

Overview of Bilbao Crystallographic server: MAXMAGN, MVISUALIZE, k- SUBGROUPSMAG, MAGNDATA database etc

Stuart Calder, ORNL

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Duke University July 20-24



U.S. DEPARTMENT
of ENERGY

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Bilbao Crystallographic Server

<https://cryst.ehu.es/>

- Tools and information on a large variety of symmetry related topics.
- Constantly updated and new features added.



Bilbao Crystallographic Server
in forthcoming schools and workshops

News:

- **New program: SPGENPOS**
06/2026: General positions of the spin point groups
- **New Article**
04/2026: Elcoro *et al.* "Automatic calculation of symmetry-adapted tensors under spin-group symmetry: STENSOR, a new tool of the Bilbao Crystallographic Server". J. Appl. Cryst (2026) 59, 640-647
- **MORPHIC EFFECTS** updates
04/2026: The magnetic-field option is now available.
- **New Article**
06/2025: Etxebarria *et al.* "Crystal tensor properties of magnetic materials with and without spin-orbit coupling. Application of spin point groups as approximate symmetries.". Acta Cryst (2025) A81, 317-338
- **New program: MINSUP for plane groups**
06/2025: Minimal supergroups of plane groups
- **New program: CollinearSpinGroups**
05/2025: Operations of Nontrivial Collinear Spin Space Groups
- **New program: STENSOR**
04/2025: Symmetry-adapted form of crystal tensors under spin point groups
- **New Article**
04/2025: Tasci *et al.* "Computational analysis tools for magnetic structures in the Bilbao Crystallographic Server". Acta Cryst (2025) B81, 181-191

bilbao crystallographic server



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some tables

Space-group symmetry

Space Groups

Magnetic Symmetry and Applications

Plane Groups

Group-Subgroup Relations of Space Groups

Layer Groups

Representations and Applications

Rod Groups

Solid State Theory Applications

Frieze Groups

Structure Utilities

2D Point Groups

3D Point Groups

Topological Quantum Chemistry

Magnetic Space
Groups

Subperiodic Groups: Layer, Rod and Frieze Groups

Structure Databases

Raman and Hyper-Raman scattering

Point-group symmetry

Plane-group symmetry

Double point and space groups

Bilbao Crystallographic Server:

Magnetic Symmetry and Applications

bilbao crystallographic server

- This workshop will mainly use the “**Magnetic-Symmetry and Applications**” section

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

MAGNDATA

bilbao crystallographic server

Contact us About us Publications How to cite the server

Space-group symmetry

Magnetic Symmetry and Applications

Magnetic groups	
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MKVEC	The k-vector types and Brillouin zones of Magnetic Space Groups
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k-SUBGROUPS	Magnetic subgroups consistent with some given propagation vector(s) or a space group
MAGNDATA	A collection of magnetic structures with portable cif-type files
MVISUALIZE	3D visualization of magnetic structures with Bilbao Crystallographic Server
MTENSOR	Symmetry-adapted form of crystal tensors in magnetic phases
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Spin groups	
SPGENPOS ⚠	General positions of spin point groups
STENSOR ⚠	Symmetry-adapted form of crystal tensors under spin point groups
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MAGNDATA: A Collection of magnetic structures with portable cif-type files

MAGNDATA: A Collection of magnetic structures with portable cif-type files

MAGNDATA: A collection of magnetic structures with portable cif-type files

A database of more than 2000 published commensurate and incommensurate magnetic structures can be found here. The structures are described using magnetic symmetry (Shubnikov magnetic space groups) in the BNS setting for commensurate structures, and magnetic superspace groups for incommensurate structures. Symmetry is applied both for magnetic moments and atomic positions. The information provided is sufficient to define unambiguously the positions and magnetic moments (if any) of all atoms in the structure. A non-standard setting consistent with the setting of the paramagnetic phase is often used (this setting does not necessarily coincide with the one used in the original reference). A cif-like (.mcif) file of each entry can be downloaded. mcif files are supported by: ISOCIF, ISODISTORT, VESTA, Jmol, JANA2006 and FullProf. ISOCIF can be used to generate an alternative mcif file in a standard setting, as required by ISODISTORT. Vesta files for visualization of a single magnetic unit cell are also available. Any entry can be directly downloaded in StrConvert for editing, visualization, generation of various files, etc. The magnetic structure corresponding to each entry can also be 3D visualized online with Jmol.

Tutorial of MAGNDATA: [download](#)

Examples and further information can be found in the following papers:

1. Samuel V. Gallego, J. Manuel Perez-Mato, Luis Elcoro, Emre S. Tasci, Robert M. Hanson, Koichi Momma, Mois I. Aroyo and Gotzon Madariaga
J. Appl. Cryst. (2016). 49, 1750-1776

[Link to the paper on Journal of Applied Crystallography.](#)

2. Samuel V. Gallego, J. Manuel Perez-Mato, Luis Elcoro, Emre S. Tasci, Robert M. Hanson, Mois I. Aroyo and Gotzon Madariaga
J. Appl. Cryst. (2016). 49, 1941-1956

[Link to the paper on Journal of Applied Crystallography.](#)

which can be used to cite this program.

See also:

J.M. Perez-Mato, S.V. Gallego, E.S. Tasci, L. Elcoro, G. de la Flor, and M.I. Aroyo
Annu. Rev. Mater. Res. (2015), 45:13.1-13.32

[View Full Database](#)

Element search (separate with space or comma): ☒ AND ☐ OR

Enter the label of the structure:

[Advanced Search](#)

To submit any published structure
click [HERE](#)

To submit any published structure click [HERE](#)

Element search (separate with space or comma): ☒ AND ☐ OR

Enter the label of the structure:

COMMENSURATE STRUCTURES

Zero propagation vector -- Total :1154
Non-zero propagation vector (magnetic space groups of Type I or Type III) -- Total :60
Non-zero propagation vector (magnetic space groups of Type IV) -- Total :882
Two propagation vectors -- Total :118
Three or more propagation vectors -- Total :30
Partial Total: 2244

INCOMMENSURATE STRUCTURES

One propagation vector -- Total :163
Two propagation vectors -- Total :3
Three propagation vectors -- Total :1
Partial Total: 167

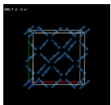
Total number of entries in the MAGNDATA database: 2411

COMMENSURATE STRUCTURES

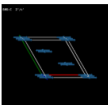
Zero propagation vector



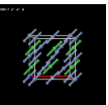
0.1 LaMnO₃



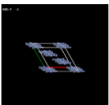
0.2 Cd₂O₉₂O₇



0.3 Ca₃LuO₉O₈



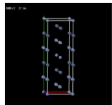
0.4 NiCr₂O₄



0.5 Cr₂S₃

[Click to expand/shrink back the rest](#)

Non-zero propagation vector (magnetic space groups of Type I or Type III)



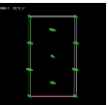
1.0.1 Ag₂CrO₂



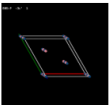
1.0.2 URu_{0.96}Rh_{0.04}Si₂



1.0.3 CuCoBr₃



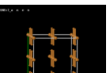
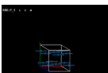
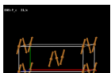
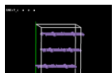
1.0.4 CuNiCl₃



1.0.5 Sr₃CoIrO₆

[Click to expand/shrink back the rest](#)

Non-zero propagation vector (magnetic space groups of Type IV)



NaOsO₃ (#0.25)

[view in Jmol](#)
[Download mcif file](#)
[Download vesta file \(all atoms\)](#)
[Download vesta file \(magnetic atoms only\)](#)

[submit to STRCONVERT](#)

Reference: S. Calder, V.O. Garlea, D.F. McMorro, M.D. Lumsden, M.B. Stone, J.C. Lang, J.-W. Kim, J.A. Schlueter, Y.G. Shi, K. Yamura, Y.S. Sun, Y. Tsumoto and A.D. Christianson, *Physical Review Letters* (2012) 108, 087201
DOI: 10.1103/physrevlett.108.257209
Atomic positions from: Shi et al., *Phys. Rev. B* (2009) 80, 161104(R)

