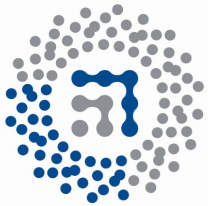

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Universidad del País Vasco
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Symmetry description of magnetic structures: Magnetic space groups

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

Annu. Rev. Mater. Res. 2015. 45:217–48

Symmetry-Based Computational Tools for Magnetic Crystallography

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

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

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

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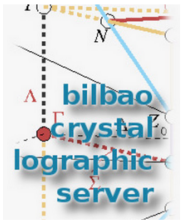


Crystallography Online: Workshop on the use of the structural and magnetic tools of the Bilbao Crystallographic Server
September 2021, Leioa (Spain)

Forthcoming schools and workshops

News:

- **New Article in Nature**
  10/2020: Xu *et al.* "High-throughput calculations of magnetic topological materials" *Nature* (2020) **586**, 702-707.
- New programs: **MBANDREP**, **COREPRESENTATIONS**, **COREPRESENTATIONS PG**, **MCOMPREL**, **MSITESYM**, **MKVEC**, **Check Topological Magnetic Mat**
  10/2020: new tools in the sections "Magnetic Symmetry and Applications" and "Representations and Applications". **More info**

Space-group symmetry

Magnetic Symmetry and Applications

Group-Subgroup Relations of Space Groups

Representations and Applications

Solid State Theory Applications

Structure Utilities

Topological Quantum Chemistry

Subperiodic Groups: Layer, Rod and Frieze Groups

Structure Databases

Raman and Hyper-Raman scattering

Point-group symmetry

Quick access to some tables

- Space Groups
- Plane Groups
- Layer Groups
- Rod Groups
- Frieze Groups
- 2D Point Groups
- 3D Point Groups
- Magnetic Space Groups

Reminder of symmetry in non-magnetic structures

SPACE GROUPS:

Group of operations {**R** | **t**} transforming any point **r** in space in the following form:

If **r** = x **a** + y **b** + z **c** (**a** ,**b**, **c**): set of vectors defining a basis/unit cell

r = (x,y,z)

$$\begin{bmatrix} x' \\ y' \\ z' \end{bmatrix} = \mathbf{R} \begin{bmatrix} x \\ y \\ z \end{bmatrix} + \mathbf{t}$$

R: 3x3 matrix. Proper rotation or improper (rotation+inversion)
[det(**R**)= +1 or -1]

t: translation $(t_1,t_2,t_3) = t_1\,\mathbf{a} + t_2\,\mathbf{b} + t_3\,\mathbf{c}$

Lattice periodicity: Subgroup of lattice translations: { 1 || **T** }, **T** = $n_1\,\mathbf{a} + n_2\,\mathbf{b} + n_3\,\mathbf{c}$, n_i integers

rotation 360º/2 around (100) (a-axis)

inversion

mirror plane perpendicular to (010) direction (b-axis)

rotation 360º/3 around (001) (c- axis)

Notations (Seitz and xyz form):

$\{2_{100} \mid ½\ ½\ ½\}$	x+1/2,-y+1/2,-z+1/2 (for an orthogonal unit cell)
{-1|000}	-x,-y,-z
$\{m_{010} \mid 0\ ½\ 0\}$	x,-y+1/2,z (for an orthogonal unit cell)
$\{3^+_{001} \mid 0\ 0\ 1/3\}$	-y,x-y,z+1/3 (for a trigonal unit cell)

Reminder of symmetry in non-magnetic structures

space group symmetry: $\rho(\mathbf{r}) = \rho(\{\mathbf{R} \mid \mathbf{t}\}^{-1}\mathbf{r})$ $\rho(\mathbf{r})$: particle density

$\rho(\mathbf{r} + \mathbf{T}) = \rho(\mathbf{r})$ lattice periodicty

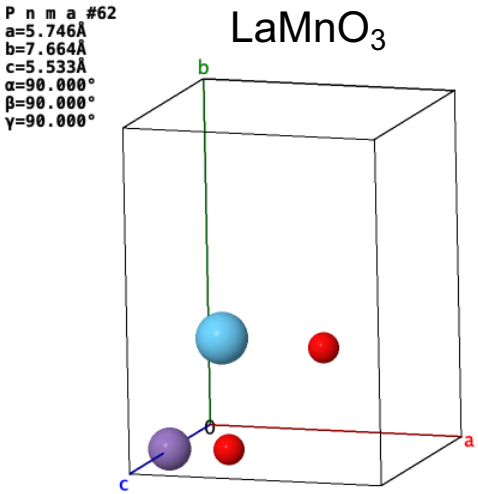
Space Group:
Pnma

Lattice parameters:
5.7461 7.6637 5.5333 90.000 90.000 90.000

asymmetric unit

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



“standard setting” of SG *Pnma*

General Position of the Group *Pnma* (No. 62)

Click here to get the general position in text format

from **GENPOS** in the Bilbao server

No.	(x,y,z) form	Matrix form	Symmetry operation	
			ITA	Seitz
1	x,y,z	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	1	{ 1 | 0 }
2	-x+1/2,-y,z+1/2	$\begin{pmatrix} -1 & 0 & 0 & 1/2 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 1/2 \end{pmatrix}$	2 (0,0,1/2) 1/4,0,z	{ 2_{001} | 1/2 0 1/2 }
3	-x,y+1/2,-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	{ 2_{010} | 0 1/2 0 }
4	x+1/2,-y+1/2,-z+1/2	$\begin{pmatrix} 1 & 0 & 0 & 1/2 \\ 0 & -1 & 0 & 1/2 \\ 0 & 0 & -1 & 1/2 \end{pmatrix}$	2 (1/2,0,0) x,1/4,1/4	{ 2_{100} | 1/2 1/2 1/2 }
5	-x,-y,-z	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \end{pmatrix}$	-1 0,0,0	{ -1 | 0 }
6	x+1/2,y,-z+1/2	$\begin{pmatrix} 1 & 0 & 0 & 1/2 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 1/2 \end{pmatrix}$	a x,y,1/4	{ m_{001} | 1/2 0 1/2 }
7	x,-y+1/2,z	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 1/2 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	m x,1/4,z	{ m_{010} | 0 1/2 0 }
8	-x+1/2,y+1/2,z+1/2	$\begin{pmatrix} -1 & 0 & 0 & 1/2 \\ 0 & 1 & 0 & 1/2 \\ 0 & 0 & 1 & 1/2 \end{pmatrix}$	n (0,1/2,1/2) 1/4,y,z	{ m_{100} | 1/2 1/2 1/2 }

xyz notation

Seitz notation

Reminder of symmetry in non-magnetic structures

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Pnma

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5.7461 7.6637 5.5333 90.000 90.000 90.000

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Atomic positions of asymmetric unit:

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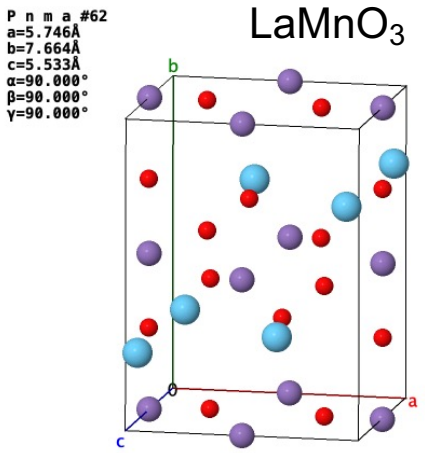
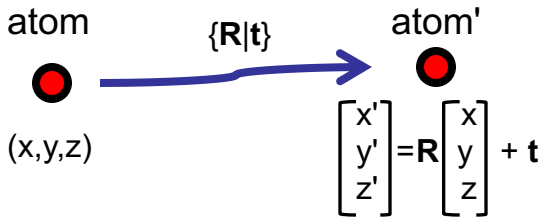


