- **MGPOS**: General Positions of Magnetic Space Groups
- **MWYKPOS**: 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

#### Table: Standard/Default Setting

<table>
<thead>
<tr>
<th>N</th>
<th>(x,y,z) form</th>
<th>Matrix form</th>
<th>Geom. interp.</th>
<th>Selz notation</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>x, y, z, +1</td>
<td>m_x, m_y, m_z</td>
<td>1 +1</td>
<td>(1</td>
</tr>
<tr>
<td>2</td>
<td>-x, -y, -z, +1</td>
<td>m_x, m_y, m_z</td>
<td>-1 0,0, 0 +1</td>
<td>(-1</td>
</tr>
<tr>
<td>3</td>
<td>-x, y+1/2, -z, +1</td>
<td>m_x, m_y, m_z</td>
<td>2 (0,1/2,0) 0,0, +1</td>
<td>(2</td>
</tr>
<tr>
<td>4</td>
<td>x, -y+1/2, z, +1</td>
<td>m_x, m_y, m_z</td>
<td>m x,1/4,z +1</td>
<td>(m</td>
</tr>
<tr>
<td>5</td>
<td>x+1/2, -y+1/2, -z+1/2, -1</td>
<td>m_x, m_y, m_z</td>
<td>2 (1/2,0,0) x,1/4,1/4 +1</td>
<td>(2</td>
</tr>
<tr>
<td>6</td>
<td>-x+1/2, -y, z+1/2, -1</td>
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<td>2 (0,0,1/2) 1/4,0,z -1</td>
<td>(2</td>
</tr>
<tr>
<td>7</td>
<td>-x+1/2, y+1/2, z+1/2, -1</td>
<td>m_x, m_y, m_z</td>
<td>n (0,1/2,1/2) 1/4,y,z -1</td>
<td>(m</td>
</tr>
<tr>
<td>8</td>
<td>x+1/2, y, -z+1/2, -1</td>
<td>m_x, m_y, m_z</td>
<td>a x,y,1/4 -1</td>
<td>(m</td>
</tr>
</tbody>
</table>

---

**Example**

LaMnO₃

Pn’ma’ (62.448)
Wyckoff Positions of the Group \( \text{Pn}'ma' \) (#62.448)

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

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<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))</td>
</tr>
<tr>
<td></td>
<td></td>
<td>((-x, y+1/2, z \mid -m_x, m_y, m_z)) ((-x+1/2, y+1/2, z+1/2 \mid m_x, -m_y, m_z))</td>
</tr>
<tr>
<td></td>
<td></td>
<td>((-x, y+1/2, z \mid m_x, m_y, m_z)) ((-x+1/2, y+1/2, z+1/2 \mid -m_x, m_y, m_z))</td>
</tr>
<tr>
<td></td>
<td></td>
<td>((x, y+1/2, z \mid -m_x, m_y, m_z)) ((x+1/2, y+1/2, z+1/2 \mid m_x, m_y, m_z))</td>
</tr>
</tbody>
</table>

Site Symmetries of the Wyckoff Positions

<table>
<thead>
<tr>
<th>WP</th>
<th>Representative</th>
<th>Site symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>4a</td>
<td>((0,0,0 \mid m_x, m_y, m_z))</td>
<td>-1</td>
</tr>
<tr>
<td>4b</td>
<td>((0,0,1/2 \mid m_x, m_y, m_z))</td>
<td>-1</td>
</tr>
<tr>
<td>4c</td>
<td>((x,1/4,z \mid 0,m_y,0))</td>
<td>.m.</td>
</tr>
<tr>
<td>8d</td>
<td>((x,y,z \mid m_x, m_y, m_z))</td>
<td>1</td>
</tr>
</tbody>
</table>
### Magnetic Space Groups