Parent space group (paramagnetic phase): *P6₃/mmc* (#62)
Propagation vector: k1 (0, 0, 0)

Transition Temperature: 410 K
Experiment Temperature: 200 K

Lattice parameters of the magnetic unit cell:
5.3842 7.5804 5.3282 90.0000 90.0000 90.0000
Transformation from parent structure: (a,b,c,0,0,0)
[\[View matrix form\]](#)

BNS Magnetic Space Group: *Primal* (#62.448) (standard setting)
[\[View symmetry operations\]](#)
Systematic absences for this Magnetic Space Group via [MAGNEX](#)

Magnetic Point Group: *m'm'm* (8.4.27)
[\[View symmetry operations\]](#)
Symmetry-adapted form of material tensors via [MTENSOR](#)
Symmetry-adapted form of material tensors for domain-related equivalent structures via [MTENSOR](#)

Positions and magnetic moments of symmetry independent atoms:
From now on, magnetic atoms are in boldface and colored in red. Magnetic moments are expressed in units of μ_B

[\[Show only magnetic atoms\]](#) [\[Show all the atoms\]](#) [Go to standard](#) [Use MVSUALIZE to:](#) [\[Change setting\]](#) [\[Domain-related equivalent descriptions\]](#)

Label	Atom type	x	y	z	Multiplicity	Symmetry constraints on M	M _x	M _y	M _z	M
Os1	Os	0.00000	0.00000	0.50000	4	m_x, m_y, m_z	0.0	0.0	1.0(1)	1.00

[\[Show all magnetic atoms in unit cell and their moment relations\]](#)

Active Irreps: [Irrep decomposition via](#) [\[Get irreps\]](#)

Comments:

- NPD

Comments (symmetry):

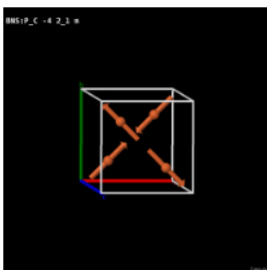
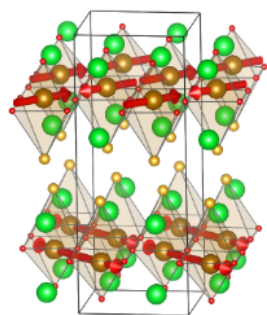
- 1k magnetic structure
- k-normal magnetic symmetry
- 1-dim irrep
- At FeO₂
- possible weak ferromagnetism along y

Everytime you publish a
magnetic structure, add it
to the database
(it is very straightforward)

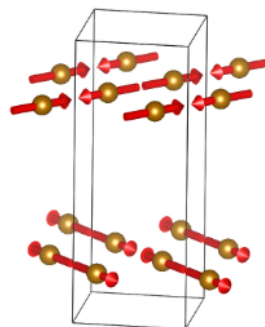
Magnetic crystallographic information files: mcif

Previous entry

Next entry

**Sr₂FeO₃Cl (#1.845)**[view in Jmol](#)[Download mcif file](#)[Download vesta file \(all atoms\)](#)[Download vesta file \(magnetic atoms only\)](#)[submit to STRCONVERT](#)

Magnetic structure with all atoms



Magnetic structure with only magnetic atoms

Reference: Andrew F. May, George Yumnam, Raphael P. Hermann, Stuart Calder, Benjamin M. Lefler, Steven J. May, Zachary E. Brubaker, Matthew Brahmek, Xiaodong Xu, Dmitry Ovchinnikov, Michael A. McGuire, *PHYSICAL REVIEW MATERIALS* (2025) **9** 034002

DOI: [10.1103/PhysRevMaterials.9.034002](https://doi.org/10.1103/PhysRevMaterials.9.034002)

Atomic positions from: same reference

Parent space group (paramagnetic phase): *P4/nmm* (#129)

Propagation vector: *k*₁ (1/2, 1/2, 0)

Transition Temperature: 311 K

Experiment Temperature: 4 K

Lattice parameters of the magnetic unit cell:

5.54985(13) 5.54985(13) 14.2902(4) 90.0000 90.0000 90.0000

Transformation from parent structure: (*a*+*b*, -*a*+*b*, *c*); -1/4, 1/4, 0)

[\[View matrix form\]](#)

BNS Magnetic Space Group: *P*_C-42₁*m* (#113.273) (standard setting)

[\[View symmetry operations\]](#)

Transformation to a standard setting: (*a*, *b*, *c*); 0, 0, 0)

[\[View matrix form\]](#)

Systematic absences for this Magnetic Space Group via [MAGNEXT](#)

1.845_Sr2FeO3Cl.mcif

Magnetic Point Group: -42*m*1' (14.2.49)

[\[View symmetry operations\]](#)

Symmetry-adapted form of material tensors via [MTENSOR](#)

Symmetry-adapted form of material tensors for domain-related equivalent structures via [MTENSOR](#)

Positions and magnetic moments of symmetry independent atoms:

From now on, magnetic atoms are in boldface and colored in red. Magnetic moments are expressed in units of μ_B

[\[Show only magnetic atoms\]](#)

[\[Show all the atoms\]](#)

[Go to standard](#)

Use MVSUALIZE to:

[Change setting](#)

[Domain-related equivalent descriptions](#)

Label	Atom type	x	y	z	Multiplicity	Symmetry constraints on M	M _x	M _y	M _z	M
Fe1	Fe	0.25000	0.25000	0.20731(14)	4	<i>m_x, m_x, 0</i>	2.778(14)	2.778(14)	0.0	3.93

[\[Show all magnetic atoms in unit cell and their moment relations\]](#)

Active Irreps:

Irrep decomposition via [Get_mirreps](#)

label	dim. full irrep	dim. small irrep	direction	action	number of modes
mM1	2	2	special	primary	1

Comments:

- NPD
- Structure described in standard setting of the MSG

Comments (symmetry):

- 1k magnetic structure
- k-maximal magnetic symmetry
- 2-dim irrep along a special direction


```

1  \CIF 2.0
2  # Created by the Bilbao Crystallographic Server
3  # http://www.crysl.ehu.es
4  # Date: 04/03/2025
5
6  data_5yOhtAoR
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8  _audit_creation_method    "Bilbao Crystallographic Server"
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10 _chemical_name_systematic
11 ;
12 ;
13 _chemical_name_common      ?
14 _chemical_formula_moiety    ?
15 _chemical_formula_structural ?
16 _chemical_formula_analytical ?
17 _chemical_formula_iupac     ?
18 _chemical_formula_sum       "Ca2 Fe1 O3 Cl1"
19 _chemical_formula_weight     ?
20 _chemical_melting_point     ?
21 _chemical_compound_source    ?
22 _chemical_absolute_configuration ?
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29 _citation_article_id          034002
30 _citation_year                2025
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36 "George Yumnam"
37 "Raphael P. Hermann"
38 "Stuart Calder"
39 "Benjamin M. Lefler"
40 "Steven J. May"
41 "Zachary E. Brubaker"
42 "Matthew Brahlek"
43 "Xiaodong Xu"
44 "Dmitry Ovchinnikov"
45 "Michael A. McGuire"
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63 _irrep_action
64 _irrep_modes_number
65 _irrep_presence
66 mM1 2 2 special primary 1 .
67
68 _exptl_crystal_magnetic_properties_details
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70 NPD
71 Structure described in standard setting of the MSG
72 ;
73

