Magnetic Symmetry and the Bilbao Crystallographic Server

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Symmetry-Based Computational Tools for Magnetic Crystallography

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Magnetic Section

FCT/ZTF

bilbao crystallographic server

UPV EHU

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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

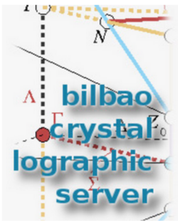
Structure Databases

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



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**

Three main tutorials on the programs of the BCS Magnetic Section can be directly downloaded from the webpages of the programs :

Tutorial_magnetic_section_BCS_1

Tutorial_magnetic_section_BCS_3

Tutorial_magnetic_section_BCS_2

Magnetic Symmetry and Applications	
MGENPOS	General Positions of Magnetic Space Groups
MWYCKPOS	Wyckoff Positions of Magnetic Space Groups
MKVEC	The k-vector types and Brillouin zones of Magnetic Space Groups
IDENTIFY MAGNETIC GROUP	Identification of a Magnetic Space Group from a set of generators in an arbitrary setting
BNS2OG	Transformation of symmetry operations between BNS and OG settings
mCIF2PCR	Transformation from mCIF to PCR format (FullProf).
MPOINT	Magnetic Point Group Tables
MAGNEXT	Extinction Rules of Magnetic Space Groups
MAXMAGN	Maximal magnetic space groups for a given space group and a propagation vector
MAGMODELIZE	Magnetic structure models for any given magnetic symmetry
STRCONVERT	Convert & Edit Structure Data (supports the CIF, mCIF, VESTA, VASP formats -- with magnetic information where available)
k-SUBGROUPSMAG	Magnetic subgroups consistent with some given propagation vector(s) or a supercell
MAGNDATA	A collection of magnetic structures with portable cif-type files
MVISUALIZE	3D Visualization of magnetic structures with Jmol
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

Tutorial-MAXMAGN (3 versions)

Tutorial-k-SUBGROUPSMAG

Reminder of symmetry in non-magnetic structures

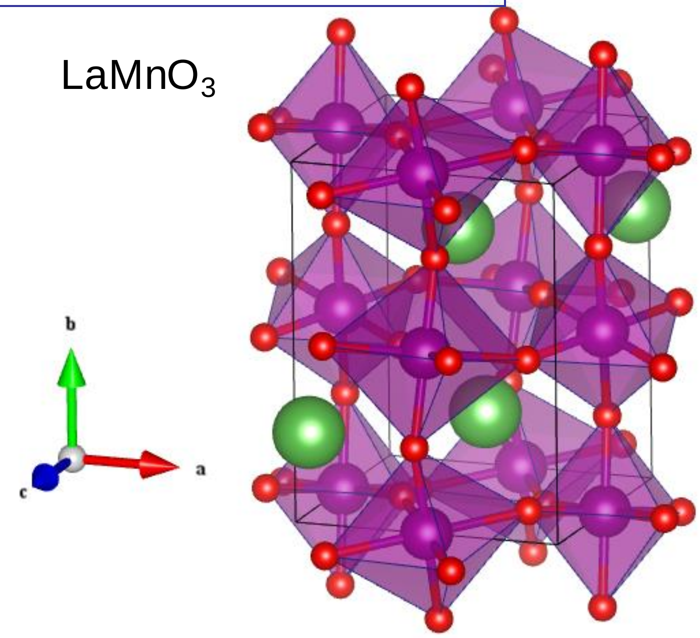
asymmetric unit

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

$LaMnO_3$



Reminder of symmetry in non-magnetic structures

asymmetric unit →

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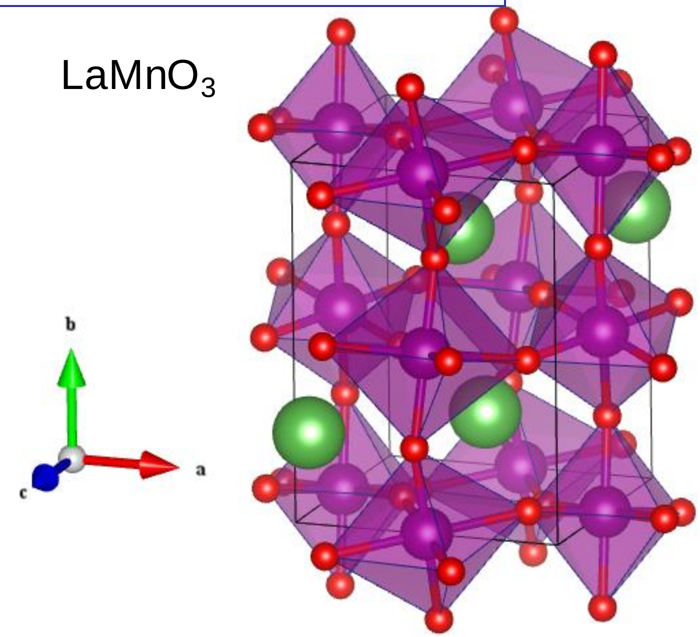

Space Group: set of operations {R|t}

for all atoms:

atom (x,y,z) $\xrightarrow{\{\mathbf{R}|\mathbf{t}\}}$ atom'

