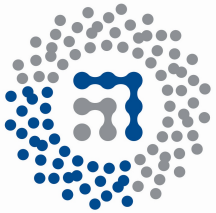

ZTF-FCT
Zientzia eta Teknologia Fakultatea
Facultad de Ciencia y Tecnología

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Universidad del País Vasco
Euskal Herriko Unibertsitatea

Symmetry description of magnetic structures: Magnetic space groups

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Symmetry-Based Computational Tools for Magnetic Crystallography

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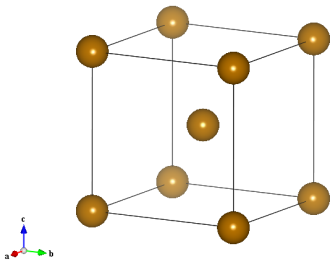
Symmetry and Physics:

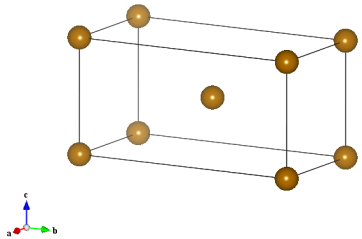
A symmetry property in a solid is **NOT ONLY** some mathematical property. It is a **PHYSICAL PROPERTY!**

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.



a=b=c symmetry property



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

Symmetry and Physics:

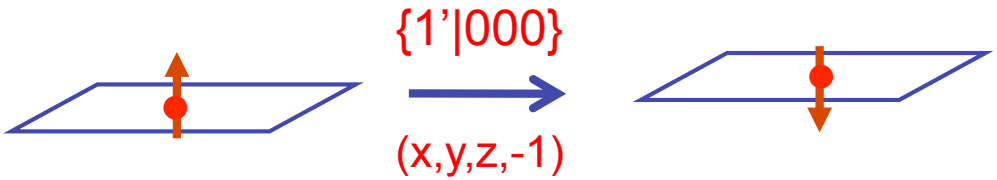
Group of all possible combinations of **rotations**
translations
space inversion

(They all keep the **ENERGY of the system invariant….**)

The symmetry group of the 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:

Definition of time reversal: {1'|0,0,0}:
- Does not change nuclear variables
- Changes sign of ALL atomic (average) magnetic moments



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

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

Magnetic symmetry groups:

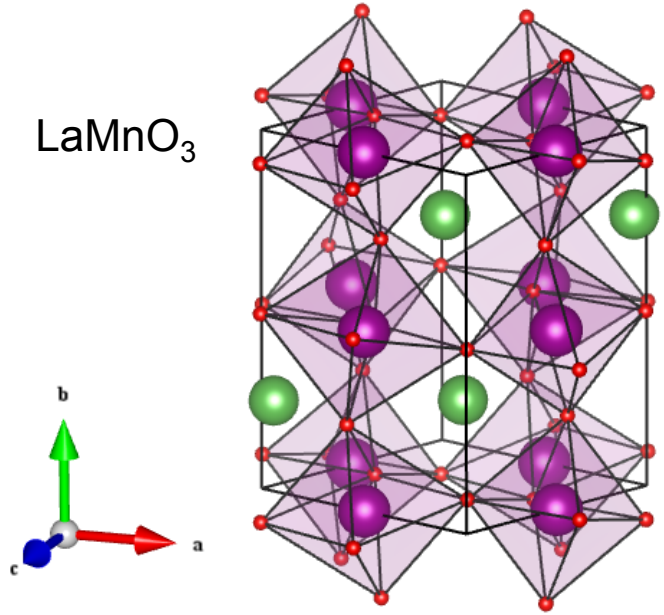
We do not add but SUBSTRACT symmetry operations !

A symmetry operation 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

$LaMnO_3$



Pnma1'

(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:

Pnma1' = 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**}

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

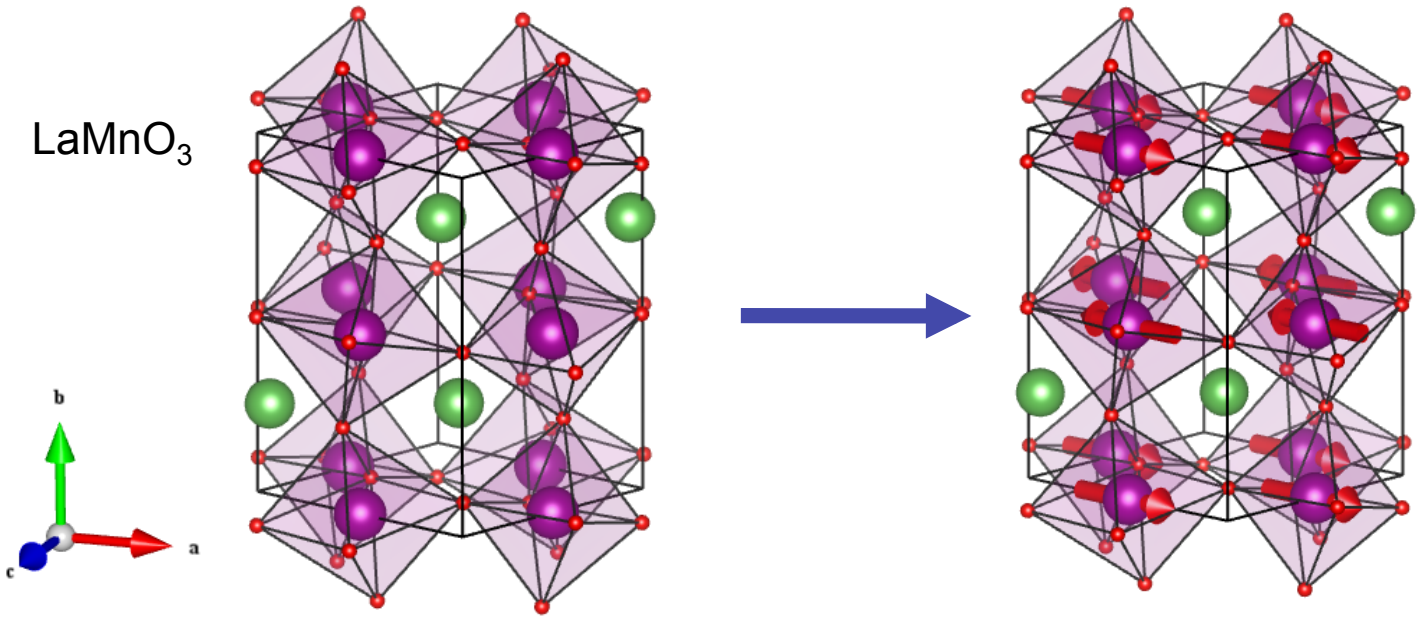
Seitz notation

Magnetic ordering is a SYMMETRY BREAKING PROCESS

Magnetically ordered phases:

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

$LaMnO_3$



Pnma1'

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

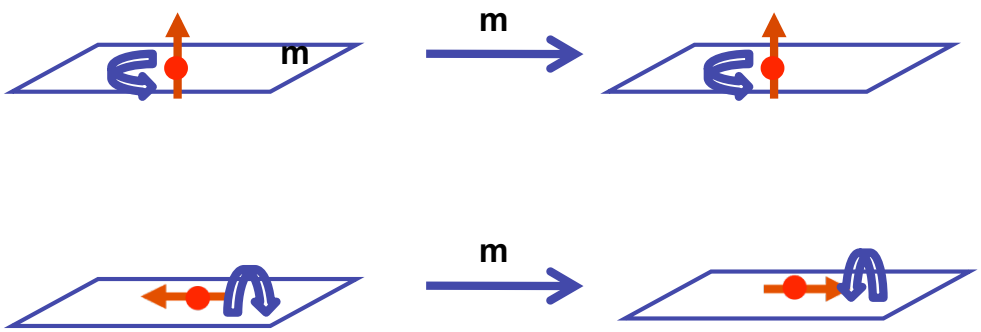
(-x,-y,-z,+1) (x+1/2,y,-z+1/2 ?2,y+1/2,z+1/2,+1)

