The MAGNDATA database and how to properly report a magnetic structure

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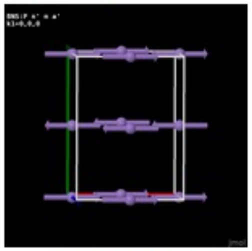
MAGNDATA: A Collection of magnetic structures with portable cif-type files

Element search (separate with space or comma): ◉ AND ○ OR Search

312 structures found

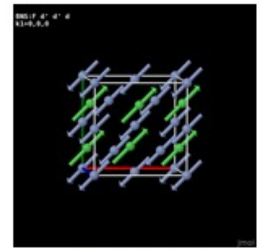
Update: by Qct 2025 it contains about 2350 structures

Zero propagation vector


0.1 $LaMnO_3$


0.2 $Cd_2Os_2O_7$


0.3 Ca_3LiOsO_6


0.4 $NiCr_2O_4$

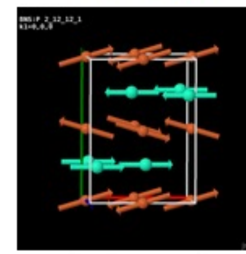

0.5 Cr_2S_3


0.6 $YMnO_3$


0.7 $ScMnO_3$


0.8 $ScMnO_3$


0.9 GdB_4


0.10 $DyFeO_3$





MAGNDATA: A collective endeavour

- ***Bilbao:*** **Samuel V. Gallego, J. Manuel Perez-Mato, L. Elcoro, G. Madariaga, Mois I. Aroyo**
- ***Ankara:*** **Emre S. Tasci**
- ***Tsukuba:*** **Koichi Momma (VESTA)**
- ***Northfield, MN:*** **Robert M. Hanson (Jmol)**

J. Appl. Cryst. (2016) 49, 1750-1776 (Commensurate structures)

J. Appl. Cryst. (2016) 49, 1941-1956 (Incommensurate structures)

At present it keeps running through the work of:

Emre S. Tasci, Gotzon Madariaga, Luis Elcoro & J. M. Perez-Mato

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MAGNDATA: towards a database of magnetic structures. I. The commensurate case

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Keywords: magnetic structures database; *MAGNDATA*; commensurate magnetic structures; magnetic space groups; Bilbao Crystallographic Server; magnetic symmetry; irreducible representations.

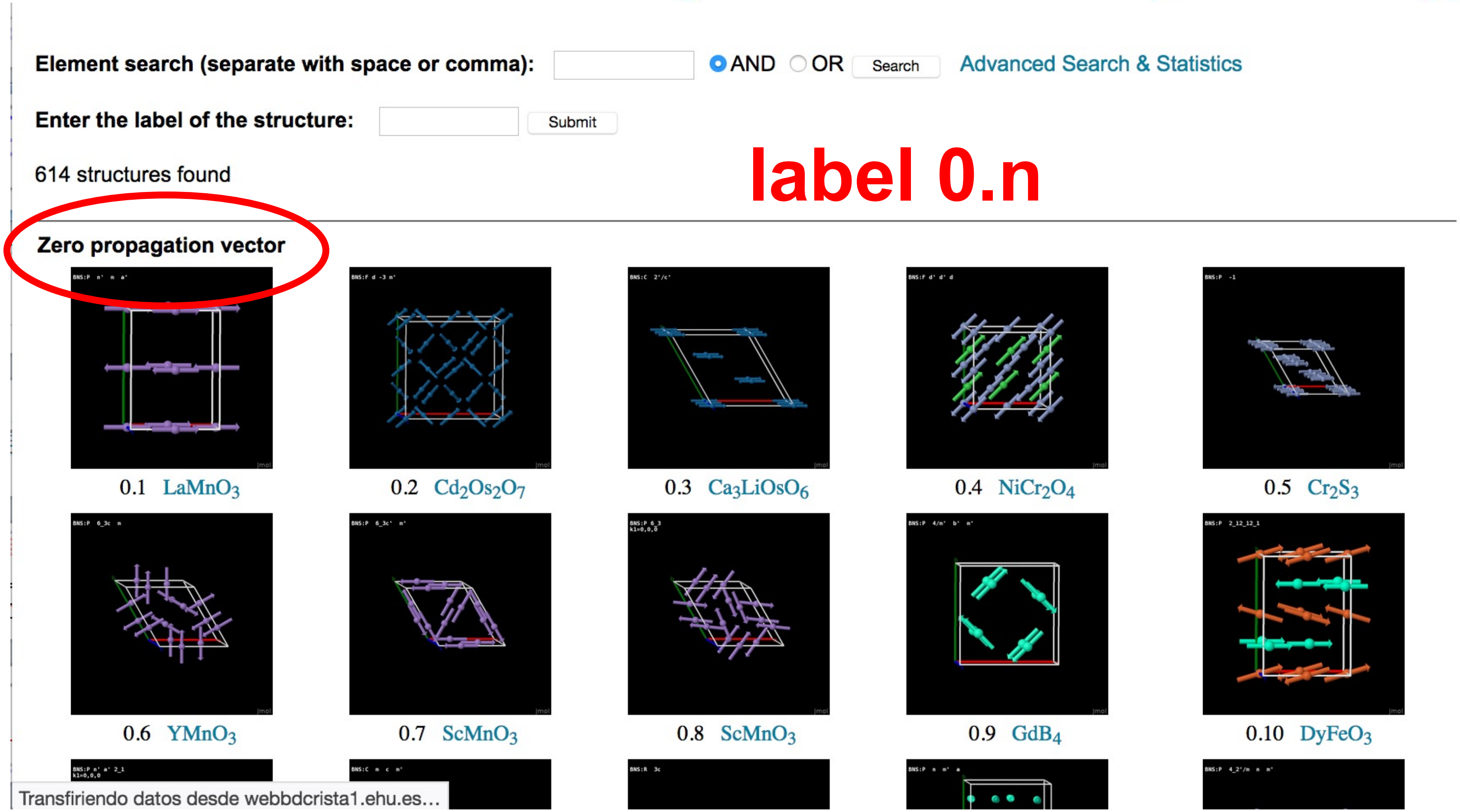
A free web page under the name *MAGNDATA*, which provides detailed quantitative information on more than 400 published magnetic structures, has been developed and is available at the Bilbao Crystallographic Server (http://www.cryst.ehu.es). It includes both commensurate and incommensurate structures. This first article is devoted to explaining the information available on commensurate magnetic structures. Each magnetic structure is described using magnetic symmetry, *i.e.* a magnetic space group (or Shubnikov group). This ensures a robust and unambiguous description of both atomic positions and magnetic moments within a common unique formalism. A non-standard setting of the magnetic space group is often used in order to keep the origin and unit-cell orientation of the paramagnetic phase, but a description in any desired setting is possible. Domain-related equivalent structures can also be downloaded. For each structure its magnetic point group is given, and the resulting constraints on any macroscopic tensor property of interest can be consulted. Any entry can be retrieved as a magCIF file, a file format under development by