Space Group: set of operations {R|t}

for all atoms:



{**R**|**t**}: **R -** rotation or rotation+plus inversion
t - translation

Pnma:

1 x,y,z	{1|000}
2 x+1/2,-y+1/2,-z+1/2	$\{2_{100} \mid ½\ ½\ ½\}$
3 -x,y+1/2,-z,	$\{2_{010} \mid 0\ ½\ 0\}$
4 -x+1/2,-y,z+1/2	$\{2_{001} \mid ½\ 0\ ½\}$
5 -x,-y,-z	{-1|000}
6 -x+1/2,y+1/2,z+1/2	$\{m_{100} \mid ½\ ½\ ½\}$
7 x,-y+1/2,z	$\{m_{010} \mid 0\ ½\ 0\}$
8 x+1/2,y,-z+1/2	$\{m_{001} \mid ½\ 0\ ½\}$

Special positions:

Pnma: 8 related positions for a general position:

Seitz Notation

(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| ½ ½ ½ }
(-x,-y,-z) (x+1/2,y,-z+1/2) (x,-y+1/2,z) (-x+1/2,y+1/2,z+1/2) == {m_x| ½ ½ ½ }

4 related positions for a special position of type (x, ¼, z):

(x,1/4,z) (-x+1/2,3/4,z+1/2) (-x,3/4,-z) (x+1/2,1/4,-z+1/2)

special positions are tabulated:
Wyckoff positions or orbits

From WYCKPOS in the BCS:

Wyckoff Positions of Group *Pnma* (No. 62)

Multiplicity	Wyckoff letter	Site symmetry	Coordinates
8	d	1	(x,y,z) (-x+1/2,-y,z+1/2) (-x,y+1/2,-z) (x+1/2,-y+1/2,-z+1/2) (-x,-y,-z) (x+1/2,y,-z+1/2) (x,-y+1/2,z) (-x+1/2,y+1/2,z+1/2)
4	c	.m.	(x,1/4,z) (-x+1/2,3/4,z+1/2) (-x,3/4,-z) (x+1/2,1/4,-z+1/2)
4	b	-1	(0,0,1/2) (1/2,0,0) (0,1/2,1/2) (1/2,1/2,0)
4	a	-1	(0,0,0) (1/2,0,1/2) (0,1/2,0) (1/2,1/2,1/2)

Reminder of symmetry in non-magnetic structures

Space Group:
Pnma

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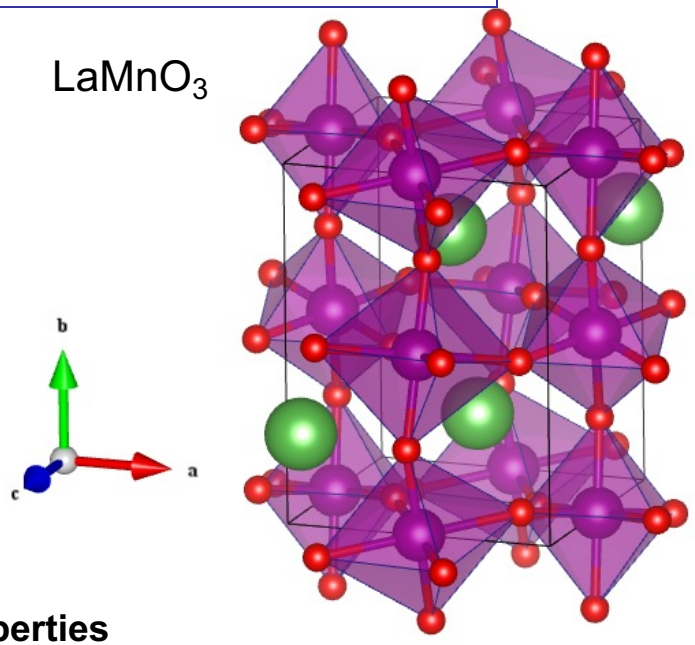
O2	0.30850	0.04080	0.72270

$LaMnO_3$



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 (with a different symmetry)

```
data_sv4w48Eo
_audit_creation_date                    2012-11-23
_audit_creation_method                  "Bilbao Crystallograph
_symmetry_Int_Tables_number             62
_symmetry_space_group_name_H-M          "Pnma"
_cell_length_a                          5.7461
_cell_length_b                          7.6637
_cell_length_c                          5.5333
_cell_angle_alpha                       90.0000
_cell_angle_beta                        90.0000
_cell_angle_gamma                       90.0000

loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
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   2   -x,y+1/2,-z
   3   -x,-y,-z
   4   x,-y+1/2,z
   5   x+1/2,-y+1/2,-z+1/2
   6   -x+1/2,-y,z+1/2
   7   -x+1/2,y+1/2,z+1/2
   8   x+1/2,y,-z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
La La 0.05130 0.25000 -0.00950 1.0000
Mn Mn 0.00000 0.00000 0.50000 1.0000
O1 O 0.48490 0.25000 0.07770 1.0000
O2 O 0.30850 0.04080 0.72270 1.0000
```

SG

unit cell

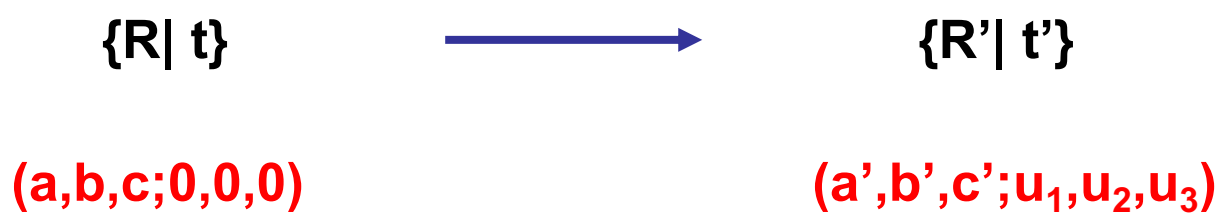
SG operations

asymm. unit

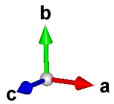
Crystallographic Information Framework (CIF)

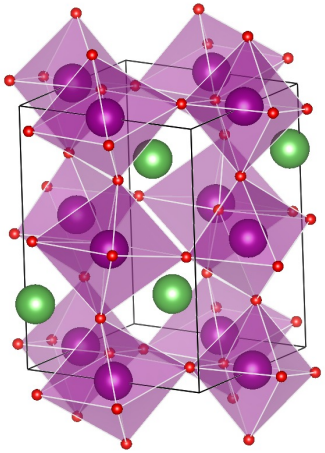
The CIF files

The form of the symmetry operations depend on the basis used

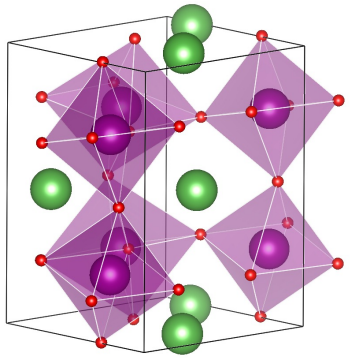


LaMnO3: same structure with SG in a different setting





Pnma



standard setting

1 x,y,z
2 x+1/2,-y+1/2,-z+1/2
3 -x,y+1/2,-z,
4 -x+1/2,-y,z+1/2
5 -x,-y,-z
6 -x+1/2,y+1/2,z+1/2
7 x,-y+1/2,z
8 x+1/2,y,-z+1/2

non-standard setting

1 x,y,z
2 -x,-y,z+1/2
3 -x+1/2,y+1/2,-z+1/2
4 x+1/2,-y+1/2,-z
5 -x+1/2,-y+1/2,-z
6 x+1/2,y+1/2,-z+1/2
7 x,-y,z+1/2
8 -x,y,z

IDENTIFY GROUP: Identification of a Space Group from a set of generators in an arbitrary setting.

