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Zientzia eta Teknologia Fakultatea
Facultad de Ciencia y Tecnología

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Universidad del País Vasco
Euskal Herriko Unibertsitatea

I. Magnetic symmetry

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BILBAO, SPAIN

Symmetry-Based Computational Tools for Magnetic Crystallography

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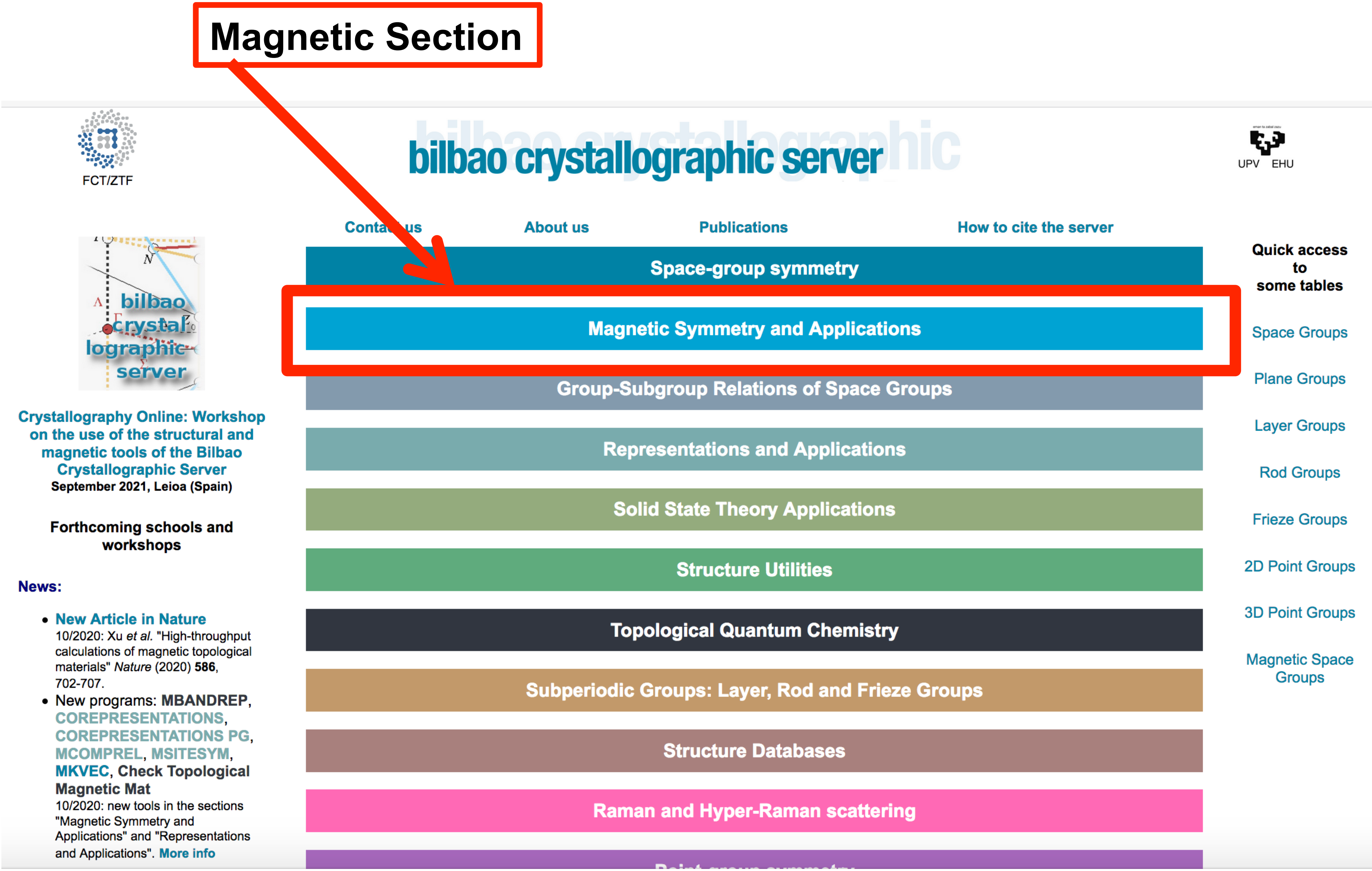
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bilbao crystallographic server
Crystallography Online: Workshop on the use of the structural and magnetic tools of the Bilbao Crystallographic Server
September 2021, Leioa (Spain)
Forthcoming schools and workshops
News:
New Article in Nature
10/2020: 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)