<table>
<thead>
<tr>
<th></th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>MGEPON</td>
<td>General Positions of Magnetic Space Groups</td>
</tr>
<tr>
<td>MWYCKPOS</td>
<td>Wyckoff Positions of Magnetic Space Groups</td>
</tr>
<tr>
<td>MAGNEXT</td>
<td>Extinction Rules of Magnetic Space Groups</td>
</tr>
</tbody>
</table>

**MAGNEXT**

**MAGNEXT: Magnetic Systematic Absences**

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**

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 $H$ is proportional to the component of $F_M(H)$ perpendicular to $H$

$$H = ha^* + kb^* + lc^* = (h,k,l)$$

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

non-magnetic: $F(H) = e^{i2\pi H.t} F(H.R)$ \hspace{1cm} Intensity$(H.R)$ = Intensity$(H)$

magnetic: $F_M(H) = \theta \det(R) e^{i2\pi H.t} R \cdot F_M(H.R)$ \hspace{1cm} Intensity$(H.R)$ = Intensity$(H)$

$$H.t = ht_1 + kt_2 + lt_3$$

$$H.R = (h,k,l).R$$
Diffraction symmetry (non-polarized) and systematic absences

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

**Extinction rules: (“trivial” cases)**

- \( \{1' | 0 0 0 \} \) (non-magnetic structures)
  
  \[ F(H) = e^{i2\pi H.t} F(H.R) \]
  
  \[ F(H) = F(H) \]

- \( \{1' | 0 0 1/2 \} \) (type IV MSG)
  
  \[ F(H) = e^{i\pi l} F(H) \]  
  
  \[ F_M(H) = e^{i\pi l} F_M(H) \]

**Nuclear diffraction:** absent \( l = \text{odd} \)

**Magnetic diffraction:** absent \( l = \text{even} \)
Diffraction symmetry (non-polarized) and systematic absences

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

Extinction rules:

For \( \{2_z \mid 0 \ 0 \ 0 \} \):

- \( H = (0, 0, l) \)
- \( H \cdot 2_z = H \)

\[ F(H) = e^{i2\pi H.t} F(H) \quad \rightarrow \quad F(H) = F(H) \]

\[ F_M(H) = \theta \det(2_z) e^{i2\pi H.t} 2_z. F_M(H) \quad \rightarrow \quad F_M(H) = 2_z. F_M(H) \]

\( F_M = (0, 0, Fz) // H \) absence for all \((0, 0, l)\)

For \( \{2_z \mid 0 \ 0 \ \frac{1}{2} \} \):

- \( H = (0, 0, l) \)
- \( H \cdot 2_z = H \)

\[ F(H) = e^{i2\pi H.t} F(H) \quad \rightarrow \quad F(H) = e^{i\pi/l} F(H) \]

\[ F_M(H) = \theta \det(2_z) e^{i2\pi H.t} 2_z. F_M(H) \quad \rightarrow \quad F_M(H) = e^{i\pi/l} 2_z. F_M(H) \]

- \( l = \text{even} \): \( F_M = (0, 0, Fz) // H \) absence
- \( l = \text{odd} \): \( F_M = (Fx, Fy, 0) \) not parallel to \( H \) presence

Systematic absences for \( \{2'_z \mid 0 \ 0 \ \frac{1}{2} \} \)?
5. Using MAGNEXT in its option B, we re-obtain the systematic absences for the symmetry operations \{2z | 0 0 0 \}; and for \{2z | 0 0 ½ \}, and obtain those for the corresponding primed operations.