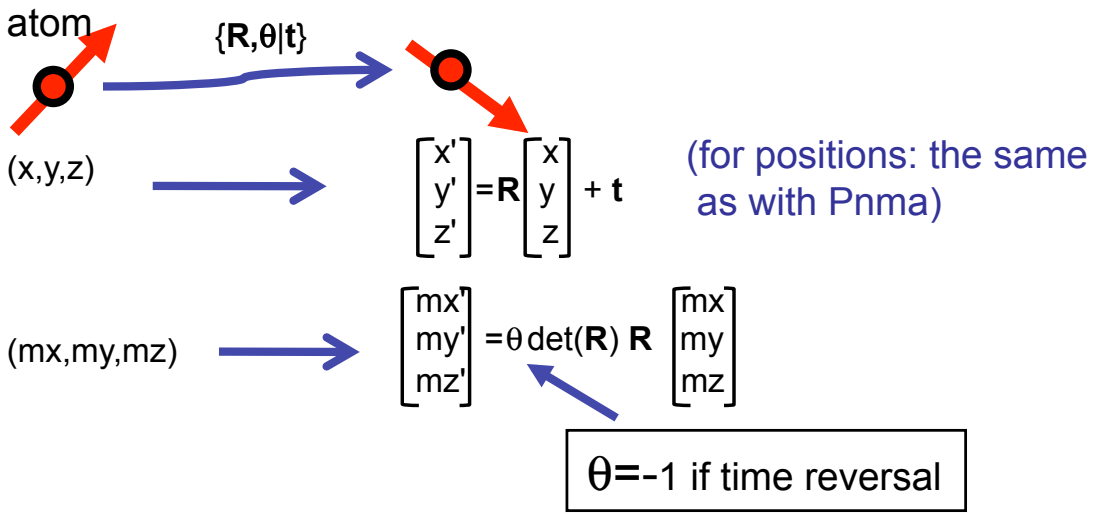
~~(x,y,z,-1)~~ (-x+1/2,-y,z+1/2 ?,-y+1/2,-z+1/2,-1)

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

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

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





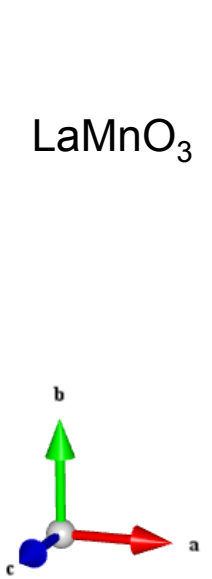
(for positions: the same as with Pnma)

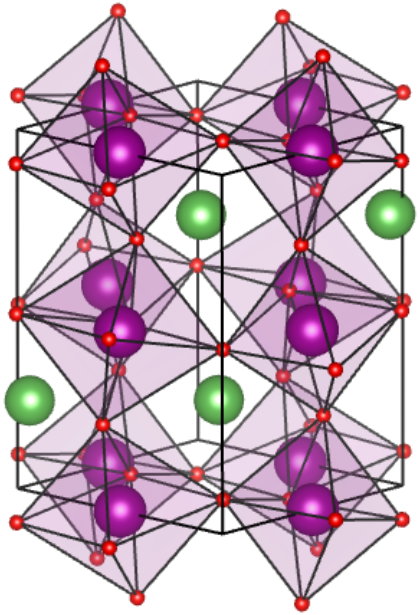
Magnetic ordering is a symmetry breaking process

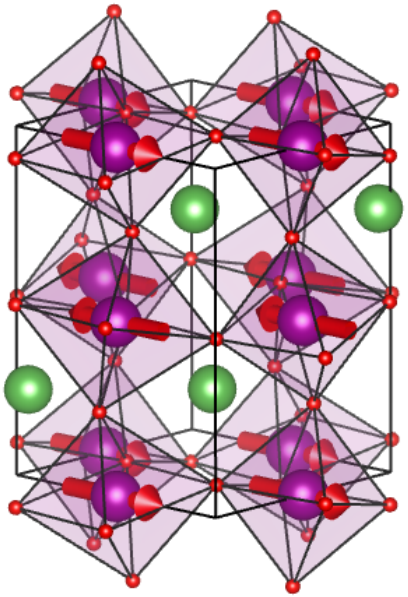
Magnetically ordered phases:

Time reversal {1'|0 0 0} is LOST but operations including time reversal can be mantained

$LaMnO_3$







Pnma1'

(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)

Types of magnetic space groups:

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

F subgroup of G
F ≤ G

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

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

antitranslation / anticentering

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

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

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 and lists 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

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. (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. "

BNS No.	BNS	OG No.	OG	UNI MSG	UNI MPG
2.7	$P_S\bar{1}$	2.4.7	$P_{2s}\bar{1}$	$P\bar{1}.1'_c[P\bar{1}]$	$\bar{1}.1'$
42.223	F_Smm2	25.9.163	P_Imm2	$Fmm2.1'_I[Pmm2]$	$mm2.1'$
161.72	R_I3c	160.5.1299	R_R3m'	$R3c.1'_c[R3m]$	$3m.1'$
218.84	$P_I\bar{4}3n$	217.5.1584	$I_P\bar{4}'3m'$	$P\bar{4}3n.1'_I[I\bar{4}3m]$	$\bar{4}3m.1'$
140.550	I_c4/mcm	123.19.1017	$P_I4/mm'm'$	$I4/mcm.1'_c[rP4/mmm]$	$4/mmm.1'$
28.96	P_Bma2	39.7.284	A_Pbm2	$Pma2.1'_B[Bma2]$	$mm2.1'$

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

Example of type III MSG

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]

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

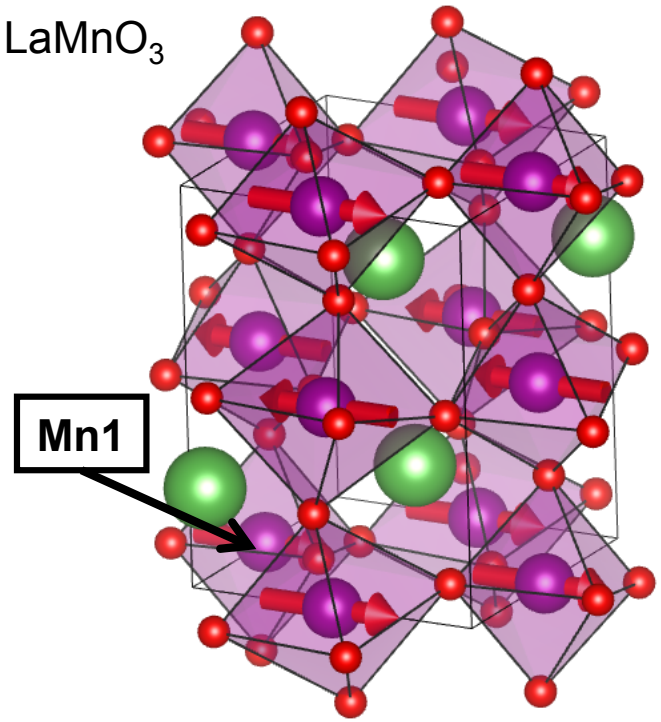
Example of type IV MSG

Propagation vector k≠0

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

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

special position: coordinates are symmetry- forced

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

Mn1 3.87 0.0 0.0 (mx,my,mz)

special position BUT 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

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, GSAS, 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

Wyckoff positions in a magnetic structure…

Magn. Space Group:
Pn'ma'

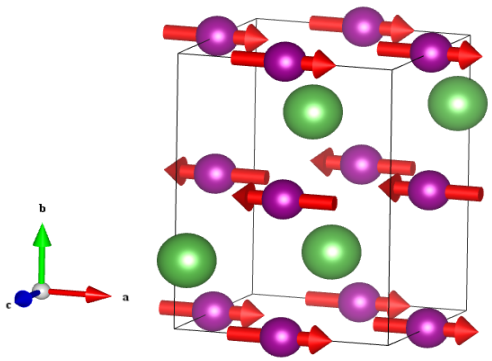
$LaMnO_3$

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

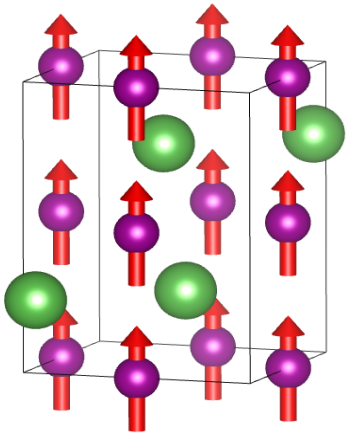
Output of MWYCKPOS in BCS

La

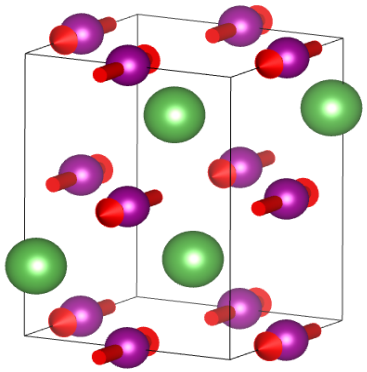
Mn



mode along x (A_x)



mode along y (F_y)
weak ferromagnet



mode along z (G_z)

- **The description of a magnetic structure using its MSG of the structure is a direct simple extension of ordinary crystallography and therefore:**

Simple, Compact and Robust…

This is the description used in the CIF file format, extended to magnetic structures (magCIF), which is now supported by many programs.