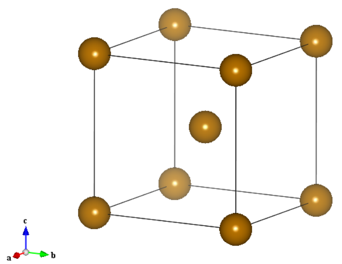
Tutorial-k-SUBGROUPSMAG (3 versions)

Symmetry and Physics:

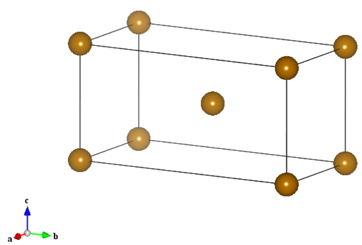
A symmetry property in a solid is **NOT ONLY** some mathematical property. It is a **PHYSICAL PROPERTY**!

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

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).* here comes the Physics:

Symmetry and Physics:

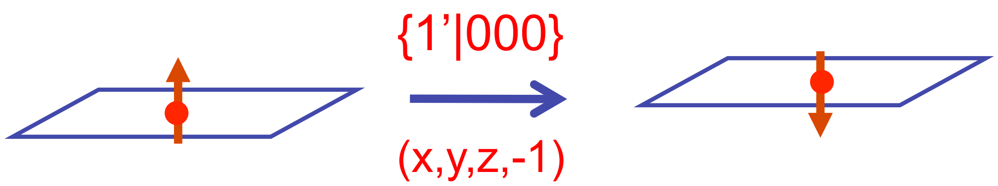
Group of all possible combinations of **rotations**
translations
space inversion

(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:

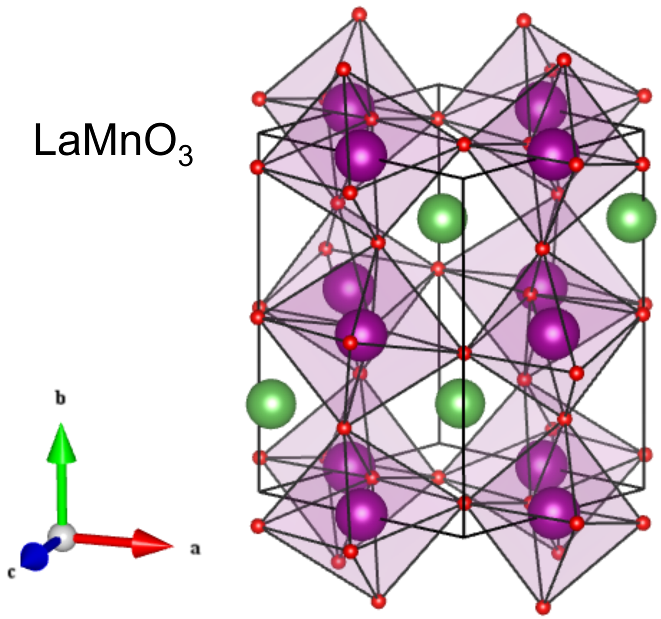
We do not add but SUBSTRACT symmetry operations !

