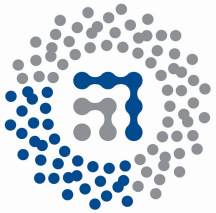

ZTF-FCT
Zientzia eta Teknologia Fakultatea
Facultad de Ciencia y Tecnología

eman ta zabal zazu

Universidad del País Vasco
Euskal Herriko Unibertsitatea

Symmetry of commensurate magnetic structures: Magnetic space groups

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Facultad de Ciencia y Tecnología
Universidad del País Vasco, UPV-EHU
BILBAO, SPAIN

WHAT IS SYMMETRY?

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

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

"symmetry-forced" means : "forced for a thermodynamic phase
"symmetry-allowed" means : "allowed within a thermodynamic phase"

Symmetry-dictated properties can be considered symmetry "protected"

Reminder of symmetry in non-magnetic structures

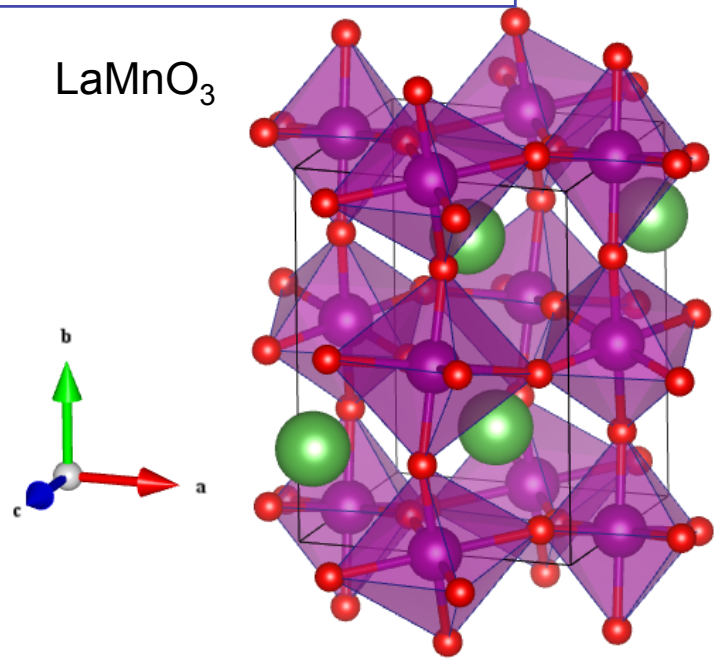
Space Group:
Pnma

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
O2	0.30850	0.04080	0.72270

$LaMnO_3$



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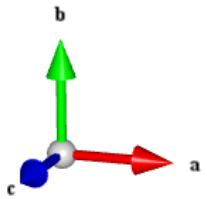
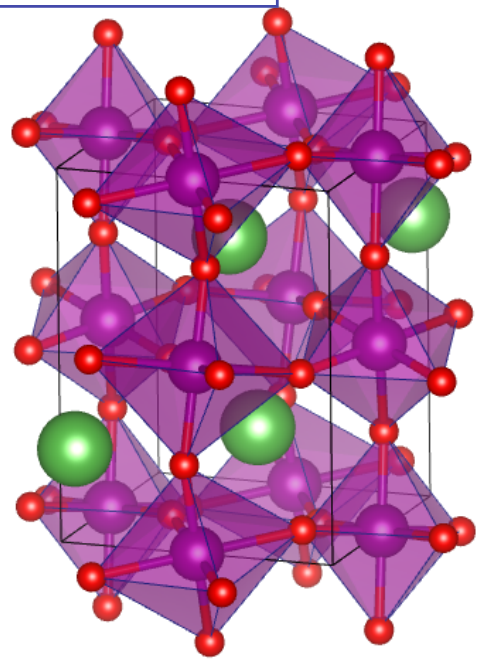
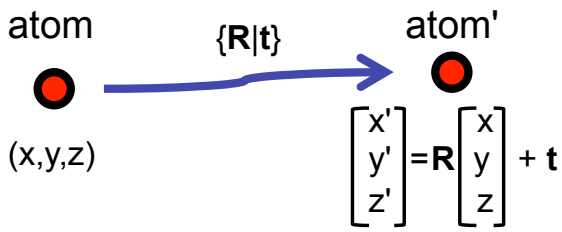




Space Group: set of operations {R|t}

for all atoms:



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

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

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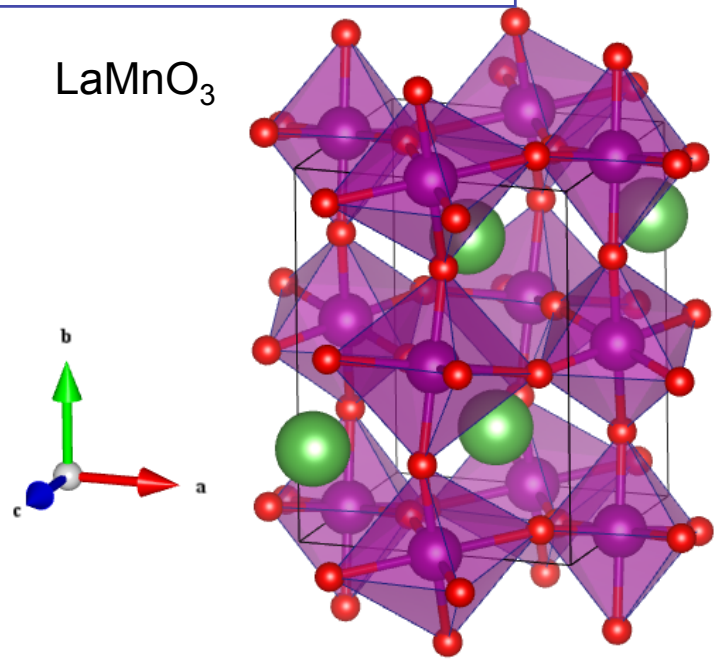

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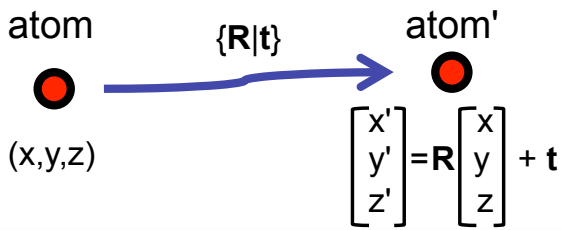

{**R**|**t**}: **R -** rotation or rotation+plus inversion
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Pnma: 8 related positions for a general position:

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): ***special positions are tabulated***:

(x,1/4,z) (-x+1/2,3/4,z+1/2) (-x,3/4,-z) (x+1/2,1/4,-z+1/2) **Wyckoff positions or orbits**

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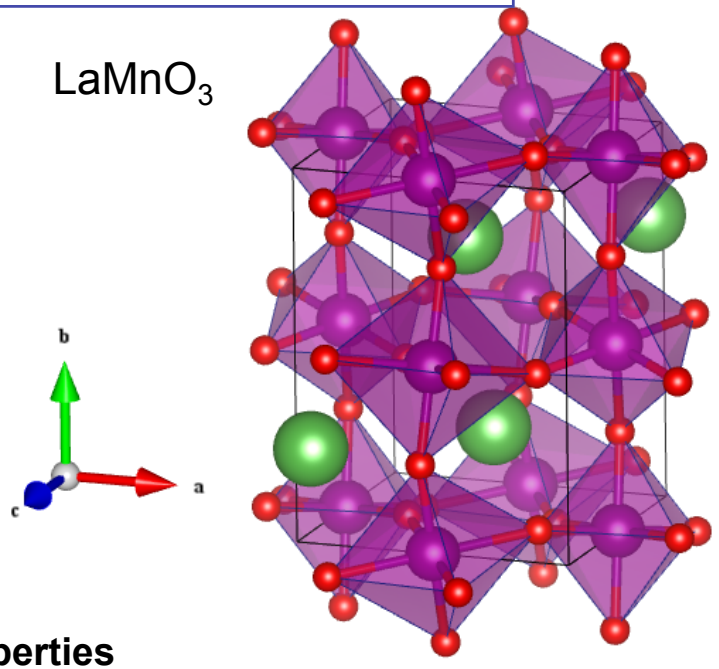

Relations among atoms from the space group:
more than "geometrical", they are "thermodynamic" properties

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

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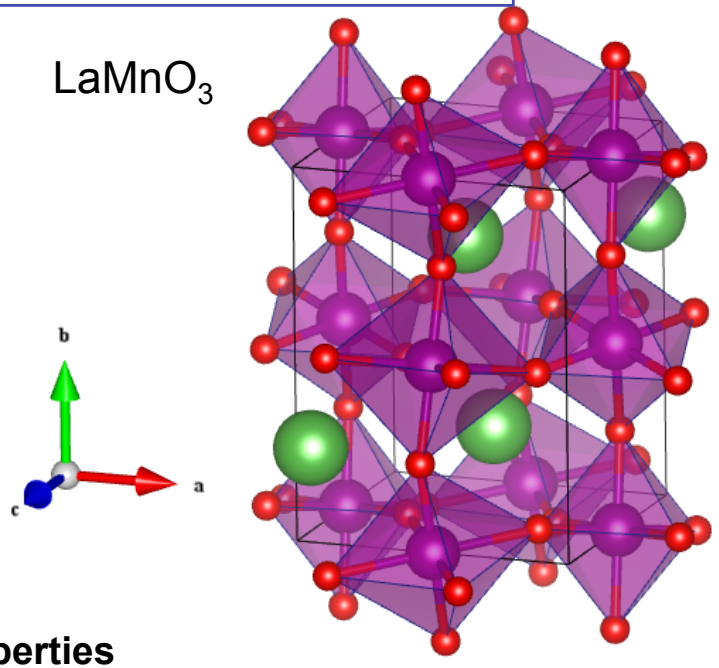

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¼ rigorously fulfilled – if broken, it means a different phase

Whatever microscopic model of atomic forces, if consistently applied, it will yield:

F_y (La1)= 0.000000 (exact!)