6. Using MAGNEXT we obtain the systematic absences that should fulfill the magnetic diffraction of LaMnO3 (space group Pn’ma’, moments along x)
Magnetic diffraction Systematic Absences for the group \( Pn\text{'}ma\text{'} (#62.448) \)

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

Values of \( h, k, l \): \( h \text{ integer}, k \text{ integer}, l \text{ integer} \)

Systematic absences for special reflections:

Diffraction vector type: \((0 \ k \ 0)\)  \(\rightarrow\)  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: \((h \ 0 \ 0)\)  \(\rightarrow\)  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: \((0 \ 0 \ l)\)  \(\rightarrow\)  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 \( Pn\text{'}ma\text{'} (#62.448) \) [OG: \( Pn\text{'}ma\text{'} (#62.8.509) \)]
Go to the list of the Wyckoff Positions of the Group \( Pn\text{'}ma\text{'} (#62.448) \) [OG: \( Pn\text{'}ma\text{'} (#62.8.509) \)]

[Show systematic absences in a different setting]
Symmetry-adapted form of the Structure Factors

Magnetic Space Group: \textit{Pn}'ma' (\#62.448) [OG: \textit{Pn}'ma' (\#62.8.509)]

Values of \( h, k, l \): \( h \) integer, \( k \) integer, \( l \) integer

Structure factors for general reflections (produced by centring):

\[
\text{Diffraction vector type: } h,k,l \\
\text{For any } h,k,l: \quad I = 0 \quad F = (F_x,F_y,F_z)
\]

Structure factors for special reflections:

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

\[
\text{Diffraction vector type: } 0,k,0 \\
\text{For } k = 1: \quad I = 0 \quad F = (F_x,0,0) \\
\text{For } k = 2: \quad I = 0 \quad F = (0,F_y,0)
\]

\[
\text{Diffraction vector type: } h,0,l \\
\text{For } h = 1, \; l = 1: \quad I = 0 \quad F = (0,F_y,0) \\
\text{For } h = 1, \; l = 2: \quad I = 0 \quad F = (0,F_y,0) \\
\text{For } h = 2, \; l = 1: \quad I = 0 \quad F = (0,F_y,0) \\
\text{For } h = 2, \; l = 2: \quad I = 0 \quad F = (0,F_y,0)
\]

\[
\text{Diffraction vector type: } h,0,0 \\
\text{For } h = 1: \quad I = 0 \quad F = (0,0,0) \\
\text{For } h = 2: \quad I = 0 \quad F = (0,F_y,0)
\]

\[
\text{Diffraction vector type: } 0,0,l \\
\text{For } l = 1: \quad I = 0 \quad F = (0,0,0) \\
\text{For } l = 2: \quad I = 0 \quad F = (0,F_y,0)
\]
For more subtle systematic absences in LaMnO$_3$ (due to the special position of the magnetic atoms), see:

Reflection (2, -1, 3)

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)

\[ \text{Ba}_5\text{Co}_5\text{ClO}_{13} \]
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

Structure factor is necessarily of the form:

- $(0,0,Fz)$

Absences that permit to distinguish the two MSGs

- $(0,k,l)$ $k+l$ odd
- $(h,0,l)$ $h+l$ odd
- $(0,Fx,0)$
- $(0,Fy,0)$
<table>
<thead>
<tr>
<th>Command</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>MGENPOS</td>
<td>General Positions of Magnetic Space Groups</td>
</tr>
<tr>
<td>Mwyckpos</td>
<td>Wyckoff Positions of Magnetic Space Groups</td>
</tr>
<tr>
<td>Magnetext</td>
<td>Extinction Rules of Magnetic Space Groups</td>
</tr>
<tr>
<td>Identify magnetic group</td>
<td>Identification of a Magnetic Space Group from a set of generators in an</td>
</tr>
<tr>
<td></td>
<td>arbitrary setting</td>
</tr>
<tr>
<td>Mpoint</td>
<td>Magnetic Point Group Tables</td>
</tr>
<tr>
<td>Maxmagn</td>
<td>Maximal magnetic space groups for a given a propagation vector and resulting</td>
</tr>
<tr>
<td></td>
<td>magnetic structural models</td>
</tr>
<tr>
<td>Magmodelize</td>
<td>Magnetic structure models for any given magnetic symmetry</td>
</tr>
<tr>
<td>K-subgroups mag</td>
<td>Magnetic subgroups consistent with some given propagation vector(s) or a</td>
</tr>
<tr>
<td></td>
<td>supercell</td>
</tr>
<tr>
<td>Magndata</td>
<td>A collection of magnetic structures with transportable cif-type files</td>
</tr>
<tr>
<td>Mvisualize</td>
<td>3D Visualization of magnetic structures with Jmol</td>
</tr>
<tr>
<td>Mtensor</td>
<td>Symmetry-adapted form of magnetic crystal tensors</td>
</tr>
</tbody>
</table>
MAXMAGN: Maximal magnetic space groups for a given a propagation vector and resulting magnetic structural models