```

Experiment and publication info

Irrep details

```

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76 1k magnetic structure
77 k-maximal magnetic symmetry
78 2-dim irrep along a special direction
79 ;
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81 _parent_space_group.name_H-M_alt 'P 4/n m m'
82 _parent_space_group.IT_number    129
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85 loop_
86 _parent_propagation_vector.id
87 _parent_propagation_vector.kxkykz
88 k1 1/2 1/2 0
89
90 _parent_space_group.child_transform_Fp_abc 'a+b,-a+b,c;-1/4,1/4,0'
91 _space_group_magn.transform_BNS_Fp_abc 'a,b,c;0,0,0'
92
93 _space_group_magn.number_BNS 113.273
94 _space_group_magn.name_BNS "P_C -4 2_1 m"
95 _space_group_magn.point_group_name "-42m.1"
96 _space_group_magn.point_group_number "14.2.49"
97 _cell_length_a 5.54985(13)
98 _cell_length_b 5.54985(13)
99 _cell_length_c 14.2902(4)
100 _cell_angle_alpha 90.0000
101 _cell_angle_beta 90.0000
102 _cell_angle_gamma 90.0000
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104 loop_
105 _space_group_symop_magn_operation.id
106 _space_group_symop_magn_operation.xyz
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108 2 y,x,z,-1
109 3 -y,-x,z,-1
110 4 -x,y,-z,-1
111 5 x,-y,-z,-1
112 6 -y,x,-z,+1
113 7 -x,-y,z,+1
114 8 y,-x,-z,+1
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116 loop_
117 _space_group_symop_magn_centering.id
118 _space_group_symop_magn_centering.xyz
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120 2 x+1/2,y+1/2,z,-1
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122 loop_
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124 _atom_site_type_symbol
125 _atom_site_fract_x
126 _atom_site_fract_y
127 _atom_site_fract_z
128 _atom_site_occupancy
129 Fe1 Fe 0.25000 0.25000 0.20731(14) 1
130 Sr1 Sr 0.25000 0.75000 0.09557(18) 1
131 Sr2 Sr 0.25000 0.75000 0.3469(2) 1
132 O1_1 O 0.00000 0.00000 0.2332(6) 1
133 O1_2 O 0.00000 0.50000 0.2299(6) 1
134 O2 O 0.25000 0.25000 0.0753(2) 1
135 Cl1 Cl 0.25000 0.25000 0.42569(14) 1
136
137 loop_
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139 _atom_site_moment.crystalaxis_x
140 _atom_site_moment.crystalaxis_y
141 _atom_site_moment.crystalaxis_z
142 _atom_site_moment.symmform
143 _atom_site_moment.magnitude
144 _atom_site_moment.spherical_azimuthal
145 _atom_site_moment.spherical_polar
146 Fe1 2.778(14) 2.778(14) 0.0 mx,mx,0 3.929(14) 45 90

```

Irrep summary

Parent space group

K-vector

Transformation to magnetic cell

Magnetic space group and point group

Magnetic symmetry operations

Magnetic centering translations

Atomic positions

Magnetic direction and magnitude

- mcifs are output during refinements with all the software we'll use this week.
- Including an mcif with your publication and using it to add to MAGNDATA is straightforward and strongly encouraged.

MAGNDATA: A Collection of magnetic structures with portable cif-type files

[View Full Database](#)

Element search (separate with space or comma):

☒ AND ☐ OR

Enter the label of the structure:

[Advanced Search](#)

**To submit any published structure
click [HERE](#)**

The necessary submission process is limited to a zip file containing two files, that are:

1. A PDF file of the publication, where the magnetic structure was reported.
2. A CIF file of the magnetic structure using the magCIF format and having ".mcif" as its extension. This .mcif file must have certain features and information to be appropriate for MAGNDATA.

Overview of Magnetic Space Group Approach

Magnetic Space Groups

- Extension of crystallographic space groups to include spin
- Includes symmetry of all magnetic/non-magnetic atoms
- Incommensurate recently added through supersymmetry description

Magnetic space groups (Shubnikov groups)

- Natural extension of the crystallographic space group description.
 - But only recently became widely used for magnetism.

1929: Heesch, introduces the antiidentity operation properties: $u^2 = 1$, $ut = tu$ for all $t \in T$

- aka time reversal group = $\{1, 1'\}$ (Z. Krist. 71, 95)

1945: Shubnikov re-introduces concept of bi-colour point groups

1951: Shubnikov describes and illustrates all of the bicolor point groups ($\rightarrow$ Shubnikov groups)

1955: Belov, Neronova, Smirnova (BNS) - first complete listing of the Shubnikov groups (Sov. Phys. Cryst 1, 487-488)

1957: Zamorzaev, group theoretical derivation of Shubnikov groups (Kristallografiya 2, 15 (Sov. Phys. Cryst., 3, 401))

1965: Opechowski and Guccione (OG), first complete derivation and enumeration of the Shubnikov groups

2001: Litvin, corrected Opechowski-Guccione symbols (Acta Cryst. A57, 729-730)

2010: Magnetic Space Groups on computer programs (Stokes and Campbell, BYU)

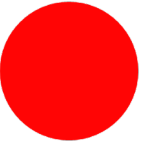
2012: Incommensurate magnetic space group approach standardized and added to software tools

Alexey Vasilyevich Shubnikov 1887-1970



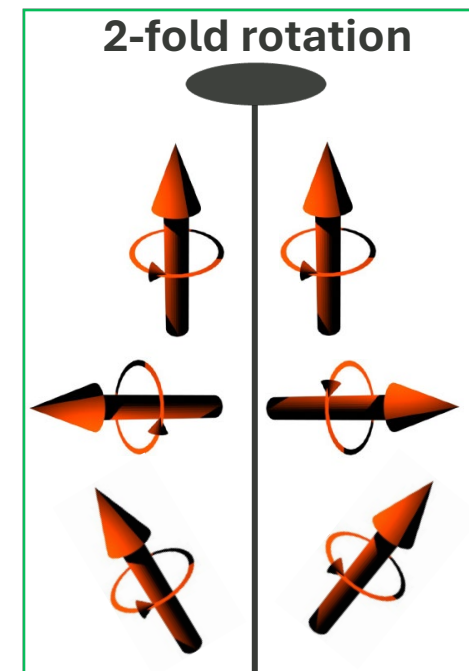
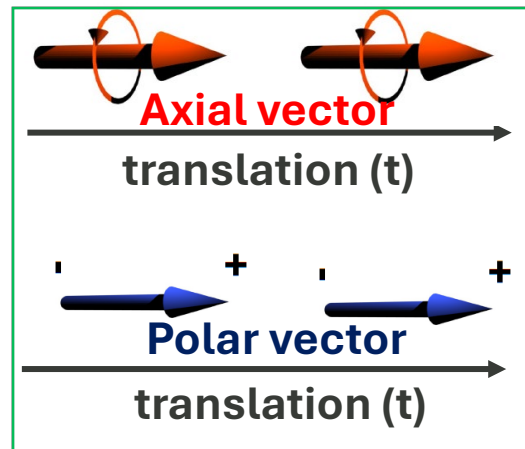
Extend Space Group Approach to include magnetism

- 230 crystallographic space groups:
 - Atoms considered as simple points at a certain location, then apply symmetry operations.
- Now add magnetic moments:
 - Underlying crystal lattice unchanged, with moments at atomic positions.
 - BUT moments are not points, they are vectors ... **axial vectors**.
 - **Location and orientation need to be considered when applying symmetry operations.**
- **Symmetry operations for crystal space groups not enough to describe magnetic structures.**