Magnetic Symmetry:

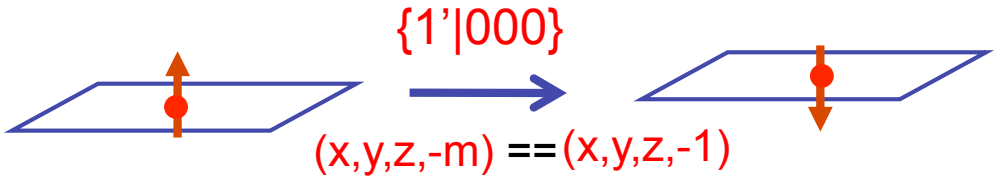
Symmetry is only detected when it does not exist!

We do not add but substract symmetry operations !

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

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

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



Magnetic structures only have symmetry operations where time reversal 1' is combined with other transformations, or is not present at all:

{1'|t} = {1'|0,0,0} {1|t}
{m'| t}= {1'|0,0,0} {m|t}
{2'|t} = {1'|0,0,0}{2|t}
{3'$^{+}$|t} = {1'|0,0,0}{3^{+}|t}, etc.

But **{1'|0,0,0}** alone is never a symmetry operation of a magn. struct.

All NON-magnetic structures have time inversion symmetry

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

Actual symmetry of the non-magnetic phase:

Pnma1' = Pnma + {1'|000}x ***Pnma*** (grey group)

16 operations:

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

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

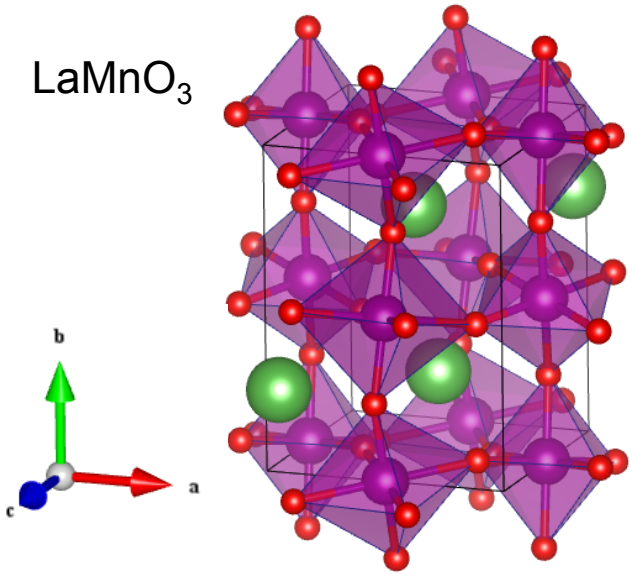
Notation: (x+1/2,-y+1/2,-z+1/2,+1) == {2x| ½ ½ ½ } {R|**t**}
(x+1/2,-y+1/2,-z+1/2,-1) == {2x'| ½ ½ ½ } {R'|**t**}

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

magnetic ordering breaks symmetry of time inversion

Magnetic ordered phases:

$LaMnO_3$



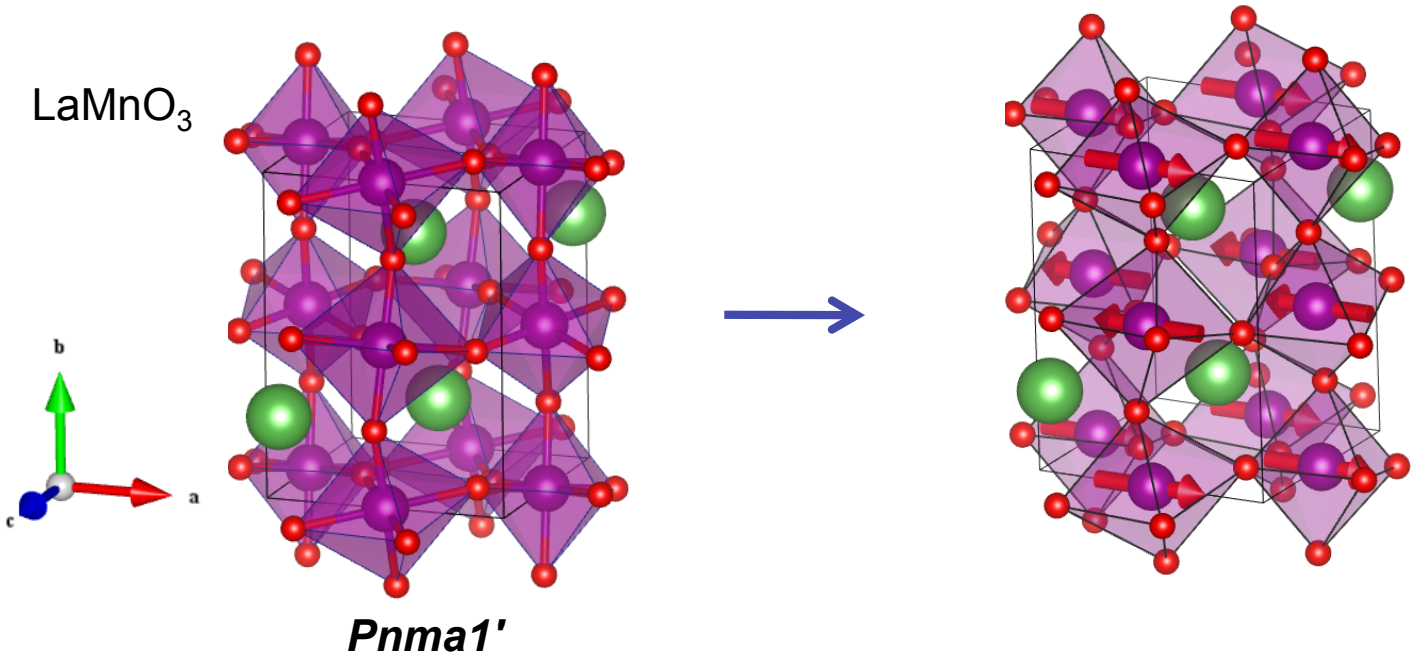
Pnma1'

(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)

magnetic ordering breaks symmetry of time inversion

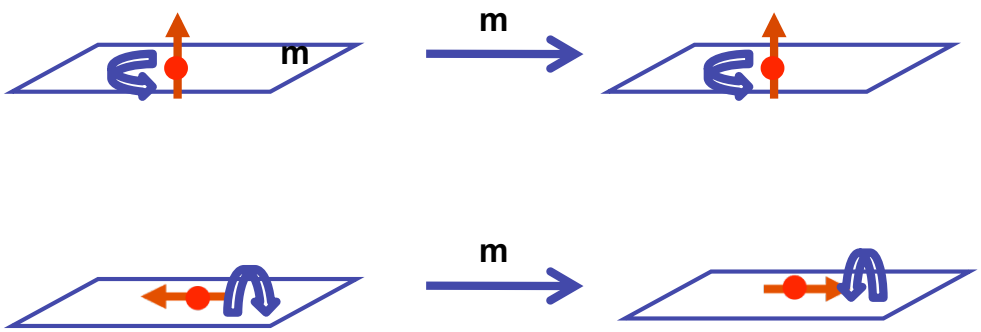
Magnetic ordered phases:

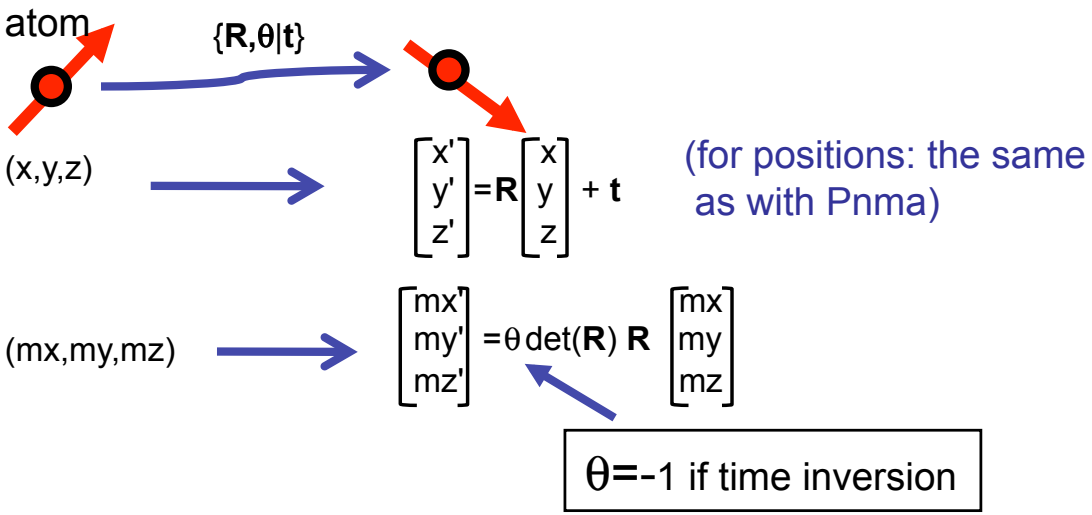
Time inversion {1'|0 0 0} is NOT a symmetry operation of a magnetic phase



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

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





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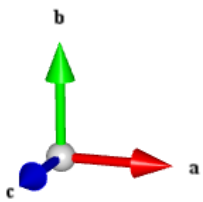