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

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

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

Reminder of symmetry in non-magnetic structures

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
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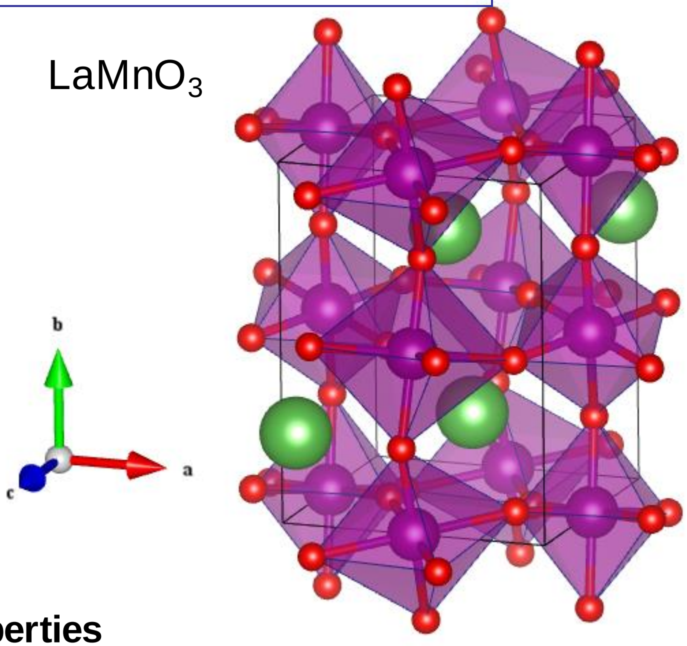
$LaMnO_3$



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)

Symmetry and Physics:

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

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.**

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

Symmetry and Physics:

Space Group: Group of all possible combinations of

rotations
translations
space inversion

which keep the crystal undistinguishable

Symmetry and Physics:

Group of all possible combinations of **rotations**
translations
space inversion

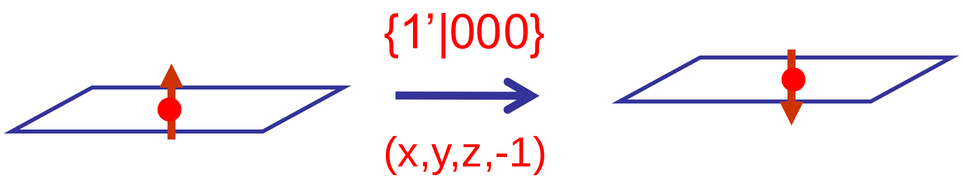
(They all keep the <u>ENERGY of the system invariant….)</u>

(hamiltonian/free energy invariant…)

The symmetry group of the crystal is formed by all operations that, keeping the <u>ENERGY invariant,</u> ALSO maintain the system undistinguishable after applying the operation.

The time reversal operation also keeps energy invariant:

Definition of time reversal: {1’|0,0,0}:
- Does NOT change nuclear positional variables
- Changes sign of ALL atomic magnetic moments
- Changes sign of momenta (not relevant for magnetic structures)



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

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

Actual symmetry of the non-magnetic phase of LaMnO3:

Pnma.1' = Pnma + {1'|000}x ***Pnma*** (gray 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 } $\{R|\mathbf{t}\}$

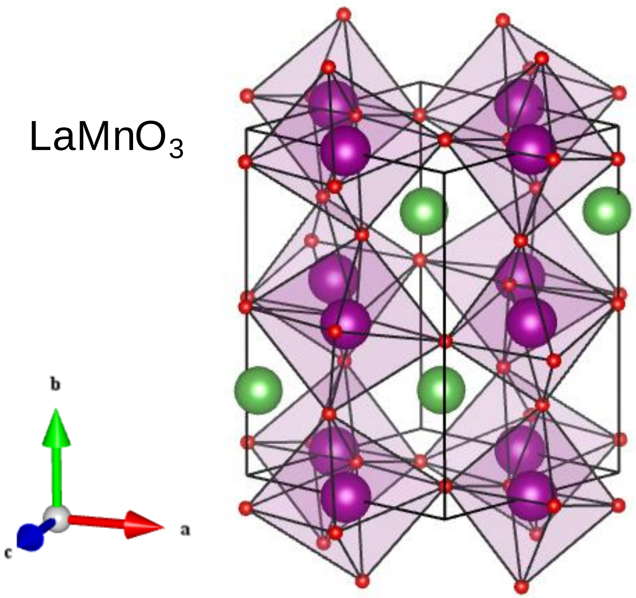
(x+1/2,-y+1/2,-z+1/2,-1) == {2x'| ½ ½ ½ } $\{R'|\mathbf{t}\}$

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

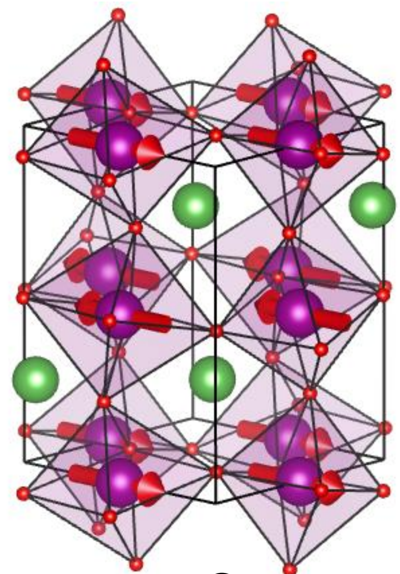
Magnetic ordering is a symmetry breaking process