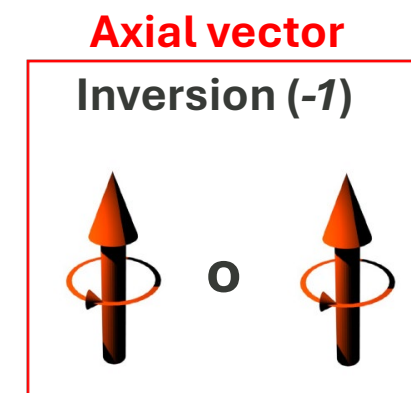
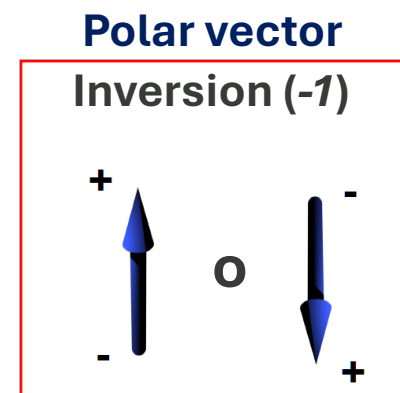
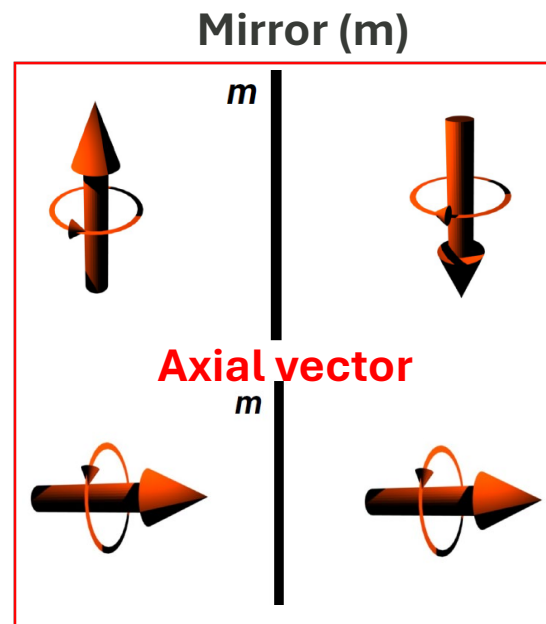
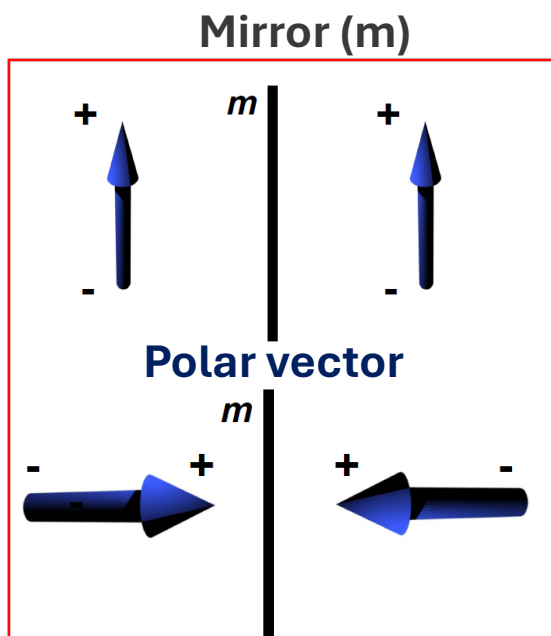


Magnetic space groups: Spins are axial vectors

- Translation (t) and 2-fold rotation are the same for axial and polar vectors.



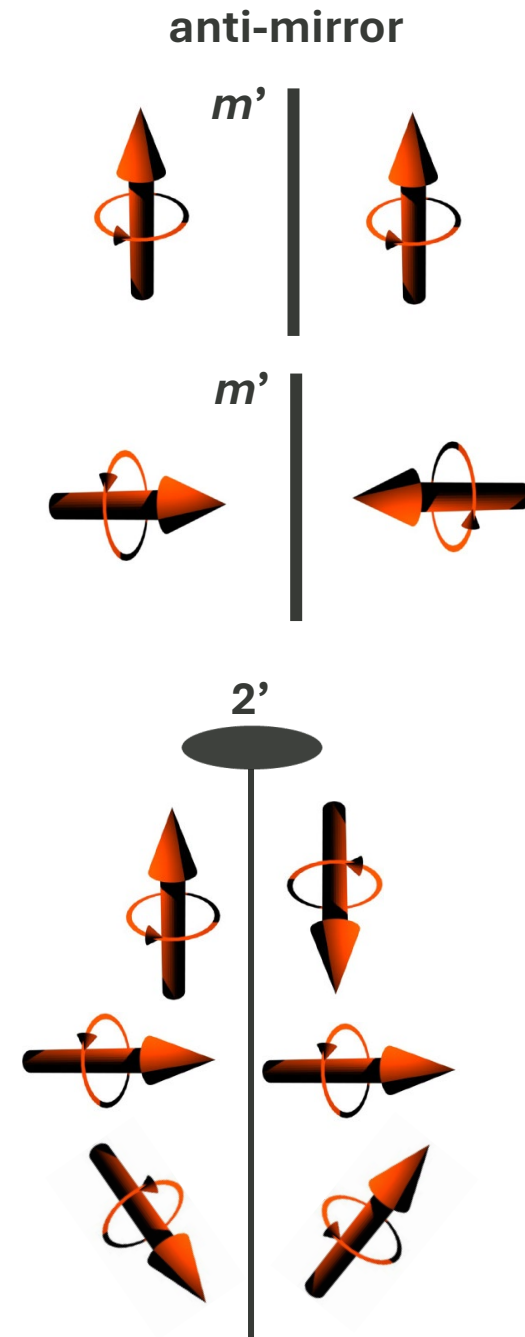
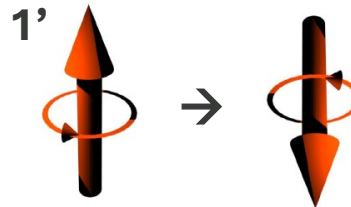
- Inversion and mirror (m) are different for axial and polar.



Magnetic space groups: Time-reversal

- To describe magnetic moments fully a new operator is added
 - Time reversal or prime ($1'$)
 - Reverses the final current loop to allow a further set of symmetry operations.
- m' (anti-mirror) behaves like polar vector
- $2'$ (anti-rotation) inverts axial vector
- t' (anti-translation)
- **All magnetic structures can be described by a combination of primed and unprimed symmetry operators**

Time reversal = spin reversal
(changes the sense of the current)