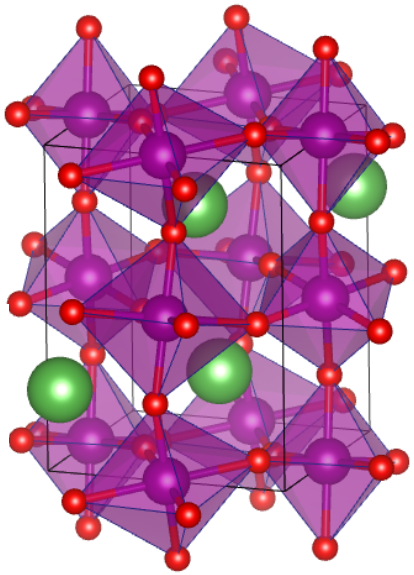

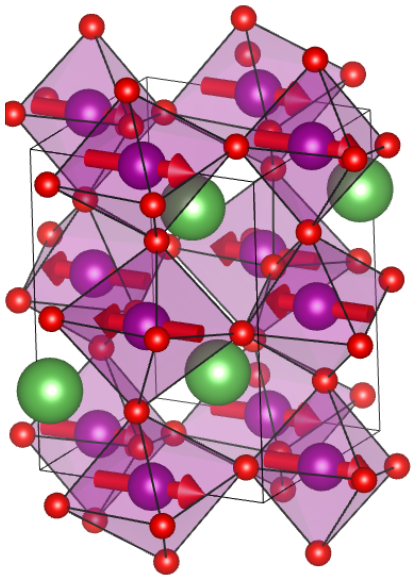

Pnma1'

(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)

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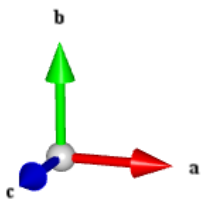

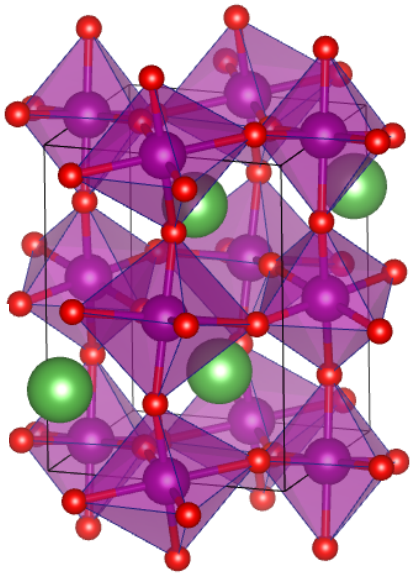

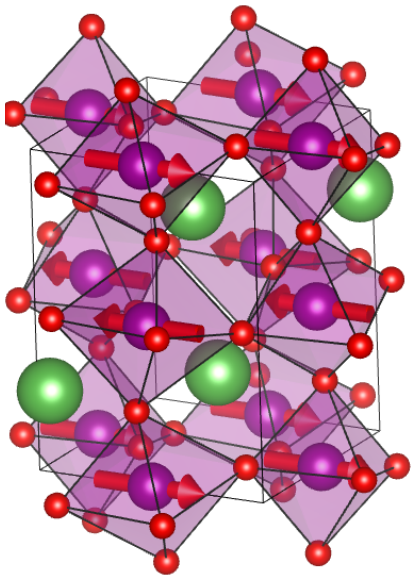

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~~(-x,-y,-z,-1)~~ (x+1/2,y,-z+1/2,-1)

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

MAGNETIC SYMMETRY IN COMMENSURATE CRYSTALS

A symmetry operation fullfills:

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

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

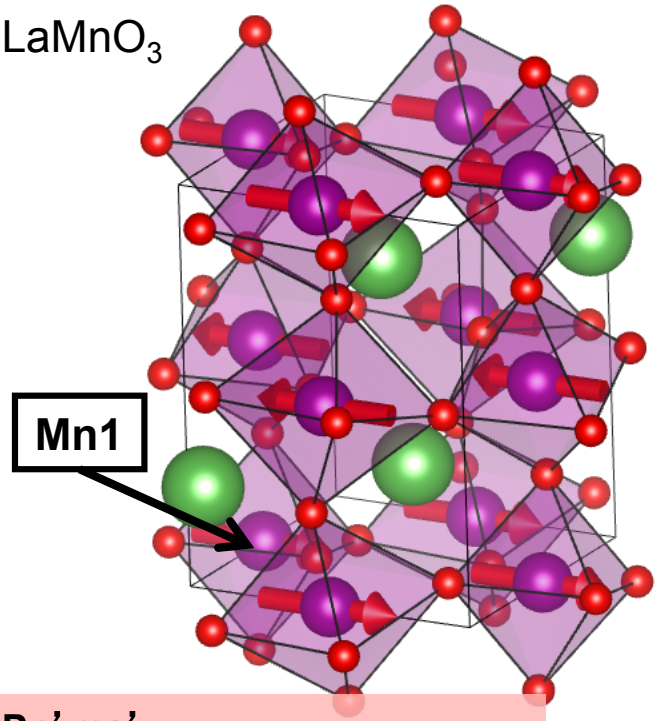
Symmetry operations in commensurate magnetic crystals:

magnetic space group: $\{ \{\mathbf{R}_i | \mathbf{t}_i\} , \{\mathbf{R'}_j | \mathbf{t}_j\} \}$

or $\{ \{\mathbf{R}_i , \theta | \mathbf{t}_i\}\}$ θ= +1 without time reversal
θ= -1 with time reversal

Description of a magnetic structure in a crystallographic form:

$LaMnO_3$



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

Symmetry operations are relevant both for positions and moments

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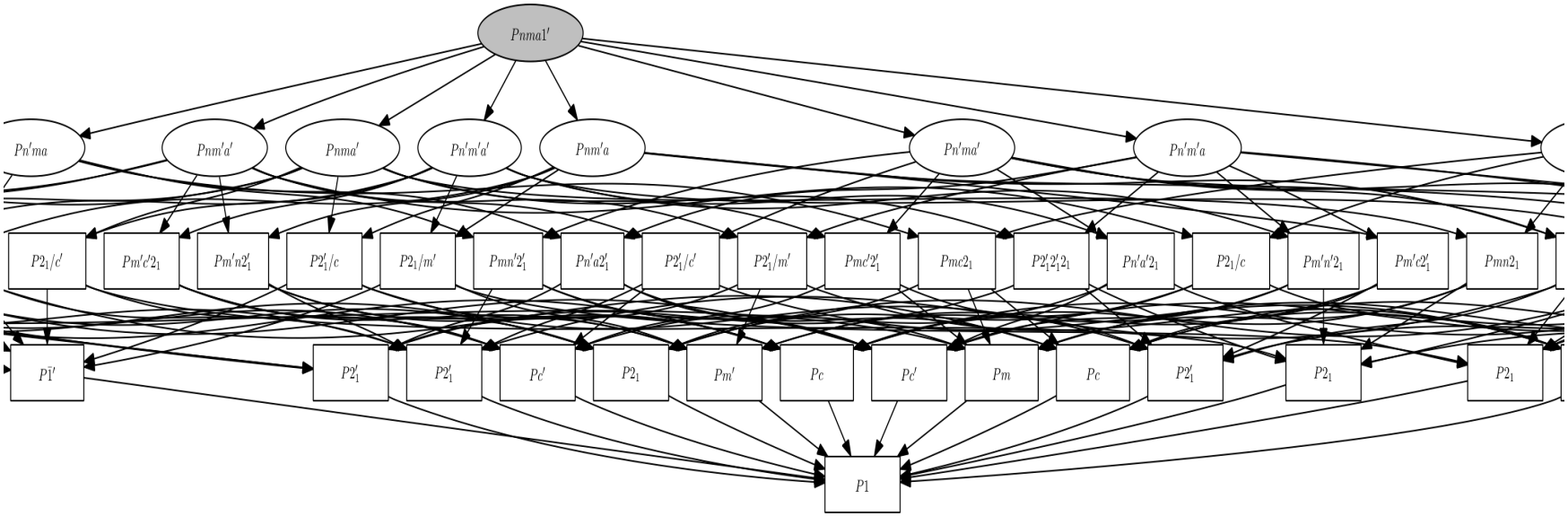
O2 0.30850 0.04080 0.72270

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

Parent symmetry Pnma1’

Possible symmetries for a k=0 magnetic ordering:



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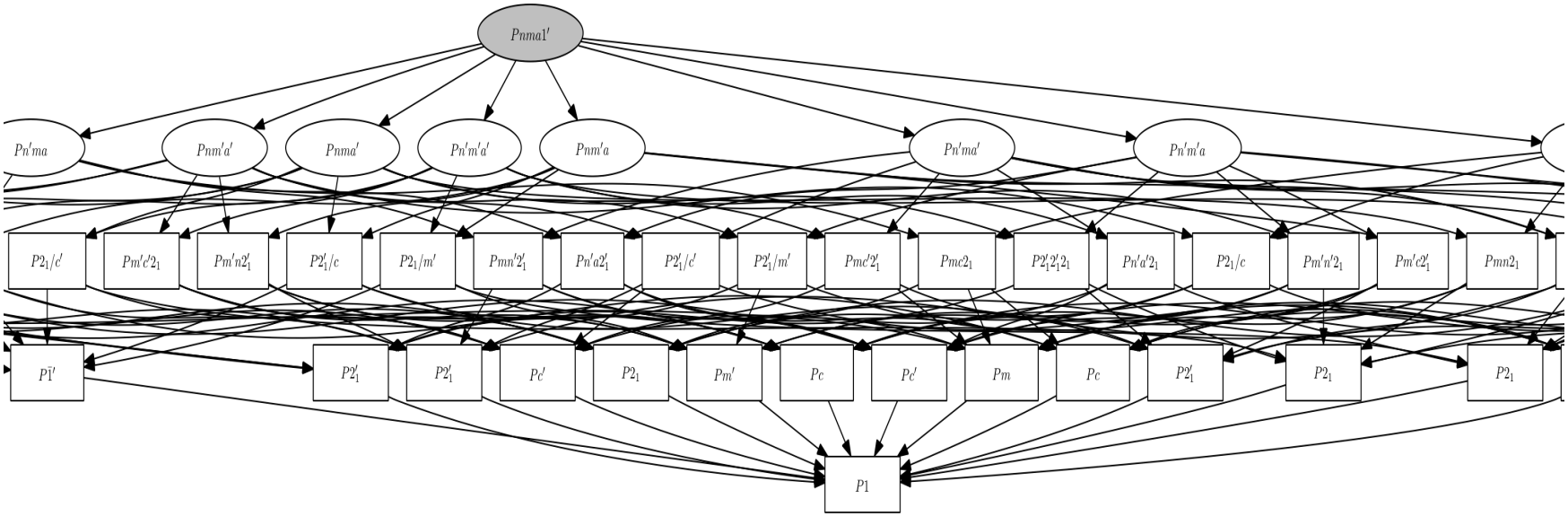
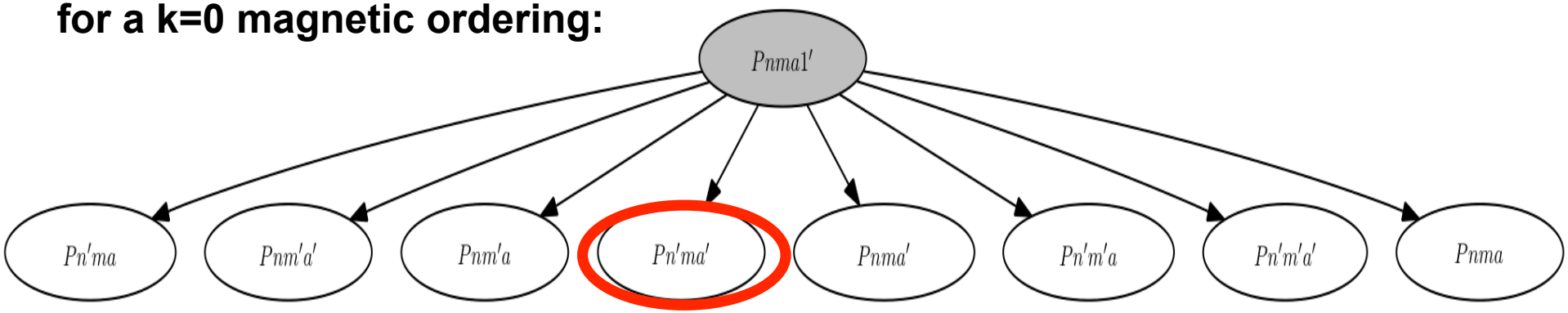