IDENTIFY GROUP: Identifies a Space Group given a set of generators

IDENTIFY GROUP identifies a Space Group given a set of generators and shows the transformation matrix to a standard or reference (default) description of the Space Group.

Help

Enter the generators of the Space Group in the box below, given in any basis of the lattice, as in the example:

x+1/2,y+1/2,z

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

Assumed lattice translations:
x + 1 , y , z
x , y + 1 , z
x , y , z + 1

```
x,y,z
−x,−y,z+1/2
−x+1/2,y+1/2,−z+1/2
x+1/2,−y+1/2,−z
−x+1/2,−y+1/2,−z
x+1/2,y+1/2,−z+1/2
x,−y,z+1/2
−x,y,z
```

Submit

From IDENTIFY GROUP:

The Space Group has been identified as *Pnma* (No. 62)

Transformation Matrix to the standard/default setting

$$\begin{pmatrix} 0 & -1 & 0 & 1/4 \\ 0 & 0 & 1 & 1/4 \\ -1 & 0 & 0 & 0 \end{pmatrix}$$

Check an alternative Transformation Matrix

(P,p) transformation to standard of the SG

P = 3x3 matrix

p = (p_1, p_2, p_3)

General positions of the Space Group *Pnma* in the given setting

1 x,y,z
2 -x+1/2,y+1/2,-z+1/2
3 x+1/2,-y+1/2,-z
4 -x,-y,z+1/2
5 -x+1/2,-y+1/2,-z
6 x,-y,z+1/2
7 -x,y,z
8 x+1/2,y+1/2,-z+1/2

$(a^s,b^s,c^s)= (a,b,c).P$, $O^s = O + p_1\, a + p_2\, b + p_3\, c$

(**c,a,b;**1/4,1/4,0)

SG in its standard setting

Pnma (**c,a,b;**1/4,1/4,0)

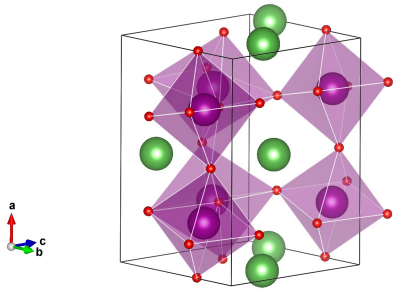
Transformation to standard setting:

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:

$$\begin{pmatrix} x^s \\ y^s \\ z^s \\ 1 \end{pmatrix} = \left(\begin{array}{ccc|c} & \mathbf{P} & & \mathbf{p} \\ \hline 0 & 0 & 0 & 1 \end{array}\right)^{-1} \begin{pmatrix} x \\ y \\ z \\ 1 \end{pmatrix}$$



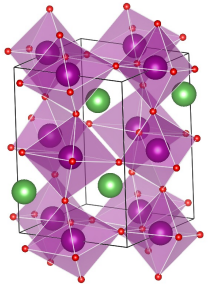
non-standard setting

Pnma **(c,a,b;**1/4,1/4,0)

Different choice of unit cell and origin shift:

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

$$\mathbf{(P,p)} = \left(\begin{array}{ccc|c} 0 & 1 & 0 & ¼ \\ 0 & 0 & 1 & ¼ \\ 1 & 0 & 0 & 0 \end{array}\right)$$



standard setting

Pnma

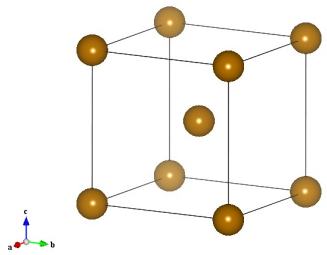
Symmetry and Physics:

A symmetry property in a solid is **NOT ONLY** some mathematical property. It is a **PHYSICAL PROPERTY!**

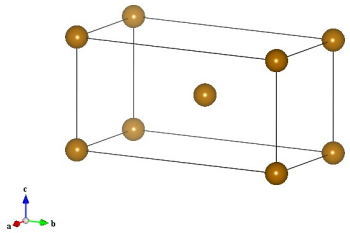
A welldefined symmetry operation in a thermodynamic system or in a ground state must be maintained when scalar fields (temperature, pressure,…) or Hamiltonian scalar parameters are continuously changed (**except if a phase transition takes place).**

The change of symmetry of a crystal necessarily implies a phase transition.

Example of a nice geometric relation, which is NOT a "symmetry" relation:



a=b=c symmetry property



a = c
b = 2a "nice" but not a symmetry property

Defining the symmetry of a crystal

1st step. ***We define a set of operations/transformations on the system: rotations, translations, space inversion, ETC. (they form a mathematical group)***

2nd step. ***On the previous group of operations we look for the subset (subgroup) of operations, which keep the crystal INVARIANT or UNDISTINGUISHABLE . This is the symmetry group of the crystal.***

But what is the group of operations that we define or choose in the first step above? *(Once this group is chosen, there is no ambigüity on the symmetry group of the system).* And here comes the Physics…:

Symmetry and Physics:

We search the symmetry operation among all possible combinations of **rotations**
translations
space inversion

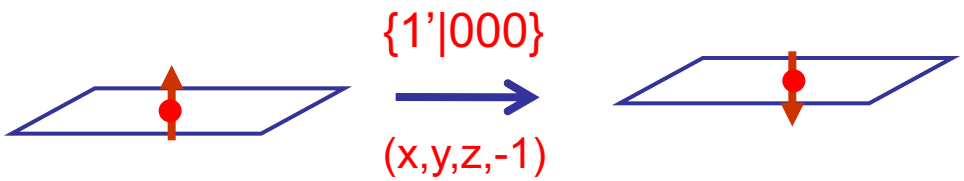
(What they have in common? :

They all keep the **ENERGY of the system invariant**
(the hamiltonian or the free energy)

The symmetry group of a solid is formed by all operations **that keeping the ENERGY invariant ALSO** maintain the system undistinguishable after applying the operation.

The time reversal operation also keeps energy invariant:

Ttime reversal operation: {1'|0,0,0}:
- Does not change nuclear variables
- Changes sign of ALL atomic (average) magnetic moments
- Changes sign of momenta (not relevant here)



If all average atomic moments are zero, the system is invariant for the time reversal operation:

Time reversal symmetry is present as symmetry operation in non-magnetic structures but it is ABSENT in magnetically ordered ones!

Magnetic symmetry groups:

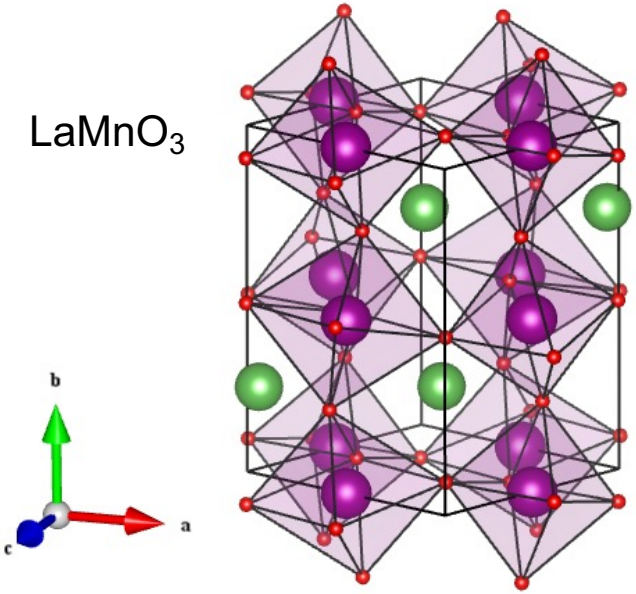
We do not add but SUBSTRACT symmetry operations !

