Symmetry of commensurate magnetic structures: Magnetic space groups

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A symmetry operation in a solid IS NOT only a more or less complex transformation leaving the system invariant. But it MUST fulfill that the resulting constraints can only be broken through a phase transition.

A well defined symmetry operation (in a thermodynamic system) must be maintained when scalar fields (temperature, pressure, ...) are changed, except if a phase transition takes place.

“symmetry-forced” means: “forced for a thermodynamic phase”
“symmetry-allowed” means: “allowed within a thermodynamic phase”

Symmetry-dictated properties can be considered symmetry “protected”
Space Group:
Pnma

Lattice parameters:
5.7461 7.6637 5.5333 90.000 90.000 90.000

Atomic positions of asymmetric unit:
La1  0.05130 0.25000 -0.00950
Mn1  0.00000 0.00000 0.50000
O1   0.48490 0.25000 0.07770
O2   0.30850 0.04080 0.72270

Reminder of symmetry in non-magnetic structures
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Reminder of symmetry in non-magnetic structures

Space Group: set of operations \( \{R|t\} \)
for all atoms:

\[
\begin{bmatrix}
  x' \\
  y' \\
  z'
\end{bmatrix} = R \begin{bmatrix}
  x \\
  y \\
  z
\end{bmatrix} + t
\]

\( R \): rotation or rotation+plus inversion
\( t \): translation
**LaMnO$_3$**

**Space Group:**
- Pnma

**Lattice parameters:**
- 5.7461 7.6637 5.5333 90.000 90.000 90.000

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**Space Group: set of operations** \{R|t\}

For all atoms:

- \( (x, y, z) \)
- \( (x', y', z') = R \begin{pmatrix} x \\ y \\ z \end{pmatrix} + t \)

**Pnma:**

- 8 related positions for a general position:
  - \( (x, y, z) \)
  - \( (-x+1/2, -y, z+1/2) \)
  - \( (-x, y+1/2, -z) \)
  - \( (x+1/2, -y+1/2, z+1/2) \) = \{2x \ 1/2 \ 1/2 \}

- 4 related positions for a special position of type \((x, 1/4, z)\): **special positions are tabulated:**
  - \( (x, 1/4, z) \)
  - \( (-x+1/2, 3/4, z+1/2) \)
  - \( (-x, 3/4, -z) \)
  - \( (x+1/2, 1/4, -z+1/2) \) **Wyckoff positions or orbits**
Space Group: Pnma

Lattice parameters: 5.7461 7.6637 5.5333 90.000 90.000 90.000

Atomic positions of asymmetric unit:
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Reminder of symmetry in non-magnetic structures

LaMnO₃

Relations among atoms from the space group: more than "geometrical", they are "thermodynamic" properties

they may be zero within experimental resolution but this is NOT symmetry forced.

La1 (≈ 0.0 0.25000 ≈ 0.0)

¼ rigorously fulfilled – if broken, it means a different phase
Space Group:
Pnma

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5.7461 7.6637 5.5333 90.000 90.000 90.000

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Relations among atoms from the space group:
much more than "geometrical", they are "thermodynamic" properties

they may be zero within experimental resolution but this is NOT symmetry forced.

La1 (≈ 0.0 0.25000 ≈0.0) ¼ rigorously fulfilled – if broken, it means a different phase

Whatever microscopic model of atomic forces, if consistently applied, it will yield:
\[ F_y (La1) = 0.000000 \text{ (exact!)} \]
Magnetic Symmetry: *Symmetry is only detected when it does not exist! We do not add but substract symmetry operations!*

Symmetry operation to be considered:
(always present in non-magnetic structures but ABSENT in magnetically ordered ones!)

Time inversion/reversal: \{1'|0,0,0\}

- Does not change nuclear variables
- Changes sign of ALL atomic magnetic moments

\[
\begin{align*}
\{1'|000\} \\
(x,y,z,-m) &= (x,y,z,-1)
\end{align*}
\]

Magnetic structures only have symmetry operations where time reversal 1’ is combined with other transformations, or is not present at all:
\[
\begin{align*}
\{1'|t\} &= \{1'|0,0,0\} \{1|t\} \\
\{m'| t\} &= \{1'|0,0,0\} \{m|t\} \\
\{2'|t\} &= \{1'|0,0,0\}\{2|t\} \\
\{3^+|t\} &= \{1'|0,0,0\}\{3^+|t\}, \text{ etc.}
\end{align*}
\]

But \{1'|0,0,0\} alone is never a symmetry operation of a magn. struct.
All NON-magnetic structures have time inversion symmetry

If all atomic magnetic moments are zero, time inversion is a (trivial) symmetry operation of the structure:

**Actual symmetry of the non-magnetic phase:**

\[ Pnma1' = Pnma + \{1'|000\} \times Pnma \]  
(grey group)

16 operations:

\[
\begin{align*}
(x,y,z,+1) & \quad (-x+1/2,-y,z+1/2,+1) & \quad (-x,y+1/2,-z,+1) & \quad (x+1/2,-y+1/2,-z+1/2,+1) \\
(-x,-y,-z,+1) & \quad (x+1/2,y,-z+1/2,+1) & \quad (x,-y+1/2,z,+1) & \quad (-x+1/2,y+1/2,z+1/2,+1)
\end{align*}
\]

\[
\begin{align*}
(x,y,z,-1) & \quad (-x+1/2,-y,z+1/2,-1) & \quad (-x,y+1/2,-z,-1) & \quad (x+1/2,-y+1/2,-z+1/2,-1) \\
(-x,-y,-z,-1) & \quad (x+1/2,y,-z+1/2,-1) & \quad (x,-y+1/2,z,-1) & \quad (-x+1/2,y+1/2,z+1/2,-1)
\end{align*}
\]