Possible maximal symmetries for a k=0 magnetic ordering:



Magnetic Symmetry and Applications

MGENPOS General Positions of Magnetic Space Groups

MWYCKPOS Wyckoff Positions of Magnetic Space Groups

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 in BCS

Magnetic point group: m'mm'

Parameters to describe a magnetic structure…

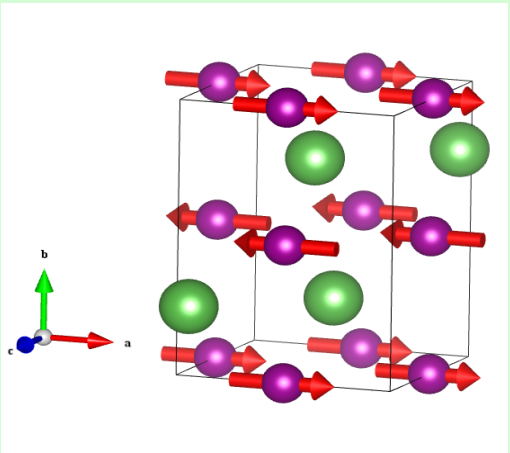
Space Group:
Pn'ma'

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)

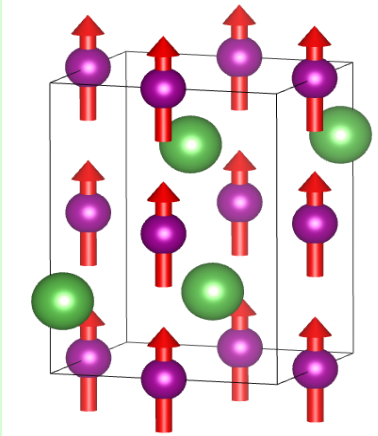
Output of MWYCKPOS in BCS

La

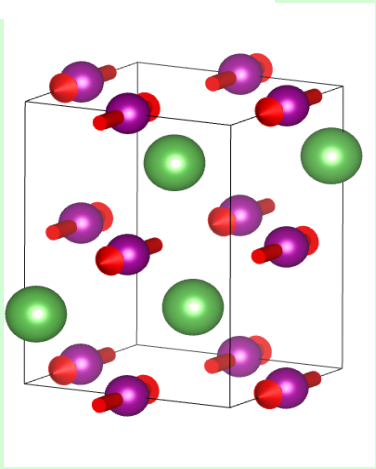
Mn



mode along x (A_x)



mode along y (F_y)
weak ferromagnet



mode along z (G_z)

Description in terms of irrep modes

Pn’ma’ === mB_{2g}

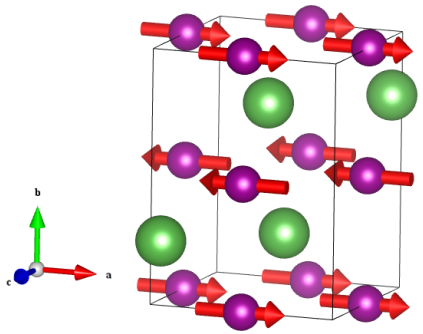
(Irrep = irreducible representation)

Character Table

D_{2h}(mmm)	#	1	2_z	2_y	2_x	-1	m_z	m_y	m_x	**1’**
mA_g	Γ_1^+	1	1	1	1	1	1	1	1	-1
mB_{1g}	Γ_3^+	1	1	-1	-1	1	1	-1	-1	-1
mB_{2g}	Γ_2^+	1	-1	1	-1	1	-1	1	-1	-1
mB_{3g}	Γ_4^+	1	-1	-1	1	1	-1	-1	1	-1
mA_u	Γ_1^-	1	1	1	1	-1	-1	-1	-1	-1
mB_{1u}	Γ_3^-	1	1	-1	-1	-1	-1	1	1	-1
mB_{2u}	Γ_2^-	1	-1	1	-1	-1	1	-1	1	-1
mB_{3u}	Γ_4^-	1	-1	-1	1	-1	1	1	-1	-1

Pn’ma’

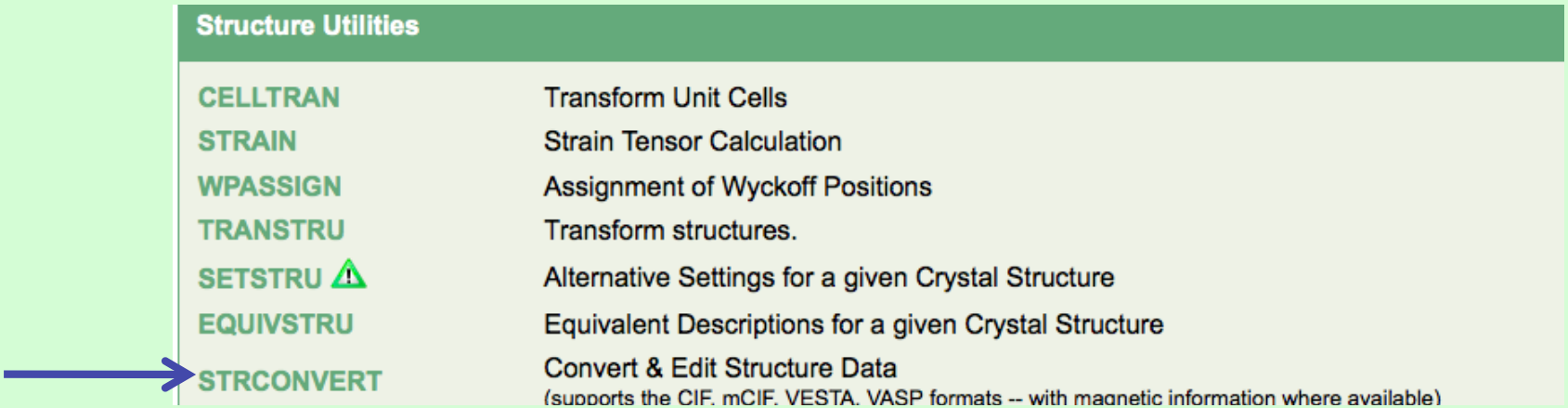
2_z’	2_y’	2_x’	-1’	m_z’	m_y’	m_x’
1	-1	1	-1	1	-1	1



one mB_{2g} spin mode (or basis function)

Building up the model of the magnetic structure of LaMnO3 using STRCONVERT

1. Upload the cif file of $LaMnO_3$ in STRCONVERT. Change to magnetic option. Transform to P1 to produce the whole set of atomic positions within the unit cell. Introduce magnetic moments along x of the four listed Mn atoms according to the sign relations: 1,-1,-1,1. Use findsym to find the MSG, and the description using this MSG. Visualize the magnetic structure with MVISUALIZE. With the back button come back in the STRCONVERT to the page in P1, and introduce a non-zero component my at the single symmetry-independent Mn atom, and transform again to P1 to observe that the resulting my values for 4 Mn atoms within the unit cell have the same sign (expected weak FM along y). Create an mcif file of the structure with STRCONVERT, open it with a text editor and localize the different data items: unit cell, atomic positions, symmetry operations. Download the mcif file in VESTA and visualize the structure with this tool. (file required: *1.LaMnO3_parent.cif*)



Structure Data Converter & Editor

Please submit a structure file:

Browse... No file selected. Upload the file

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

Symmetry

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

Lattice Parameters

a: 11.670 Å b: 7.360 Å c: 5.2572 Å

α 90.000° β: 90.000° γ: 90.000°

Symmetry Operations [Show/Hide]

Recognized formats:

1. x,y,z mx,my,mz +1
x,y,z mx,my,mz +1
x,y,z
x,y,z,+1
1 'x, y, z'
1 x,y,z

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

Update the symmetry operators with the above Apply

Symmetry operations have been parsed from the file/form

Populate with operators from database

Structure Data Converter & Editor

Atomic Positions & Magnetic Moments

Switch to the treatment of the vectors as: displacements Go!