Time reversal symmetry is detected when it does NOT exist !

All NON-magnetic structures have time reversal symmetry!

All symmetry operations are **(implicitly)** duplicated: with and without time reversal

$LaMnO_3$



Pnma.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,-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,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,-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)

All NON-magnetic structures have time reversal 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:

Pnma.1' = Pnma + {1'|000}x ***Pnma*** (grey group)

16 operations:

(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,-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,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,-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)

Notation: (x+1/2,-y+1/2,-z+1/2,+1) == {2x| ½ ½ ½ } {R|**t**}
(x+1/2,-y+1/2,-z+1/2,-1) == {2x'| ½ ½ ½ } {R'|**t**}

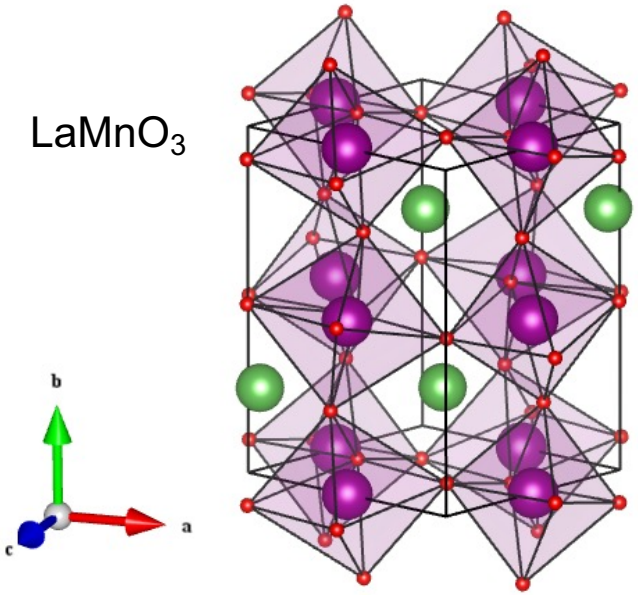
$\{R,\theta|\mathbf{t}\}$ → $\theta=1$, $\theta=-1$

Magnetic ordering is a symmetry breaking process

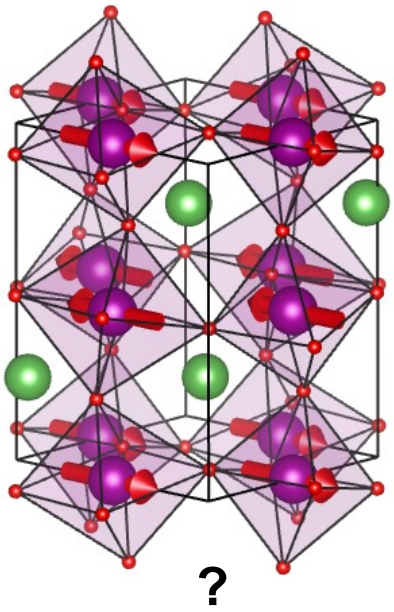
Magnetically ordered phases:

Time reversal {1'|0 0 0} is LOST

$LaMnO_3$



Pnma.1'

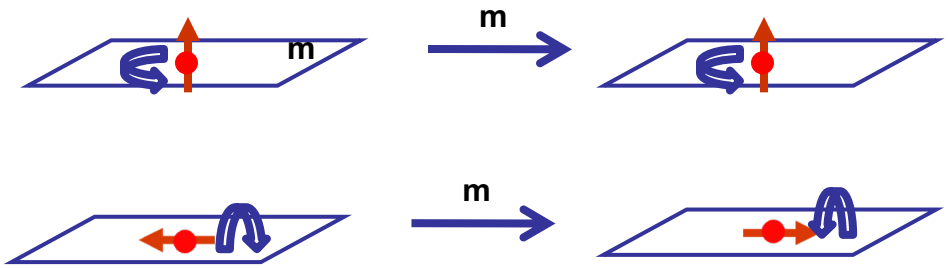


?

(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,-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,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,-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)

For space operations, the magnetic moments transform as pseudovectors or axial vectors:

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



To keep the energy invariant (SOC≠0) the magn. moments must transform together with the atomic position:

atom $\{\mathbf{R},\theta|\mathbf{t}\}$ (for positions: the same as with Pnma)

(x,y,z) $\rightarrow \begin{bmatrix} x' \\ y' \\ z' \end{bmatrix} = \mathbf{R} \begin{bmatrix} x \\ y \\ z \end{bmatrix} + \mathbf{t}$

(mx,my,mz) $\rightarrow \begin{bmatrix} mx' \\ my' \\ mz' \end{bmatrix} = \theta \det(\mathbf{R})\ \mathbf{R} \begin{bmatrix} mx \\ my \\ mz \end{bmatrix}$

θ=-1 if time reversal

operation on the magn. moments

$$\{\theta \det(\mathbf{R})\ \mathbf{R} \,||\, \mathbf{R} \,|\, \mathbf{t}\}$$

operation on the positions

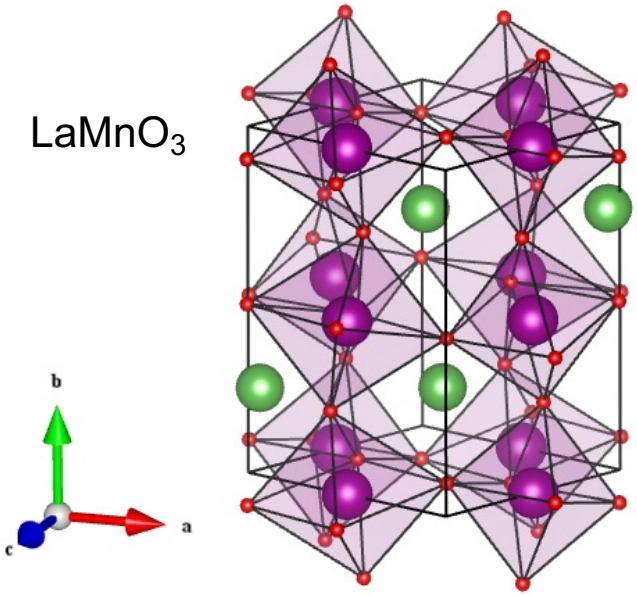
$\{\mathbf{R}, \theta \,|\, \mathbf{t}\}$: contains all the necessary information

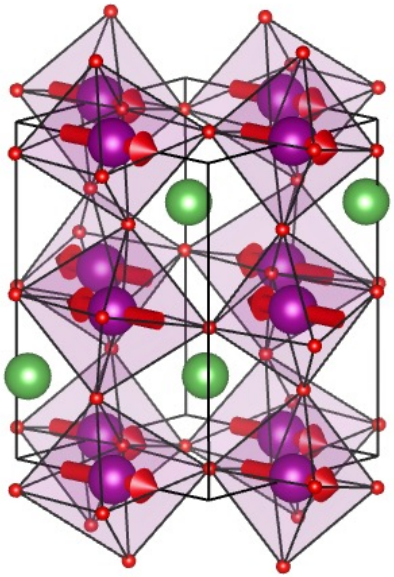
Magnetic ordering is a symmetry breaking process