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)

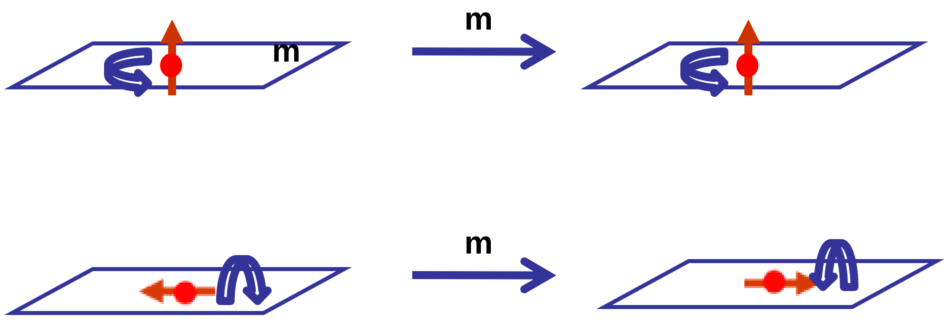
~~(x,y,z,-1)~~ (-x+1/2,-y,z+1/2,-1) (-x,y+1/2,-z,-1) (x+1/2,-y+1/2,-z+1/2,-1)

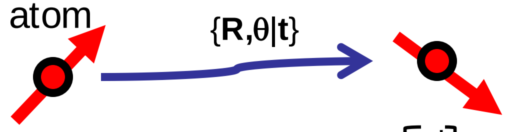
(-x,-y,-z,-1) (x+1/2,y,-z+1/2,-1) (x,-y+1/2,z,-1) (-x+1/2,y+1/2,z+1/2,-1)

?

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

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





(x,y,z) $\begin{bmatrix} x' \\ y' \\ z' \end{bmatrix} = \mathbf{R} \begin{bmatrix} x \\ y \\ z \end{bmatrix} + \mathbf{t}$ (for positions: the same as with Pnma)

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

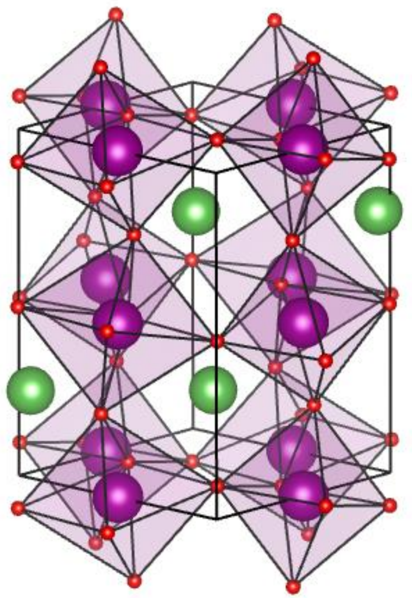
θ=-1 if time reversal

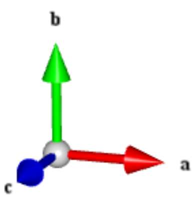
Magnetic ordering is a symmetry breaking process

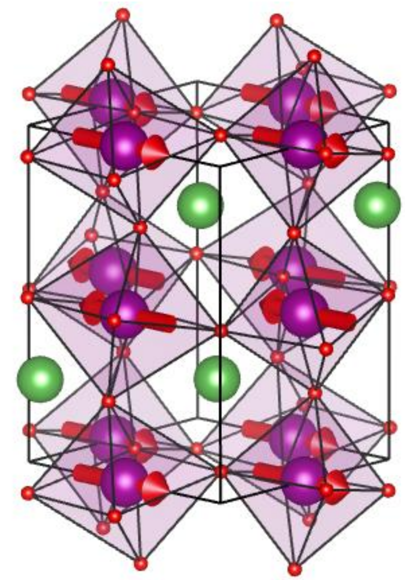
Magnetically ordered phases:

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

$LaMnO_3$







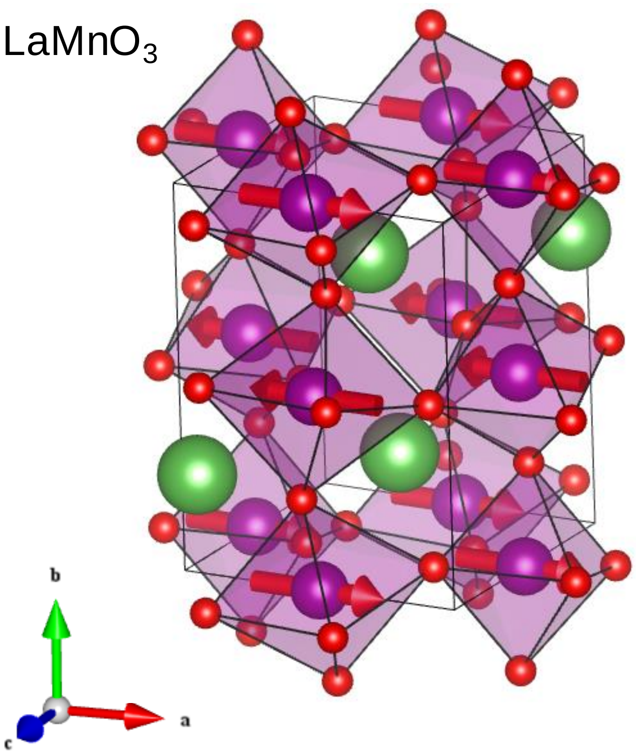
Pnma.1'