Tutorial_magnetic_section_BCS_3

Only section 3

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

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

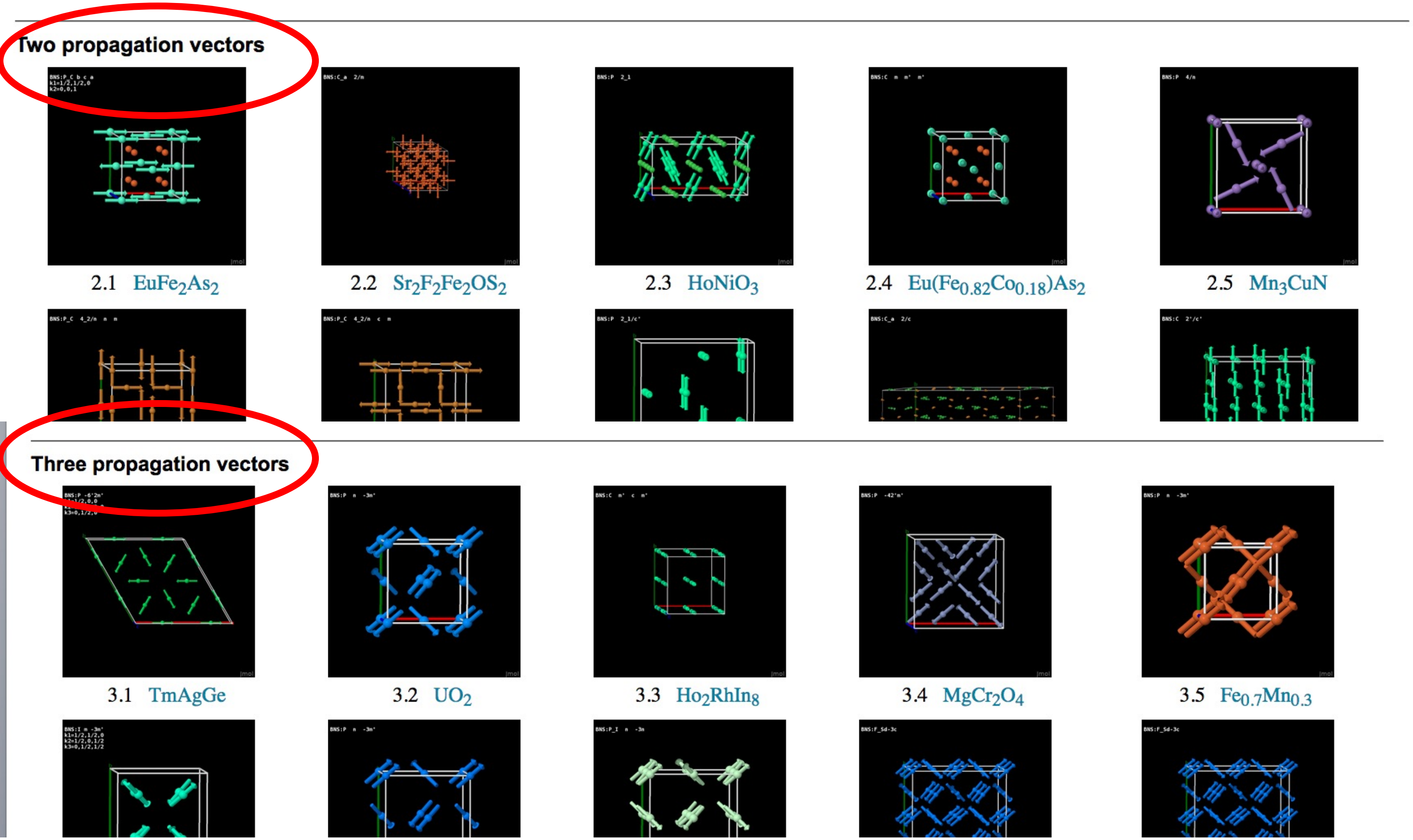


label 0.n

k=(0,0,0) → (no antitranslation)

k=0 – structures (**Type I or III MSG symmetry**). The most interesting ones for magneto-structural properties! (magnetic point group without time reversal)

labels 2.n and 3.n



2k and ≥3k structures

All types of MSG symmetries (with and without antitranslations)

Search optional filters

Advanced search

◉ All structures ○ Commensurate structures ○ Incommensurate structures

Element search
(separate with space or comma)

◉ AND ○ OR

Total number of species

Author

Search in comments

Crystal system
Magnetic (super)space group (All)
Parent space group (All)

Standard setting
Magnetic (super)space group (All)
Parent space group (All)

Class (propagation vector type)

- ☑ Class 0
- ☑ Class 2
- ☑ Class 1.0
- ☑ Class 3
- ☑ Class 1
- ☑ Class 1.1 (incomm)

Temperatures
Minimum transition temperature
Minimum experiment temperature

Properties
(magnetic super(space) group)
k-maximal? (All)
Centrosymmetric? (All)

Properties
(magnetic point group)
Polar? (All)
Ferromagnetic? (All)

Properties
(magnetic phase)
Possibly multiferroic type I? (All)
Possibly multiferroic type II? (All)

Properties
(Phase transition)
Number of wave vectors? (All)