It has allowed the development of a database of magnetic structures as MAGNDATA

Magnetic ordering is a symmetry breaking process

To define it fully one has to describe the Group-subgroup relation between the two symmetries

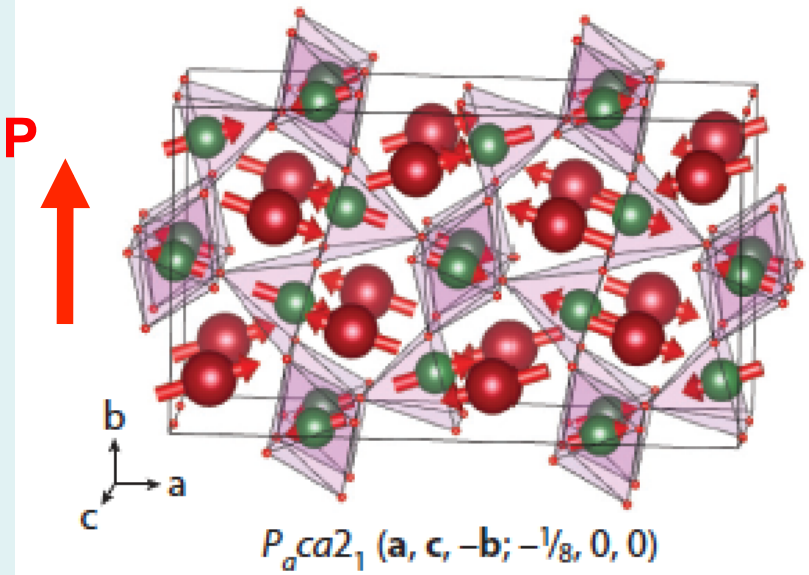
Gd_2MnO_5 (magndata 1.54)

k=(1/2,0,0) → *unit cell: (2a,b,c)*

Pbam1' → **$P_a ca2_1$**(2a,c,-b;-1/4,0,0)

Possible electr. polarization

polar along the binary axis b



loop_
_space_group_symop_magn_operation.id
_space_group_symop_magn_operation.xyz
1 x,y,z,+1
2 -x+3/4,y+1/2,-z,+1
3 -x+1/4,y+1/2,z,+1
4 x+1/2,y,-z,+1

unit cell: (2a,b,c)

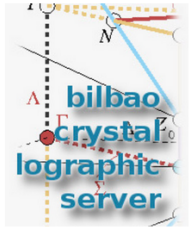
loop_
_space_group_symop_magn_centering.id
_space_group_symop_magn_centering.xyz
1 x,y,z,+1
2 x+1/2,y,z,-1

Magnetic Section

FCT/ZTF

bilbao crystallographic server

UPV EHU



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**

Quick access to some tables

IDENTIFY MAGNETIC SPACE GROUP : Identifies the MSG defined by a set of operations in an arbitrary setting

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

IDENTIFY MAGNETIC SPACE GROUP : Identifies the MSG defined by a set of operations in an arbitrary setting

The Magnetic Space Group has been identified as P_aca2_1 (No. 29.104) in the BNS setting

Transformation Matrix to the standard/default BNS setting

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

Check an alternative Transformation Matrix

General positions of the Magnetic Space Group P_aca2_1 in the given BNS setting

Input generators

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

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

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

Pbam1' → **P_aca2_1**(2a,c,-b;-1/4,0,0)

One should not confuse:

When describing a subgroup of the parent group:

Parent Pbam unit cell ($\mathbf{a}_p$, $\mathbf{b}_p$, $\mathbf{c}_p$;0,0,0):

Pbam1' → **$P_a ca2_1$**(2a,c,-b;-1/4,0,0)

transformation to standard from the parent setting of *Pnma*

description of the subgroup by its type of MSG and a unit cell and origin with respect to the parent unit cell where it WOULD adquire its standard form

When describing a magnetic structure under this MSG using a non-standard setting:

Unit cell used (2$\mathbf{a}_p$, $\mathbf{b}_p$, $\mathbf{c}_p$;0,0,0):

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

transformation to standard from the setting **USED** for the MSG.

Alternative unit cell and origin with respect to the unit cell used where the MSG WOULD adquire its standard form

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

Number of independent coefficients: 3

Group 622 (#24.1.87)

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

Number of independent coefficients: 2

Group 62'2' (#24.4.90)

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

Number of independent coefficients: 1

Group 6mm (#25.1.91)

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

Number of independent coefficients: 1

Group 6m'm' (#25.4.94)

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

Number of independent coefficients: 2

Group -6'm'2 (#26.3.97)

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

Number of independent coefficients: 2

Group -6'm2' (#26.4.98)

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

Number of independent coefficients: 1

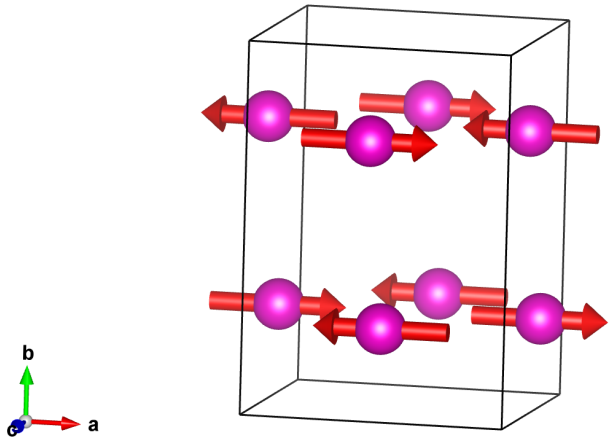
Group 6/m'mm (#27.3.102)

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

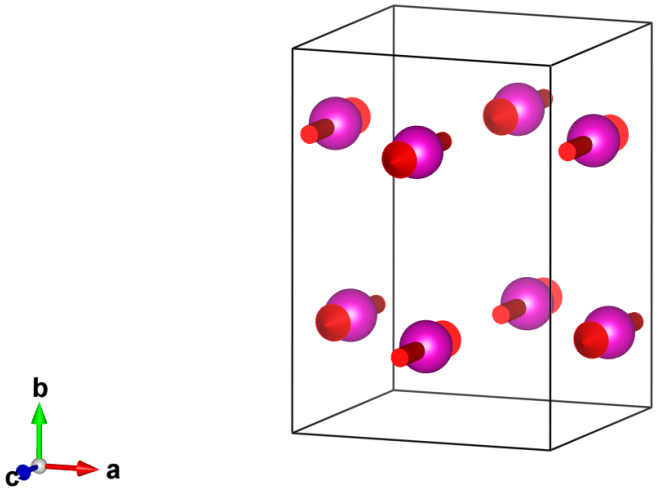
Number of independent coefficients: 1

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: $P_i=\alpha^T_{ij}H_j$
- Relates Magnetic field **H** with Polarization **P**
- Intrinsic symmetry symbol: aeV^2

Output of MTENSOR

Table of tensor components

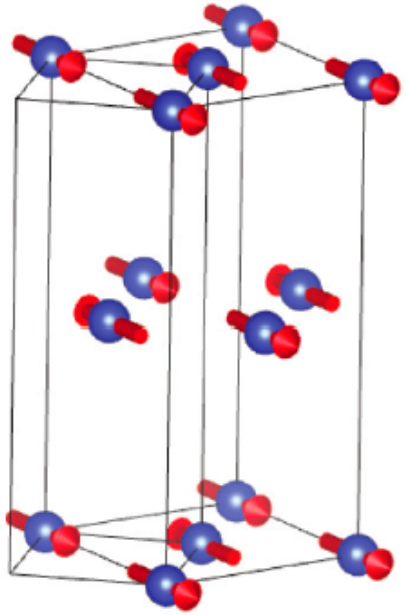
α^T_{ij}		j		
		1	*2*	*3*
	1	α^T_{11}	0	0
	2	0	α^T_{22}	0
	3	0	0	α^T_{33}