Pn'ma'

(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)

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

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)

$P12_1/m1$

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 $\underline{+1}$	{ 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 $\underline{+1}$	{ 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 $\underline{+1}$	{ -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 $\underline{+1}$	{ 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 $\underline{-1}$	{ $2'_{100}$ | 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 $\underline{-1}$	{ $2'_{001}$ | 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 $\underline{-1}$	{ 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 $\underline{-1}$	{ 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 3 MSG

Magnetic point group: m' mm'

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

Types of magnetic space groups:

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

F subgroup of G
$F \leq G$

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:

Type 1 **some may allow ferromagnetic order**	**F**
Type 3 **some may allow ferromagnetic order**	**F + {R'|t}F**
Type 4 **antiferromagnetic order** **(ferromagnetism not allowed)**	**F + {1' |t}F**

antitranslation / anticentering

(Type 2 are the grey groups of the non-magnetically ordered systems):

Type 2 **non-magnetic structures**	**F + {1' |0}F**

Tables of magnetic space groups (in "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 actual lattice of the system.

NEW MSG SYMBOLS

Acta Cryst A
FOUNDATIONS ADVANCES
ISSN 2053-2733

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]

Acta Cryst. A (2022). A78, 99–106

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

Acta Cryst B
STRUCTURAL SCIENCE
CRYSTAL ENGINEERING
MATERIALS
ISSN 2052-5206

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]

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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.

Acta Cryst. B (2024). B80, 401–408

Types of magnetic space groups:

(for a commensurate magnetic structure resulting from a paramagnetic phase having a gray 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:

Type 1 — **F**

some may allow ferromagnetic order

Type 3 — **F** + $\{$**R'**$|$**t**$\}$**F**

some may allow ferromagnetic order

Type 4 — **F** + $\{1'|$**t**$\}$**F**

antiferromagnetic order
(ferromagnetism not allowed)

antitranslation / anticentering

(Type 2 are the grey groups of the non-magnetically ordered systems):

Type 2 — **F** + $\{1'|$**0**$\}$**F**

non-magnetic structures

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 }

Example of type 1 MSG

Output of MGENPOS

Magnetic point group: mmm.1

Pnma == Pnma (operations without time reversal)

New UNI symbol:
Pnma.1

Example of type 4 MSG

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 }

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

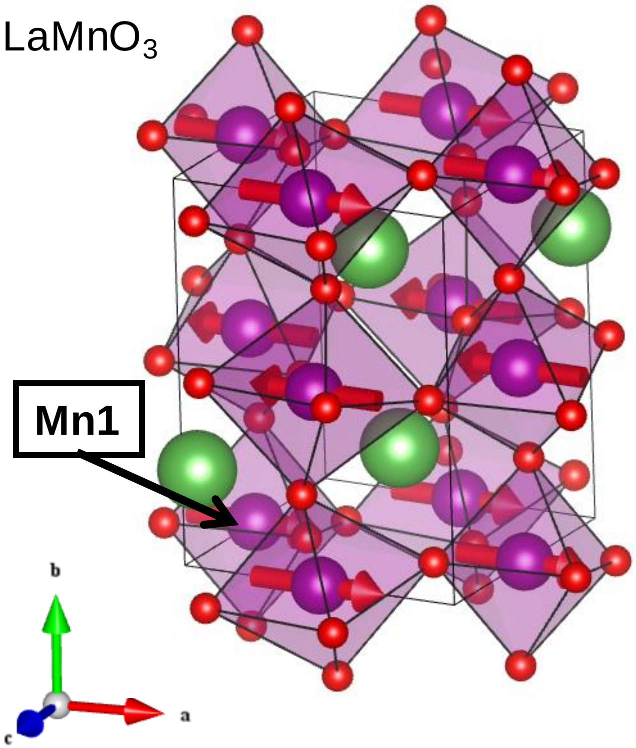
Output of MGENPOS

Propagation vector k≠0

Magnetic point group: mm2.1'

New UNI symbol:
$Pmn2_1.1'_b$

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::