Notation:

\[
\begin{align*}
(x+1/2,-y+1/2,-z+1/2,+1) & \quad \{2x|\frac{1}{2} \frac{1}{2} \frac{1}{2}\} \quad \{R|t\} \\
(x+1/2,-y+1/2,-z+1/2,-1) & \quad \{2x'|\frac{1}{2} \frac{1}{2} \frac{1}{2}\} \quad \{R'|t\}
\end{align*}
\]

\[
\begin{align*}
\theta=1 \\
\theta=-1
\end{align*}
\]
magnetic ordering breaks symmetry of time inversion

Magnetic ordered phases:

LaMnO$_3$

$Pnma1'$

(x,y,z,+1)  (-x+1/2,-y,z+1/2,+1)  (-x+1/2,-y,z+1/2,-1)  (-x, y+1/2, z+1/2,+1)  (-x+1/2, y+1/2, z+1/2,+1)

(-x,-y,-z,+1)  (x+1/2,y,-z+1/2,+1)  (x,-y+1/2,z,+1)  (-x+1/2,y+1/2,z+1/2,+1)  (-x+1/2,y+1/2,z+1/2,-1)

(x,y,z,-1)  (-x+1/2,-y,z+1/2,-1)  (-x+1/2,-y,z+1/2, -1)  (-x, y+1/2, z+1/2,-1)  (-x+1/2, y+1/2, z+1/2,-1)

(-x,-y,-z,-1)  (x+1/2,y,-z+1/2,-1)  (x,-y+1/2,z,-1)  (-x+1/2,y+1/2,z+1/2,-1)  (-x+1/2,y+1/2,z+1/2,-1)
magnetic ordering breaks symmetry of time inversion

Magnetic ordered phases:

Time inversion \( \{1'|0 \ 0 \ 0\} \) is NOT a symmetry operation of a magnetic phase

LaMnO\(_3\)

\(Pnma1'\)
For space operations, the magnetic moments transform as pseudovectors or axial vectors:

\[ T_{\text{axial}}(R) = \det[R] R \]

(for positions: the same as with Pnma)

\[ \theta = -1 \text{ if time inversion} \]
magnetic ordering breaks symmetry of time inversion

Magnetic ordered phases:

Time inversion $\{1'|0 \ 0 \ 0\}$ is NOT a symmetry operation of a magnetic phase

LaMnO$_3$

Pnma$1'$

$$(x,y,z,+1) \quad (-x+1/2,y,-z+1/2,+1) \quad (-x,y+1/2,-z,+1) \quad (x+1/2,-y+1/2,-z+1/2,+1)$$

$$(-x,-y,-z,+1) \quad (x+1/2,y,-z+1/2,-1) \quad (x,-y+1/2,z,+1) \quad (-x+1/2,y+1/2,z+1/2,+1)$$

$$(-x,y,z,-1) \quad (-x+1/2,-y,z+1/2,-1) \quad (-x,y+1/2,-z,-1) \quad (x+1/2,-y+1/2,-z+1/2,-1)$$

$$(-x,-y,-z,-1) \quad (x+1/2,y,-z+1/2,-1) \quad (x,-y+1/2,z,-1) \quad (-x+1/2,y+1/2,z+1/2,-1)$$
magnetic ordering breaks symmetry of time inversion

Magnetic ordered phases:

Time inversion \( \{1'|0 0 0\} \) is NOT a symmetry operation of a magnetic phase
A symmetry operation fulfills:

- the operation belongs to the set of transformations that keep the **energy invariant**: rotations, translations, space inversion, time reversal.

- the system is **undistinguishable** after the transformation.

Symmetry operations in commensurate magnetic crystals:

- magnetic space group: \( \{ \{ R_i \mid t_i \} , \{ R'_j \mid t_j \} \} \)

  or \( \{ \{ R_i , \theta \mid t_i \} \} \)

  \( \theta = +1 \) without time reversal

  \( \theta = -1 \) with time reversal
Description of a magnetic structure in a crystallographic form:

Magnetic space Group: 
Pn'ma'

Lattice parameters:  
5.7461 7.6637 5.5333 90.000 90.000 90.000

Atomic positions of asymmetric unit:  
La1   0.05130 0.25000 -0.00950  
Mn1  0.00000 0.00000 0.50000  
O1    0.48490 0.25000 0.07770  
O2    0.30850 0.04080 0.72270  

Magnetic moments of the asymmetric unit (µB):  
Mn1   3.87 0.0 0.0

Symmetry operations are relevant both for positions and moments.

Pn’ ma’:  
1 x,y,z,+1  
2 -x,y+1/2,-z,+1  
3 -x,-y,-z,+1  
4 x,-y+1/2,z,+1  
5 x+1/2,-y+1/2,-z+1/2,-1  
6 -x+1/2,-y,z+1/2,-1  
7 -x+1/2,y+1/2,z+1/2,-1  
8 x+1/2,y,-z+1/2,-1

Parent symmetry Pnma1’

Possible symmetries for a k=0 magnetic ordering:
Possible maximal symmetries for a k=0 magnetic ordering:

Parent symmetry Pnma1'

Possible symmetries for a k=0 magnetic ordering:
### Magnetic Symmetry and Applications

#### MGENPOS
**General Positions of Magnetic Space Groups**

#### MWYCKPOS
**Wyckoff Positions of Magnetic Space Groups**

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**General Positions of the Group \textit{Pnnm'} (#62.448)**