Magnetically ordered phases:

Time reversal {1'|0 0 0} is LOST but some operations including time reversal are mantained

$LaMnO_3$





Pnma.1'

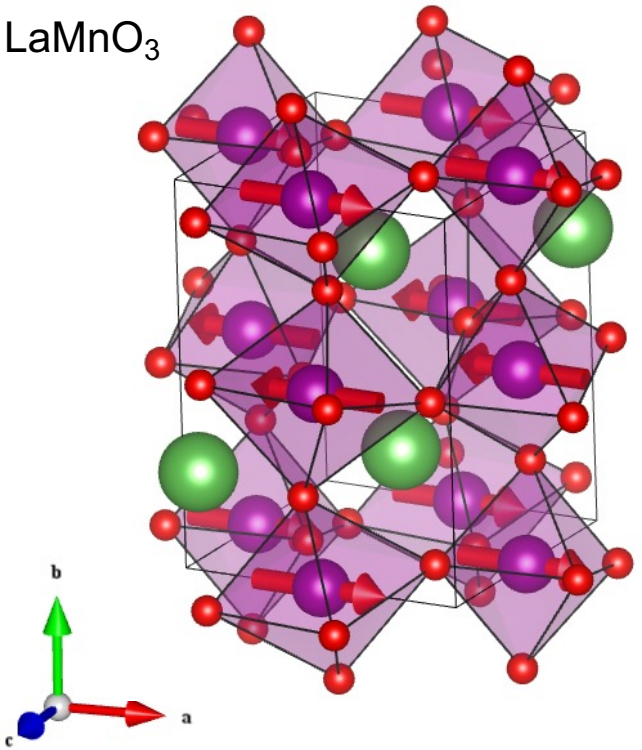
(x,y,z,+1) ~~(-x+1/2,-y,z+1/2,+1)~~
(-x,-y,-z,+1) ~~(x+1/2,y,-z+1/2,+1)~~
~~(x,y,z,-1)~~ (-x+1/2,-y,z+1/2,-1)
~~(-x,-y,-z,-1)~~ (x+1/2,y,-z+1/2,-1)

Pn'ma'

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

Description of a magnetic structure in a crystallographic form using its MSG:

$LaMnO_3$



Magnetic space Group:
Pn'ma'

Pn'ma':

x,y,z,+1	{1|000}
x+1/2,-y+1/2,-z+1/2,-1	$\{2'_{100} \mid ½\ ½\ ½\}$
-x,y+1/2,-z,+1	$\{2_{010} \mid 0\ ½\ 0\}$
-x+1/2,-y,z+1/2,-1	$\{2'_{001} \mid ½\ 0\ ½\}$
-x,-y,-z,+1	{-1|000}
-x+1/2,y+1/2,z+1/2,-1	$\{m'_{100} \mid ½\ ½\ ½\}$
x,-y+1/2,z,+1	$\{m_{010} \mid 0\ ½\ 0\}$
x+1/2,y,-z+1/2,-1	$\{m'_{001} \mid ½\ 0\ ½\}$

Operations {**R**, θ | **t**}: they contain all the necessary information including how the magn. moments transform

In the language of spin space groups, the operations are: $\{\theta \det(\mathbf{R})\ \mathbf{R} \parallel \mathbf{R} \mid \mathbf{t}\}$

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

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 }
2	-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_{010} | 0 1/2 0 }
3	-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 }
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_{010} | 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	{ $2'_{100}$ | 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	{ $2'_{001}$ | 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'_{100} | 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'_{001} | 1/2 0 1/2 }

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)

Output of MGENPOS

type III MSG

Magnetic point group: m’mm’

coset decomposition:

$$Pn'ma' = P12_1/m1 + \{2'_{100}|1/2,1/2,1/2\}\ P12_1/m1$$

Types of magnetic space groups:

(for a commensurate magnetic structure resulting from a paramagnetic phase having a grey magnetic group G.1')

F subgroup of G
F ≤ G

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

	magn. **space** group:	magn. **point** groups:
Type I **some may allow ferromagnetic order**	$\mathbf{F}$	$\mathbf{P_F}$
		black and white group
Type III **some may allow ferromagnetic order**	$\mathbf{F} + \{\mathbf{R'}|\mathbf{t}\}\mathbf{F}$	$\mathbf{P_F} + \mathbf{R'P_F}$
		grey group
Type IV **antiferromagnetic order (ferromagnetism not allowed)**	$\mathbf{F} + \{1'|\mathbf{t}\}\mathbf{F}$	$\mathbf{P_F} + \mathbf{1'}\ \mathbf{P_F}$

antitranslation / anticentering

(Type II are the grey groups of the non-magnetically ordered systems):

Type II **non-magnetic structures**	$\mathbf{F} + \{1'|\mathbf{0}\}\mathbf{F}$	$\mathbf{P_F} + \mathbf{1'}\ \mathbf{P_F}$

Tables of magnetic space groups ("standard" settings)

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

Litvin DB. 2013. *Magnetic Group Tables: 1-, 2- and 3-Dimensional Magnetic Subperiodic Groups and Magnetic Space Groups*. Chester, UK: Int. Union Crystallogr. http://www.iucr.org/publ/978-0-9553602-2-0

(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

(downloadable files using BNS and OG settings)

3.- Web online listing: Bilbao crystallographic server (www.cryst.ehu.es)

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

(listings using BNS and OG settings)

(So far) only software using BNS setting exists

Fundamental difference of the OG description:
For type IV MSGs it uses a unit cell which does NOT describe the lattice of the system.

ON THE NEW MSG SYMBOLS

Acta Cryst A FOUNDATIONS ADVANCES
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Introducing a unified magnetic space-group symbol

Branton J. Campbell,[a]* Harold T. Stokes,[a] J. Manuel Perez-Mato[b] and Juan Rodríguez-Carvajal[c]

"…., a new unified (UNI) MSG symbol is introduced, which combines a modified BNS symbol with essential information from the OG symbol. "

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STRUCTURAL SCIENCE
CRYSTAL ENGINEERING
MATERIALS

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A recapitulation of magnetic space groups and their UNI symbols

B. J. Campbell,[a]* H. T. Stokes,[a] J. M. Perez-Mato[b] and J. Rodriguez-Carvajal[c]

[a]Department of Physics and Astronomy, Brigham Young University, Provo, UT 84602, USA, [b]Facultad de Ciencia y Tecnología, Universidad del País Vasco, UPV/EHU, Apartado 644, 48080 Bilbao, Spain, and [c]Institut Laue-Langevin (ILL), 71 avenue des Martyrs, 38042 Grenoble, France. *Correspondence e-mail: branton_campbell@byu.edu

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This article is part of a focused issue on Magnetic Structures.

The mathematical structure, description and classification of magnetic space groups is briefly reviewed, with special emphasis on the recently proposed notation, the so-called UNI symbols [Campbell *et al.* (2022). *Acta Cryst.* A**78**, 99–106]. As illustrative examples, very simple magnetic space groups from each of the four possible types are described in detail.