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 $k = (1, 0, 0)$

<table>
<thead>
<tr>
<th>Group (BSN)</th>
<th>Transformation matrix</th>
<th>General positions</th>
<th>Systematic absences</th>
<th>Magnetic structure</th>
</tr>
</thead>
<tbody>
<tr>
<td>$P_{6mm}$ (#62,455)</td>
<td>$\begin{pmatrix} 0 &amp; 1 &amp; 0 &amp; 1/4 \ -1 &amp; 0 &amp; 0 &amp; 1/4 \ 0 &amp; 0 &amp; 1 &amp; 0 \end{pmatrix}$</td>
<td>Show</td>
<td>Show</td>
<td>Show</td>
</tr>
<tr>
<td>Alternatives (twin-related)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$P_{bca}$ (#51,439)</td>
<td>$\begin{pmatrix} 1 &amp; 0 &amp; 0 &amp; 0 \ 0 &amp; 1 &amp; 0 &amp; 1/4 \ 0 &amp; 0 &amp; 1 &amp; 0 \end{pmatrix}$</td>
<td>Show</td>
<td>Show</td>
<td>Show</td>
</tr>
<tr>
<td>Alternatives (twin-related)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$P_{bcn}$ (#60,429)</td>
<td>$\begin{pmatrix} 0 &amp; 1 &amp; 0 &amp; 1/4 \ 0 &amp; 0 &amp; 1 &amp; 1/4 \ 1 &amp; 0 &amp; 0 &amp; 0 \end{pmatrix}$</td>
<td>Show</td>
<td>Show</td>
<td>Show</td>
</tr>
<tr>
<td>Alternatives (twin-related)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$P_{bcm}$ (#57,390)</td>
<td>$\begin{pmatrix} 0 &amp; 0 &amp; 1 &amp; 1/4 \ 1 &amp; 0 &amp; 0 &amp; 1/4 \ 0 &amp; 1 &amp; 0 &amp; 0 \end{pmatrix}$</td>
<td>Show</td>
<td>Show</td>
<td>Show</td>
</tr>
<tr>
<td>Alternatives (twin-related)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$P_{accn}$ (#58,374)</td>
<td>$\begin{pmatrix} 0 &amp; 1 &amp; 0 &amp; 1/2 \ 0 &amp; 0 &amp; 1 &amp; 0 \ 1 &amp; 0 &amp; 0 &amp; 0 \end{pmatrix}$</td>
<td>Show</td>
<td>Show</td>
<td>Show</td>
</tr>
<tr>
<td>Alternatives (twin-related)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$P_{barn}$ (#55,362)</td>
<td>$\begin{pmatrix} 0 &amp; 0 &amp; 1 &amp; 0 \ 0 &amp; -1 &amp; 0 &amp; 0 \ 1 &amp; 0 &amp; 0 &amp; 0 \end{pmatrix}$</td>
<td>Show</td>
<td>Show</td>
<td>Show</td>
</tr>
<tr>
<td>Alternatives (twin-related)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$P_{acc}$ (#54,349)</td>
<td>$\begin{pmatrix} 0 &amp; 1 &amp; 0 &amp; 1/4 \ 0 &amp; 0 &amp; 1 &amp; 1/4 \ 1 &amp; 0 &amp; 0 &amp; 0 \end{pmatrix}$</td>
<td>Show</td>
<td>Show</td>
<td>Show</td>
</tr>
<tr>
<td>Alternatives (twin-related)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$P_{cma}$ (#53,335)</td>
<td>$\begin{pmatrix} 1 &amp; 0 &amp; 0 &amp; 0 \ 0 &amp; 1 &amp; 0 &amp; 0 \ 0 &amp; 0 &amp; 1 &amp; 0 \end{pmatrix}$</td>
<td>Show</td>
<td>Show</td>
<td>Show</td>
</tr>
<tr>
<td>Alternatives (twin-related)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