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 (#1.398)

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



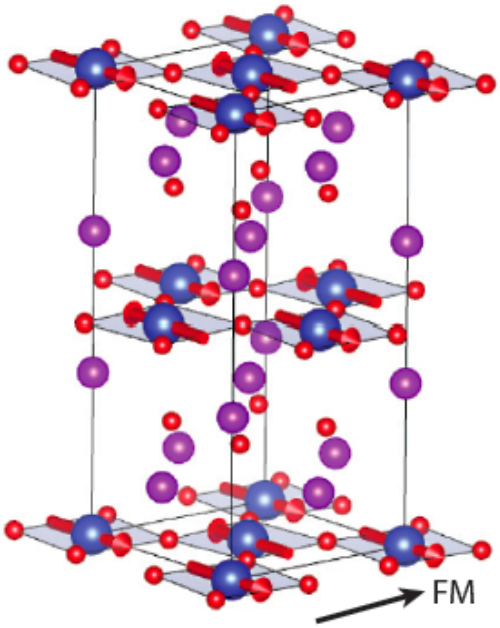
C_Accm

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

Point group: mmm1'

Gd_2CuO_4(#0.82)

Cmce, k=(0,0,0)



$Cm'ca'$

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

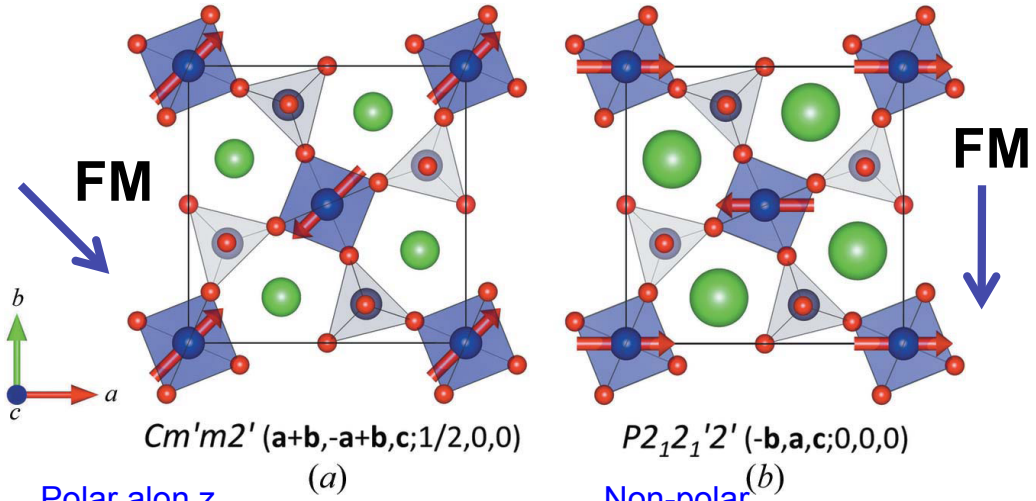
Point group: m' mm'

(weak ferromagnetism**)**

Consequences of symmetry

$Ba_2CoGe_2O_7$ (#0.56)

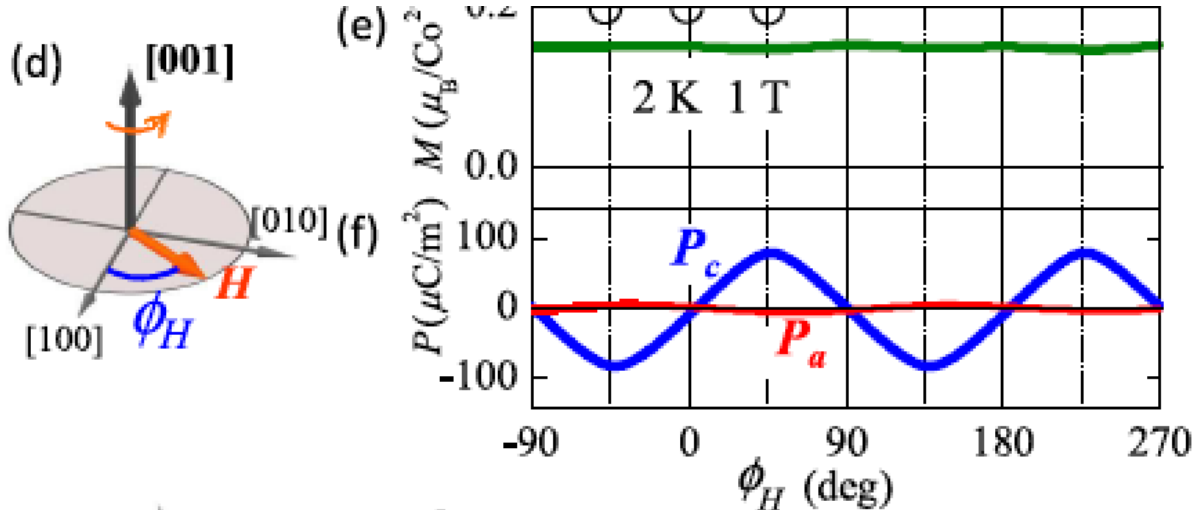
parent SG: P-42$_1$m



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

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

Murakawa et al. PRL (2010):

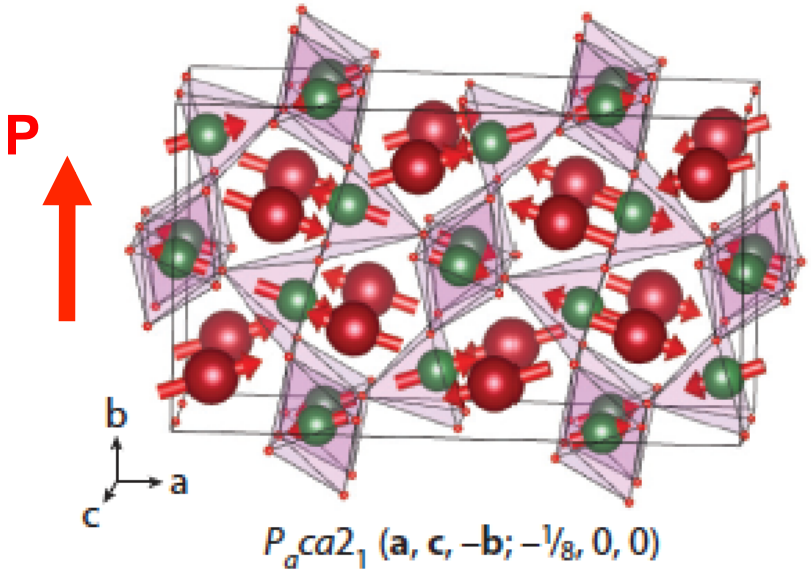


The knowledge of the MSG allows the systematic enumeration and description of all domain-related configurations:

Gd_2MnO_5 (magndata 1.54)