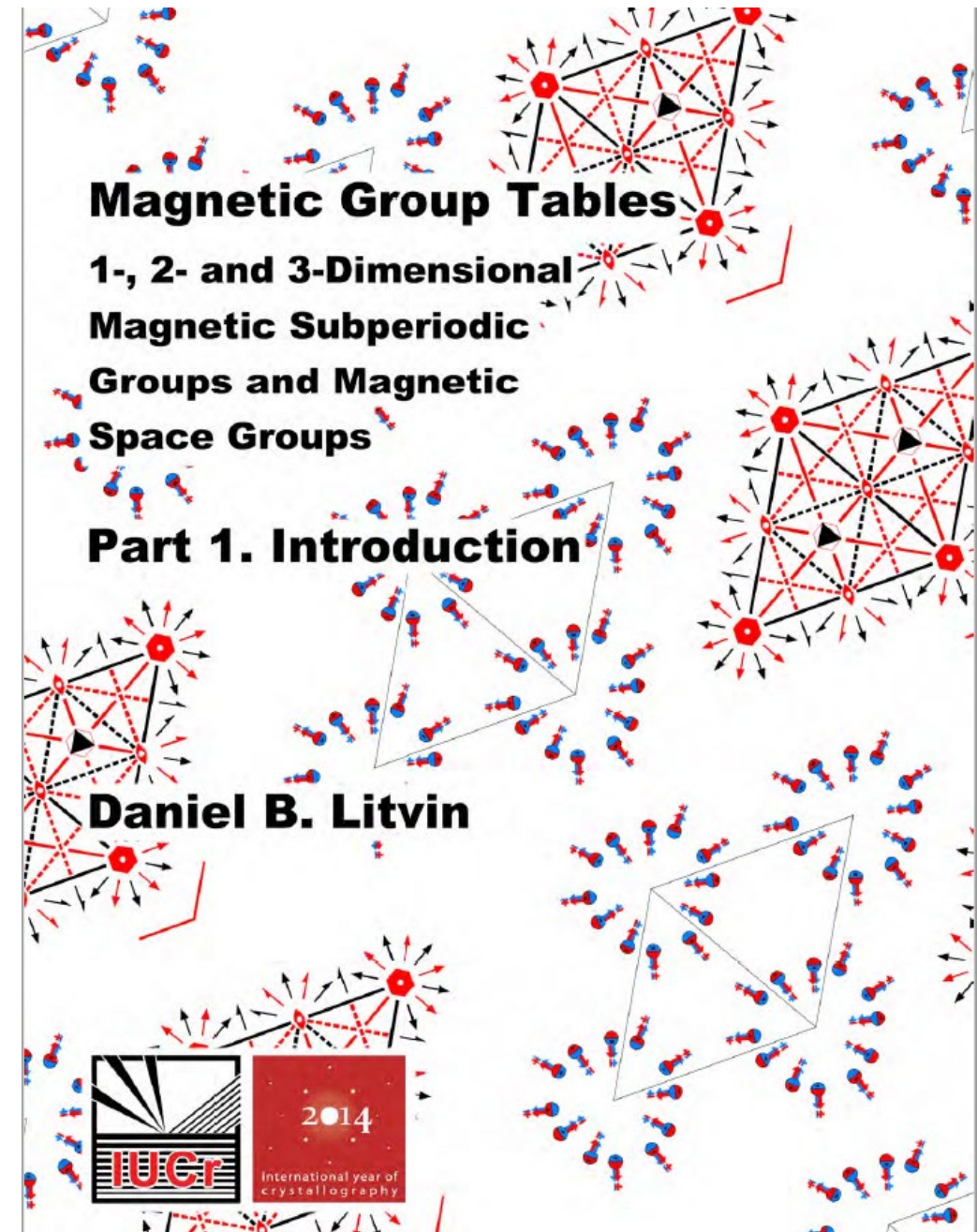
Building the magnetic space groups

- By associating the $1'$ spin operator with a color change (black to white or black to red) the magnetic symmetry theory was termed black-white symmetry.
- **The original 230 space groups are included as colorless groups and keep their standard labels**
 - e.g. ***Pmmm***
- A further 230 groups are created by adding the $1'$ operator as an extra symmetry operation
 - e.g. *Pmmm1'*
 - These correspond to paramagnetic states and are termed grey (each magnetic site is both black and white = grey)
- **The remaining 1191 magnetic space groups are created by combining the $1'$ operator with one or more of the symmetry operation in each of the 230 crystallographic space groups**
 - e.g. *Pm'mm* where the mirror plane perpendicular to *a* is now an anti-mirror and the other two are unchanged.

→ Combining all possibilities leads to 1651 magnetic space groups

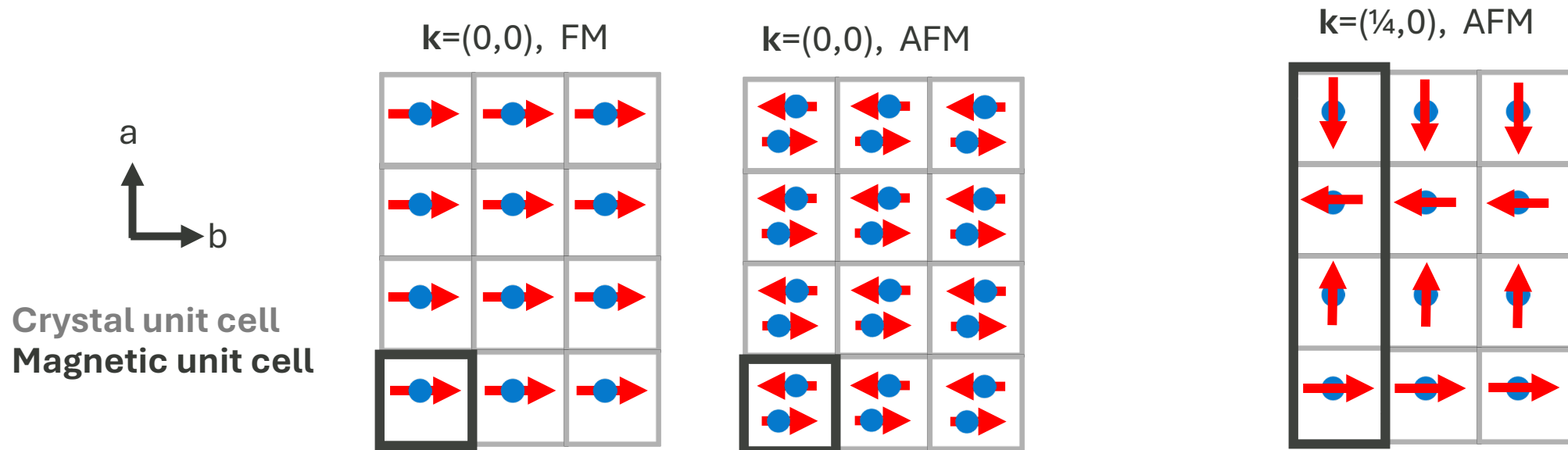
Magnetic space groups

- Full description of all Magnetic Space groups produced.
 - Acta Cryst A57, 729-730 (2001)
 - Acta Cryst. (2008). A64, 419-424 (2008)
- Utilized in analysis tools
 - Isodistort, Bilbao (GSAS-II), Fullprof, JANA, etc



Magnetic propagation vector: Magnetic space groups

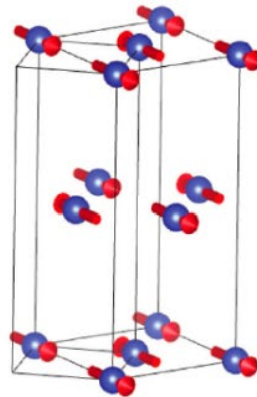
- Magnetic Space groups: $\mathbf{k}$ -vector is directly incorporated into the magnetic unit cell.
- Consider a paramagnetic crystal unit cell of $\mathbf{a}$ and $\mathbf{b}$.
 - If $\mathbf{k}=(0, 0) \rightarrow$ magnetic space group unit cell is unchanged: $\mathbf{a}$ and $\mathbf{b}$
 - If $\mathbf{k}=(1/4, 0) \rightarrow$ magnetic space group unit cell is: $4\mathbf{a}$ and $\mathbf{b}$
- Need to keep track of this in refinements, cif/mCIF files, reflections and reporting of results.



Magnetic space groups: all atoms

- The non-magnetic atoms are also often important in the physics
- Magnetic space groups contain all information on crystal and magnetic symmetry of whole structure
- The same spin arrangement can produce different magnetic space groups (and different physical properties, e.g. ferroic) depending on the symmetry of the parent

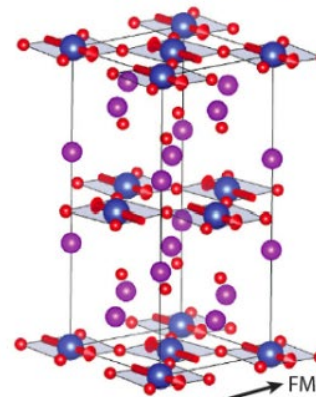
$I4/mmm$, $k=(1/2, 1/2, 0)$



$C_{4v}ccm$
($c, a-b, a+b; 1/4, 3/4, 1/4$)

Pr_2CuO_4

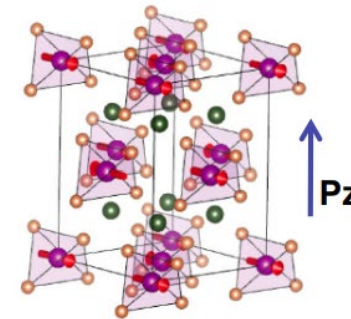
$Cmce$, $k=(0, 0, 0)$



$Cm'ca'$
($c, a-b, a+b; 0, 0, 0$)