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**}

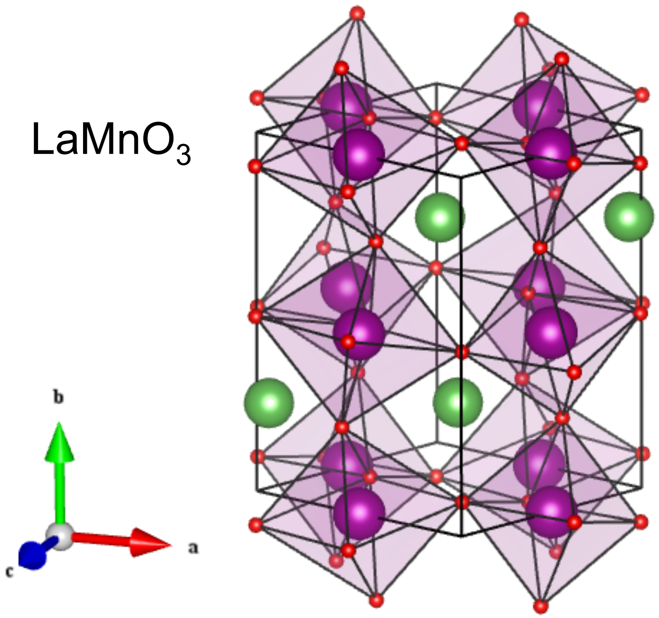
{R,θ|**t**} $\theta=1$ $\theta=-1$

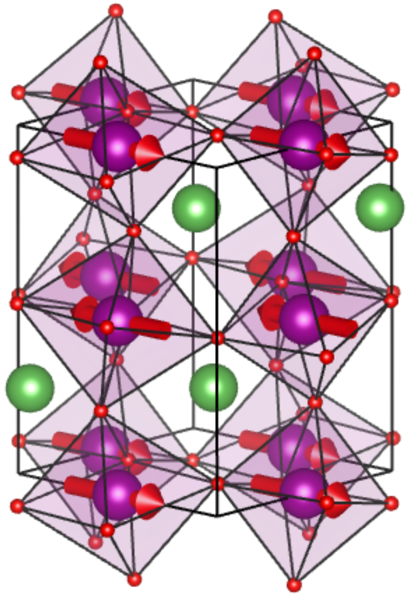
Magnetic ordering is a symmetry breaking process

Magnetically ordered phases:

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

LaMnO$_3$





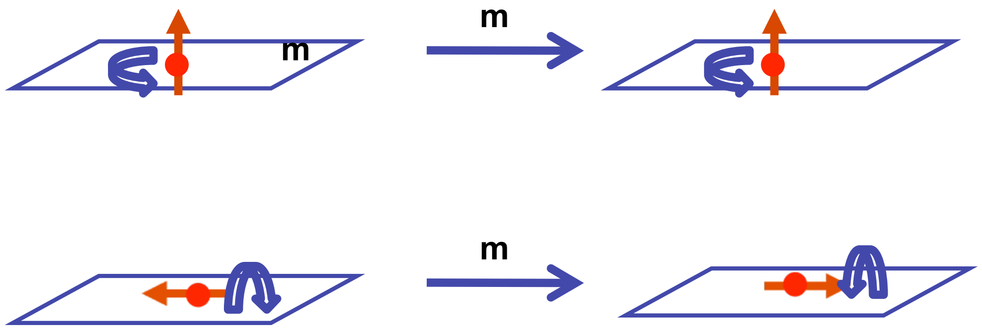
Pnma1'

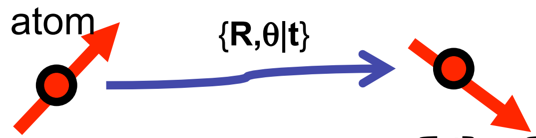
(x,y,z,+1) (-x+1/2,-y,z+1/2 … 2,-y+1/2,-z+1/2,+1)
(-x,-y,-z,+1) (x+1/2,y,-z+1/2 … /2,y+1/2,z+1/2,+1)
~~(x,y,z,-1)~~ (-x+1/2,-y,z+1/2 … ,-y+1/2,-z+1/2,-1)
(-x,-y,-z,-1) (x+1/2,y,-z+1/2, … 2,y+1/2,z+1/2,-1)

?

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

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





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

(for positions: the same as with Pnma)

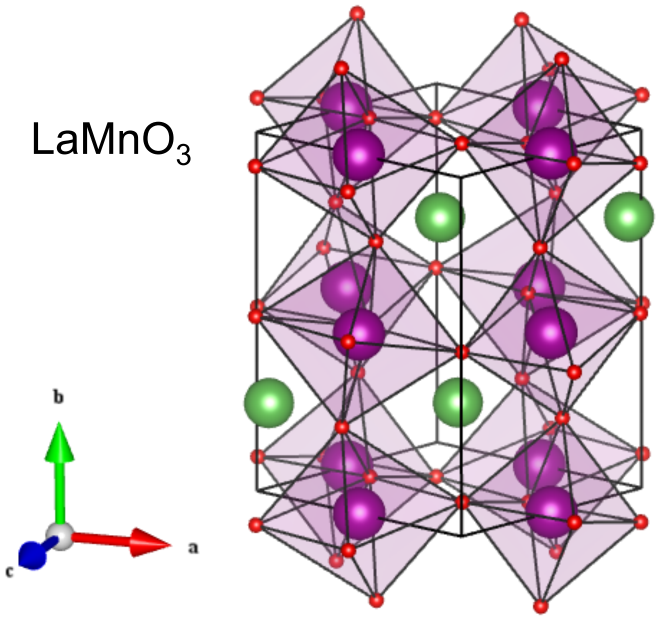
(mx,my,mz) $\longrightarrow$ $\begin{bmatrix} mx' \\ my' \\ mz' \end{bmatrix} = \theta \det(\mathbf{R})\ \mathbf{R} \begin{bmatrix} mx \\ my \\ mz \end{bmatrix}$