Pbam1' → **P_aca2_1**(2a,c,-b;-1/4,0,0)

polar along the binary axis



P_aca2_1 (**a**, **c**, –**b**; –⅛, 0, 0)

```
loop_
_space_group_symop_magn_operation.id
_space_group_symop_magn_operation.xyz
1 x,y,z,+1
2 -x+3/4,y+1/2,-z,+1
3 -x+1/4,y+1/2,z,+1
4 x+1/2,y,-z,+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
```

coset decomposition

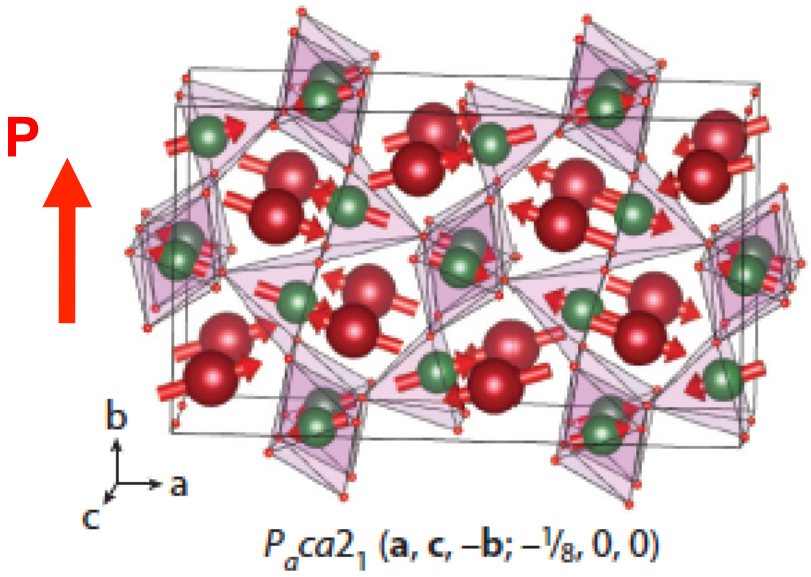
Pbam1' = P_aca2_1 + {1'|0,0,0} P_aca2_1 + {-1|0,0,0}P_aca2_1 + {-1'|0,0,0}P_aca2_1

The knowledge of the MSG allows the systematic enumeration and description of all domain-related configurations:

Gd_2MnO_5 (magndata 1.54)

Pbam1' → **P_aca2_1**(2a,c,-b;-1/4,0,0)

polar along the binary axis



P_aca2_1 (**a**, **c**, –**b**; –1/8, 0, 0)

```
loop_
_space_group_symop_magn_operation.id
_space_group_symop_magn_operation.xyz
1 x,y,z,+1
2 -x+3/4,y+1/2,-z,+1
3 -x+1/4,y+1/2,z,+1
4 x+1/2,y,-z,+1
```

{1'|1/2,0,0} →

```
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
```

coset decomposition

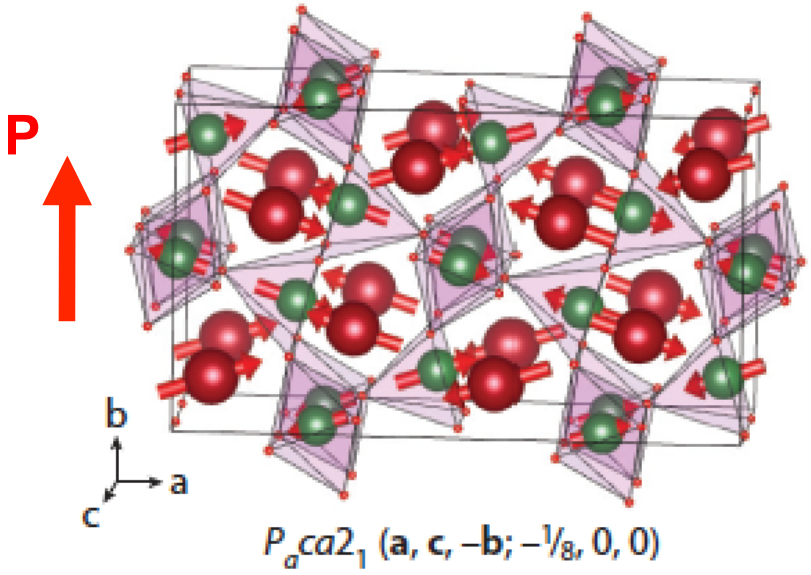
Pbam1' = P_aca2_1 + {1'|0,0,0} P_aca2_1 + {-1|0,0,0}P_aca2_1 + {-1'|0,0,0}P_aca2_1

The knowledge of the MSG allows the systematic enumeration and description of all domain-related configurations:

Gd_2MnO_5 (magndata 1.54)

Pbam1' → **P_aca2_1**(2a,c,-b;-1/4,0,0)

polar along the binary axis



P_aca2_1 (**a**, **c**, –**b**; –⅛, 0, 0)

```
loop_
_space_group_symop_magn_operation.id
_space_group_symop_magn_operation.xyz
1 x,y,z,+1
2 -x+3/4,y+1/2,-z,+1
3 -x+1/4,y+1/2,z,+1
4 x+1/2,y,-z,+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
```

coset decomposition

Pbam1' = P_aca2_1 + {1'|0,0,0} P_aca2_1 + {-1|0,0,0}P_aca2_1 + {-1'|0,0,0}P_aca2_1

$$\text{index of } P_aca2_1 = \frac{\text{Number of operations of Pbam1'}}{\text{Number of operations of } P_aca2_1} = 4$$

Different EQUIVALENT domain-related descriptions that will fit equally well your data: how many and which ones?

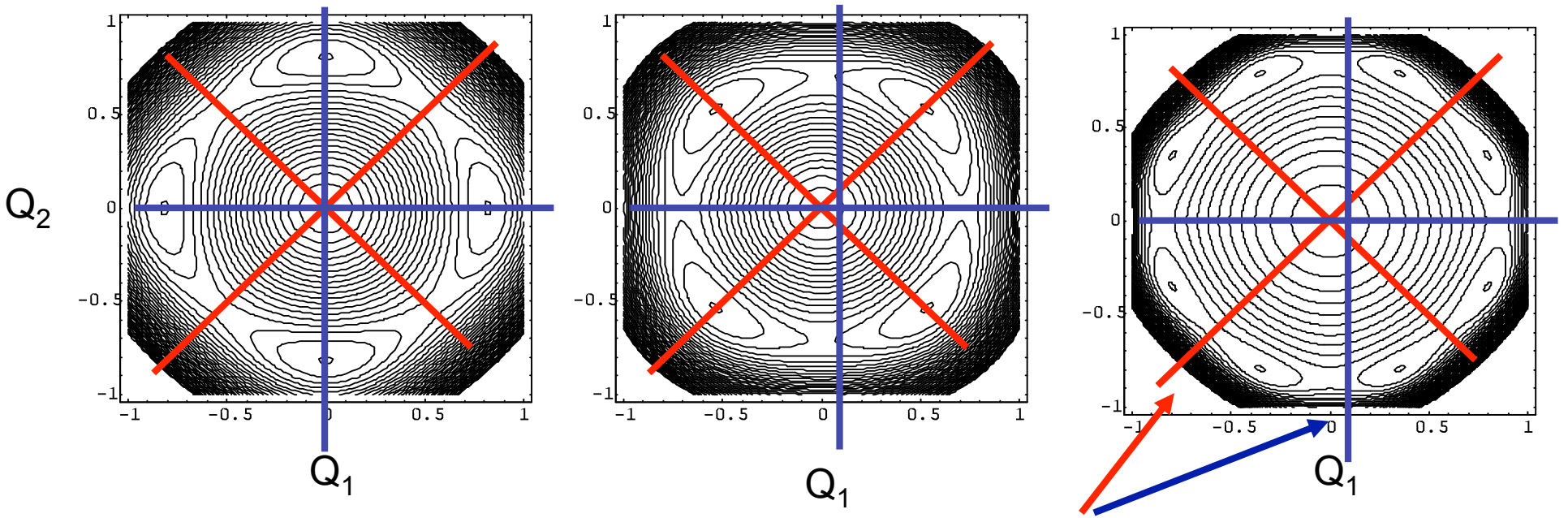
$$G \longrightarrow F$$

F subgroup of G

$$\text{Number of domains} = \text{index of F} = \frac{\text{Number of operations of G}}{\text{Number of operations of F}}$$

$$\text{index of F} = \frac{\text{N. lattice oper. of G}}{\text{N. lattice oper. of F}} \times \frac{\text{N. point group oper. of G}}{\text{N. point group oper. of F}}$$