	Label	Element	x	y	z	Occ.	m_x	m_y	m_z
☐	Ho	Ho	0.04195	0.25000	0.98250	1.00000	0.00000	0.00000	0.00000
☐	Ho_1	Ho	0.95805	0.75000	0.01750	1.00000	0.00000	0.00000	0.00000
☐	Mn	Mn	0.00000	0.00000	0.50000	1.00000	3.87000	0.00000	0.00000
☐	O1	O	0.23110	0.25000	0.11130	1.00000	0.00000	0.00000	0.00000
☐	O1_1	O	0.76890	0.75000	0.88870	1.00000	0.00000	0.00000	0.00000
☐	O2	O	0.16405	0.05340	0.70130	1.00000	0.00000	0.00000	0.00000
☐	O2_1	O	0.83595	0.55340	0.29870	1.00000	0.00000	0.00000	0.00000

Add atoms more. || Remove selected atoms || Change the selected atoms' symbol to

Select the atoms with the symbol: || Select all atoms || Unselect all atoms

Longest Arrow size: 1.314 [for VESTA format export: Å *(Default: min(a,b,c)/4)]*
[for Jmol visualize: a proportional coefficient]

Export to BCS format | Export to VESTA format
Export to Standard CIF format | Export to MCIF format
Export to VASP format | Transform the structure to P1 setting
Remove the magnetic information | Re-order the sites | Visualize

a CIF-type file can be produced:

```
_magnetic_space_group_BNS_number 31.129
_magnetic_space_group_BNS_name "P_bmn2_1"
_magnetic_cell_length_a 11.67080
_magnetic_cell_length_b 7.36060
_magnetic_cell_length_c 5.25720
_magnetic_cell_angle_alpha 90.00
_magnetic_cell_angle_beta 90.00
_magnetic_cell_angle_gamma 90.00

loop_
_magnetic_space_group_symop_id
_magnetic_space_group_symop_operation_xyz
_magnetic_space_group_symop_operation_mxmymz
_magnetic_space_group_symop_operation_timereversal
1 x,y,z mx,my,mz +1
2 -x+1/4,-y,z+1/2 -mx,-my,mz +1
3 x,-y+1/2,z -mx,my,-mz +1
4 -x+1/4,y+1/2,z+1/2 mx,-my,-mz +1
5 x+1/2,y,z -mx,-my,-mz -1
6 -x+3/4,-y,z+1/2 mx,my,-mz -1
7 x+1/2,-y+1/2,z mx,-my,mz -1
8 -x+3/4,y+1/2,z+1/2 -mx,my,mz -1

loop_
_magnetic_atom_site_label
_magnetic_atom_site_type_symbol
_magnetic_atom_site_fract_x
_magnetic_atom_site_fract_y
_magnetic_atom_site_fract_z
Ho Ho 0.04195 0.25000 0.98250
Ho_1 Ho 0.95805 0.75000 0.01750
Mn Mn 0.00000 0.00000 0.50000
O1 O 0.23110 0.25000 0.11130
O1_1 O 0.7689 0.75000 0.88870
O2 O  0.16405 0.05340 0.70130
O2_1 O 0.83595 0.55340 0.29870

loop_
_magnetic_atom_site_moment_label
_magnetic_atom_site_moment_crystalaxis_mx
_magnetic_atom_site_moment_crystalaxis_my
_magnetic_atom_site_moment_crystalaxis_mz
Mn 3.87 0.00000 0.00000
```

These files permit the different alternative models to be analyzed, refined, shown graphically, transported to ab-initio codes etc., with programs as ISODISTORT, JANA2006, STRCONVERT, etc. A controlled descent to lower symmetries is also possible.

http://stokes.byu.edu/iso/isotropy.php

ISOTROPY Software Suite

Harold T. Stokes, Dorian M. Hatch, and Branton J. Campbell, Department of Physics and Astronomy, Brigham Young University, Provo, Utah 84606, USA, stokesh@byu.edu

Description: The ISOTROPY software suite is a collection of software which applies group theoretical methods to the analysis of phase transitions in crystalline solids.
How to cite: ISOTROPY Software Suite, iso.byu.edu.

References and Resources

Isotropy subgroups and distortions

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

Space groups and irreducible representations

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

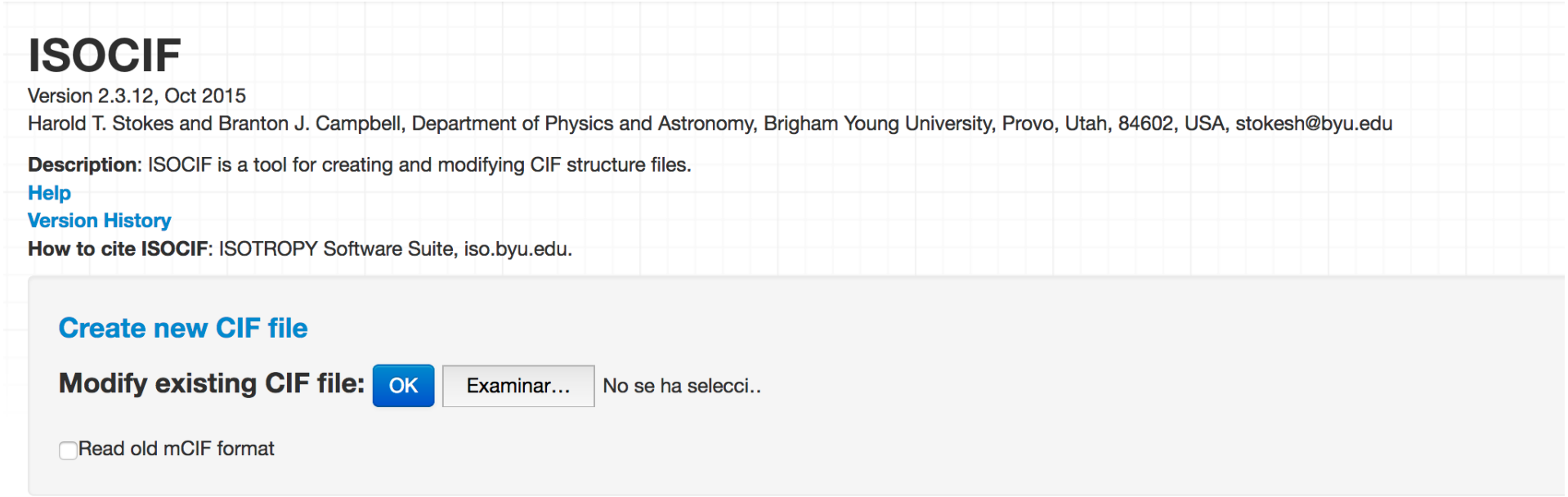
Superspace Groups

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

Phase Transitions

- **COPL**: Find a complete list of order parameters for a phase transition, given the space-group symmetries of the parent and subgroup phases.
- **INVARIANTS**: Generate invariant polynomials of the components of order parameters.
- **COMSUBS**: Find common subgroups of two structures in a reconstructive phase transition

Other CIF (and mCIF) file editor



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

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 grey magnetic group G1')

F subgroup of G
F ≤ G

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

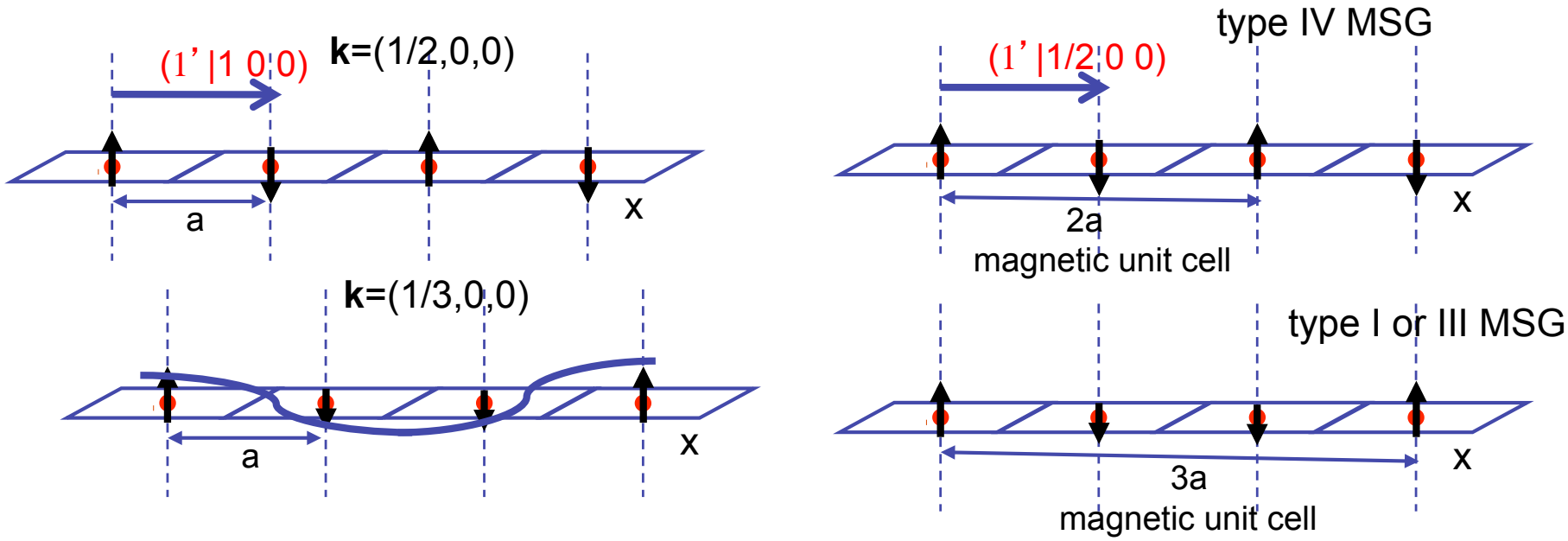
	magn. **space** group:	magn. **point** groups:	nuclear space group: (space group)
Type I some may allow ferromagnetic order	**F**	$\mathbf{P_F}$	**F**
Type III some may allow ferromagnetic order	$\mathbf{F + \{R'|t\}F}$	black and white group $\mathbf{P_F + R'P_F}$	$\mathbf{F + \{R|t\}F = H}$
Type IV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

antitranslation / anticentering

(Type II are the grey groups ……)