Magnetic Symmetry and Applications

Magnetic groups	
MGENPOS	General Positions of Magnetic Space Groups
MWYCKPOS	Wyckoff Positions of Magnetic Space Groups
MKVEC	The k-vector types and Brillouin zones of Magnetic Space Groups
IDENTIFY MAGNETIC GROUP	Identification of a Magnetic Space Group from a set of generators in an arbitrary setting
BNS2OG	Transformation of symmetry operations between BNS and OG settings
mCIF2PCR	Transformation from mCIF to PCR format (FullProf).
MPOINT	Magnetic Point Group Tables
MAGNEXT	Extinction Rules of Magnetic Space Groups
MAXMAGN	Maximal magnetic space groups for a given space group and a propagation vector
MAGMODELIZE	Magnetic structure models for any given magnetic symmetry
STRCONVERT	Convert & Edit Structure Data (supports the CIF, mCIF, VESTA, VASP formats -- with magnetic information where available)
k-SUBGROUPSMAG	Magnetic subgroups consistent with some given propagation vector(s) or a supercell
MAGNDATA	A collection of magnetic structures with portable cif-type files
MVISUALIZE	3D Visualization of magnetic structures with Jmol
MTENSOR	Symmetry-adapted form of crystal tensors in magnetic phases
MAGNETIC REP.	Decomposition of the magnetic representation into irreps
Get_mirreps	Irreps and order parameters in a paramagnetic space group-magnetic subgroup phase transition
Spin groups	
STENSOR ⚠	Symmetry-adapted form of crystal tensors under spin point groups
CollinearSpinGroups ⚠	Operations of Nontrivial Collinear Spin Space Groups

General Positions of the Group *Pnma* (#62.441)

62.441 *Pnma.1* (UNI symbol)

For this space group, BNS and OG settings coincide.
Its label in the OG setting is given as: Pnma (#62.1.502)

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 }
2	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_{100} | 1/2 1/2 1/2 }
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_{010} | 0 1/2 0 }
4	-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_{001} | 1/2 0 1/2 }
5	-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 }
6	-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_{100} | 1/2 1/2 1/2 }
7	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_{010} | 0 1/2 0 }
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_{001} | 1/2 0 1/2 }

Output of MGENPOS

Example of TYPE I

Magnetic point group: mmm.1

Pnma → Pnma.1 UNI symbol

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 }
2	-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_{010} | 0 1/2 0 }
3	-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 }
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_{010} | 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	{ $2'_{100}$ | 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	{ $2'_{001}$ | 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'_{100} | 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'_{001} | 1/2 0 1/2 }

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)

Output of MGENPOS

Example of TYPE III

Magnetic point group: m' mm'

Pn' ma' = $P12_1/m1$ + {$2'_{100}$|1/2,1/2,1/2} $P12_1/m1$

General Positions of the Group P_bmn2_1 (#31.129) [BNS setting]

31.129 $Pmn2_1.1'_b[Pmn2_1]$ (UNI symbol)

To display the general positions in the OG setting, please follow this link: $P_{2b}mn2_1$ (#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)

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 }
2	-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_{001} | 1/2 0 1/2 }
3	-x, y, z, +1 $m_x,-m_y,-m_z$	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	m 0,y,z +1	{ m_{100} | 0 }
4	x+1/2, -y, z+1/2, +1 $-m_x,m_y,-m_z$	$\begin{pmatrix} 1 & 0 & 0 & 1/2 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 1/2 \end{pmatrix}$	n (1/2,0,1/2) x,0,z +1	{ m_{010} | 1/2 0 1/2 }
5	x, y+1/2, z, -1 $-m_x,-m_y,-m_z$	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1/2 \\ 0 & 0 & 1 & 0 \end{pmatrix}'$	t (0,1/2,0) -1	{ 1' | 0 1/2 0 }
6	-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 (0,0,1/2) 1/4,1/4,z -1	{ $2'_{001}$ | 1/2 1/2 1/2 }
7	-x, y+1/2, z, -1 $-m_x,m_y,m_z$	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1/2 \\ 0 & 0 & 1 & 0 \end{pmatrix}'$	b 0,y,z -1	{ m'_{100} | 0 1/2 0 }
8	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 (1/2,0,1/2) x,1/4,z -1	{ m'_{010} | 1/2 1/2 1/2 }

Output of MGENPOS

Example of TYPE IV

Magnetic point group: mmm.1'

UNI symbol: **$Pmn2_1.1'_b$**

$P_bmn2_1 = Pmn2_1 + \{1' | 0,1/2,0\} Pmn2_1$

General Positions of the Group P_c2_1/c (#14.82) [BNS setting]

14.82 $P2_1/c.1'_c[P2_1/m]$ (UNI symbol[1,2])

To display the general positions in the OG setting, please follow this link: $P_{2c}2_1/m'$ (#11.7.65) [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'|0,0,1/2)

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 }
2	-x, y+1/2, -z+1/2, +1 $-m_x,m_y,-m_z$	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1/2 \\ 0 & 0 & -1 & 1/2 \end{pmatrix}$	2 (0,1/2,0) 0,y,1/4 +1	{ 2_{010} | 0 1/2 1/2 }
3	-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 }
4	x, -y+1/2, z+1/2, +1 $-m_x,m_y,-m_z$	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 1/2 \\ 0 & 0 & 1 & 1/2 \end{pmatrix}$	c x,1/4,z +1	{ m_{010} | 0 1/2 1/2 }
5	x, y, z+1/2, -1 $-m_x,-m_y,-m_z$	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1/2 \end{pmatrix}'$	t (0,0,1/2) -1	{ 1' | 0 0 1/2 }
6	-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	{ $2'_{010}$ | 0 1/2 0 }
7	-x, -y, -z+1/2, -1 $-m_x,-m_y,-m_z$	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 1/2 \end{pmatrix}'$	-1 0,0,1/4 -1	{ -1' | 0 0 1/2 }
8	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'_{010} | 0 1/2 0 }

Output of MGENPOS

Another example of TYPE IV

Disregarding time reversal:

SG: $P2_1/m$

Extended UNI symbol:
$P2_1/c.1'_c$ [$P2_1/m$]

UNI symbol:
$P2_1/c.1'_c$

$P_c2_1/c = P2_1/c + \{1' \mid 0,0,½\}\ P2_1/c$

General Positions of the Group $P_{2c}2_1/m'$ (#11.7.65) [OG setting]

14.82 $P2_1/c.1'_c[P2_1/m]$ (UNI symbol[1,2])

To display the general positions in the BNS setting, please follow this link: P_c2_1/c (#14.82) [Transformation matrix]

Translation lattice generators: (1|1,0,0), (1|0,1,0), (1|0,0,2), (1|0,0,0)

Black-and-white lattice generators: (1|1,0,0), (1|0,1,0), (1'|0,0,1)

k-vector [Help] : (0, 0, 1/2)

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 }
2	-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_{010} | 0 1/2 0 }
3	-x, -y, -z+1, +1 m_x,m_y,m_z	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 1 \end{pmatrix}$	-1 0,0,1/2 +1	{ -1 | 0 0 1 }
4	x, -y+1/2, z+1, +1 $-m_x,m_y,-m_z$	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 1/2 \\ 0 & 0 & 1 & 1 \end{pmatrix}$	g (0,0,1) x,1/4,z +1	{ m_{010} | 0 1/2 1 }
5	x, y, z+1, -1 $-m_x,-m_y,-m_z$	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \end{pmatrix}'$	t (0,0,1) -1	{ 1' | 0 0 1 }
6	-x, y+1/2, -z+1, -1 $m_x,-m_y,m_z$	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1/2 \\ 0 & 0 & -1 & 1 \end{pmatrix}'$	2 (0,1/2,0) 0,y,1/2 -1	{ $2'_{010}$ | 0 1/2 1 }
7	-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 }
8	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'_{010} | 0 1/2 0 }