θ=-1 if time reversal

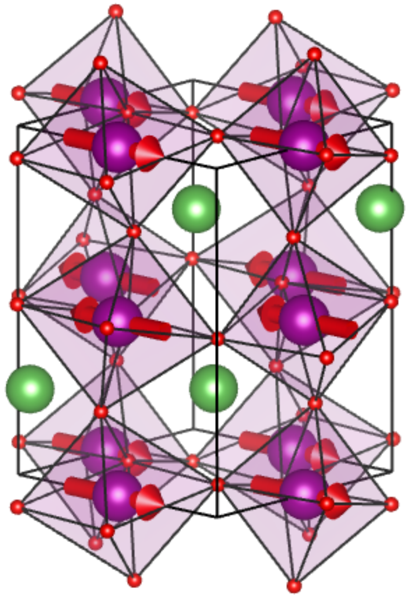
Magnetic ordering is a symmetry breaking process

Magnetically ordered phases:

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



Pnma1'



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)

Types of magnetic space groups:

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

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

F subgroup of G

F ≤ G

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

antitranslation / anticentering

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

Type II **non-magnetic structures**	**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 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. (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 $\underline{+1}$	{ 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

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 }

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

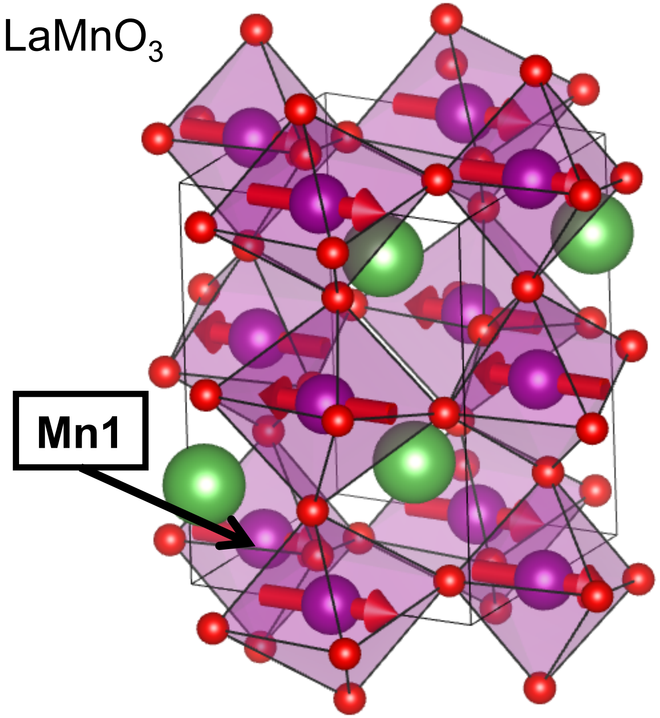
Output of MGENPOS

Example of type IV MSG

Propagation vector k≠0

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, 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