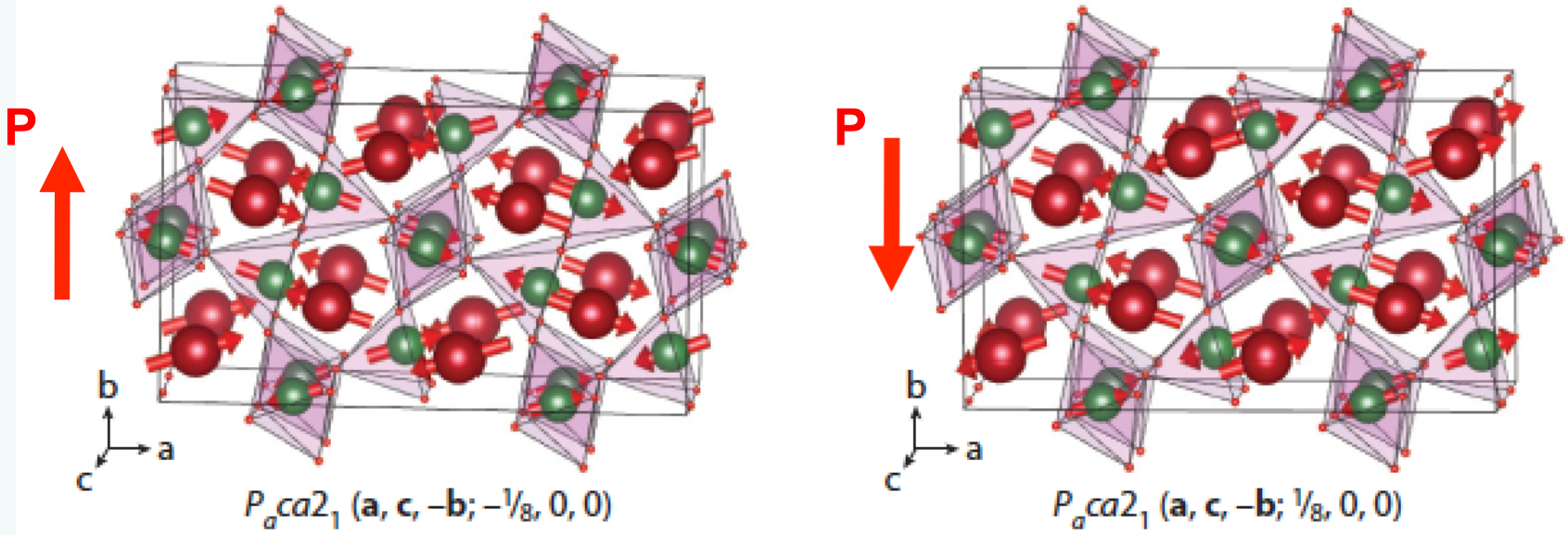
Domains/variants: symmetry related configurations (energy minima) around a higher-symmetry configuration



Q_i : Symmetry-breaking coordinates

The knowledge of the MSG allows the systematic enumeration and description of all domain-related configurations:

Gd_2MnO_5 (magndata 1.54) **Pbam1'** → **P_aca2_1**(2a,c,-b;-1/4,0,0)



twin-related spin arrangements related by space inversion, with opposite induced electric polarization.

P_aca2_1(2a,c,-b;-1/4,0,0) → **{-1|0,0,0}** **P_aca2_1**(2a,c,-b;1/8,0,0)

the MSG of domain-related structures can be a different subgroup (of the same type)

MVISUALIZE: Visualization with Jmol, but also generation of domain-related descriptions

Magnetic Symmetry and Applications	
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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
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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

Domain equivalent descriptions with MVISUALIZE

Magnetic space group $P_ac a 2_1$ (#29.104) (**a**,**c**,-**b**; -1/8,0,0)
Parent space group *Pbam* (#55) (**a**,**b**,**c**; 0,0,0)
Transformation from parent structure: (2**a**,**b**,**c**; 0,0,0)

[Magnetic Structure]

Lattice parameters: a=14.70620, b=8.53710, c=5.68070, alpha=90.00, beta=90.00, gamma=90.00

N	Atom	Occupancy	Magnetic moment constraint	Magnetic moment Values
1	Gd1_1 Gd 0.0698 0.1716 0.0000	1	$(M_x,M_y,0)$	(4.87, 1.63, 0.0)
2	Gd1_2 Gd 0.9303 0.8284 0.0000	1	$(M_x,M_y,0)$	(-4.51, -1.5, 0.0)
3	Mn1 Mn 0.0000 0.5000 0.2551	1	(M_x,M_y,M_z)	(-2.85, 0.95, 0.0)
4	Mn2_1 Mn 0.2059 0.3518 0.5000	1	$(M_x,M_y,0)$	(3.8, -1.27, 0.0)
5	Mn2_2 Mn 0.7941 0.6482 0.5000	1	$(M_x,M_y,0)$	(3.8, -1.27, 0.0)
6	O1 O 0.0000 0.0000 0.2697	1	-	-
7	O2_1 O 0.0763 0.4486 0.0000	1	-	-
8	O2_2 O 0.9237 0.5514 0.0000	1	-	-
9	O3_1 O 0.0727 0.4356 0.5000	1	-	-
10	O3_2 O 0.9273 0.5644 0.5000	1	-	-
11	O4_1 O 0.1997 0.2076 0.2450	1	-	-
12	O4_2 O 0.8003 0.7924 0.2450	1	-	-

[Show all atoms in unit cell and their moment relations]

Domain-related equivalent structures: coset representatives and conjugated subgroups

The transformation matrices of the table are from the parent space group to the standard setting of the listed magnetic space groups
The coset representatives used to derive the domain-related equivalent structures are expressed in the setting of the parent group

N	Coset representatives (x,y,z) form	Coset representatives Seitz notation	Transformation matrix	Magnetic Structure
1	x,y,z,+1	$\{1\mid 0\}$	$\begin{pmatrix} 2 & 0 & 0 & 7/4 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$	Show
2	-x,-y,z,+1	$\{2_{001}\mid 0\}$	$\begin{pmatrix} -2 & 0 & 0 & 1/4 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$	Show

The MSG of the transformed structure is of the same type but different subgroup!

equivalent

Pbam1' = $P_ac a 2_1$ + {1'|0,0,0} $P_ac a 2_1$ + {-1|0,0,0}$P_ac a 2_1$ + {-1'|0,0,0}$P_ac a 2_1$

Domain equivalent descriptions with MVISUALIZE

coset representative
$\{2_{001}|0,0,0\}$

(same as $\{-1'|0,0,0\}$)

mCIF file of the transformed structure

Domain-related equivalent description

Selected parent symmetry operation transforming the initial structure: 2- $\{ 2_{001} \mid 0 \}$

Magnetic space group *$P_a ca2_1$* (#29.104) (**-a,c,b**; 1/8,0,0)
Parent space group *Pbam* (#55) (**a,b,c**; 0,0,0)

Setting (**2a,b,c**; 0,0,0) from parent group

Go to standard setting Change setting

[Transformed Magnetic Structure]

Lattice parameters: a=14.7062, b=8.5371, c=5.6807, alpha=90.00, beta=90.00, gamma=90.00

N	Atom	Occupancy	Magnetic moment constraint	Magnetic moment Values
1	Gd1_1 Gd 0.0698 0.1716 0.0000	1	$(M_x,M_y,0)$	(4.5100, 1.5000, 0.0000)
2	Gd1_2 Gd 0.9303 0.8284 0.0000	1	$(M_x,M_y,0)$	(-4.8700, -1.6300, 0.0000)
3	Mn1 Mn 0.0000 0.5000 0.2551	1	(M_x,M_y,M_z)	(2.8500, -0.9500, 0.0000)
4	Mn2_1 Mn 0.2059 0.3518 0.5000	1	$(M_x,M_y,0)$	(-3.8000, 1.2700, 0.0000)
5	Mn2_2 Mn 0.7941 0.6482 0.5000	1	$(M_x,M_y,0)$	(-3.8000, 1.2700, 0.0000)
6	O1 O 0.0000 0.0000 0.2697	1	-	-
7	O2_1 O 0.0763 0.4486 0.0000	1	-	-
8	O2_2 O 0.9237 0.5514 0.0000	1	-	-
9	O3_1 O 0.0727 0.4356 0.5000	1	-	-
10	O3_2 O 0.9273 0.5644 0.5000	1	-	-
11	O4_1 O 0.1997 0.2076 0.2450	1	-	-
12	O4_2 O 0.8003 0.7924 0.2450	1	-	-