Output of MGENPOS

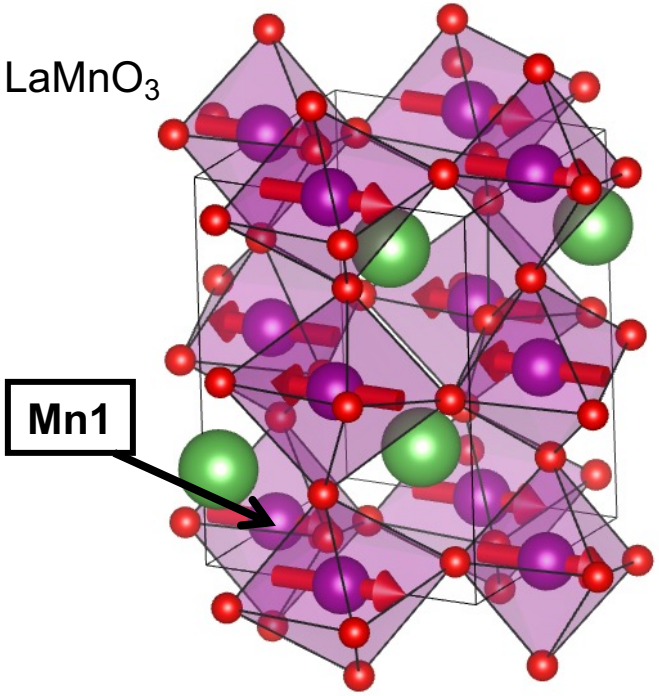
Same MSG in OG setting

Disregarding time reversal:

SG: $P2_1/m$

Extended UNI symbol:
$P2_1/c.1'_c[P2_1/m]$

Description of a magnetic structure in a crystallographic form using its MSG:



Magnetic space Group:
Pn'ma'

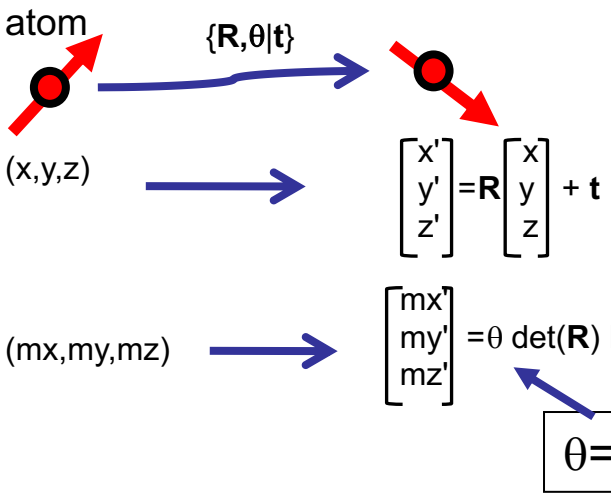
Lattice parameters:
5.7461 7.6637 5.5333 90.000 90.000 90.000

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) and symmetry constraints::

Mn1 3.87 0.0 0.0 (mx,my,mz)

Symmetry operations are relevant both for positions and moments



MSG

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

Wyckoff positions of a MSG

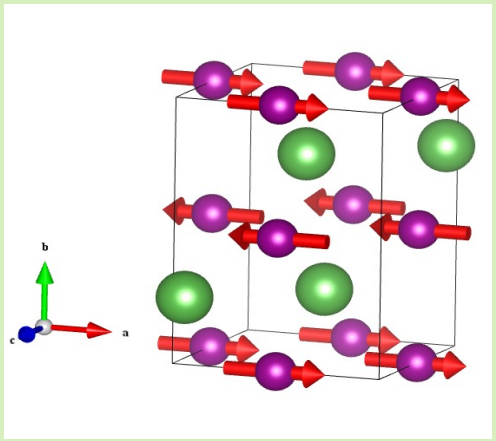
Space Group:
Pn'ma'

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

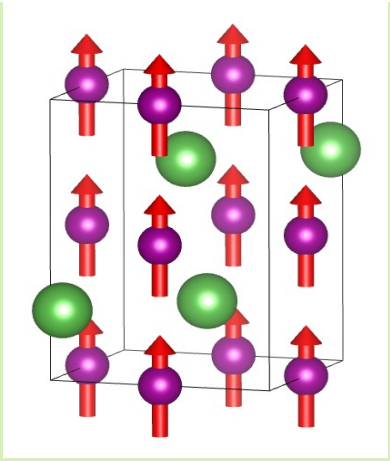
Output of MWYCKPOS

La

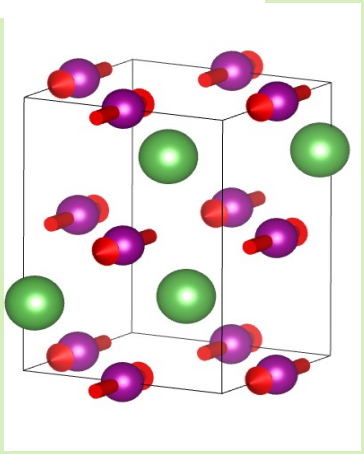
Mn



mode along x (A_x)



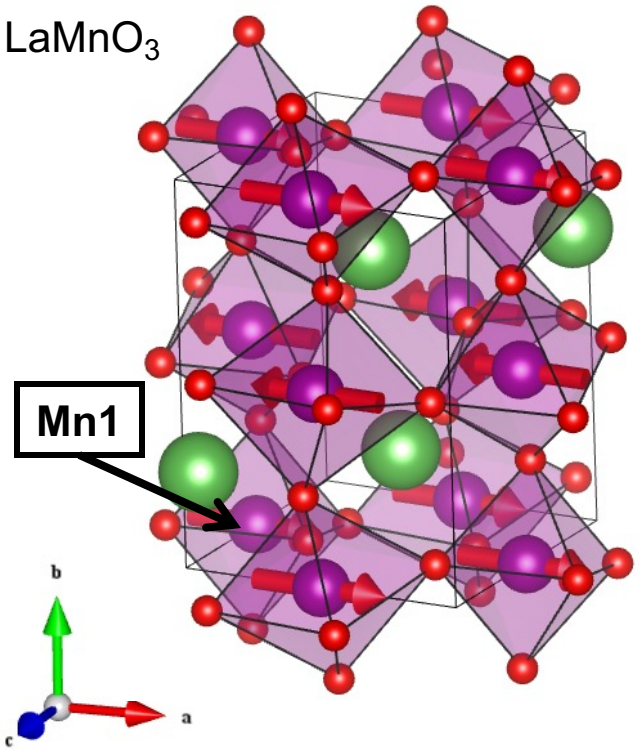
mode along y (F_y)
weak ferromagnet



mode along z (G_z)

Description of a magnetic structure in a crystallographic form using its MSG:

$LaMnO_3$



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

special positions: coordinates are symmetry- forced

Magnetic moments of the asymmetric unit (μB) and symmetry constraints::

Mn1 3.87 0.0 0.0 (mx,my,mz)

zero components are NOT symmetry-forced

Ferromagnetic component along y is symmetry permitted
(weak FM)

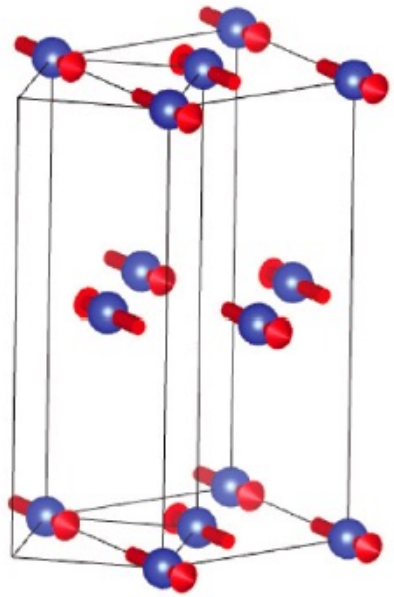
Pn' ma' :
1 x,y,z,+1
2 -x,y+1/2,-z,+1
3 -x,-y,-z,+1
4 x,-y+1/2,z,+1
5 x+1/2,-y+1/2,-z+1/2,-1
6 -x+1/2,-y,z+1/2,-1
7 -x+1/2,y+1/2,z+1/2,-1
8 x+1/2,y,-z+1/2,-1