Same point group than parent? (All)

Nonzero tensors

((None)
◉ AND ○ OR
(None))
◉ AND ○ OR
(None)

Irreducible representations

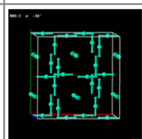
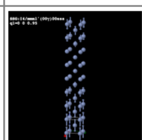
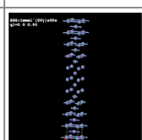
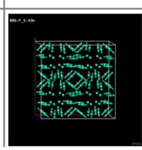
Number of irreps (All)
Multidimensional full irreps? (All)
Multidimensional small irreps? (All)
Primary irreps with: (All)
Irrep general or special direction? (All)

> 1 primary irreps? (All)
Secondary irreps allowed? (All)
Secondary irreps present? (All)
"Secondary irreps" mentioned in comments? (All)

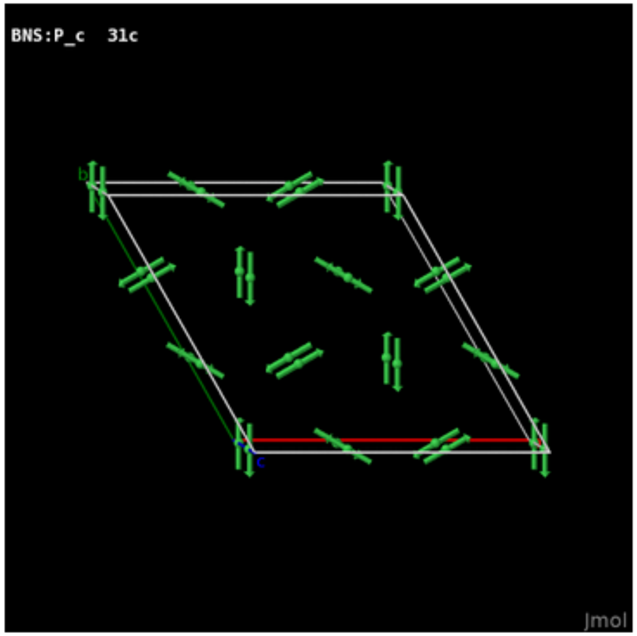
Search

ordering according to parent space group

Other optional orderings

Entry	Structure	Propagation vector(s)	Parent space group	Transformation from parent	Magnetic (super)space group	Magnetic point group
0.127 $Dy_3Al_5O_{12}$		0,0,0	Ia-3d (230) (standard)	(**a**,**b**,**c**;0,0,0)	Ia-3d' (230.148) (standard)	m-3m' (32.4.121)
1.1.4 Cr		0.000000,0.000000,0.950000	Im-3m (229) (standard)	(**a**,**b**,**c**;0,0,0)	I4/mmm1'(00g)00sss	4/mmm1' (15.2.54)
1.1.3 Cr		0.000000,0.000000,0.950000	Im-3m (229) (standard)	(**a**,**b**,**c**;0,0,0)	Immm1'(00g)s00s	mmm1' (8.2.25)
3.16 $Gd_2Ti_2O_7$		1/2,1/2,1/2 -1/2,1/2,1/2 1/2,-1/2,1/2 1/2,1/2,-1/2	Fd-3m (227) (standard)	(2**a**,2**b**,2**c**;15/8,3/8,15/8)	F_S-43m (216.77) (standard)	-43m1' (31.2.116)