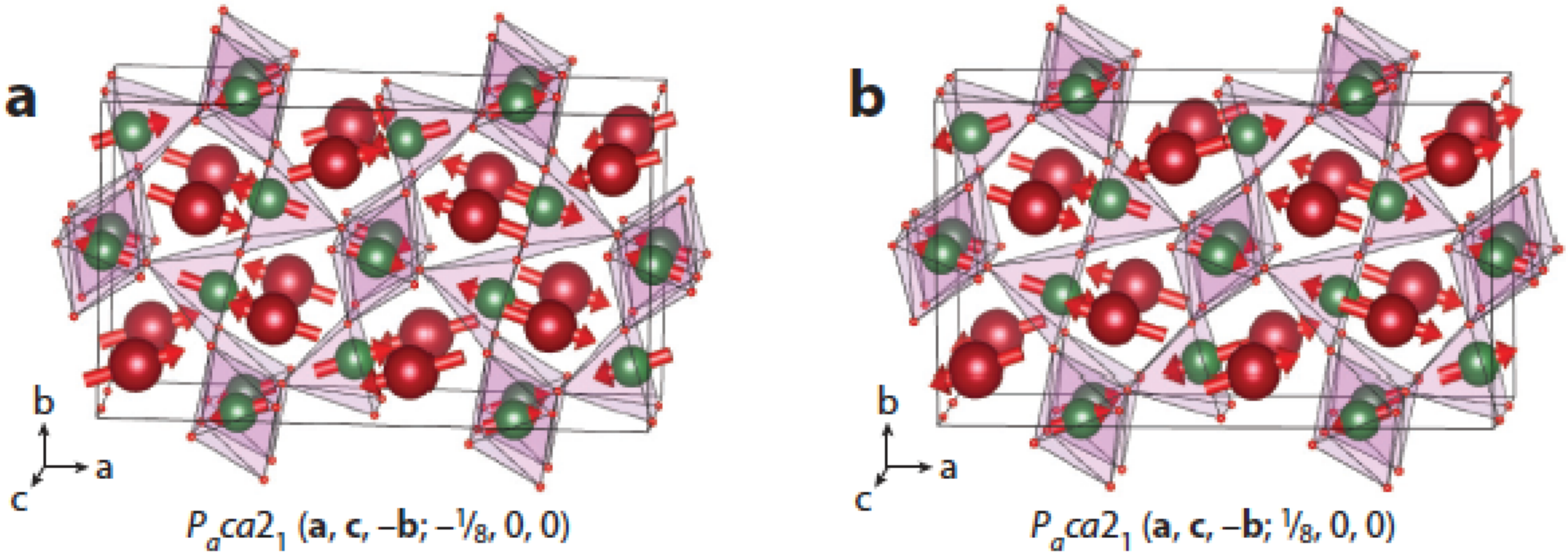
MSG

asymmetric unit

magnetic moments in the asymmetric unit

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

Gd_2MnO_5 (magndata 1.54)



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

Consequences of symmetry

Von Neumann principle:

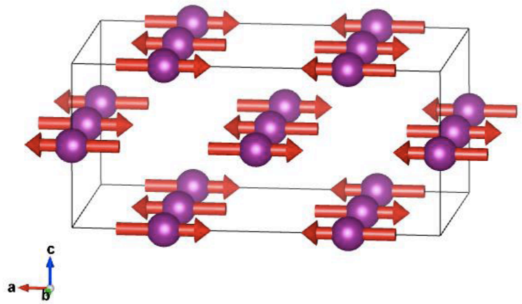
- all variables/parameters/degrees of freedom compatible with the symmetry will be present (their magnitude may be small or large, but not necessarily zero.

- 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)

$HoMnO_3$

unit cell: $2a_p$, b_p, c_p



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

WP	**+ (1' |1/2 0 0)**
8b	(x, y, z | m_x, m_y, m_z), (-x+1/4, -y, z+1/2 | $-m_x$, $-m_y$, m_z), (x, -y+1/2, z | $-m_x$, m_y, $-m_z$), (-x+1/4, y+1/2, z+1/2 | m_x, $-m_y$, $-m_z$)
4a	(x, 1/4, z| 0, m_y, 0), (-x+1/4, 3/4, z+1/2 | 0, $-m_y$, 0)

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

Atomic positions of asymmetric unit:

Ho1 4a 0.04195 0.25000 0.98250
Ho2 4a 0.95805 0.75000 0.01750
Mn1 8b 0.00000 0.00000 0.50000
O1 4a 0.23110 0.25000 0.11130
O12 4a 0.76890 0.75000 0.88870
O2 8b 0.16405 0.05340 0.70130
O22 8b 0.83595 0.55340 0.29870

Split independent positions in the lower symmetry

General position:
x, y, z not restricted by symmetry!