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

<table>
<thead>
<tr>
<th>N</th>
<th>((x,y,z)) form</th>
<th>Matrix form</th>
<th>Geom. interp.</th>
<th>Seitz notation</th>
</tr>
</thead>
</table>
| 1  | \(x, y, z, +1\)  | \[
\begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
\end{pmatrix}
\] | \(1 +1\) | \(\{1 | 0\}\) |
| 2  | \(-x, y, +1/2, -z, +1\) | \[
\begin{pmatrix}
-1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & -1 & 0 \\
\end{pmatrix}
\] | \(2 (0,1/2,0) x, 0, y, 0 \pm 1\) | \(\{2_{010} | 0 \ 1/2 \ 0\}\) |
| 3  | \(-x, -y, -z, +1\) | \[
\begin{pmatrix}
-1 & 0 & 0 & 0 \\
0 & -1 & 0 & 0 \\
0 & 0 & -1 & 0 \\
\end{pmatrix}
\] | \(-1 \ 0,0,0 \pm 1\) | \(\{-1 | 0\}\) |
| 4  | \(x, -y, +1/2, z, +1\) | \[
\begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & -1 & 0 & 0 \\
0 & 0 & 1/2 & 0 \\
\end{pmatrix}
\] | \(m x, 1/4, z \pm 1\) | \(\{m_{010} | 0 \ 1/2 \ 0\}\) |
| 5  | \(x+1/2, -y+1/2, -z+1/2, -1\) | \[
\begin{pmatrix}
1 & 0 & 0 & 1/2 \\
0 & -1 & 0 & 0 \\
0 & 0 & 1/2 & 0 \\
\end{pmatrix}
\] | \(2 (1/2,0,0) x, 1/4, 1/4 \pm 1\) | \(\{Z_{100} | 1/2 \ 1/2 \ 1/2\}\) |
| 6  | \(-x+1/2, -y, z+1/2, -1\) | \[
\begin{pmatrix}
-1 & 0 & 0 & 1/2 \\
0 & -1 & 0 & 0 \\
0 & 0 & 1/2 & 0 \\
\end{pmatrix}
\] | \(2 (0,1/2) 1/4, 0, z \pm 1\) | \(\{Z_{001} | 1/2 \ 0 \ 1/2\}\) |
| 7  | \(-x+1/2, y+1/2, z+1/2, -1\) | \[
\begin{pmatrix}
-1 & 0 & 0 & 1/2 \\
0 & 1 & 0 & 0 \\
0 & 0 & 1/2 & 0 \\
\end{pmatrix}
\] | \(h (0,1/2,1/2) 1/4, y, z \pm 1\) | \(\{m'_{100} | 1/2 \ 1/2 \ 1/2\}\) |
| 8  | \(x+1/2, y, -z+1/2, -1\) | \[
\begin{pmatrix}
1 & 0 & 0 & 1/2 \\
0 & 1 & 0 & 0 \\
0 & 0 & -1 & 0 \\
\end{pmatrix}
\] | \(a x, y, 1/4 \pm 1\) | \(\{m'_{001} | 1/2 \ 0 \ 1/2\}\) |

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Magnetic point group: \textit{m'm'm'}

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Go to the list of the Wyckoff Positions of the Group \textit{Pnnm'} (#62.448)

Go to the Systematic Absences for the Group \textit{Pnnm'} (#62.448)
Parameters to describe a magnetic structure...

Space Group: Pn'ma'

<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</td>
</tr>
<tr>
<td>4</td>
<td>c</td>
<td>((x,1/4,z</td>
</tr>
<tr>
<td>4</td>
<td>b</td>
<td>((0,0,1/2</td>
</tr>
<tr>
<td>4</td>
<td>a</td>
<td>((0,0,0</td>
</tr>
</tbody>
</table>

Output of MWYCKPOS in BCS

La
Mn

Mode along x \(A_x\)
Mode along y \(F_y\)
Weak ferromagnet
Mode along z \(G_z\)
Description in terms of irrep modes

\[ \text{Pn'}\text{ma'} \implies mB_{2g} \]  

(Irrep = irreducible representation)

<table>
<thead>
<tr>
<th>(D_{2h}(mmm))</th>
<th>#</th>
<th>(1)</th>
<th>(2_z)</th>
<th>(2_y)</th>
<th>(2_x)</th>
<th>(-1)</th>
<th>(m_z)</th>
<th>(m_y)</th>
<th>(m_x)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(m_{A_g})</td>
<td>(\Gamma_1^+)</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>-1</td>
</tr>
<tr>
<td>(m_{B_{1g}})</td>
<td>(\Gamma_3^+)</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>-1</td>
</tr>
<tr>
<td>(m_{B_{2g}})</td>
<td>(\Gamma_2^+)</td>
<td>1</td>
<td>-1</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
</tr>
<tr>
<td>(m_{B_{3g}})</td>
<td>(\Gamma_4^+)</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>1</td>
<td>-1</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
</tr>
<tr>
<td>(m_{A_u})</td>
<td>(\Gamma_1^-)</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>-1</td>
<td>-1</td>
<td>-1</td>
</tr>
<tr>
<td>(m_{B_{1u}})</td>
<td>(\Gamma_3^-)</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>-1</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>(m_{B_{2u}})</td>
<td>(\Gamma_2^-)</td>
<td>1</td>
<td>-1</td>
<td>1</td>
<td>-1</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>-1</td>
</tr>
<tr>
<td>(m_{B_{3u}})</td>
<td>(\Gamma_4^-)</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>1</td>
<td>-1</td>
<td>1</td>
<td>1</td>
<td>-1</td>
</tr>
</tbody>
</table>