Heading of an entry:



$Ba_3Nb_2NiO_9$ (#1.13)

view in Jmol

Download mcif file

Download vesta file (all atoms)

Download vesta file (magnetic atoms only)

submit to STRCONVERT

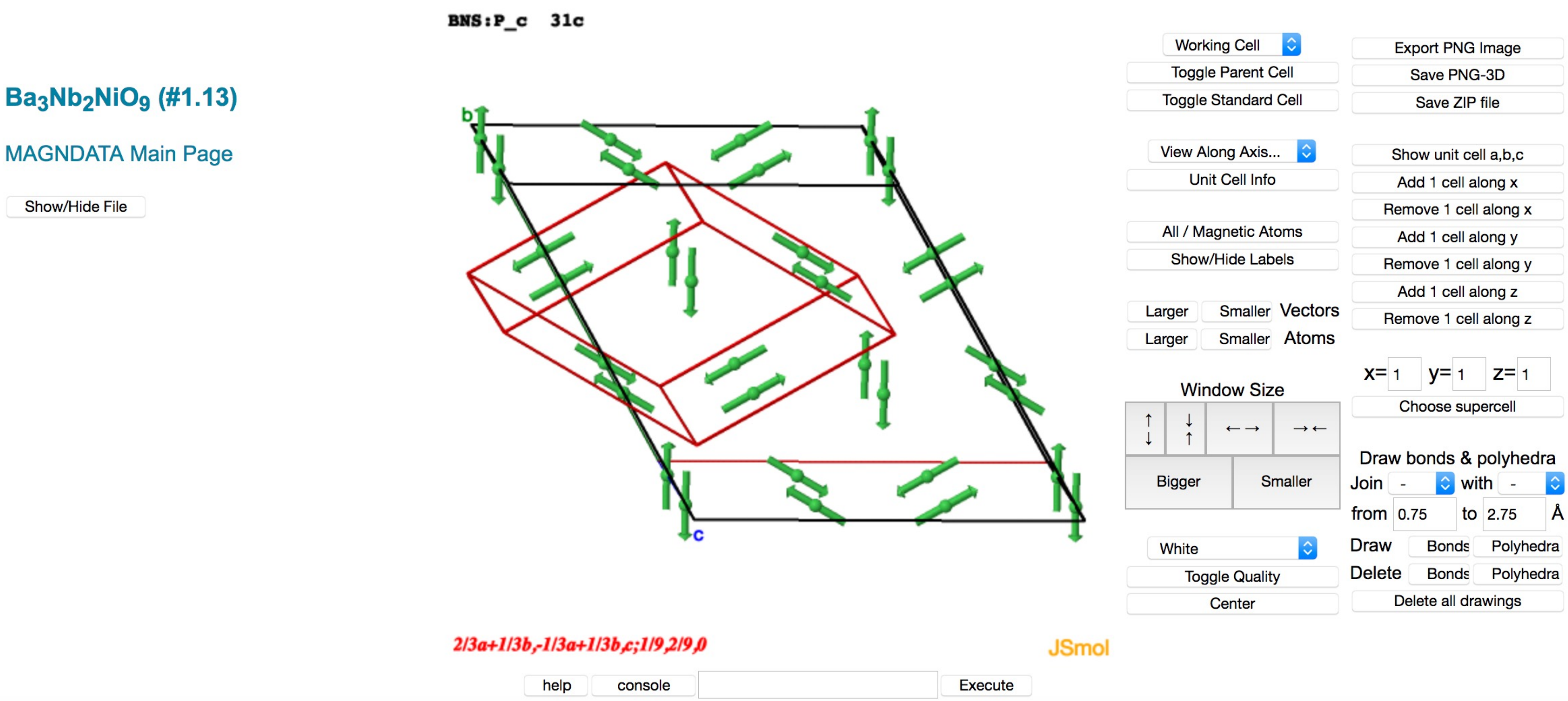
for 3D online visualization

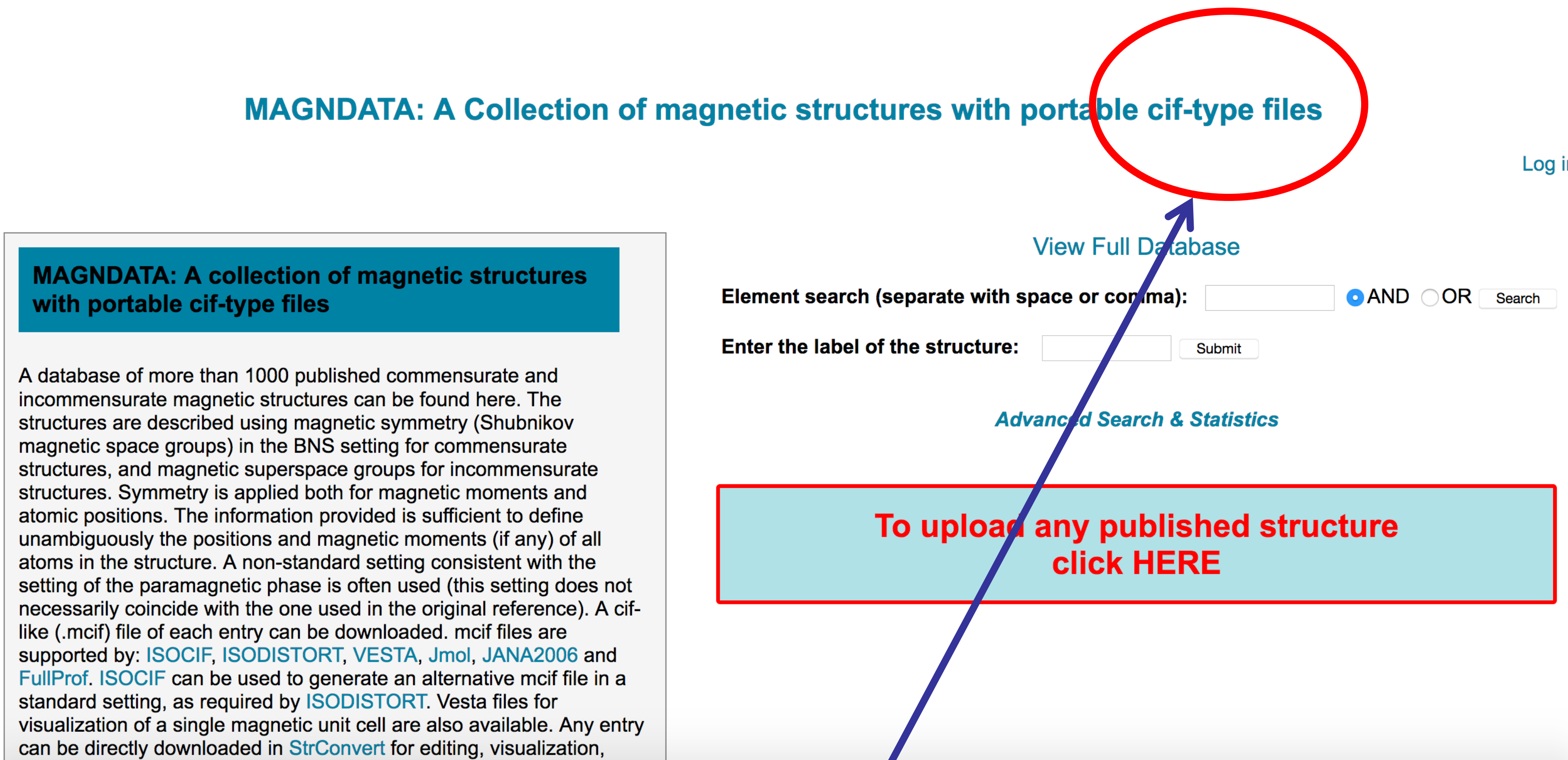
magCIF file

for editing

JSmol online 3D visualization

MAGNDATA Structure Viewer: 3D Visualization of magnetic structures with Jmol





CIF: Crystal Information File/Framework

magCIF: Format extension to magnetic structures

Developed by the IUCr Commission on Magnetic Structures under the direction of Branton Campbell.

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

A database of more than 1000 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,

magCIF file

```
_space_group_magn.transform_BNS_Pp_abc  '2/3a+1/3b,-1/3a+1/3b,c;1/9,2/9,0'
_space_group_magn.number_BNS  159.64
_space_group_magn.name_BNS  "P_c  31c"
_space_group_magn.point_group_name  "3m1'"
_space_group_magn.point_group_number  "19.2.69"
_cell_length_a                17.2650
_cell_length_b                17.2650
_cell_length_c                14.1312
_cell_angle_alpha             90.0000
_cell_angle_beta              90.0000
_cell_angle_gamma             120.0000

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

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

transformation to standard

MSG type identification

unit cell (magnetic)

Magnetic space group (MSG)

magCIF file