Magnetic moments of the asymmetric unit (μB):

Mn1 3.87 ≈0.0 ≈0.0

zero values are not symmetry "protected"

Magnetic Point Group: **mm21'**

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

Magnetic Symmetry and Applications	
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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		
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

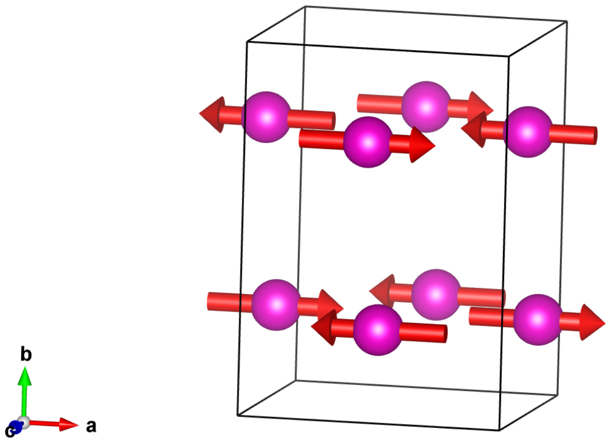
Group 6/m'mm (#27.3.102)

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

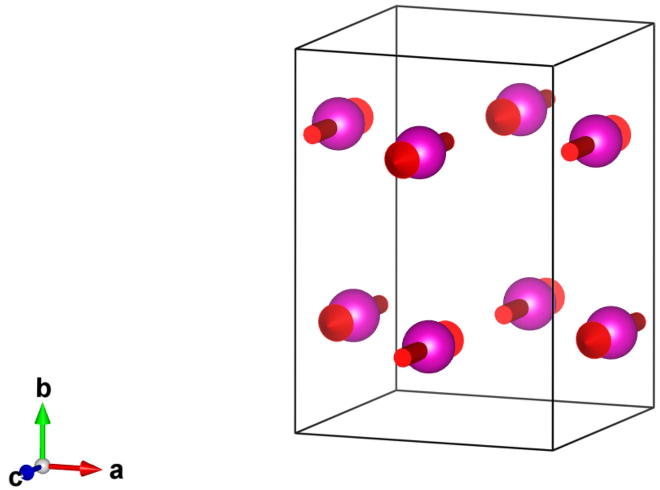
Number of independent coefficients: 1

Consequences of symmetry

$EuZrO_3$: magndata #0.146 & 0.147



Pnm'a



Pn'm'a'

Table of tensor components

α^T_{ij}	j		
i	*1*	*2*	*3*
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

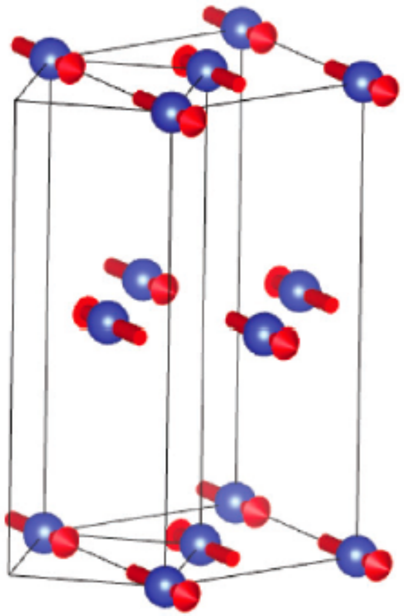
$^T_{ij}$	j		
	1	*2*	*3*
1	α^T_{11}	0	0
2	0	α^T_{22}	0
3	0	0	α^T_{33}

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

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



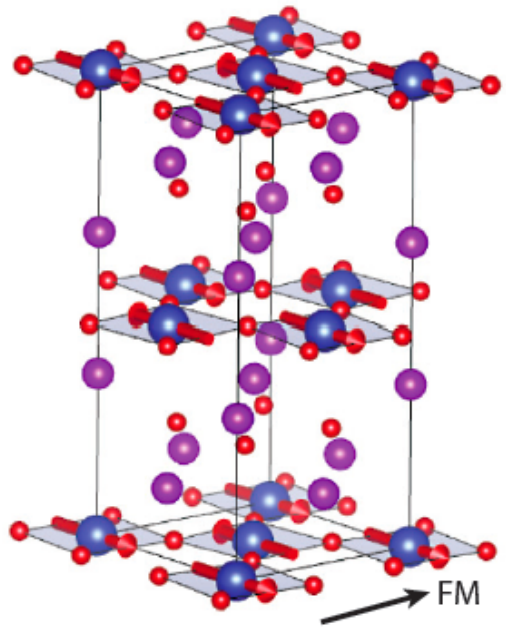
$C_A ccm$

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

Point group: mmm1'