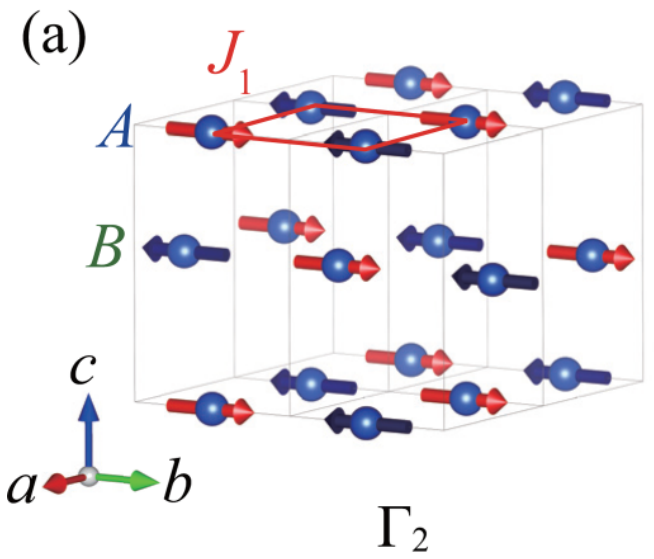
[Show all atoms in unit cell and their moment relations]

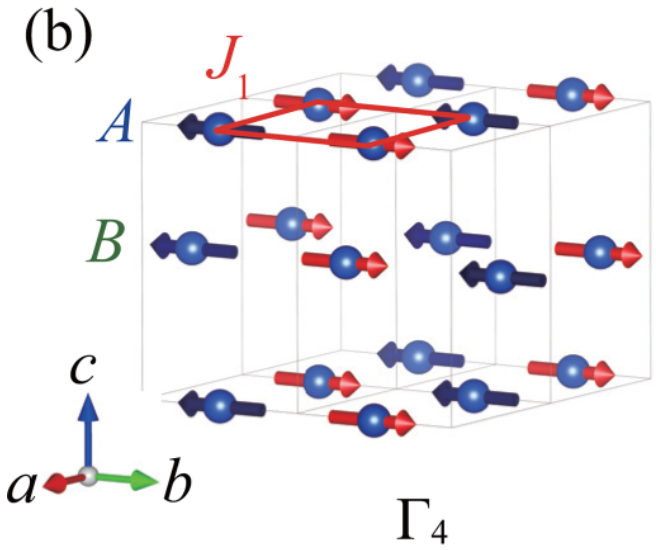
Visualize this magnetic structure in 3D using Jmol: Visualize

Download mCIF file: bcs_file.mcif
[The preview text below is non-editable, only copy-allowed]

```
#\#CIF_2.0
# Created by the Bilbao Crystallographic Server
# http://www.cryst.ehu.es
# Date: 27/01/2023
# Domain-related equivalent description. Coset representative: -x,-y,z,+1

data_5yOhtAoR
_audit_creation_date              27/01/2023
_audit_creation_method            "Bilbao Crystallographic Server"

_citation_journal_abbrev          PHYSICAL REVIEW LETTERS
_citation_journal_volume          110
_citation_page_first              ?
_citation_page_last               ?
_citation_article_id              137203
_citation_year                    2013
_citation_DOI                     10.1103/physrevlett.110.137203

loop_
```

The confusion between EQUIVALENT (domain-related) magnetic structures and DIFFERENT models fitting equally the diffraction data





$SrLaCuSbO_6$ (MAGNDATA #1.674)

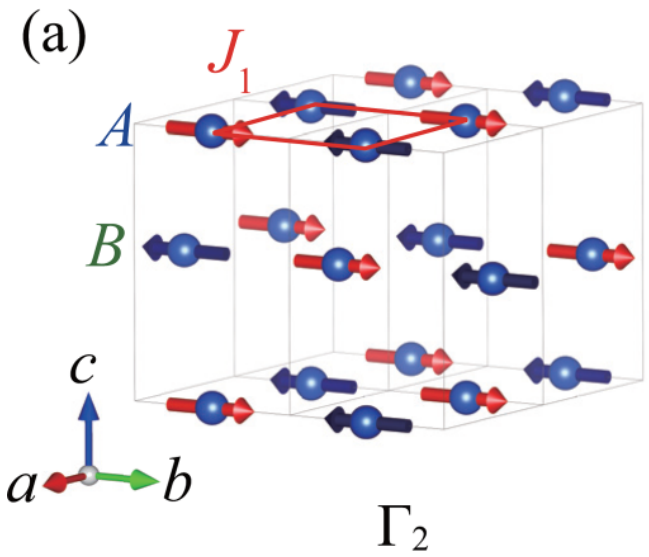
Phys. Rev. B (2022) **k**=(½ ½ 0)

These two arrangements are reported to fit equally well the data….They are claimed to correspond to two different irreps and represent two different alternative models…

BUT in fact: … they are the SAME magnetic structure!

They are related by some of the lost symmetry operations. They represent the two forms that the same magnetic ordering can be realized in the parent structure, forming twin domains

The two irreps are complex conjugate: they cannot yield different REAL magnetic arrangements! They form a SINGLE PHYSICALLY irreducible representation



$SrLaCuSbO_6$ (MAGNDATA #1.674)

k=(½ ½ 0)

$P2_1/n1' \longrightarrow P_S\text{-}1$

index= 2 x 2 = 4

N. of domains = 4

Pairs of domains are trivially related by time reversal

Number of non-trivial domains = 2

MVISUALIZE has an option to generate all domains that are non-trivial

- **The identification and assignment the magnetic space group (MSG) should be a "must"**

- Whatever the method employed to determine a commensurate magnetic structure, its MSG must be identified and reported.

- For a full identification of the MSG the transformation from the unit cell used to one where the MSG has its standard form must also be reported or even better list of the symmetry operations of the MSG in the origin and unit cell used.

- The magnetic point group (MPG) can be derived from the MSG, but it is so important that it is recommendable to report it explictly.

- **If you fear that the referees will think your paper is not enough "cutting hedge" research, because it includes too much detail and Tables, you can always submit the information as supplemental material, and your magnetic structure will be fully unambiguous, and easily portable for other studies.**

You know your structure but you do not know its MSG?

- Then construct by hand or make that your refinement program produces a magCIF file of your structure under MSG P1

Get from your refinement program a simple mCIF file in the lowest MSG P1, which only includes the lattice periodicity as symmetry and lists all atoms and moments within the unit cell.

If the program does not have this option, but you know your structure you should be able to prepare this file either manually or with some computer script

A template file can be downloaded from MAGNDATA

All atoms in the unit cell, also the non-magnetic ones!