```
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Ba1_1 Ba 0.11111 0.22222 0.83190 1
Ba1_2 Ba 0.44444 0.22222 0.83190 1
Ba1_3 Ba 0.88889 0.77778 0.16810 1
Ba2_1 Ba 0.00000 0.00000 0.00000 1
Ni1 Ni 0.00000 0.00000 0.25000 1
Nb2_1 Nb 0.11111 0.22222 0.08850 1
Nb2_2 Nb 0.44444 0.22222 0.08850 1
Nb2_3 Nb 0.88889 0.77778 0.91150 1
O1_1 O 0.16667 0.00000 0.00000 1
O1_2 O 0.83333 0.66667 0.00000 1
O2_1 O 0.05660 0.94340 0.16312 1
O2_2 O 0.05660 0.11320 0.16312 1
O2_3 O 0.11320 0.05660 0.83688 1
O2_4 O 0.94340 0.88680 0.83688 1

loop_
_atom_site_moment.label
_atom_site_moment.crystalaxis_x
_atom_site_moment.crystalaxis_y
_atom_site_moment.crystalaxis_z
_atom_site_moment.symmform
_atom_site_moment.magnitude
_atom_site_moment.spherical_azimuthal
_atom_site_moment.spherical_polar
Ni1 1.04 2.08 0.0 mx,2mx,mz 1.8 ? ?
```

symmetry-independent atomic positions (split by the lowering of symmetry)

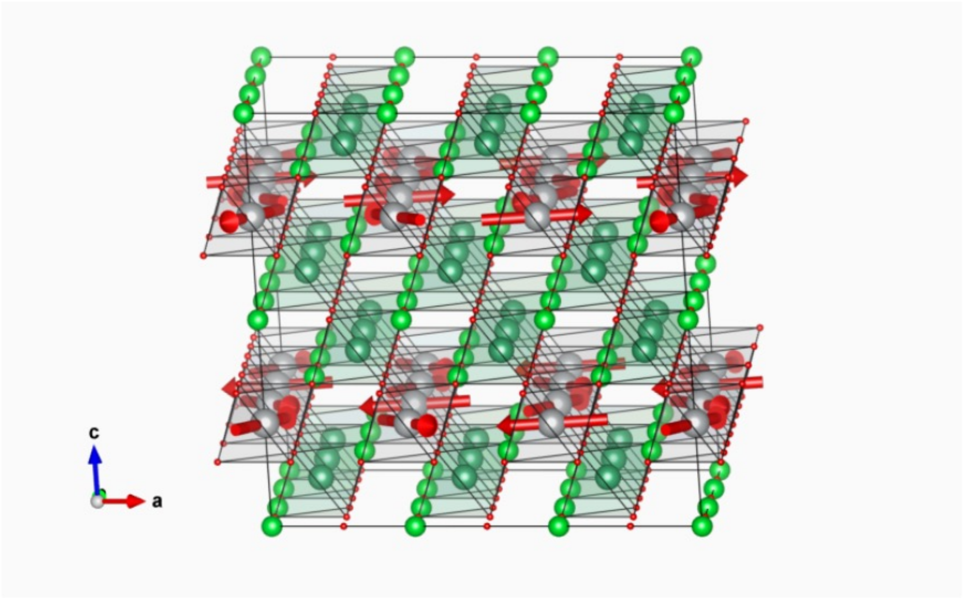
symmetry-independent magnetic moments

components

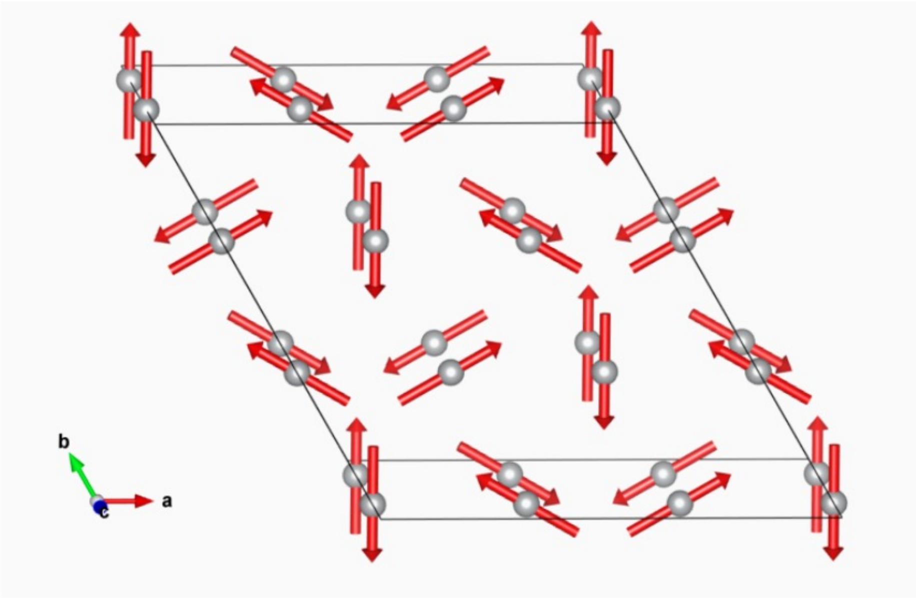
symmetry constraints

modulus

spherical coordinates (not supported by most programs!)



Magnetic structure with all atoms



Magnetic structure with only magnetic atoms

Reference: J. Hwang, E.S. Choi, F. Ye, C.R.D. Cruz, Y. Xin, H.D. Zhou and P. Schlottmann, *Physical Review Letters* (2012) **109**.
DOI: 10.1103/physrevlett.109.257205
Atomic positions from: ICSD #240280

it includes a direct link to the reference (DOI)

Parent space group (paramagnetic phase): P-3m1 (#164)