One \(mB_{2g}\) spin mode  
(or basis function)
Building up the model of the magnetic structure of LaMnO$_3$ using **STRCONVERT**

1. Upload the cif file of LaMnO$_3$ in STRCONVERT. Change to magnetic option. Transform to P1 to produce the whole set of atomic positions within the unit cell. Introduce magnetic moments along x of the four listed Mn atoms according to the sign relations: 1,-1,-1,1. Use findsym to find the MSG, and the description using this MSG. Visualize the magnetic structure with MVISUALIZE. With the back button come back in the STRCONVERT to the page in P1, and introduce a non-zero component my at the single symmetry-independent Mn atom, and transform again to P1 to observe that the resulting my values for 4 Mn atoms within the unit cell have the same sign (expected weak FM along y). Create an mcif file of the structure with STRCONVERT, open it with a text editor and localize the different data items: unit cell, atomic positions, symmetry operations. Download the mcif file in VESTA and visualize the structure with this tool. (file required: *1.LaMnO3_parent.cif*)
Structure Data Converter & Editor

Please submit a structure file:
Browse... No file selected. Upload the file

[Supported file formats: CIF, mCIF, VESTA, VASP]

Symmetry
Magnetic Space Group # (BNS): 31.129  (P_bmn2_1)  Type: IV

Lattice Parameters
a: 11.670 Å  b: 7.360Å  c: 5.257Å
α: 90.00°  β: 90.00°  γ: 90.00°

Symmetry Operations [Show/Hide]

Recognized formats:
1. x,y,z mx,my,mz +1
   x,y,z
   x,y,z +1
   1 'x , y , z'
   1 x,y,z

- x+1/4, - y, z+1/2, +1
- x+y/2, z, +1
- x+1/4, y+1/2, z1/2, +1
x+1/2, y, z1/2
- x+3/4, - y, z+1/2, -1
x+1/2, - y+1/2, z, -1
- x+3/4, y+1/2, z1/2, -1

☐ Update the symmetry operators with the above  Apply

Symmetry operations have been parsed from the file
Populate with operators from database
### Atomic Positions & Magnetic Moments

Switch to the treatment of the vectors as: 

<table>
<thead>
<tr>
<th>Label</th>
<th>Element</th>
<th>x</th>
<th>y</th>
<th>z</th>
<th>Occ.</th>
<th>mx</th>
<th>my</th>
<th>mz</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ho</td>
<td>Ho</td>
<td>0.04195</td>
<td>0.25000</td>
<td>0.98250</td>
<td>1.00000</td>
<td>0.00000</td>
<td>0.00000</td>
<td>0.00000</td>
</tr>
<tr>
<td>Ho_1</td>
<td>Ho</td>
<td>0.95805</td>
<td>0.75000</td>
<td>0.01750</td>
<td>1.00000</td>
<td>0.00000</td>
<td>0.00000</td>
<td>0.00000</td>
</tr>
<tr>
<td>Mn</td>
<td>Mn</td>
<td>0.00000</td>
<td>0.00000</td>
<td>0.50000</td>
<td>1.00000</td>
<td>3.87000</td>
<td>0.00000</td>
<td>0.00000</td>
</tr>
<tr>
<td>O1</td>
<td>O</td>
<td>0.23110</td>
<td>0.25000</td>
<td>0.11130</td>
<td>1.00000</td>
<td>0.00000</td>
<td>0.00000</td>
<td>0.00000</td>
</tr>
<tr>
<td>O1_1</td>
<td>O</td>
<td>0.76890</td>
<td>0.75000</td>
<td>0.88870</td>
<td>1.00000</td>
<td>0.00000</td>
<td>0.00000</td>
<td>0.00000</td>
</tr>
<tr>
<td>O2</td>
<td>O</td>
<td>0.16405</td>
<td>0.05340</td>
<td>0.70130</td>
<td>1.00000</td>
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<td>0.00000</td>
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</tr>
<tr>
<td>O2_1</td>
<td>O</td>
<td>0.83595</td>
<td>0.55340</td>
<td>0.29870</td>
<td>1.00000</td>
<td>0.00000</td>
<td>0.00000</td>
<td>0.00000</td>
</tr>
</tbody>
</table>

---

**Longest Arrow size:** 1.314

[for VESTA format export: Å (Default: \(min(a,b,c)/4\))]
[for Jmol visualize: a proportional coefficient]

- Export to BCS format
- Export to VESTA format
- Export to Standard CIF format
- Export to CIF format
- Export to VASP format
- Transform the structure to P1 setting
- Remove the magnetic information
- Re-order the sites
- Visualize
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.
ISOTROPY Software Suite
Harold T. Stokes, Dorian M. Hatch, and Branton J. Campbell, Department of Physics and Astronomy, Brigham Young University, Provo, Utah 84606, USA, stokes@byu.edu

Description: The ISOTROPY software suite is a collection of software which applies group theoretical methods to the analysis of phase transitions in crystalline solids.

How to cite: ISOTROPY Software Suite, iso.byu.edu.

References and Resources

Isotropy subgroups and distortions
- **ISODISTORT**: Explore and visualize distortions of crystalline structures. Possible distortions include atomic displacements, atomic ordering, strain, and magnetic moments.
- **New! ISOSUBGROUP**: Interactive program using user-friendly interface to list isotropy subgroups.
- **ISOTROPY**: Interactive program using command lines to explore isotropy subgroups and their associated distortions.
- **SMODES**: Find the displacement modes in a crystal which brings the dynamical matrix to block-diagonal form, with the smallest possible blocks.
- **FROZSL**: Calculate phonon frequencies and displacement modes using the method of frozen phonons.