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

MAXMAGN

bilbao crystallographic server

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Space-group symmetry

Magnetic Symmetry and Applications

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

Bilboa Crystallographic Server: Pyrochlore example

Maximal magnetic space groups for the parent space group $Fd-3m$ (No. 227) and the propagation vector $k = (0, 0, 0)$

N	Group (BNS)	Transformation matrix	General positions	Properties	Magnetic structure
1	$Fd-3'm'$ (#227.132) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
2	$Fd-3m'$ (#227.131) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
3	$Fd-3'm$ (#227.130) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
4	$Fd-3m$ (#227.128) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
5	$I4_1/am'd$ (#141.557) Go to a subgroup	$\begin{pmatrix} 0 & 0 & -1 & 1/4 \\ 1/2 & 1/2 & 0 & 1/4 \\ 1/2 & -1/2 & 0 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
6	$I4_1/a'm'd$ (#141.556) Go to a subgroup	$\begin{pmatrix} 0 & 0 & -1 & 1/4 \\ 1/2 & 1/2 & 0 & 1/4 \\ 1/2 & -1/2 & 0 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
7	$I4_1/amd$ (#141.555) Go to a subgroup	$\begin{pmatrix} 0 & 0 & 1 & 0 \\ 1/2 & 1/2 & 0 & 1/4 \\ -1/2 & 1/2 & 0 & 1/4 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
8	$I4_1/a'md$ (#141.553) Go to a subgroup	$\begin{pmatrix} 0 & 0 & -1 & 1/4 \\ 1/2 & 1/2 & 0 & 1/4 \\ 1/2 & -1/2 & 0 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
9	$Imm'a'$ (#74.559) Go to a subgroup	$\begin{pmatrix} 1/2 & 1/2 & 0 & 0 \\ -1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
10	$Im'ma$ (#74.556) Go to a subgroup	$\begin{pmatrix} 1/2 & 1/2 & 0 & 0 \\ -1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show

Magnetic Structure

Selected magnetic space group: 2- $Fd-3m'$ (#227.131)

Setting of the parent group

Parent space group $Fd-3m$ (No. 227)

Lattice parameters: a=10.09060, b=10.09060, c=10.09060, alpha=90.0000, beta=90.0000, gamma=90.0000

[\[Go to setting standard \(a, b, c ; 0, 0, 0\)\]](#)

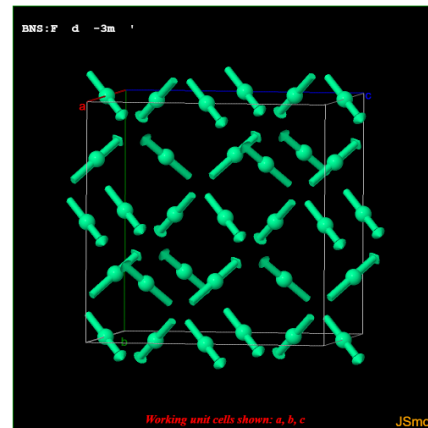
[\[Go to an alternative setting\]](#)

[Export data to MCIF file/Visualize](#) [Go to a subgroup](#)

Atomic positions, Wyckoff positions and Magnetic Moments

N	Atom	Occupancy	New WP	Multiplicity	Magnetic moment	Values of M_x, M_y, M_z
1	Ho1 Ho	0.50000 0.50000 0.50000	1.	16	(M_x, M_x, M_x)	$M_x = 1$
2	Ti1 Ti					

MVISUALIZE: 3D Visualization of magnetic structures



All-in, all-out magnetic structure

K-SUBGROUPSMAG

bilbao crystallographic server

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Space-group symmetry

Magnetic Symmetry and Applications

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CollinearSpinGroups ⚠	Operations of Nontrivial Collinear Spin Space Groups

K-SUBGROUPSMAG

- Allows you to check all magnetic space groups compatible with the parent space group and k-vector.

Enter the serial number of the space group of the parent paramagnetic phase:

[Choose an alternative magnetic group](#)

Introduce the magnetic wave vector(s)

(Give the components of the wave vectors in a fractional form, n/m)

k_{1x} k_{1y} k_{1z}

[Show the independent vectors of the star](#)

☐ Choose the whole star of the propagation vector

☒ Include the subgroups compatible with intermediate cells.
(It is not applied when only the maximal subgroups are calculated)

Optional: refine further the subgroups of the output giving the Wyckoff positions of the atoms
Give the Wyckoff positions

☒ **Optional:** Show only subgroups that can be the result of a Landau-type transition (single irrep order parameter).

Optional: refine further the subgroups of the output giving a set of irreps
Choose the irreps

Optional: possible limitations of the subgroup list
(Check only one option on the left and the specific value on the right)

☒ Lowest space group to consider

☐ Lowest point group to consider

☐ Lowest crystal system to consider

☐ Only maximal subgroups

Optional: further limitations considering physical properties of the point groups

☐ Only centrosymmetric / non-centrosymmetric groups

☐ Only polar / non-polar groups

☒ List of subgroups ☐ Graph of subgroups

Input data

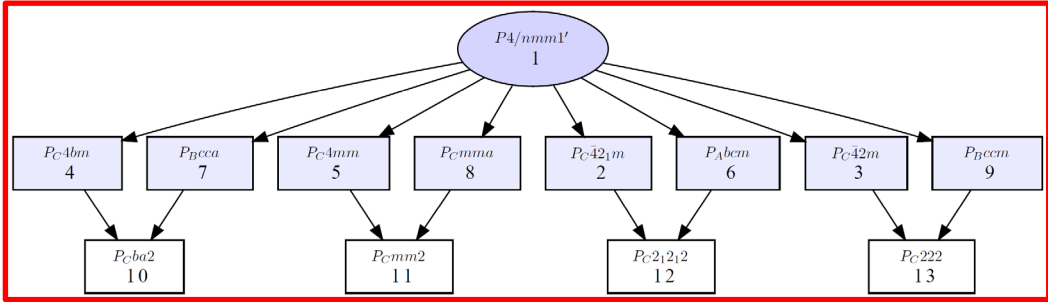
Subgroups of the paramagnetic space group :
Lowest magnetic space group to consider:
Magnetic propagation wave-vectors
Subgroups compatible with intermediate cells included
Only subgroups compatible with a Landau-type transition

P4/nmm1' (N. 129)
P1 (N. 1.1)
(0.5,0.5,0)

List of subgroups that can be the result of a Landau-type transition

Get the subgroup-graph

N	Group Symbol	Transformation matrix	Group-Subgroup index	Other members of the Conjugacy Class	irreps	Magnetic structure models (MAGMODELIZE)
1	<i>P4/nmm1'</i> (No. 129.412)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	1=1x1	Conjugacy Class	Get irreps	☐
2	<i>P_C4₂1m</i> (No. 113.273)	$\begin{pmatrix} 1 & -1 & 0 & 1/4 \\ 1 & 1 & 0 & -1/4 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps	☐
3	<i>P_C4₂m</i> (No. 111.257)	$\begin{pmatrix} 1 & -1 & 0 & -1/4 \\ 1 & 1 & 0 & 1/4 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps	☐
4	<i>P_C4bm</i> (No. 100.177)	$\begin{pmatrix} 1 & -1 & 0 & -1/4 \\ 1 & 1 & 0 & -1/4 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps	☐
5	<i>P_C4mm</i> (No. 99.169)	$\begin{pmatrix} 1 & -1 & 0 & -1/4 \\ 1 & 1 & 0 & -1/4 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps	☐
6	<i>P_Abcm</i> (No. 57.389)	$\begin{pmatrix} 0 & 1 & -1 & 0 \\ 0 & 1 & 1 & 1/2 \\ 1 & 0 & 0 & 0 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps	☐
7	<i>P_Bcca</i> (No. 54.350)	$\begin{pmatrix} 1 & 0 & 1 & 0 \\ -1 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps	☐
8	<i>P_Cmma</i> (No. 51.303)	$\begin{pmatrix} 1 & 1 & 0 & 0 \\ -1 & 1 & 0 & 1/2 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps	☐
9	<i>P_Bccm</i> (No. 49.274)	$\begin{pmatrix} 1 & 0 & -1 & 0 \\ -1 & 0 & -1 & 1/2 \\ 0 & 1 & 0 & 0 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps	☐
10	<i>P_Cba2</i> (No. 32.141)	$\begin{pmatrix} 1 & -1 & 0 & 1/4 \\ 1 & 1 & 0 & 1/4 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	8=2x4	Conjugacy Class	Get irreps	☐
11	<i>P_Cmm2</i> (No. 25.63)	$\begin{pmatrix} 1 & -1 & 0 & 1/4 \\ 1 & 1 & 0 & 1/4 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	8=2x4	Conjugacy Class	Get irreps	☐
12	<i>P_C2₁2₁2</i> (No. 18.23)	$\begin{pmatrix} 1 & 1 & 0 & -1/4 \\ -1 & 1 & 0 & 1/4 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	8=2x4	Conjugacy Class	Get irreps	☐
13	<i>P_C222</i> (No. 16.5)	$\begin{pmatrix} 1 & -1 & 0 & -1/4 \\ 1 & 1 & 0 & 1/4 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	8=2x4	Conjugacy Class	Get irreps	☐