MSG

Word of caution: The same spin arrangement can produce different MSGs (and different constraints on the physical properties !) *(The non magnetic atoms are also important for the magnetic symmetry!)*

Pr_2CuO_4

I4/mmm, k=(1/2,1/2,0)



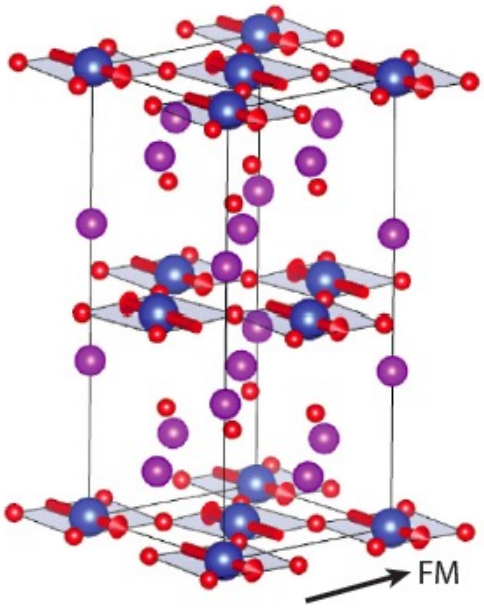
C_Accm

(**c**, **a** – **b**, **a** + **b**; 1/4, 3/4, 1/4)

Point group: mmm.1'

Gd_2CuO_4

Cmce, k=(0,0,0)



$Cm'ca'$

(**c,b,-a,0,0,0**)

Point group: m' mm'

(weak ferromagnetism**)**

magCIF file for $HoMnO_3$

magCIF Format

Official extension of the CIF format to communicate magnetic structures

(developed by the Commission on magnetic structures of the IUCr)

These files permit the different alternative models to be analyzed, refined, shown graphically, transported to ab-initio codes etc., with various programs as ISODISTORT, JANA2006, STRCONVERT, FullProf, VESTA, Jmol, etc.

The magCIF format supports incommensurate magnetic structures !

```
_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"
_space_group_magn.point_group_name  "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_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
_atom_site_occupancy
Ho1_1 Ho 0.04195 0.25000 0.98250 1
Ho1_2 Ho 0.95805 0.75000 0.01750 1
Mn1 Mn1 0.00000 0.00000 0.50000 1
O1_1 O 0.23110 0.25000 0.11130 1
O1_2 O 0.7689 0.75000 0.88870 1
O2_1 O 0.16405 0.05340 0.70130 1
O2_2 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
_atom_site_moment.symmform
Mn1 3.87 0.0 0.0 mx,my,mz
```

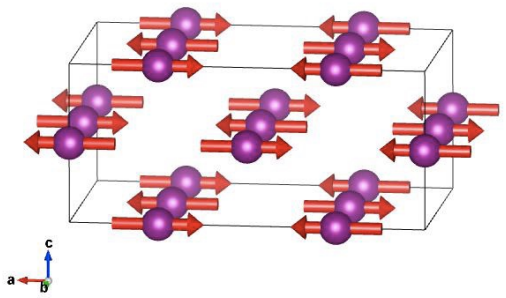
unit cell

MSG

asymmetric unit

magnetic moments in the asymmetric unit

$HoMnO_3$ (magndata 1.20)



_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

Atomic positions of asymmetric unit:

Ho1_1	4a	0.04195	0.25000	0.98250
Ho1_2	4a	0.95805	0.75000	0.01750
Mn1	8b	0.00000	0.00000	0.50000
O1_1	4a	0.23110	0.25000	0.11130
O1_2	4a	0.76890	0.75000	0.88870
O2_1	8b	0.16405	0.05340	0.70130
O2_2	8b	0.83595	0.55340	0.29870

MSG:

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

Magnetic moments of atoms in the asymmetric unit:

Mn1 3.87 0.0 0.0 mx,my,mz

non-standard setting of the MSG

```
_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
```

equivalent to the listing of the operations

```
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
```

MSG of HoMnO3 in the unit cell and origin used:

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
5 x+1/2,y,z,-1
6 -x+3/4,-y,z+1/2,-1
7 x+1/2,-y+1/2,z,-1
8 -x+3/4,y+1/2,z+1/2,-1

P_bmn2_1 (**-b,a,c;**1/8,1/4,0)

Different choice of unit cell and origin shift:

(**-b,a,c;**1/8,1/4,0)

MSG: P_bmn2_1 (31.129) in its standard setting:

1 x,y,z,+1
2 -x+1/2,-y,z+1/2,+1
3 -x,y,z,+1
4 x+1/2,-y,z+1/2,+1
5 x,y+1/2,z,-1
6 -x+1/2,-y+1/2,z+1/2,-1
7 -x,y+1/2,z,-1
8 x+1/2,-y+1/2,z+1/2,-1

P_bmn2_1 (**a,b,c;**0,0,0)

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:

$$\begin{pmatrix} m_x^s/a^s \\ m_y^s/b^s \\ m_z^s/c^s \end{pmatrix} = \mathbf{P}^{-1} \begin{pmatrix} m_x/a \\ m_y/b \\ m_z/c \end{pmatrix}$$

IDENTIFY MAGNETIC GROUP: Identification of a Magnetic Space Group from a set of generators in an arbitrary setting.

IDENTIFY MAGNETIC GROUP: Identifies a Magnetic Space Group given a set of generators

IDENTIFY MAGNETIC GROUP identifies a Magnetic Space Group given a set of generators and shows the transformation matrix to a standard or reference (default) description of the Magnetic Space Group. The groups can given in the BNS or OG setting.

Tutorial of IDENTIFY MAGNETIC GROUP: download

Help

Enter the generators of the Magnetic Space Group in the box below, given in any basis of the lattice, as in the example:

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

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

When the symmetry operations are given in the BNS setting, the following translations are assumed:

x + 1 , y , z ,+1
x , y + 1 , z ,+1
x , y , z + 1 ,+1

When the symmetry operations are given in the OG setting, the following translations should be explicitly given:

x + 1 , y , z ,+-1
x , y + 1 , z ,+-1
x , y , z + 1 ,+-1

(•) BNS setting ( ) OG setting

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

Submit

The Magnetic Space Group has been identified as P_bmn2_1 (No. 31.129) in the BNS setting

Transformation Matrix to the standard/default BNS setting

$$\begin{pmatrix} 0 & 1 & 0 & 1/8 \\ -1 & 0 & 0 & 1/4 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

Check an alternative Transformation Matrix

(P,p) transformation to standard of the MSG

P = 3x3 matrix

p = (p_1, p_2, p_3)

General positions of the Magnetic Space Group P_bmn2_1 in the given BNS setting

Input generators

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

$(a^s,b^s,c^s)= (a,b,c).P$, $O^s = O + p_1\,a + p_2\,b + p_3\,c$

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
5	x+1/2,y,z,-1
6	-x+3/4,-y,z+1/2,-1
7	x+1/2,-y+1/2,z,-1
8	-x+3/4,y+1/2,z+1/2,-1

(**-b,a,c;**1/8,1/4,0) → MSG in its standard Standard setting

P_bmn2_1 (-b,a,c;1/8,1/4,0)

```
_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
```

important information on the relation with the parent paramagnetic structure

```
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
```