Gd_2CuO_4

Cmce, k=(0,0,0)



Cm'ca'

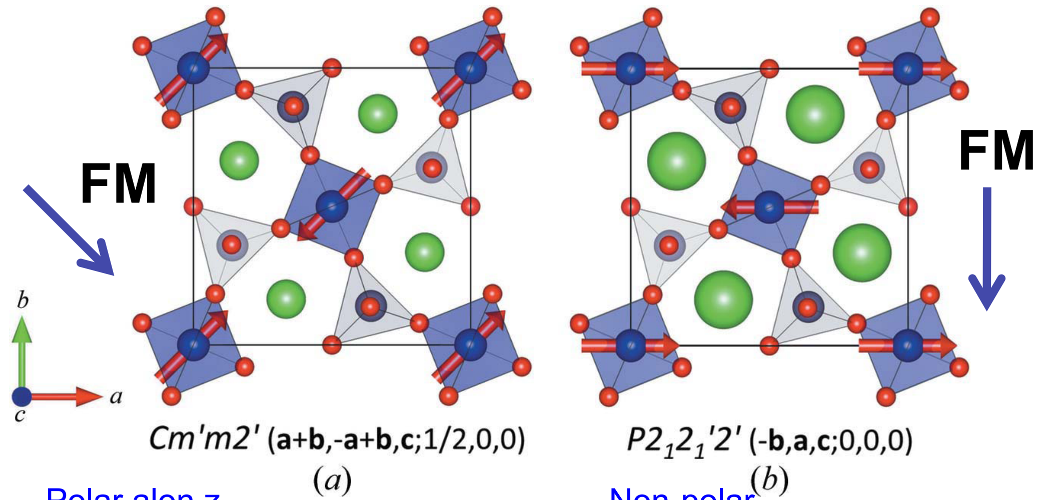
(c,b,-a,0,0,0)

Point group: m'mm'

(weak ferromagnetism)

Consequences of symmetry

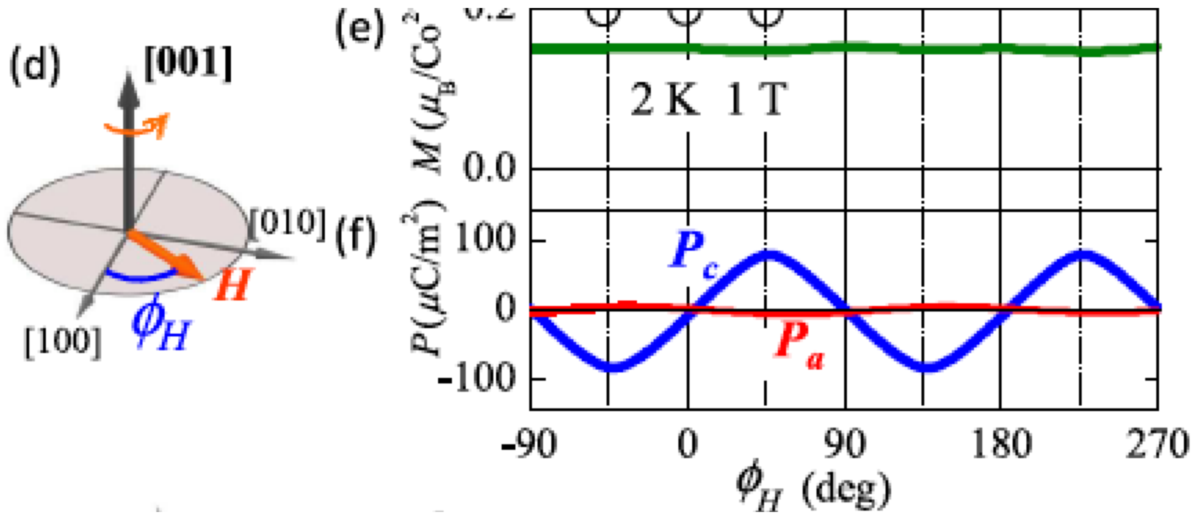
$Ba_2CoGe_2O_7$ **parent SG: P-42_1m**



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

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