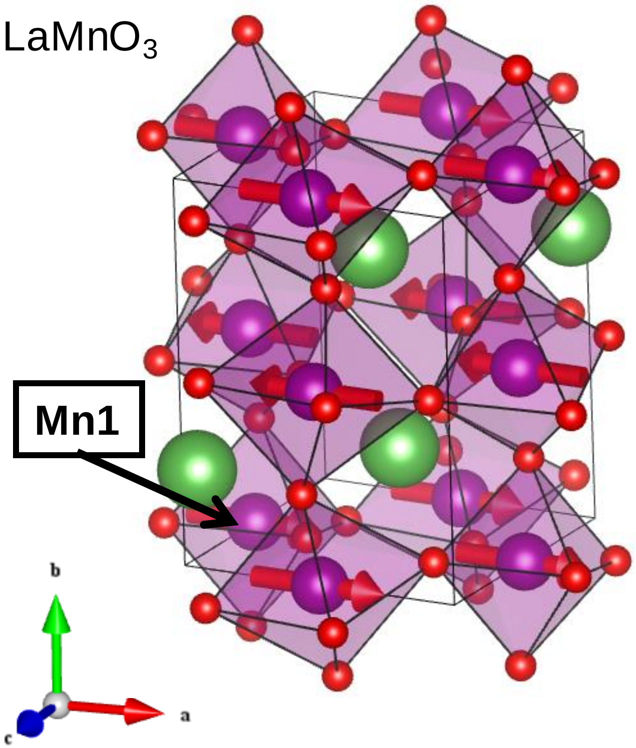
Mn1 3.87 0.0 0.0 (mx,my,mz)

Symmetry operations are relevant both for positions and moments

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

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

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

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

MSG

Parameters to describe a magnetic structure…

Space Group:

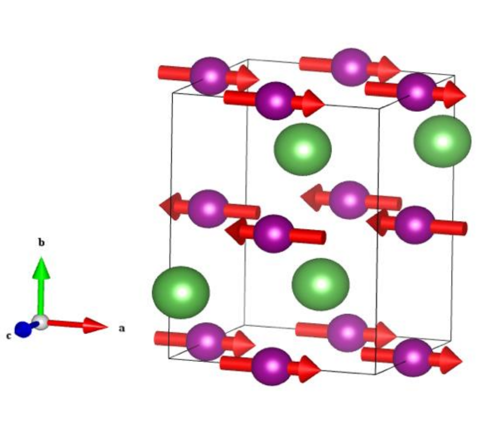
Pn'ma'

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)

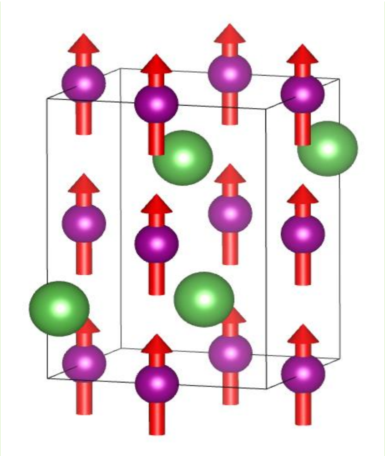
Output of MWYCKPOS

La

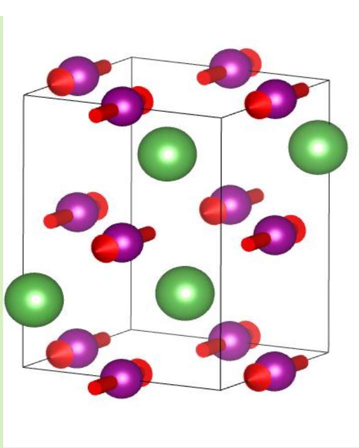
Mn



mode along x (A_x)



mode along y (F_y)
weak ferromagnet



mode along z (G_z)

magCIF Format

Official extension of the CIF format to communicate magnetic structures

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

(magCIF file for $HoMnO_3$) →

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.