Can check maximal and subgroups.

Select/Deselect all subgroups
☒ Include structure data of the parent phase

Submit selected subgroups to MAGMODELIZE:

*Warning: Submitting many subgroups to MAGMODELIZE, when the 'include structure' option is selected may take too long -- it is recommended to check at most 5 structures at a time

Subgroups of the paramagnetic space group :

Lowest magnetic space group to consider:

Magnetic propagation wave-vectors

Subgroups compatible with intermediate cells included

Only subgroups compatible with a Landau-type transition

 $P4/nmm1'$ (N. 129) $P1$ (N. 1.1)

(0.5,0.5,0)

List of subgroups that can be the result of a Landau-type transition

Get the subgroup-graph

N	Group Symbol	Transformation matrix	Group-Subgroup index	Other members of the Conjugacy Class	irreps	Magnetic structure models (MAGMODELIZE)
1	$P4/nmm1'$ (No. 129.412)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	1=1x1	Conjugacy Class	Get irreps	☐
2	$P_C\bar{4}2_1m$ (No. 113.273)	$\begin{pmatrix} 1 & -1 & 0 & 1/4 \\ 1 & 1 & 0 & -1/4 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps	☒
3	$P_C\bar{4}2m$ (No. 111.257)	$\begin{pmatrix} 1 & -1 & 0 & -1/4 \\ 1 & 1 & 0 & 1/4 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps	☐
4	P_C4bm (No. 100.177)	$\begin{pmatrix} 1 & -1 & 0 & -1/4 \\ 1 & 1 & 0 & -1/4 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps	☐
5	P_C4mm (No. 99.169)	$\begin{pmatrix} 1 & -1 & 0 & -1/4 \\ 1 & 1 & 0 & -1/4 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps	☐
6	P_Abcm (No. 57.389)	$\begin{pmatrix} 0 & 1 & -1 & 0 \\ 0 & 1 & 1 & 1/2 \\ 1 & 0 & 0 & 0 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps	☐
7	P_Bcca (No. 54.350)	$\begin{pmatrix} 1 & 0 & 1 & 0 \\ -1 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps	☐
8	P_Cmma (No. 51.303)	$\begin{pmatrix} 1 & 1 & 0 & 0 \\ -1 & 1 & 0 & 1/2 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps	☐
9	P_Bccm (No. 49.274)	$\begin{pmatrix} 1 & 0 & -1 & 0 \\ -1 & 0 & -1 & 1/2 \\ 0 & 1 & 0 & 0 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps	☐
10	P_Cba2 (No. 32.141)	$\begin{pmatrix} 1 & -1 & 0 & 1/4 \\ 1 & 1 & 0 & 1/4 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	8=2x4	Conjugacy Class	Get irreps	☐
11	P_Cmm2 (No. 25.63)	$\begin{pmatrix} 1 & -1 & 0 & 1/4 \\ 1 & 1 & 0 & 1/4 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	8=2x4	Conjugacy Class	Get irreps	☐
12	$P_C2_12_12$ (No. 18.23)	$\begin{pmatrix} 1 & 1 & 0 & -1/4 \\ -1 & 1 & 0 & 1/4 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	8=2x4	Conjugacy Class	Get irreps	☐
13	P_C222 (No. 16.5)	$\begin{pmatrix} 1 & -1 & 0 & -1/4 \\ 1 & 1 & 0 & 1/4 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	8=2x4	Conjugacy Class	Get irreps	☐

Select/Deselect all subgroups

☒ Include structure data of the parent phaseSubmit selected subgroups to MAGMODELIZE:

*Warning: Submitting many subgroups to MAGMODELIZE, when the 'include structure' option is selected may take too long -- it is recommended to check at most 5 structures at a time

Parent paramagnetic structure cif file

Option 1: Please submit a structure file (CIF format):

 Sr2FeO3Cl.cif

Note: The space group of the cif file will supersede any previous one.

Option 2: Specify structure data by hand:

Space Group: $P4/nmm$ (No. 129)

Lattice parameters (Angstroms and degrees):

a=b= c= alpha=90 beta=90 gamma=90Number of unique atomic positions:

Parent phase structure data: Magnetic Atoms

Parent space group: $P4/nmm$ (No. 129)

Lattice parameters (Angstroms and degrees): a=3.92390, b=3.92390, c=14.29760, alpha=90.000000, beta=90.000000, gamma=90.000000

Atoms: Please select the magnetic ones

N	Atom name	Atom type	Wyckoff Position	Coordinates	Magnetic?
1	Fe1	Fe	2c	0.25000 0.25000 0.29252	☒
2	Sr1	Sr	2c	0.25000 0.25000 0.59641	☐
3	Sr2	Sr	2c	0.25000 0.25000 0.84513	☐
4	O1	O	4f	0.75000 0.25000 0.26885	☐
5	O2	O	2c	0.25000 0.25000 0.42467	☐
6	Cl1	Cl	2c	0.25000 0.25000 0.07478	☐

Selected magnetic space subgroup for the parent space group $P4/nmm$ (No. 129)

Maximal subgroups which allow non-zero magnetic moments for at least one atom are coloured

N	Group (BNS)	Transformation matrix	General positions	Properties	Magnetic structure
1	$P_C\bar{4}2_1m$ (#113.273) Go to a subgroup	$\begin{pmatrix} 1 & -1 & 0 & 1/4 \\ 1 & 1 & 0 & 7/4 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	<input checked="" type="button" value="Show"/>

List of subgroups that can be the result of a Landau-type transition

[Get the subgroup-graph](#)