Space groups and irreducible representations
- **ISOCIF**: Create or modify CIF files.
- **FINDSYM**: Identify the space group of a crystal, given the positions of the atoms in a unit cell.
- **ISO-IR**: Tables of irreducible Representations. The 2011 version of IR matrices.
- **ISO-MAG**: Tables of magnetic space groups, both in human-readable and computer-readable forms.

Superspace Groups
- **ISO(3+1d)**: (3+d)-Dimensional Superspace Groups for d=1,2,3
- **ISO(3+1l)**: Isotropy Subgroups for Incommensurately Modulated Distortions in Crystalline Solids: A Complete List for One-Dimensional Modulations
- **FINDSSG**: Identify the superspace group symmetry given a list of symmetry operators.
- **TRANSFORMSSG**: Transform a superspace group to a new setting.

Phase Transitions
- **COPL**: Find a complete list of order parameters for a phase transition, given the space-group symmetries of the parent and subgroup phases.
- **INVARINT**: Generate invariant polynomials of the components of order parameters.
- **COMSUBS**: Find common subgroups of two structures in a reconstructive phase transition.
Other CIF (and mCIF) file editor

ISOCIF
Version 2.3.12, Oct 2015
Harold T. Stokes and Branton J. Campbell, Department of Physics and Astronomy, Brigham Young University, Provo, Utah, 84602, USA, stokesh@byu.edu

Description: ISOCIF is a tool for creating and modifying CIF structure files.

Help
Version History
How to cite ISOCIF: ISOTROPY Software Suite, iso.byu.edu.

Create new CIF file
Modify existing CIF file: OK Examinar… No se ha selecci..

Read old mCIF format
## 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 point group: m′mm′

<table>
<thead>
<tr>
<th>N</th>
<th>(x,y,z) form</th>
<th>Matrix form</th>
<th>Geom. interp.</th>
<th>Selitz notation</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>x, y, z, +1</td>
<td>( 1 0 0 0</td>
<td>1+1</td>
<td>{1</td>
</tr>
<tr>
<td></td>
<td>m_x,m_y,m_z</td>
<td>0 0 0 1</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>0 0 1 0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>-x, y+1/2, -z, +1</td>
<td>( -1 0 0 0</td>
<td>2 (0,1/2,0) 0,0,0</td>
<td>{201</td>
</tr>
<tr>
<td></td>
<td>m_x,m_y,m_z</td>
<td>0 0 1 0/2</td>
<td>0,0,0</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>0 0 0 1/2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>-x, -y, -z, +1</td>
<td>( -1 0 0 0</td>
<td>-1 0,0,0,0</td>
<td>{-1</td>
</tr>
<tr>
<td></td>
<td>m_x,m_y,m_z</td>
<td>0 0 1 0</td>
<td>-1,0,0,0</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>0 0 1 0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>x, -y+1/2, z, +1</td>
<td>( 1 0 0 0</td>
<td>m_x,1/4,z, +1</td>
<td>{m01</td>
</tr>
<tr>
<td></td>
<td>m_x,m_y,m_z</td>
<td>0 0 1 0/2</td>
<td>m_x,1/4,0,0</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>0 0 1 0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>x+1/2, -y+1/2, -z+1/2, -1</td>
<td>1/2 0 1/2</td>
<td>2 (1/2,0,0) x,1/4,1/4, -1</td>
<td>{2</td>
</tr>
<tr>
<td></td>
<td>m_x,m_y,m_z</td>
<td>0 0 -1 1/2</td>
<td>2,1/2,0,0</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>0 0 -1 1/2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>-x+1/2, -y, z+1/2, -1</td>
<td>( -1 0 0 0</td>
<td>2 (0,0,1/2) 1/4,0,2, -1</td>
<td>{2</td>
</tr>
<tr>
<td></td>
<td>m_x,m_y,m_z</td>
<td>0 0 -1 1/2</td>
<td>2,0,1/2,0</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>0 0 -1 1/2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>-x+1/2, y+1/2, z+1/2, -1</td>
<td>-1 0 0 1/2</td>
<td>n(0,1/2,1/2) 1/4,y,z, -1</td>
<td>{m</td>
</tr>
<tr>
<td></td>
<td>m_x,m_y,m_z</td>
<td>0 0 0 -1/2</td>
<td>n(0,1/2,1/2)</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>0 0 0 -1/2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>x+1/2, y, -z+1/2, -1</td>
<td>( 1 0 0 0</td>
<td>a x,y,1/4, -1</td>
<td>{a01</td>
</tr>
<tr>
<td></td>
<td>m_x,m_y,m_z</td>
<td>0 0 0 1/2</td>
<td>a x,y,1/4, -1</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>0 0 0 1/2</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Go to the list of the Wyckoff Positions of the Group Pn′ma′ (#62.448)
Go to the Systematic Absences for the Group Pn′ma′ (#62.448)

Pn′ma′ = P12₁/m1 + {2’,100 | 1/2,1/2,1/2} P12₁/m1
Types of magnetic space groups:

(for a commensurate magnetic structure resulting from a paramagnetic phase having a grey magnetic group $G1'$)

Time inversion $\{1' | 0 0 0\}$ is NOT a symmetry operation of magnetic structure, but combined with a translation it can be…

F subgroup of G

$F \leq G$

magn. space group:  

magn. point groups:  

nuclear space group: (space group)

F subgroup of G

F

Types of magnetic space groups:

- **Type I**
  - some may allow ferromagnetic order

  - Type III
    - some may allow ferromagnetic order

  **Type IV**
  - antiferromagnetic order (ferromagnetism not allowed)

  $F + \{1' | t\}F$

  $P_F + 1' P_F$

  $F + \{R | t\}F = H$

  (lattice duplicated)