La$_2$CuO$_4$
Selected magnetic space group: 5- P\textsubscript{4}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

<table>
<thead>
<tr>
<th>N</th>
<th>Atom</th>
<th>New WP</th>
<th>Multiplicity</th>
<th>Magnetic moment</th>
<th>Values of (M_x, M_y, M_z)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Cu1</td>
<td>(0,0,0</td>
<td>4</td>
<td>(0, M_y, M_z)</td>
<td>(M_y = 0.00000), (M_z = 0.00000)</td>
</tr>
<tr>
<td></td>
<td>Cu</td>
<td>0.000000 0.000000 0.000000</td>
<td>(0,1/2,0</td>
<td>0,-m_y,-m_z)</td>
<td>(1/2,0,1/2 \times 0,0,0)</td>
</tr>
<tr>
<td>2</td>
<td>La1</td>
<td>(0,y,0</td>
<td>8</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>La</td>
<td>0.000000 0.36110 0.00460</td>
<td>(0,1/2,0</td>
<td>0,-m_y,-m_z)</td>
<td>(1/2,0,1/2 \times 0,0,0)</td>
</tr>
<tr>
<td>3</td>
<td>O1</td>
<td>(1/4,y,0</td>
<td>8</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>O</td>
<td>0.25000 -0.00510 0.25000</td>
<td>(3/4,-y,0</td>
<td>0,-m_y,-m_z)</td>
<td>(3/4,1/2,0 \times 0,0,0)</td>
</tr>
<tr>
<td>4</td>
<td>O2</td>
<td>(0,y,0</td>
<td>8</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>O</td>
<td>0.000000 0.18300 -0.02430</td>
<td>(0,1/2,0</td>
<td>0,-m_y,-m_z)</td>
<td>(1/2,0,1/2 \times 0,0,0)</td>
</tr>
</tbody>
</table>

[Go to setting standard \((c, a, b ; 0, 0, 0)\)]
Maximal magnetic space groups for the space group 64 (Cmce) and the propagation vector $k = (1, 0, 0)$