Type of MSG depends on the propagation vector of the magnetic ordering:

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



multiple k structures: analogous situation …

General Positions of the Group P_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

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

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

(listing using BNS and OG settings)

3.- 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)

Here we will always use BNS settings for the MSGs

Magnetic symmetry tools and applications in the BCS :

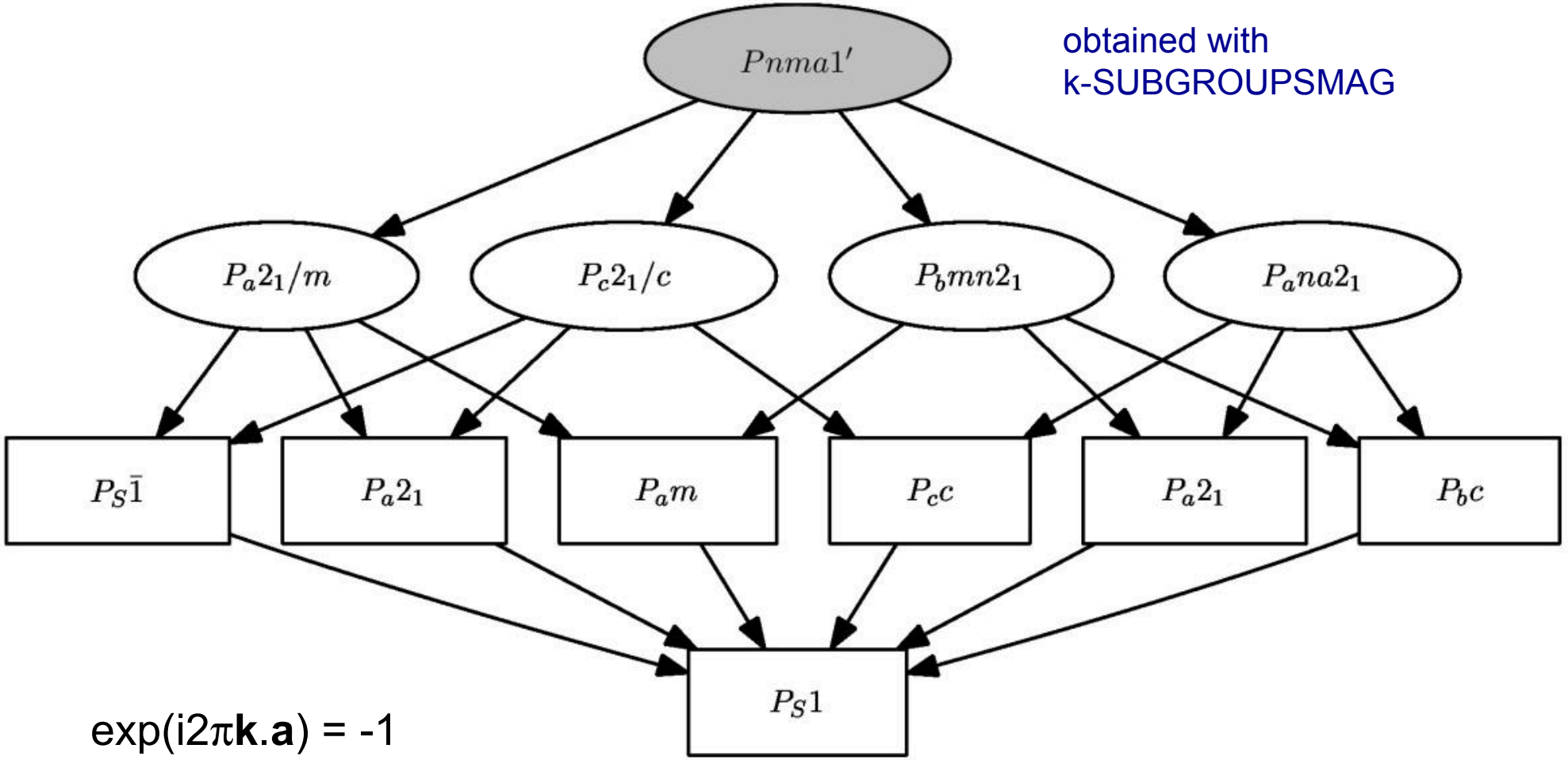
Magnetic Symmetry and Applications	
MGENPOS	General Positions of Magnetic Space Groups
MWYCKPOS	Wyckoff Positions of Magnetic Space Groups
MAGNEXT	Extinction Rules of Magnetic Space Groups
IDENTIFY MAGNETIC GROUP	Identification of a Magnetic Space Group from a set of generators in an arbitrary setting
MPOINT ⚠	Magnetic Point Group Tables
MAXMAGN	Maximal magnetic space groups for a given a propagation vector and resulting magnetic structural models
MAGMODELIZE	Magnetic structure models for any given magnetic symmetry
k-SUBGROUPSMAG	Magnetic subgroups consistent with some given propagation vector(s) or a supercell
MAGNDATA ⚠	A collection of magnetic structures with transportable cif-type files
MVISUALIZE ⚠	3D Visualization of magnetic structures with Jmol
MTENSOR ⚠	Symmetry-adapted form of magnetic crystal tensors

Obtaining all possible magnetic symmetries for a magnetic phase with propagation vector (1/2,0,0) and parent space group Pnma

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

Magnetic Symmetry and Applications	
MGENPOS	General Positions of Magnetic Space Groups
MWYCKPOS	Wyckoff Positions of Magnetic Space Groups
MAGNEXT	Extinction Rules of Magnetic Space Groups
IDENTIFY MAGNETIC GROUP	Identification of a Magnetic Space Group from a set of generators in an arbitrary setting
MPOINT ⚠	Magnetic Point Group Tables
MAXMAGN	Maximal magnetic space groups for a given a propagation vector and resulting magnetic structural models
MAGMODELIZE	Magnetic structure models for any given magnetic symmetry
k-SUBGROUPSMAG	Magnetic subgroups consistent with some given propagation vector(s) or a supercell
MAGNDATA ⚠	A collection of magnetic structures with transportable cif-type files

Possible magnetic symmetries for a magnetic phase with propagation vector (1/2,0,0) and parent space group Pnma



obtained with k-SUBGROUPSMAG

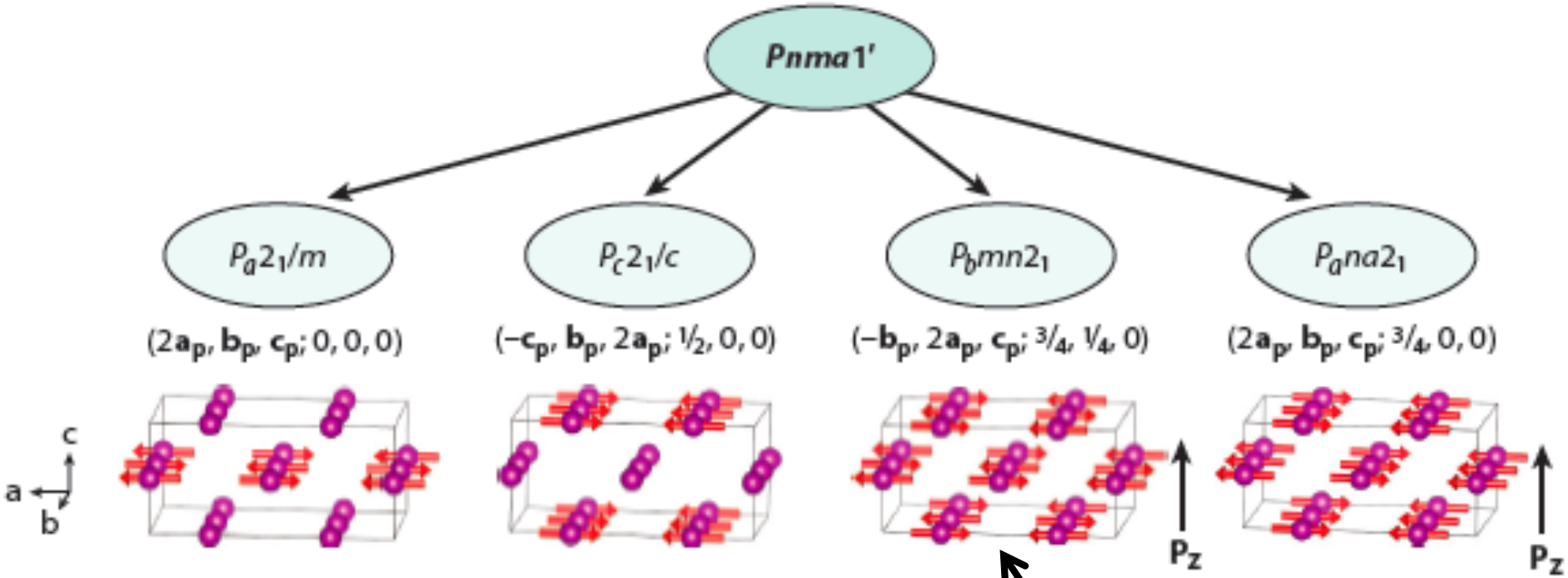
exp(i2π**k**.**a**) = -1

Symmetry operation {1'\|1/2,0,0} is present in any case: all MSGs are type IV

(magnetic cell= (2**a**$_p$,**b**$_p$,**c**$_p$))

$HoMnO_3$ An Inevitable multiferroic...