It includes incommensurate 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
```

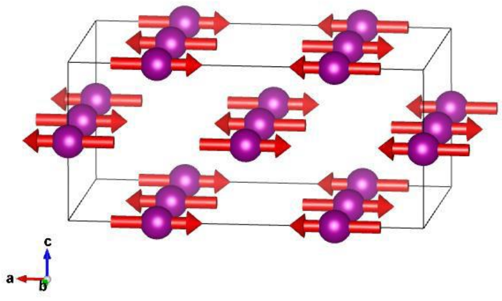
unit cell

MSG

asymmetric unit

magnetic moments in the asymmetric unit

$HoMnO_3$



_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

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

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

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

[Get general positions in matrix form]

[Get general positions in plain text format]

Bilbao Crystallographic Server → IDENTIFY MAGNETIC GROUP   Help

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

(P,p) transformation to standard of the MSG

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 = 3x3 matrix

p = (p_1, p_2, p_3)

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

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

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

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)

[Get general positions in matrix form]

[Get general positions in plain text format]

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

choice of unit cell and origin shift to put the MSG operations in the standard form:

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

MSG: $P_b mn2_1$ (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

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

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:

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

magnetic moment (absolute) components:

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

Consequences of symmetry

Von Neumann principle:

- all variables/parameters/degrees of freedom compatible with the symmetry will be present (their magnitude may be small or large, but not necessarily zero.

- Tensor crystal properties are constrained by the (magnetic) point group symmetry of the crystal.

- Reversely: any tensor property allowed by the (magnetic) point group symmetry can exist (large or small, but it is not forced to be zero)

MTENSOR: Symmetry-adapted form of crystal tensors properties of magnetic crystals

Magnetic Symmetry and Applications	
MGENPOS	General Positions of Magnetic Space Groups
MWYCKPOS	Wyckoff Positions of Magnetic Space Groups
MKVEC	The k-vector types and Brillouin zones of Magnetic Space Groups
IDENTIFY MAGNETIC GROUP	Identification of a Magnetic Space Group from a set of generators in an arbitrary setting
BNS2OG	Transformation of symmetry operations between BNS and OG settings
mCIF2PCR	Transformation from mCIF to PCR format (FullProf).
MPOINT	Magnetic Point Group Tables
MAGNEXT	Extinction Rules of Magnetic Space Groups
MAXMAGN	Maximal magnetic space groups for a given space group and a propagation vector
MAGMODELIZE	Magnetic structure models for any given magnetic symmetry
STRCONVERT	Convert & Edit Structure Data (supports the CIF, mCIF, VESTA, VASP formats -- with magnetic information where available)