<table>
<thead>
<tr>
<th>Group (BNS)</th>
<th>Transformation matrix</th>
<th>General positions</th>
<th>Systematic absences</th>
<th>Magnetic structure</th>
</tr>
</thead>
<tbody>
<tr>
<td>$P_{can} (162.456)$</td>
<td>$\begin{pmatrix} 1 &amp; 0 &amp; 0 &amp; 1/4 \ -1 &amp; 0 &amp; 0 &amp; 1/4 \ 0 &amp; 1 &amp; 0 &amp; 0 \ 0 &amp; 0 &amp; 1 &amp; 0 \end{pmatrix}$</td>
<td>Show</td>
<td>Show</td>
<td>Show</td>
</tr>
<tr>
<td>$P_{bcna} (161.439)$</td>
<td>$\begin{pmatrix} 1 &amp; 0 &amp; 0 &amp; 1/4 \ 0 &amp; 1 &amp; 0 &amp; 0 \ 0 &amp; 0 &amp; 1 &amp; 0 \end{pmatrix}$</td>
<td>Show</td>
<td>Show</td>
<td>Show</td>
</tr>
<tr>
<td>$P_{abcm} (160.429)$</td>
<td>$\begin{pmatrix} 0 &amp; 0 &amp; 1 &amp; 1/4 \ 0 &amp; 1 &amp; 0 &amp; 0 \ 1 &amp; 0 &amp; 0 &amp; 0 \end{pmatrix}$</td>
<td>Show</td>
<td>Show</td>
<td>Show</td>
</tr>
<tr>
<td>$P_{abcm} (167.390)$</td>
<td>$\begin{pmatrix} 0 &amp; 0 &amp; 1 &amp; 1/4 \ 1 &amp; 0 &amp; 0 &amp; 1/4 \ 0 &amp; 1 &amp; 0 &amp; 0 \end{pmatrix}$</td>
<td>Show</td>
<td>Show</td>
<td>Show</td>
</tr>
<tr>
<td>$P_{aaccn} (56.374)$</td>
<td>$\begin{pmatrix} 0 &amp; 1 &amp; 0 &amp; 5/2 \ 0 &amp; 1 &amp; 0 &amp; 0 \ 1 &amp; 0 &amp; 0 &amp; 1/2 \end{pmatrix}$</td>
<td>Show</td>
<td>Show</td>
<td>Show</td>
</tr>
<tr>
<td>$P_{abarn} (55.362)$</td>
<td>$\begin{pmatrix} 0 &amp; 0 &amp; 1 &amp; 0 \ 0 &amp; -1 &amp; 0 &amp; 0 \ 1 &amp; 0 &amp; 0 &amp; 0 \end{pmatrix}$</td>
<td>Show</td>
<td>Show</td>
<td>Show</td>
</tr>
<tr>
<td>$P_{accn} (54.349)$</td>
<td>$\begin{pmatrix} 0 &amp; 1 &amp; 0 &amp; 1/4 \ 0 &amp; 0 &amp; 1 &amp; 1/4 \ 1 &amp; 0 &amp; 0 &amp; 0 \end{pmatrix}$</td>
<td>Show</td>
<td>Show</td>
<td>Show</td>
</tr>
<tr>
<td>$P_{cma} (53.335)$</td>
<td>$\begin{pmatrix} 1 &amp; 0 &amp; 0 &amp; 0 \ 0 &amp; 1 &amp; 0 &amp; 0 \ 0 &amp; 0 &amp; 1 &amp; 0 \end{pmatrix}$</td>
<td>Show</td>
<td>Show</td>
<td>Show</td>
</tr>
</tbody>
</table>

La$_2$CuO$_4$

$P_{aaccn}$ (56.374)

($=0, \approx0, m_z$)
Na$_2$MnF$_5$  Parent: P2$_1$/c

\[ \mathbf{k} = (0, 1/2, 0) \]

Derive the possible orderings of maximal symmetry

Tutorial MAXMAGN, example 4

7. From the knowledge of its parent space group and its propagation vector (P21/c and \( \mathbf{k}=(0,1/2,0) \)), use \texttt{k-SUBGROUPSMAG} to explore all possible symmetries of the magnetic structure of Na$_2$MnF$_5$ 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: 3.Na2MnF5_parent.cif)
\( P\bar{b}c \) \((a,2b,c;0 1/4 0)\)

\( P\bar{b}c \) \((a,2b,c;0 3/4 0)\)

\( P_\delta - 1 \) \((-a,-c,2b;0 0 0)\)

\( P_\delta - 1 \) \((-a,-c,2b;0 1/2 0)\)

Diagram:

- \( P_2/1/c \)
- \( P_\delta c \)
- \( P_\delta \bar{1} \)
- \( P_\delta 1 \)
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 \( \{2y\mid 0 \ \frac{1}{2} \ 0\} \) …

8. Using \texttt{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 for the case of \( P2_1/c \) symmetry because the binary rotation includes a non-trivial translation.
We use **MAXMAGN** to explore the four possible alternative models of maximal symmetry for HoMnO$_3$.

9. 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: 4.HoMnO3_parent.cif).