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

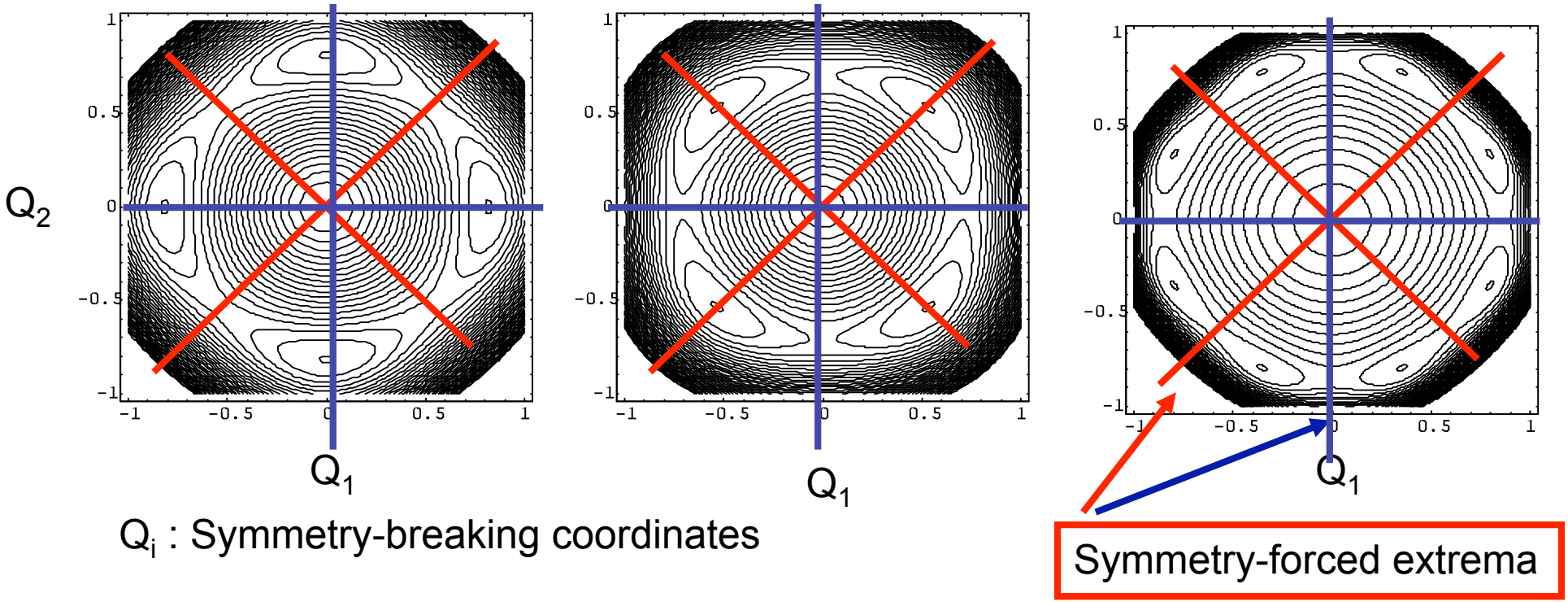


graphic models are depicted
assuming collinearity along x
(my and mz are symmetry allowed)

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

Why the (magnetic) order parameter usually takes “special” directions of higher symmetry in the irrep space?

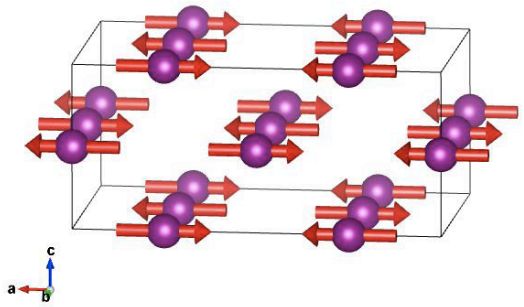
Domains/variants: symmetry related configurations around a higher-symmetry configuration



Q_i : Symmetry-breaking coordinates

$HoMnO_3$

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):

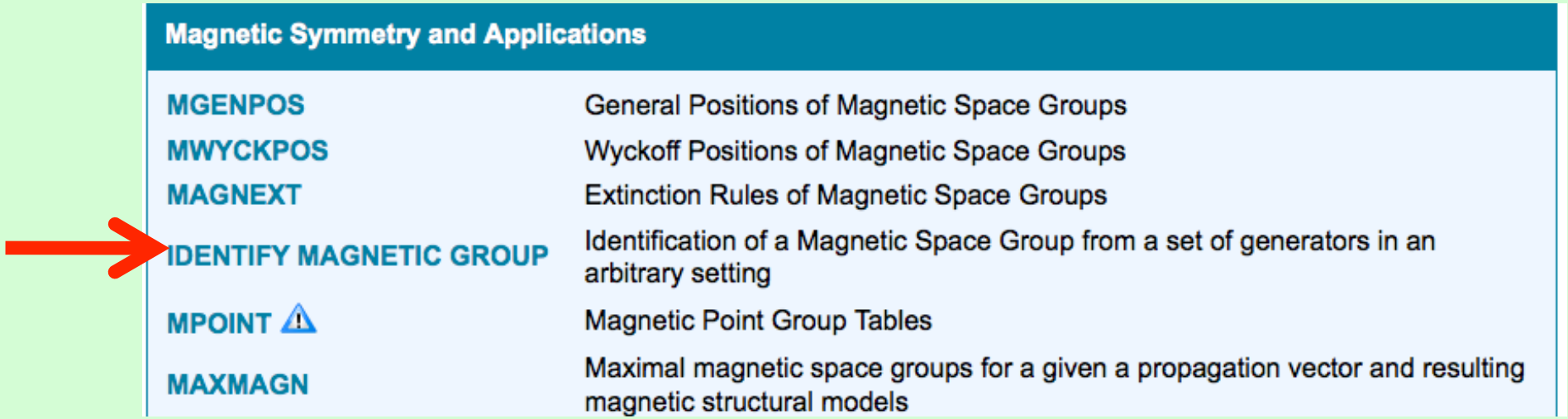
Mn1 3.87 ≈0.0 ≈0.0

zero values are not symmetry "protected"

Magnetic Point Group: **mm21'**

Checking the symmetry operations present in the magnetic structure of $HoMnO_3$.

3. Upload the mcif file of $HoMnO_3$ in STRCONVERT. Among the listed symmetry operations identify the anticentering operation {1'|1/2,0,0}. Identify also in the list the operations {2_z|3/4,0,1/2} and {2_z'|1/4,0,1/2}. Copy/paste the list of symmetry operations and introduce them in the program "IDENTIFY MAGNETIC GROUP" and check the MSG of the structure.
(file required: *2.HoMnO3.mcif*)



Subgroup of Pnma1' in a basis: $2a_p$, b_p, c_p

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

centering and "anticentering" translations:

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

Pnma1' = P_anm2_1 + (1'|000)**P_anm2_1+**(-1|000) **P_anm2_1+** (-1'|000) **P_anm2_1**

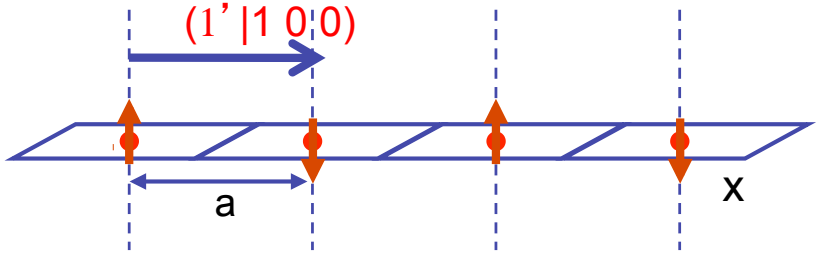
It is the MSG P_bmn2_1 (31.129) in a non-standard basis

Tranformation to its standard setting: (-**b**, **a**, **c**; 3/8,1/4,0)

Consequences of symmetry

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

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

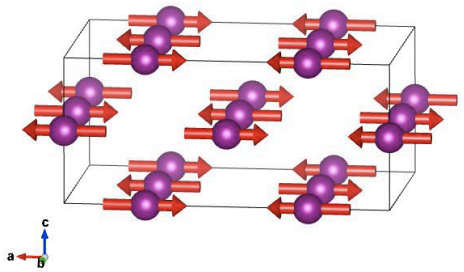


$P2/m \longrightarrow P_c2/m$

for the nuclear/lattice structure:

$P2/m \longrightarrow P2/m$

- case 2: symmetry break for “nuclear structure”



for the nuclear/lattice structure :

$Pnma \longrightarrow Pmn2_1$ (-**b**$_p$, **a**$_p$, **c**$_p$; 1/4,1/4,0)

Consequences of symmetry

Von Neumann principle:

- all variables/parameters/degrees of freedom compatible with the symmetry can be present in the total distortion

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

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

Consequences of symmetry

Symmetry-constrained tensor properties:

TABLE 1.7. HEESCH–SHUBNIKOV POINT GROUPS OF CRYSTALS WHICH MAY EXHIBIT FERROMAGNETISM AND FERROELECTRICITY

(Ascher, 1970) (from 122 point groups)

Point group	M and P
2, $m'm'2$, 3, $3m'$, 4, $4m'm'$, 6, $6m'm'$	$\mathbf{M} \parallel z$ $\mathbf{P} \parallel z$
$m'm2'$	$\mathbf{M} \parallel y$ $\mathbf{P} \parallel z$
$2'$	$\mathbf{M} \perp z$ $\mathbf{P} \parallel z$
m	$\mathbf{M} \parallel z$ $\mathbf{P} \perp z$
m'	$\mathbf{M} \perp z$ $\mathbf{P} \perp z$
1	No restriction

A. P. Cracknell, "Magnetism in crystalline materials" 1975

Consequences of symmetry

Symmetry-constrained tensor properties:

A. P. Cracknell,
B. "Magnetism in crystalline materials" 1975

TABLE 5.4. THE MAGNETOELECTRIC TENSOR

Magnetic point group	Q_{ij}
1, 1′	$\begin{bmatrix} Q_{11} & Q_{12} & Q_{13} \\ Q_{21} & Q_{22} & Q_{23} \\ Q_{31} & Q_{32} & Q_{33} \end{bmatrix}$
2, m', $2/m'$	$\begin{bmatrix} Q_{11} & Q_{12} & 0 \\ Q_{21} & Q_{22} & 0 \\ 0 & 0 & Q_{33} \end{bmatrix}$
2′, m, $2'/m$	$\begin{bmatrix} 0 & 0 & Q_{13} \\ 0 & 0 & Q_{23} \\ Q_{31} & Q_{32} & 0 \end{bmatrix}$
222, $m'm'2$, $m'm'm'$	$\begin{bmatrix} Q_{11} & 0 & 0 \\ 0 & Q_{22} & 0 \\ 0 & 0 & Q_{33} \end{bmatrix}$
22′2′, $mm2$, $(m'm2')$, $m'mm$	$\begin{bmatrix} 0 & Q_{12} & 0 \\ Q_{21} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$
4, $\bar{4}'$, $4/m'$, 3, $\bar{3}'$, 6, $\bar{6}'$, $6/m'$	$\begin{bmatrix} Q_{11} & Q_{12} & 0 \\ -Q_{12} & Q_{11} & 0 \\ 0 & 0 & Q_{33} \end{bmatrix}$

MTENSOR: Tensor calculation for Magnetic Point Groups

Tensor calculation for Magnetic Point Groups

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

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

Further information can be found here

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

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

Choose a magnetic point group:

Magnetic Point or Space Group number: Please, enter the label of the group or choose it *(point group)*

Non-conventional setting

Introduce a magnetic point group by hand:

Please, choose a tensor by one of these ways:

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)

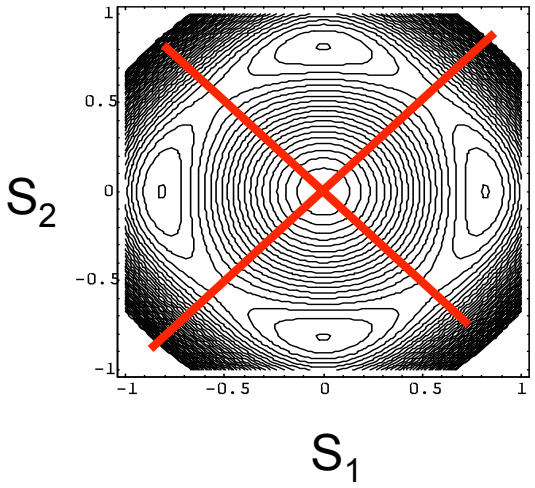
α^T_{ij}	j		
i	1	2	3
1	0	α^T_{12}	0
2	$-\alpha^T_{12}$	0	0
3	0	0	0

Number of independent coefficients: 1

Ferroic properties

A "multiferroic": improper ferroelectric

$HoMnO_3$



param. phase → antiferrom. phase

Pnma 1' → **$P_a nm2_1$** index 4 → 4 total number of domains

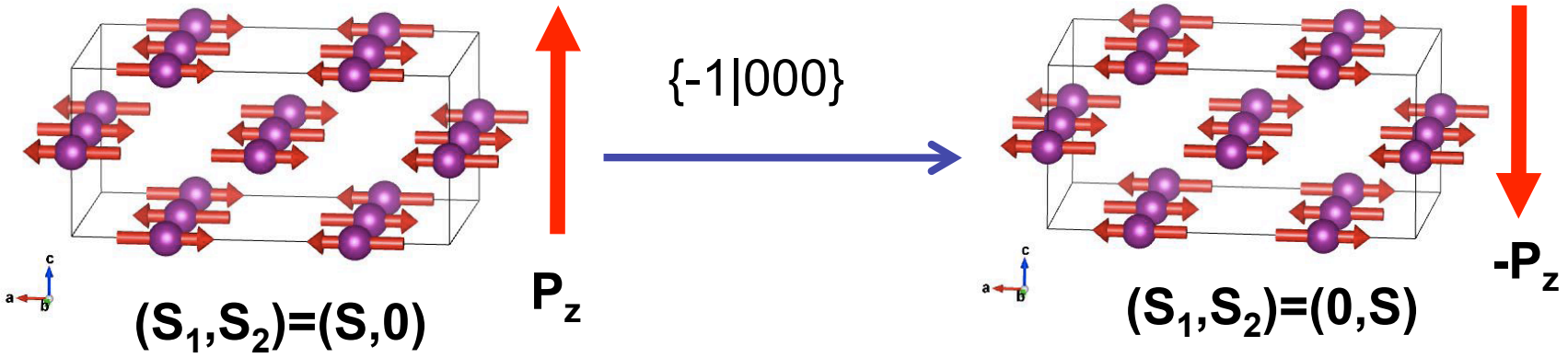
point groups

mmm1' → **mm21'** index 2 → **2 ferroic domains**

Secondary symmetry-allowed effect: spontaneous polarization: P_z

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

generators of the four domain configurations: $\{g_n\} = \{(1|000), (-1|000), (1'|000), (-1'|000)\}$



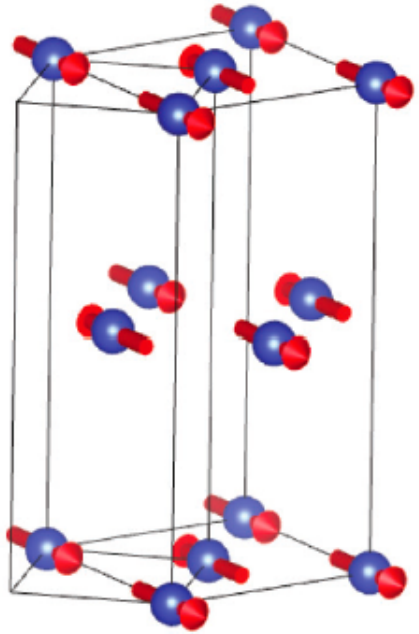
domains: equivalent energy minima

Their MSG are equivalent, but not equal in general

The importance of non-magnetic atoms:

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

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

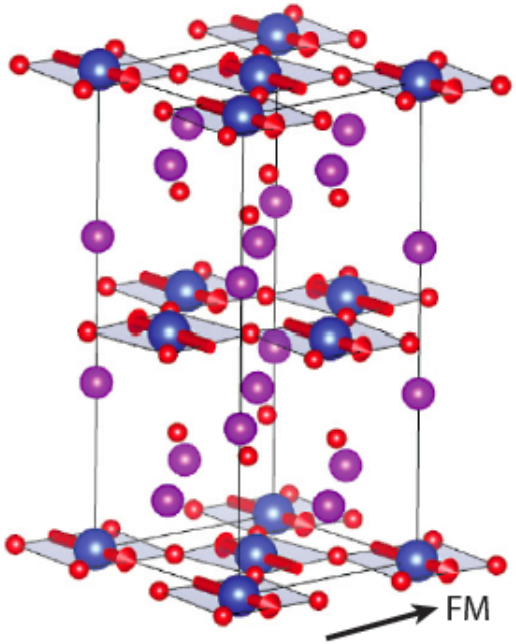


C_Accm

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

Pr_2CuO_4

Cmce, k=(0,0,0)

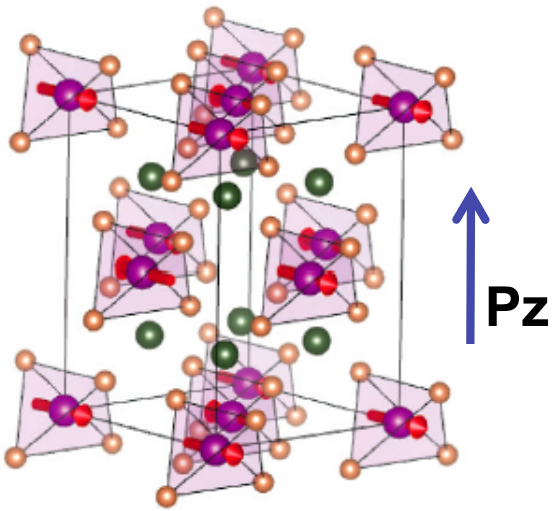


$Cm'ca'$

(**c**, **a** – **b**, **a** + **b**; 0, 0, 0)

Gd_2CuO_4

I-42m, k=(1/2,1/2,0)



A_Bma2

(**a** + **b**, –**a** + **b**, **c**; 1/2, 0, 0)

Hypothetical spin configuration on a structure of type $GaMnSe_4$

Check the symmetry restrictions on the Mn and Ho spins resulting from the symmetry of the magnetic phase of $HoMnO_3$.

4. Upload the mcif file of the magnetic structure of $HoMnO_3$ in STRCONVERT. Introduce a non-zero spin component of Ho along x or along z, and try to obtain all the atomic positions and moments within the unit cell by transforming to trivial symmetry P1. Check that the program in both cases (for Ho moment along x or z) gives and error/warning: this means that if the Ho atoms are magnetically ordered in this phase, their magnetic moments can only be directed along b. Come back to the description using the MSG using the back button of the browser and introduce now a non-zero spin component for the Ho atoms along b and transform again to P1 to observe the resulting values for the symmetry-related Ho atoms within the unit cell. Visualize the magnetic structure reading the mcif file with VESTA. Using alternatively MVISUALIZE observe the differences between the parent unit cell, the standard unit cell and the unit cell actually used in the description. (file required: *2.HoMnO3.mcif*)

Acknowledgements:

The past and present team in Bilbao of the…

bilbao crystallographic server

[The crystallographic site at the Condensed Matter Physics Dept. of the University of the Basque Country]

present:
- M. I. Aroyo
- E. Tasci
- G. de la Flor
- S. V. Gallego
- L. Elcoro
- G. Madariaga

past:
- D. Orobengoa
- C. Capillas
- E. Kroumova
- S. Ivantchev

- J.L. Ribeiro (Braga, Portugal)
- H. Stokes & B. Campbell (Provo, USA) – program ISODISTORT
- V. Petricek (Prague) - program JANA2006
- J. Rodriguez-Carvajal (Grenoble) - program FullProf