Propagation vector: k1 (1/3, 1/3, 3/2)

Transition Temperature: 4.9 K
Experiment Temperature: 2 K

Lattice parameters of the magnetic unit cell:
17.2650 17.2650 14.1312 90.0000 90.0000 120.0000
Transformation from parent structure: (3**a**,3**b**,2**c**;0,0,0)
[View matrix form]

#1.13

BNS Magnetic Space Group: P_c31c (#159.64) (non-standard)
[View symmetry operations]
Transformation to a standard setting: (2/3**a**+1/3**b**,-1/3**a**+1/3**b**,**c**;1/9,2/9,0)
[View matrix form]
Systematic absences for this Magnetic Space Group via MAGNEXT

Links to other programs of the BCS

Magnetic Point Group: 3m1' (19.2.69)
[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 μB.*

[Show only magnetic atoms]
[Show all the atoms]

Use MVISUALIZE to:
Go to standard | Change setting | Domain-related equivalent descriptions

Label	Atom type	x	y	z	Multiplicity	Symmetry constraints on M	M_x	M_y	M_z	|M|
Ni1	**Ni**	**0.00000**	**0.00000**	**0.25000**	**18**	$m_x,2m_x,m_z$	**0.85**	**1.7**	**0.0**	**1.47**

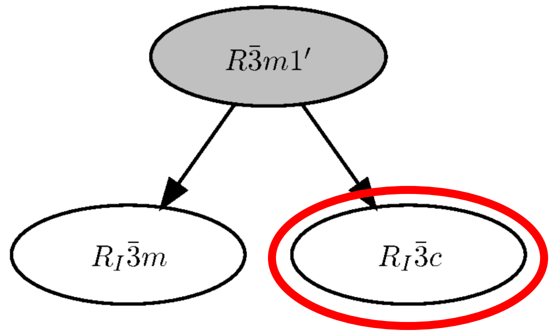
[Show all magnetic atoms in unit cell and their moment relations]

m_z is symmetry allowed, but zero

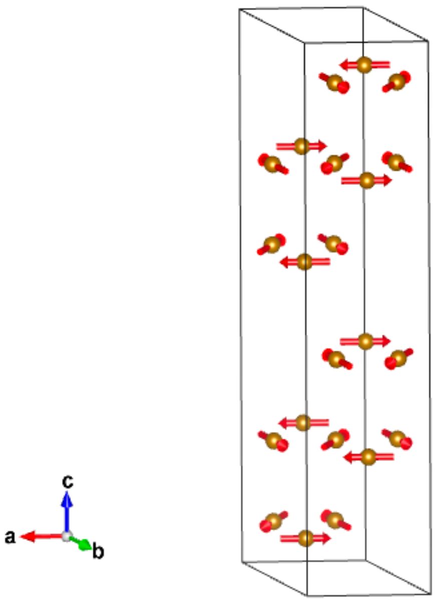
Active Irreps: *Irrep decomposition via* Get_mirreps

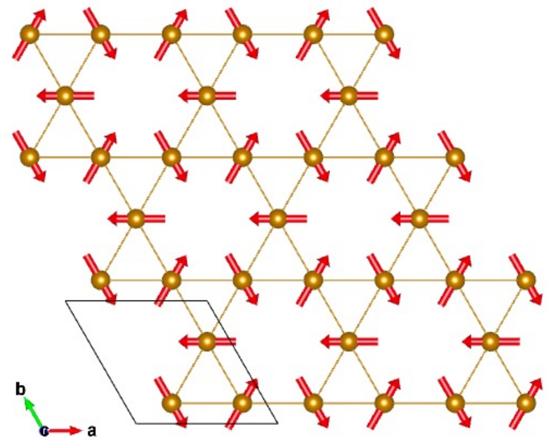
label	dim. full irrep	dim. small irrep	direction	action
mH3	4	2	special	primary

$KFe_3(OH)_6(SO_4)_2$
magndata 1.25



two possible k-maximal MSGs for a k-vector (0,0,3/2) and magnetic atom at
site 9d (0.5,0,0.5)