**Tutorial MAXMAGN, example 2**
**HoMnO$_3$** (Muñoz et al. Inorg. Chem. 2001)

Diffraction peaks:

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

<table>
<thead>
<tr>
<th>N</th>
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<th>Magnetic structure</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Pna21 (#33.149)</td>
<td>$\begin{pmatrix} -2 &amp; 0 &amp; 0 &amp; 1/4 \ 0 &amp; -1 &amp; 0 &amp; 0 \ 0 &amp; 0 &amp; 1 &amp; 0 \end{pmatrix}$</td>
<td>Show</td>
<td>Show</td>
<td>Show</td>
</tr>
<tr>
<td>2</td>
<td>Pnm21 (#31.129)</td>
<td>$\begin{pmatrix} 0 &amp; 2 &amp; 0 &amp; 1/4 \ -1 &amp; 0 &amp; 1 &amp; 1/4 \ 0 &amp; 0 &amp; 1 &amp; 1 \end{pmatrix}$</td>
<td>Show</td>
<td>Show</td>
<td>Show</td>
</tr>
<tr>
<td>3</td>
<td>P2$_1$/c (#14.82)</td>
<td>$\begin{pmatrix} -2 &amp; 0 &amp; 2 &amp; 0 \ 0 &amp; 1 &amp; 0 &amp; 0 \ -1 &amp; 0 &amp; 0 &amp; 0 \end{pmatrix}$</td>
<td>Show</td>
<td>Show</td>
<td>Show</td>
</tr>
<tr>
<td>4</td>
<td>P2$_1$/m (#11.56)</td>
<td>$\begin{pmatrix} 2 &amp; 0 &amp; 0 &amp; 0 \ 0 &amp; 1 &amp; 0 &amp; 0 \ 0 &amp; 0 &amp; 1 &amp; 0 \end{pmatrix}$</td>
<td>Show</td>
<td>Show</td>
<td>Show</td>
</tr>
</tbody>
</table>

Maximal subgroups which allow non-zero magnetic moments for at least one atom are coloured.
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: \( \text{HoMnO}_3 \) (Muñoz et al. Inorg. Chem. 2001)

Diffraction peaks:

\[
Gp = \text{Pnma}
\]

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

Point group

\[
\text{mm2 1'}
\]

Induced polarization: multiferroic

\[
\text{Pz}
\]

Symmetry operation kept: \( \{1'|1/2 \ 0 \ 0\} \)

Equivalent to a lattice translation for the positions

\[
1' \text{ belongs to the point group of the magnetic phase}
\]
**HoMnO$_3$**

unit cell: 2a, b, c

**Magnetic space group: $P_{a}nm2_1$ (31.129)**

(non-conventional setting)

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

Magnetic moments of the asymmetric unit (µB):

Mn1 3.87 ≈0.0 ≈0.0

Split independent positions in the lower symmetry

**WP**

| WP | + (1’|1/2 0 0) |
|----|--------------|
| 8b | (x, y, z | mx, my, mz), (-x+1/4, -y, z+1/2 | -mx, -my, mz), (x, -y+1/2, z | -mx, my, -mz), (-x+1/4, y+1/2, z+1/2 | mx, -my, -mz) |
| 4a | (x, 1/4, z| 0, my, 0), (-x+1/4, 3/4, z+1/2 | 0, -my, 0) |

General position:

x, y, z not restricted by symmetry!
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.
Derive the symmetry constraints on some crystal tensor properties of a magnetic phase using MTENSOR

10. Use **MTENSOR** to obtain some of the crystal tensor properties of the magnetic phase of HoMnO$_3$ (electric polarization, magnetization, linear magnetoelectric tensor, quadratic 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 5.LaMnO3.mcif)*
Use of k-SUBGROUPSMAG to explore all possible symmetries for HoMnO$_3$

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

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

(magnetic cell= \(2a_p,b_p,c_p\))