k-SUBGROUPSMAG	Magnetic subgroups consistent with some given propagation vector(s) or a supercell
MAGNDATA	A collection of magnetic structures with portable cif-type files
MVISUALIZE	3D Visualization of magnetic structures with Jmol
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

MTENSOR: Tensor calculation for Magnetic Point Groups

For the symmetry-adapted form of non-magnetic crystal tensors see TENSOR

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. On the other hand, a tensor must be defined by the user or selected from the lists of known equilibrium, optical, nonlinear optical susceptibility and transport tensors, gathered from scientific literature. If a magnetic point or space group is defined and a known tensor is selected from the lists the program will obtain the required tensor from an internal database; otherwise, the tensor is calculated live. Live calculation of tensors may take too much time and even exceed the time limit, giving an empty result, if high-rank tensors, and/or a lot of symmetry elements are introduced.

Tutorial of MTENSOR: download

Further information can be found here

If you are using this program in the preparation of an article, please cite this reference:

Gallego *et al.* "Automatic calculation of symmetry-adapted tensors in magnetic and non-magnetic materials: a new tool of the Bilbao Crystallographic Server" *Acta Cryst. A* (2019) **75**, 438-447.

Please, enter a magnetic point group or a magnetic space group:

Magnetic Point or Space Group number: choose it

Please, choose a tensor by one of these ways:

Choose a tensor from the lists

Show symmetry-adapted tensors for all the magnetic point groups in standard setting
(this overrides previous choices)

EQUILIBRIUM TENSORS

OPTICAL TENSORS

NONLINEAR OPTICAL SUSCEPTIBILITY TENSORS

TRANSPORT TENSORS

Build your own tensor

- Introduce Jahn's symbol without superscripts. Examples: (1) [[V2][V2]], (2) a{V2}*, (3) (V2[V2])*

Detailed information in. Gallego et al., Acta Cryst. A (2019) 75, 438-447.
and tutorial: Tutorial_magnetic_section_BCS_1.pdf

MTENSOR

Magnetoelectric tensor:

Group 6/m' (#23.4.85)

α^T_{ij}	j		
i	1	2	3
1	α^T_{11}	α^T_{12}	0
2	$-\alpha^T_{12}$	α^T_{11}	0
3	0	0	α^T_{33}

Number of independent coefficients: 3

Group 622 (#24.1.87)

α^T_{ij}	j		
i	1	2	3
1	α^T_{11}	0	0
2	0	α^T_{11}	0
3	0	0	α^T_{33}

Number of independent coefficients: 2

Group 62'2' (#24.4.90)

α^T_{ij}	j		
i	1	2	3
1	0	α^T_{12}	0
2	$-\alpha^T_{12}$	0	0
3	0	0	0

Number of independent coefficients: 1

Group 6mm (#25.1.91)

α^T_{ij}	j		
i	1	2	3
1	0	α^T_{12}	0
2	$-\alpha^T_{12}$	0	0
3	0	0	0

Number of independent coefficients: 1

Group 6m'm' (#25.4.94)

α^T_{ij}	j		
i	1	2	3
1	α^T_{11}	0	0
2	0	α^T_{11}	0
3	0	0	α^T_{33}

Number of independent coefficients: 2

Group -6'm'2 (#26.3.97)

α^T_{ij}	j		
i	1	2	3
1	α^T_{11}	0	0
2	0	α^T_{11}	0
3	0	0	α^T_{33}