Magnetic moments of all magnetic atoms in the unit cell

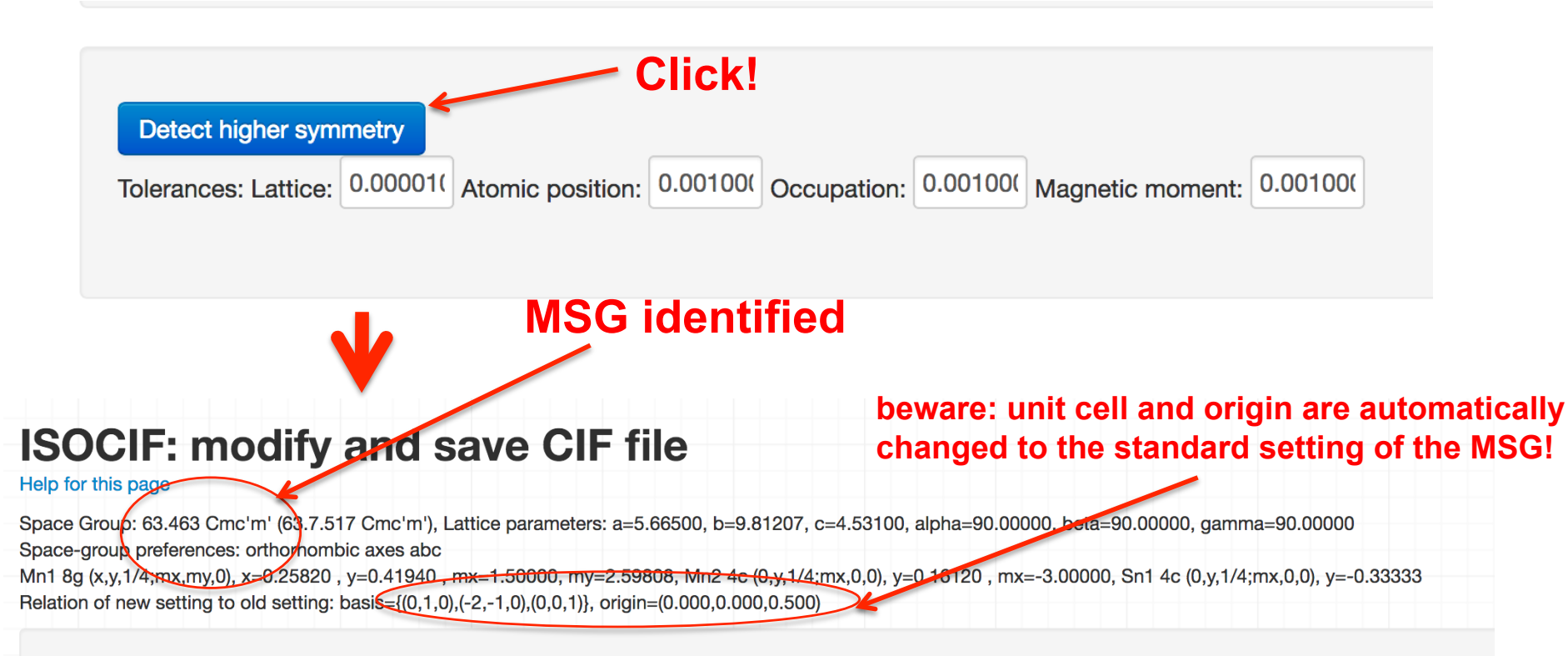
“Magnetic” unit cell

No symmetry. Only the identity

```
data_1
_cell_length_a                         5.66500
_cell_length_b                         5.66500
_cell_length_c                         4.53100
_cell_angle_alpha                      90.00000
_cell_angle_beta                       90.00000
_cell_angle_gamma                      120.00000

loop_
_space_group_symop_magn_operation.id
_space_group_symop_magn_operation.xyz
1    x,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
Mn1_1 Mn 0.83880 0.67760 0.25000 1.0000
Mn1_2 Mn 0.16120 0.83880 0.75000 1.0000
Mn1_3 Mn 0.16120 0.32240 0.75000 1.0000
Mn1_4 Mn 0.83880 0.16120 0.25000 1.0000
Mn1_5 Mn 0.32240 0.16120 0.25000 1.0000
Mn1_6 Mn 0.67760 0.83880 0.75000 1.0000
Sn1_1 Sn 0.33333 0.66667 0.25000 1.0000
Sn1_2 Sn 0.66667 0.33334 0.75000 1.0000

loop_
_atom_site_moment.label
_atom_site_moment.crystalaxis_x
_atom_site_moment.crystalaxis_y
_atom_site_moment.crystalaxis_z
Mn1_1 3.000 3.000 0.000
Mn1_2 -3.000 0.000 0.000
Mn1_3 3.000 3.000 0.000
Mn1_4 -3.000 0.000 0.000
Mn1_5 0.000 -3.000 0.000
Mn1_6 0.000 -3.000 0.000
```

You know your structure but you do not know its MSG?

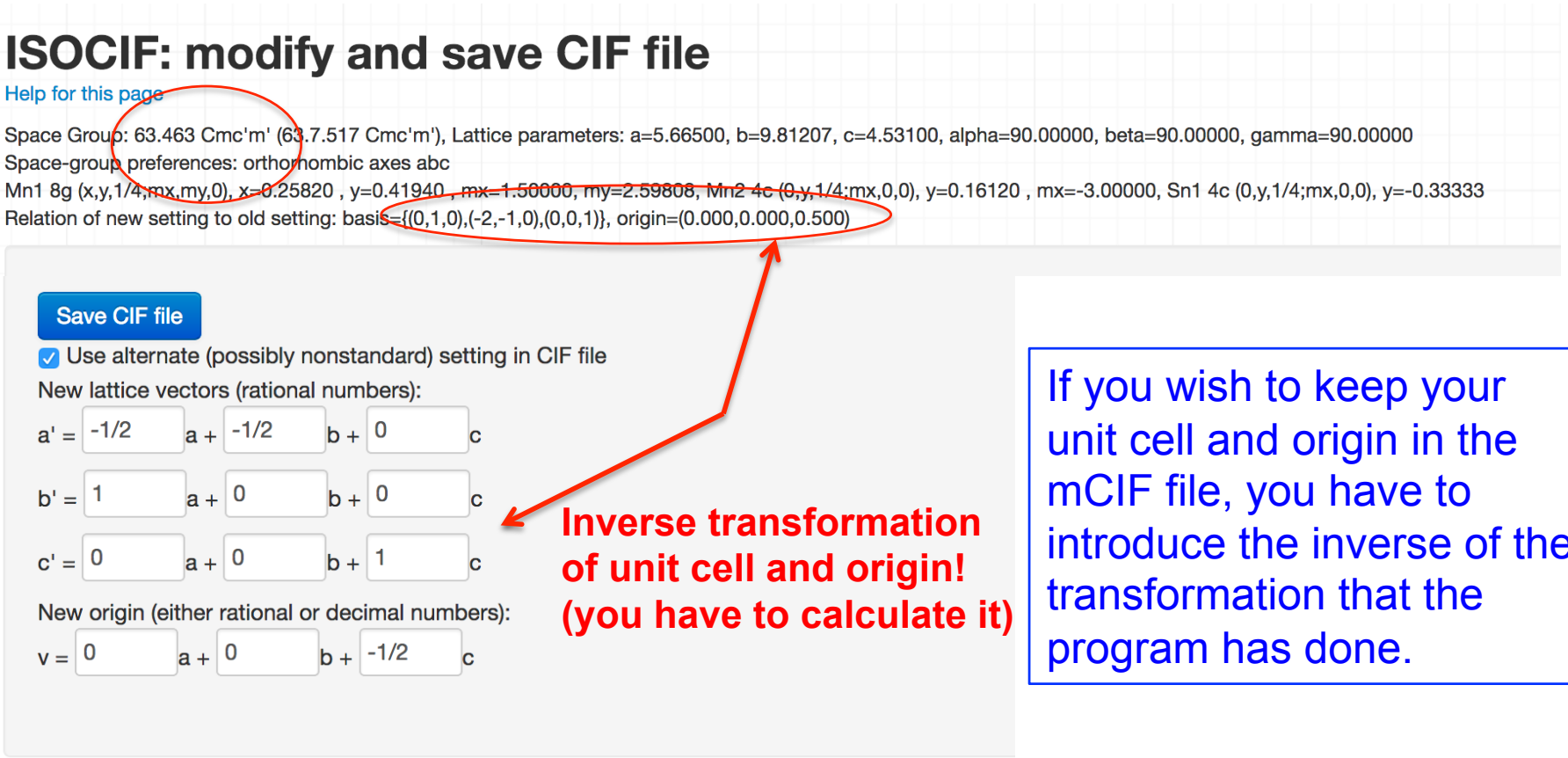
Upload the P1 mCIF file of your structure in ISOCIF available in the ISOTROPY Software Suite in the web.



You know your structure but you do not know its MSG?

Save the new mCIF file with the correct MSG detected by ISOCIF.

- To keep the origin and unit cell of the original input P1 file, care must be taken indicating the correct transformation from the standard basis chosen by the program.



Inverse transformation of unit cell and origin! (you have to calculate it)

If you wish to keep your unit cell and origin in the mCIF file, you have to introduce the inverse of the transformation that the program has done.

A new program to identify the MSG of a magnetic structure:

Condensed Matter > Materials Science

[Submitted on 28 Nov 2022]

Algorithm for deriving magnetic space-group information

Kohei Shinohara, Atsushi Togo, Isao Tanaka

A crystal symmetry search is crucial for computational crystallography and materials science. Although algorithms and implementations for the crystal symmetry search have been developed, their extension to magnetic space groups (MSGs) remains limited. In this paper, algorithms for determining magnetic symmetry operations of magnetic crystal structures, identifying magnetic space-group types of given MSGs, and symmetrizing the magnetic crystal structures using the MSGs are presented. The determination of magnetic symmetry operations is numerically stable and is implemented with minimal modifications from the existing crystal symmetry search. Magnetic space-group types are identified by combining space-group type identification and the use of affine normalizers. Point coordinates and magnetic moments of the magnetic crystal structures are symmetrized by projection operators for the MSGs. An implementation is distributed with a permissive free software license in spglib v2.0.2: this https URL.

Subjects: **Materials Science (cond-mat.mtrl-sci)**; Computational Physics (physics.comp-ph)
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Tutorial_magnetic_section_BCS_1

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