N	Group Symbol	Transformation matrix	Group-Subgroup index	Other members of the Conjugacy Class	irreps	Magnetic structure models (MAGMODELIZE)
1	$P4/nmm1'$ (No. 129.412)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$	1=1x1	Conjugacy Class	Get irreps	☐
2	$P_C\bar{4}2_1m$ (No. 113.273)	$\begin{pmatrix} 1 & -1 & 0 & 1/4 \\ 1 & 1 & 0 & -1/4 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps	☐
3	$P_C\bar{4}2m$ (No. 111.257)	$\begin{pmatrix} 1 & -1 & 0 & -1/4 \\ 1 & 1 & 0 & 1/4 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps	☐
4	P_C4bm (No. 100.177)	$\begin{pmatrix} 1 & -1 & 0 & -1/4 \\ 1 & 1 & 0 & -1/4 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps	☐
5	P_C4mm (No. 99.169)	$\begin{pmatrix} 1 & -1 & 0 & -1/4 \\ 1 & 1 & 0 & -1/4 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps	☐
6	P_Abcm (No. 57.389)	$\begin{pmatrix} 0 & 1 & -1 & 0 \\ 0 & 1 & 1 & 1/2 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps	☐
7	P_Bcca (No. 54.350)	$\begin{pmatrix} 1 & 0 & 1 & 0 \\ -1 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps	☐
8	P_Cmma (No. 51.303)	$\begin{pmatrix} 1 & 1 & 0 & 0 \\ -1 & 1 & 0 & 1/2 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps	☐
9	P_Bccm (No. 49.274)	$\begin{pmatrix} 1 & 0 & -1 & 0 \\ -1 & 0 & -1 & 1/2 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps	☐
10	P_Cba2 (No. 32.141)	$\begin{pmatrix} 1 & -1 & 0 & 1/4 \\ 1 & 1 & 0 & 1/4 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$	8=2x4	Conjugacy Class	Get irreps	☐
11	P_Cmm2 (No. 25.63)	$\begin{pmatrix} 1 & -1 & 0 & 1/4 \\ 1 & 1 & 0 & 1/4 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$	8=2x4	Conjugacy Class	Get irreps	☐
12	$P_C2_12_12$ (No. 18.23)	$\begin{pmatrix} 1 & 1 & 0 & -1/4 \\ -1 & 1 & 0 & 1/4 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$	8=2x4	Conjugacy Class	Get irreps	☐
13	P_C222 (No. 16.5)	$\begin{pmatrix} 1 & -1 & 0 & -1/4 \\ 1 & 1 & 0 & 1/4 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$	8=2x4	Conjugacy Class	Get irreps	☒

[Select/Deselect all subgroups](#)☒ Include structure data of the parent phaseSubmit selected subgroups to MAGMODELIZE: [Submit](#)Selected magnetic space subgroup for the parent space group $P4/nmm$ (No. 129)

Maximal subgroups which allow non-zero magnetic moments for at least one atom are coloured

N	Group (BNS)	Transformation matrix	General positions	Properties	Magnetic structure
1	P_C222 (#16.5) Go to a subgroup	$\begin{pmatrix} 1 & -1 & 0 & 7/4 \\ 1 & 1 & 0 & 1/4 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show

This lower symmetry has $M_x \neq M_y$,
this can be tested against data.

Magnetic Structure

Selected magnetic space group: 1- P_C222 (#16.5)Setting parent-like (**2a, 2b, c** ; 0, 0, 0)Parent space group $P4/nmm$ (No. 129)

Lattice parameters: a=7.84780, b=7.84780, c=14.29760, alpha=90.00, beta=90.00, gamma=90.00

[\[Go to setting standard \(a+b, -a+b, c ; 7/4, 1/4, 0\)\]](#)[\[Go to an alternative setting\]](#)[Export data to ICIF file/Visualize](#) [Go to a subgroup](#)

Atomic positions, Wyckoff positions and Magnetic Moments

N	Atom	New WP	Multiplicity	Magnetic moment	Values of M_x, M_y, M_z
1	Fe1 Fe 0.12500 0.12500 0.29252	(1/8, 1/8, z $m_x, m_y, 0$) (3/8, 3/8, -z $-m_y, -m_x, 0$) (1/8, 5/8, z $-m_x, -m_y, 0$) (3/8, 7/8, -z $m_y, m_x, 0$) (5/8, 1/8, z $-m_x, -m_y, 0$) (7/8, 3/8, -z $m_y, m_x, 0$) (5/8, 5/8, z $m_x, m_y, 0$) (7/8, 7/8, -z $-m_y, -m_x, 0$)	8	$(M_x, M_y, 0)$	$M_x = 0.00000$ $M_y = 0.00000$
2	Sr1 Sr 0.12500 0.12500 0.59641	(1/8, 1/8, z $m_x, m_y, 0$) (3/8, 3/8, -z $-m_y, -m_x, 0$) (1/8, 5/8, z $-m_x, -m_y, 0$) (3/8, 7/8, -z $m_y, m_x, 0$) (5/8, 1/8, z $-m_x, -m_y, 0$) (7/8, 3/8, -z $m_y, m_x, 0$) (5/8, 5/8, z $m_x, m_y, 0$) (7/8, 7/8, -z $-m_y, -m_x, 0$)	8	-	-

MVISUALIZE

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Space-group symmetry

Magnetic Symmetry and Applications

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

MVISUALIZE: 3D Visualization of magnetic structures with Jmol

MVISUALIZE Main Page

[Download complete mcif file \(including all tags needed for submission to MAGNDATA\)](#)

[Change setting](#) [Domain-related equivalent descriptions](#)

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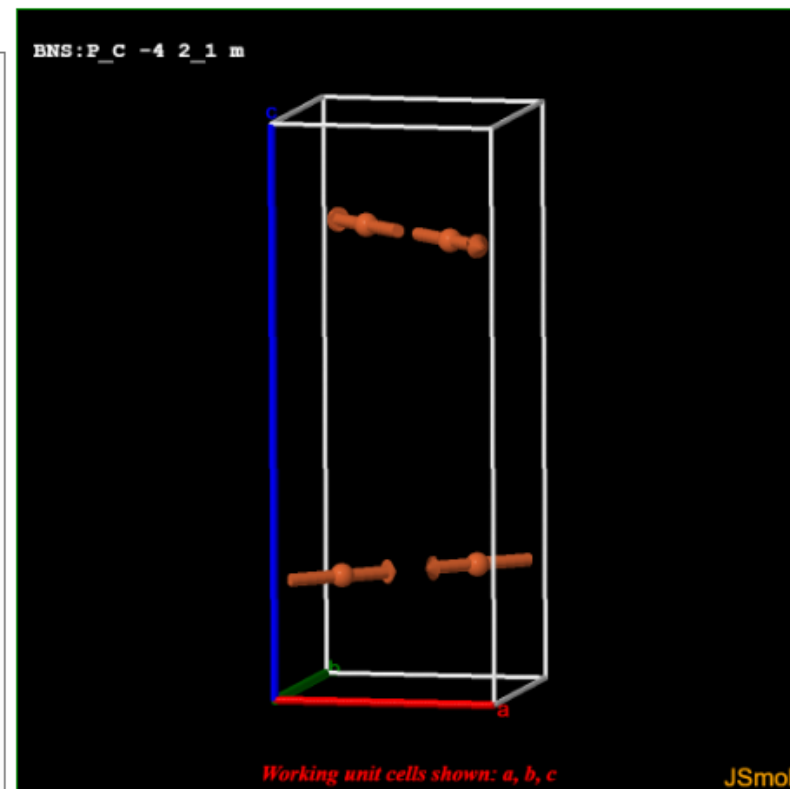
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# Created by the Bilbao Crystallographic Server
# http://www.cryst.ehu.es
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Select cell... ▼

Toggle Parent Cell

Toggle Standard Cell

View Along Axis... ▼

Unit Cell Info

All / Magnetic Atoms

Show/Hide Labels

Larger Smaller Vectors

Larger Smaller Atoms

Window Size

Bigger Smaller

Background Color ▼

Toggle Quality

Center

Export PNG Image

Save PNG-3D

Save ZIP file

Show unit cell a,b,c

Add 1 cell along x

Remove 1 cell along x

Add 1 cell along y

Remove 1 cell along y

Add 1 cell along z

Remove 1 cell along z

x=1 y=1 z=1

Choose supercell

Draw bonds & polyhedra

Join - ▼ with - ▼

from 0.75 to 2.75 Å

Draw Bonds Polyhedra

Delete Bonds Polyhedra

Clear all drawings

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Symmetry-adapted form of material tensors via [MTENSOR](#)

Symmetry-adapted form of material tensors for domain-related equivalent structures via [MTENSOR](#)

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If you still observe any malfunction, write an e-mail to cryst@wm.lc.ehu.es explaining the problem in detail.