Number of independent coefficients: 2

Group -6'm2' (#26.4.98)

α^T_{ij}	j		
i	1	2	3
1	0	α^T_{12}	0
2	$-\alpha^T_{12}$	0	0
3	0	0	0

Number of independent coefficients: 1

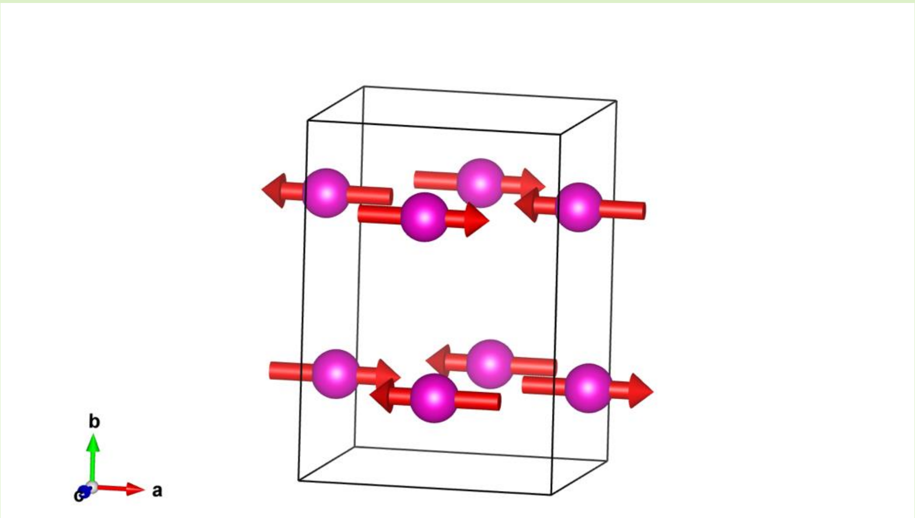
Group 6/m'mm (#27.3.102)

α^T_{ij}	j		
i	1	2	3
1	0	α^T_{12}	0
2	$-\alpha^T_{12}$	0	0
3	0	0	0

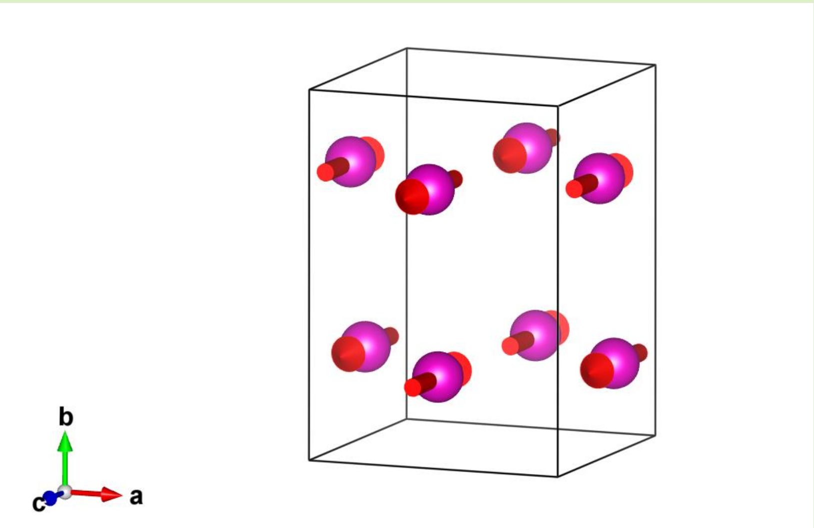
Number of independent coefficients: 1

Consequences of symmetry

$EuZrO_3$: magndata #0.146 & 0.147



Pnm'a



Pn'm'a'

Table of tensor components

α^T_{ij}		j		
		1	*2*	*3*
i	*1*	0	0	α^T_{13}
	2	0	0	0
	3	α^T_{31}	0	0

Number of independent coefficients: 2

Information about the selected tensor

- 2 nd rank Magnetoelectric tensor α^T_{ij} (inverse effect)
- Axial tensor which inverts under time-reversal symmetry operation
- Defining equation: $\mathbf{P_i=\alpha^T_{ij}H_j}$
- Relates Magnetic field **H** with Polarization **P**
- Intrinsic symmetry symbol: **aeV^2**

Output of MTENSOR

Table of tensor components

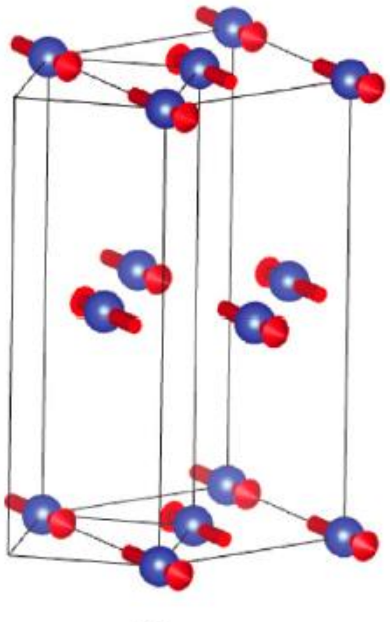
ij		j		
		1	*2*	*3*
	1	α^T_{11}	0	0
	2	0	α^T_{22}	0
	3	0	0	α^T_{33}

lumber of independent coefficients: 3

The same spin arrangement can produce different MSGs (and different ferroic properties) *(The non magnetic atoms are also important for the magnetic symmetry!)*

Pr_2CuO_4

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



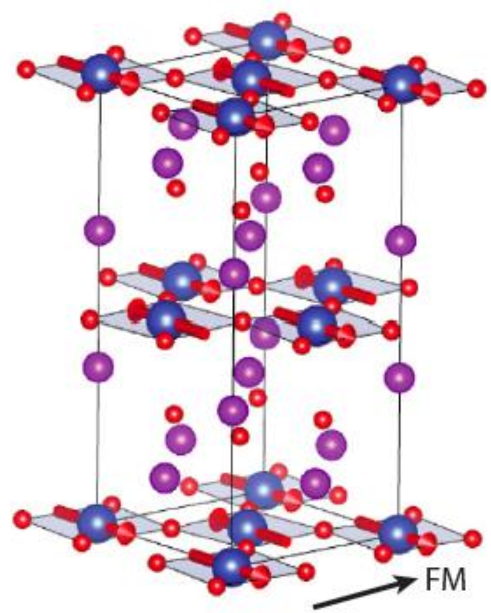
C_Accm

(**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'

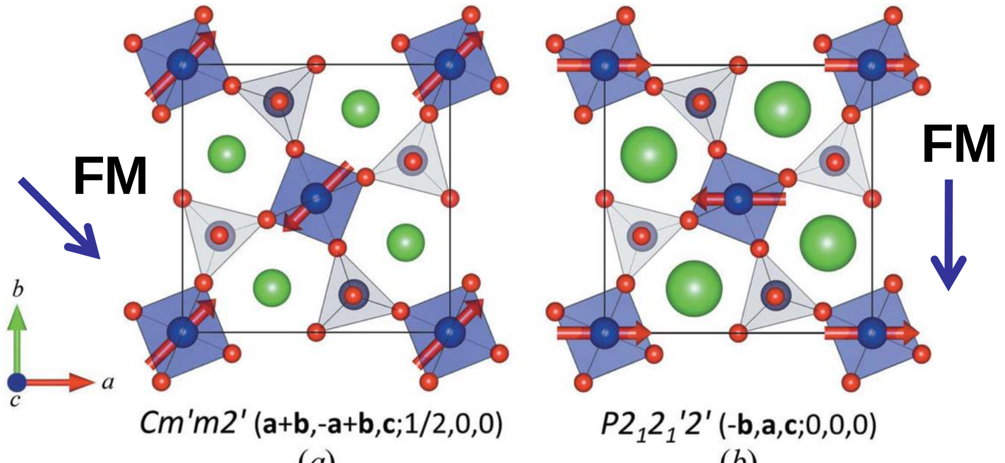
(c,b,-a,0,0,0)

Point group: m'mm'

(weak ferromagnetism**)**

Consequences of symmetry

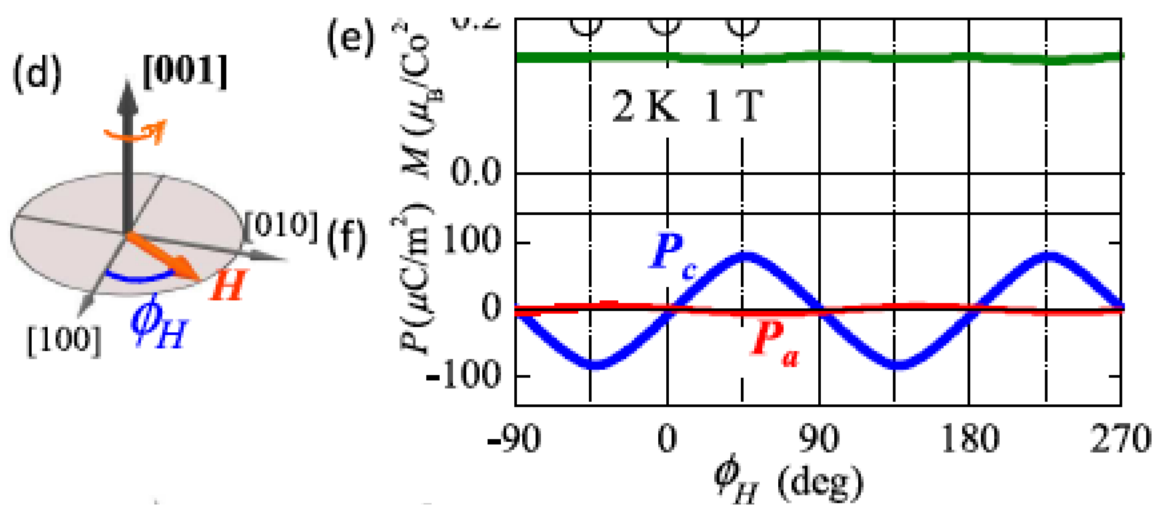
$Ba_2CoGe_2O_7$ parent SG: $P\text{-}42_1m$



Polar alon z
FM canting along (-1,1,0)

Non-polar
FM canting along (0,1,0)

Murakawa et al. PRL (2010):



Tutorial 1 :

Tutorial_magnetic_ section_BCS_1

Magnetic Symmetry and Applications	
MGENPOS	General Positions of Magnetic Space Groups
MWYCKPOS	Wyckoff Positions of Magnetic Space Groups
MKVEC	The k-vector types and Brillouin zones of Magnetic Space Groups
IDENTIFY MAGNETIC GROUP	Identification of a Magnetic Space Group from a set of generators in an arbitrary setting
BNS2OG	Transformation of symmetry operations between BNS and OG settings
mCIF2PCR	Transformation from mCIF to PCR format (FullProf).
MPOINT	Magnetic Point Group Tables
MAGNEXT	Extinction Rules of Magnetic Space Groups
MAXMAGN	Maximal magnetic space groups for a given space group and a propagation vector
MAGMODELIZE	Magnetic structure models for any given magnetic symmetry
STRCONVERT	Convert & Edit Structure Data (supports the CIF, mCIF, VESTA, VASP formats -- with magnetic information where available)
k-SUBGROUPSMAG	Magnetic subgroups consistent with some given propagation vector(s) or a supercell
MAGNDATA	A collection of magnetic structures with portable cif-type files
MVISUALIZE	3D Visualization of magnetic structures with Jmol
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