  *antitranslation / anticentering*

  (Type II are the grey groups ……)
Type of MSG depends on the propagation vector of the magnetic ordering:

- Most magn. orderings are 1k-magnetic structures.
- 1k-magnetic structures: moment changes from one unit cell to another according to a single wave vector or propagation vector $k$.
- Phase factor for unit cell $T$: $\exp(-i2\pi k.T)$
- The lattice translations such that $\exp(-i2\pi k.T)=1$ define the lattice maintained by the magnetic structure.
- The lattice translations such that $\exp(-i2\pi k.T)=-1$, are kept as antitranslations (type IV MSG). Only occur if $nk=$recipr. lattice vector with $n=$even

multiple $k$ structures: analogous situation …
### General Positions of the Group $P_{b\text{mn}2_1}$ (#31.129) [BNS setting]

To display the general positions in the OG setting, please follow this link: $P_{2\text{gem}2_1}$ (#31.6.217) [Transformation matrix]

#### Translation lattice generators:
- $(1|1,0,0)$, $(1|0,1,0)$, $(1|0,0,1)$, $(1|0,0,0)$

#### Black-and-white lattice generators:
- $(1|1,0,0)$, $(1|0,1,0)$, $(1|0,0,1)$, $(1^*|0,1/2,0)$

#### Example of type IV MSG

### Propagation vector $k \neq 0$

\[ P_{b\text{mn}2_1} = P_{\text{mn}2_1} + \{1'|0,1/2,0\} P_{\text{mn}2_1} \]

<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>$\begin{pmatrix} 1 &amp; 0 &amp; 0 \ 0 &amp; 1 &amp; 0 \ 0 &amp; 0 &amp; 1 \end{pmatrix}$</td>
<td>$1 +1$</td>
<td>${1\mid0}$</td>
</tr>
<tr>
<td>2</td>
<td>$-x+1/2, -y, z+1/2, +1$</td>
<td>$\begin{pmatrix} -1 &amp; 0 &amp; 0 \ 0 &amp; -1 &amp; 0 \ 0 &amp; 1 &amp; 1/2 \end{pmatrix}$</td>
<td>$2 (0,0,1/2) 1/4,0,z +1$</td>
<td>$(2\text{0}01 \mid 1/2 0 1/2)$</td>
</tr>
<tr>
<td>3</td>
<td>$-x, y, z, +1$</td>
<td>$\begin{pmatrix} -1 &amp; 0 &amp; 0 \ 0 &amp; 1 &amp; 0 \ 0 &amp; 0 &amp; 1 \end{pmatrix}$</td>
<td>$m_0,y,z +1$</td>
<td>${m_{100} \mid 0}$</td>
</tr>
<tr>
<td>4</td>
<td>$x+1/2, -y, z+1/2, +1$</td>
<td>$\begin{pmatrix} 1 &amp; 0 &amp; 0 \ 0 &amp; -1 &amp; 0 \ 0 &amp; 0 &amp; 1 \end{pmatrix}$</td>
<td>$n (1/2,0,1/2) x,0,z +1$</td>
<td>$(m_{010} \mid 1/2 0 1/2)$</td>
</tr>
<tr>
<td>5</td>
<td>$x, y+1/2, z, -1$</td>
<td>$\begin{pmatrix} 1 &amp; 0 &amp; 0 \ 0 &amp; 1 &amp; 0 \ 0 &amp; 0 &amp; 1/2 \end{pmatrix}$</td>
<td>$t (0,1/2,0) -1$</td>
<td>${1\mid0/2\ 0}$</td>
</tr>
<tr>
<td>6</td>
<td>$-x+1/2, -y+1/2, z+1/2, -1$</td>
<td>$\begin{pmatrix} -1 &amp; 0 &amp; 0 \ 0 &amp; -1 &amp; 0 \ 0 &amp; 1 &amp; 1/2 \end{pmatrix}$</td>
<td>$2 (0,0,1/2) 1/4,1/4,z +1$</td>
<td>$(2\text{0}01 \mid 1/2 1/2 1/2)$</td>
</tr>
<tr>
<td>7</td>
<td>$-x, y+1/2, z, -1$</td>
<td>$\begin{pmatrix} -1 &amp; 0 &amp; 0 \ 0 &amp; 1 &amp; 0 \ 0 &amp; 0 &amp; 1 \end{pmatrix}$</td>
<td>$b_0,y,z -1$</td>
<td>${m'_{100} \mid 0 1/2 0}$</td>
</tr>
<tr>
<td>8</td>
<td>$x+1/2, -y+1/2, z+1/2, -1$</td>
<td>$\begin{pmatrix} 1 &amp; 0 &amp; 0 \ 0 &amp; -1 &amp; 0 \ 0 &amp; 0 &amp; 1 \end{pmatrix}$</td>
<td>$n (1/2,0,1/2) x,1/4,z -1$</td>
<td>$(m'_{010} \mid 1/2 1/2 1/2)$</td>
</tr>
</tbody>
</table>
Tables of magnetic space groups ("standard" settings)

1.- E-book: D.B. Litvin: "Magnetic space groups" (Electronic Book)


(listing using only OG setting)

2.- Computer readable listing:

ISOTROPY webpage: http://stokes.byu.edu/iso/magneticspacegroups.html

H.T. Stokes and B.J. Campbell

(listing using BNS and OG settings)

3.- Bilbao crystallographic server (www.cryst.ehu.es)

(listings using BNS and OG settings)

Here we will always use BNS settings for the MSGs
Magnetic symmetry tools and applications in the BCS:

<table>
<thead>
<tr>
<th>Tool</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>MAGNEXT</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 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 magnetic structural models</td>
</tr>
<tr>
<td>MAGMODELIZE</td>
<td>Magnetic structure models for any given magnetic symmetry</td>
</tr>
<tr>
<td>k-SUBGROUPSMAG</td>
<td>Magnetic subgroups consistent with some given propagation vector(s) or a supercell</td>
</tr>
<tr>
<td>MAGNDATA</td>
<td>A collection of magnetic structures with transportable cif-type files</td>
</tr>
<tr>
<td>MVVISUALIZE</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>
Obtaining all possible magnetic symmetries for a magnetic phase with propagation vector \((1/2,0,0)\) and parent space group \(Pnma\)

2. Using \texttt{k-SUBGROUPSMAG} we obtain the \(k\)-maximal subgroups for the parent space group \(Pnma\) for a propagation vector \(k=(1/2,0,0)\).
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))

\[ \exp(i2\pi k \cdot a) = -1 \]

obtained with k-SUBGROUPSMAG
HoMnO$_3$  An Inevitable multiferroic...

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

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

graphic models are depicted assuming collinearity along x (my and mz are symmetry allowed)
Why the (magnetic) order parameter usually takes “special” directions of higher symmetry in the irrep space?

Domains/variants: symmetry related configurations around a higher-symmetry configuration

$Q_i$: Symmetry-breaking coordinates

Symmetry-forced extrema
**HoMnO$_3$**

unit cell: 2$a_p$, $b_p$, $c_p$

Magnetic space group: $P_bmn2_1$ (31.129)
in non-standard setting.
to transform to conventional setting:
(-$b$, $a$, $c$; 3/8,1/4,0)

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

### Atomic positions of asymmetric unit:

<p>| | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Ho1 4a</td>
<td>0.04195</td>
<td>0.25000</td>
</tr>
<tr>
<td>Ho2 4a</td>
<td>0.95805</td>
<td>0.75000</td>
</tr>
<tr>
<td>Mn1 8b</td>
<td>0.00000</td>
<td>0.00000</td>
</tr>
<tr>
<td>O1 4a</td>
<td>0.23110</td>
<td>0.25000</td>
</tr>
<tr>
<td>O12 4a</td>
<td>0.76890</td>
<td>0.75000</td>
</tr>
<tr>
<td>O2 8b</td>
<td>0.16405</td>
<td>0.05340</td>
</tr>
<tr>
<td>O22 8b</td>
<td>0.83595</td>
<td>0.55340</td>
</tr>
</tbody>
</table>

### Magnetic moments of the asymmetric unit ($\mu_B$):

<p>| | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Mn1</td>
<td>3.87</td>
<td>$\approx$0.0</td>
</tr>
</tbody>
</table>

### Magnetic Point Group: mm21'
Checking the symmetry operations present in the magnetic structure of HoMnO₃.

3. Upload the mcif file of HoMnO₃ in STRCONVERT. Among the listed symmetry operations identify the anticentering operation \{1'|1/2,0,0\}. Identify also in the list the operations \{2_z|3/4,0,1/2\} and \{2_z'|1/4,0,1/2\}. Copy/paste the list of symmetry operations and introduce them in the program “IDENTIFY MAGNETIC GROUP” and check the MSG of the structure. (file required: 2.HoMnO3.mcif)

<table>
<thead>
<tr>
<th>Magnetic Symmetry and Applications</th>
</tr>
</thead>
<tbody>
<tr>
<td>MGENPOS</td>
</tr>
<tr>
<td>MWYCKPOS</td>
</tr>
<tr>
<td>MAGNEXT</td>
</tr>
<tr>
<td>IDENTIFY MAGNETIC GROUP</td>
</tr>
<tr>
<td>MPOINT ![ ]</td>
</tr>
<tr>
<td>MAXMAGN</td>
</tr>
</tbody>
</table>
Subgroup of Pnma1’ in a basis: 2a_p, b_p, c_p

1 x,y,z,+1
2 -x+3/4,-y,z+1/2,+1
3 x,-y+1/2,z,+1
4 -x+3/4,y+1/2,z+1/2,+1

centering and “anticentering” translations:
1 x,y,z,+1
2 x+1/2,y,z,-1

Pnma1' = P_a nm2_1 + (1'|000) P_a nm2_1 + (-1|000) P_a nm2_1 + (-1'|000) P_a nm2_1

It is the MSG P_b mn2_1 (31.129) in a non-standard basis
Transformation to its standard setting: (-b, a, c; 3/8,1/4,0)
Consequences of symmetry

Effect of the magnetic ordering on the nuclear/lattice structure:

- case 1: no symmetry break for “nuclear structure”

\[ P_{2/m} \rightarrow P_{c2/m} \]

for the nuclear/lattice structure:

\[ P_{2/m} \rightarrow P_{2/m} \]

- case 2: symmetry break for “nuclear structure”

for the nuclear/lattice structure:

\[ Pnma \rightarrow Pmn2_1 (\mathbf{b}_p, \mathbf{a}_p, \mathbf{c}_p; 1/4,1/4,0) \]
Von Neumann principle:

- all variables/parameters/degrees of freedom compatible with the symmetry can be present in the total distortion
- Tensor crystal properties are constrained by the point group symmetry of the crystal.
- Reversely: any tensor property allowed by the point group symmetry can exist (large or small, but not forced to be zero)
Consequences of symmetry

Symmetry-constrained tensor properties:

<table>
<thead>
<tr>
<th>Point group</th>
<th>M and P</th>
</tr>
</thead>
<tbody>
<tr>
<td>2, m'm'2, 3, 3m', 4, 4m'm', 6, 6m'm'</td>
<td>M</td>
</tr>
<tr>
<td>m'm'2'</td>
<td>M</td>
</tr>
<tr>
<td>2'</td>
<td>M ⊥ z  P</td>
</tr>
<tr>
<td>m</td>
<td>M</td>
</tr>
<tr>
<td>m'</td>
<td>M ⊥ z  P ⊥ z</td>
</tr>
<tr>
<td>1</td>
<td>No restriction</td>
</tr>
</tbody>
</table>

Table 1.7. Heesch–Shubnikov Point Groups of Crystals which May Exhibit Ferromagnetism and Ferroelectricity
(Ascher, 1970)
(from 122 point groups)

A. P. Cracknell, "Magnetism in crystalline materials" 1975
Consequences of symmetry

Symmetry-constrained tensor properties:

A. P. Cracknell,
B. "Magnetism in crystalline materials" 1975
MTENSOR: Tensor calculation for Magnetic Point Groups

**Tensor calculation for Magnetic Point Groups**

MTENSOR provides the symmetry-adapted form of tensor properties for any magnetic point (or space) group. On the one hand, a point or space group must be selected, either in standard setting or in a non-standard setting defined by means of a transformation matrix to the standard setting or a set of generators of the magnetic point group. On the other hand, a tensor must be defined by the user or selected from the lists of known equilibrium, optical and transport tensors, gathered from scientific literature. If a standard magnetic point or space group is defined and a known tensor is selected from the lists the program will obtain the required tensor from and internal database; otherwise, the tensor is calculated live. The working setting is defined by the rules explained here. Live calculation of tensors may take too much time and even exceed the time limit, giving an empty result, if high-rank tensors, a lot of symmetry elements and/or rare settings are introduced.

Additionally, MTENSOR allows the introduction of a space group and a magnetic space subgroup in order to derive the symmetry-adapted form of tensor properties for all the corresponding domain-related equivalent structures.

Further information can be found here.

---

**Introduce a parent space group and a magnetic space subgroup and calculate tensors of the resulting domain-related equivalent structures**

**Please, enter a magnetic point group by one of these ways:**

- **Choose a magnetic point group:**
  
  **Magnetic Point or Space Group number:** Please, enter the label of the group or choose it

- **Non-conventional setting**

- **Introduce a magnetic point group by hand:**

  **Please, choose a tensor by one of these ways:**
Ferroic properties

A "multiferroic": improper ferroelectric

HoMnO$_3$

param. phase \hspace{2cm} antiferrom. phase

P$_{\text{nma}1'}$ $\overset{\text{index 4}}{\rightarrow}$ P$_{\text{a}nm2_1}$

point groups

mmm$_1'$ $\overset{\text{index 2}}{\rightarrow}$ mm$_{21'}$

Secondary symmetry-allowed effect: spontaneous polarization: $P_z$

$P_{\text{nma}1'} = P_{\text{a}nm2_1} + (1'|000)P_{\text{a}nm2_1} + (-1|000)P_{\text{a}nm2_1} + (-1'|000)P_{\text{a}nm2_1}$

generators of the four domain configurations:

$\{g_n\} = \{(1|000), (-1|000), (1'|000), (-1'|000)\}$

domains: equivalent energy minima

$(S_1,S_2) = (S,0)$ \hspace{2cm} $P_z$

$(S_1,S_2) = (0,S)$ \hspace{2cm} $-P_z$

Their MSG are equivalent, but not equal in general
The importance of non-magnetic atoms:

The same spin arrangement can produce different MSGs (and different ferroic properties) depending on the symmetry of the parent structure.

\[ \text{I4/mmm, } \mathbf{k} = (1/2, 1/2, 0) \]

\[ \text{Cmce, } \mathbf{k} = (0, 0, 0) \]

\[ \text{I-42m, } \mathbf{k} = (1/2, 1/2, 0) \]

\[ C_{\text{Accm}} \]
\[ (\mathbf{c}, \mathbf{a} - \mathbf{b}, \mathbf{a} + \mathbf{b}; 1/4, 3/4, 1/4) \]

\[ \text{Pr}_2\text{CuO}_4 \]

\[ C_{\text{mc'a'}} \]
\[ (\mathbf{c}, \mathbf{a} - \mathbf{b}, \mathbf{a} + \mathbf{b}; 0, 0, 0) \]

\[ \text{Gd}_2\text{CuO}_4 \]

\[ A_{\text{Bma2}} \]
\[ (\mathbf{a} + \mathbf{b}, -\mathbf{a} + \mathbf{b}, \mathbf{c}; 1/2, 0, 0) \]

Hypothetical spin configuration on a structure of type GaMnSe$_4$.
Check the symmetry restrictions on the Mn and Ho spins resulting from the symmetry of the magnetic phase of HoMnO$_3$.

4. Upload the mcif file of the magnetic structure of HoMnO$_3$ in STRCONVERT. Introduce a non-zero spin component of Ho along x or along z, and try to obtain all the atomic positions and moments within the unit cell by transforming to trivial symmetry P1. Check that the program in both cases (for Ho moment along x or z) gives an error/warning: this means that if the Ho atoms are magnetically ordered in this phase, their magnetic moments can only be directed along b. Come back to the description using the MSG using the back button of the browser and introduce now a non-zero spin component for the Ho atoms along b and transform again to P1 to observe the resulting values for the symmetry-related Ho atoms within the unit cell. Visualize the magnetic structure reading the mcif file with VESTA. Using alternatively MVISUALIZE observe the differences between the parent unit cell, the standard unit cell and the unit cell actually used in the description. (file required: 2.HoMnO3.mcif)
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