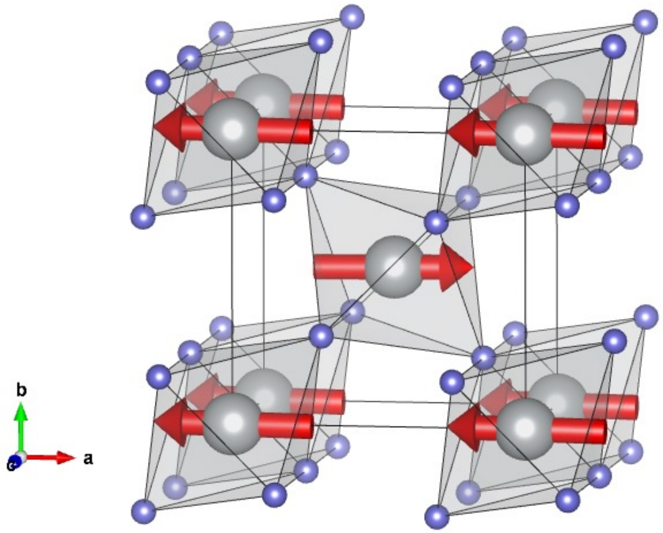


(about 70% of the structures have k-maximal symmetry)

24 possible spin arrangements were considered in the original paper!

NiF_2 magndata #0.36

"historical" weak ferromagnet



k=(0,0,0)

$P4_2/mnm1'$ → $Pnn'm'$ (b,-a,c;0,0,0**)**

k-maximal symmetry **weak FM along y**

- PNPD
- my = weak ferromagnetic component
- value of weak F component from macroscopic measurements
- **very small orthorhombic strain of the unit cell detected in other studies. A Pnnm structural model consistent with the magnetic symmetry has been reported (icsd 73728)**

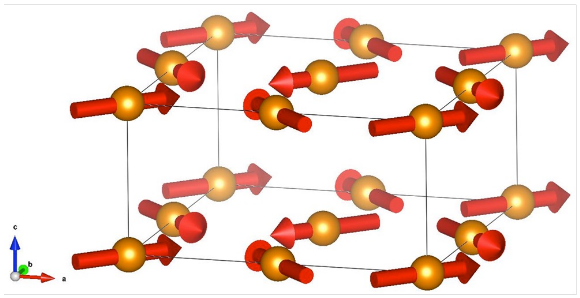
irrep mGM5 (2-dim), special direction

Label	Atom type	x	y	z	Multiplicity	Symmetry constraints on M	M_x	M_y	M_z	|M|
Ni	Ni	0.00000	0.00000	0.00000	2	$m_x,m_y,0$	-2.	0.03	0.0	2.00

FM component from a macroscopic measurement

weak FM is explained by the MSG of the structure

Multi-k structures



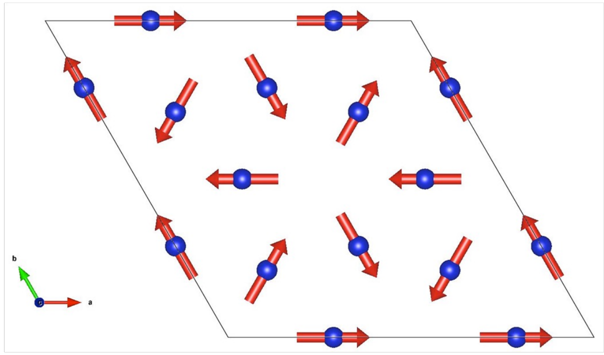
NdMg (#2.14)

Parent: *Pm-3m1'*

P_C4/nbm (2$\mathbf{a}_p$,2$\mathbf{b}_p$,$\mathbf{c}_p$; 0,0,0)

$\mathbf{k_1}$ = (1/2,0,0)

$\mathbf{k_2}$ = (0,1/2,0)



TmAgGe (#3.1)

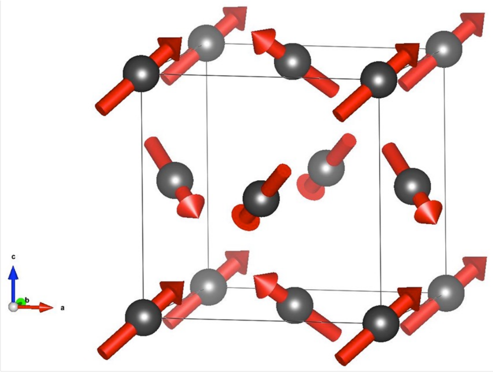
Parent: *P-62m1'*

P-6'2m' (2$\mathbf{a}_p$,2$\mathbf{b}_p$,$\mathbf{c}_p$; 0,0,0)

$\mathbf{k_1}$ = (1/2,0,0)

$\mathbf{k_2}$ = (1/2,1/2,0)

$\mathbf{k_3}$ = (0,1/2,0)



NpBi (#3.7)

Parent: *Fm-3m1'*

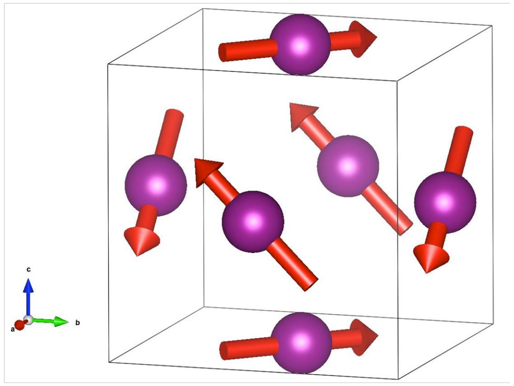
Pn-3m' ($\mathbf{a}_p$,$\mathbf{b}_p$,$\mathbf{c}_p$; 0,0,0)

$\mathbf{k_1}$ = (1,0,0)

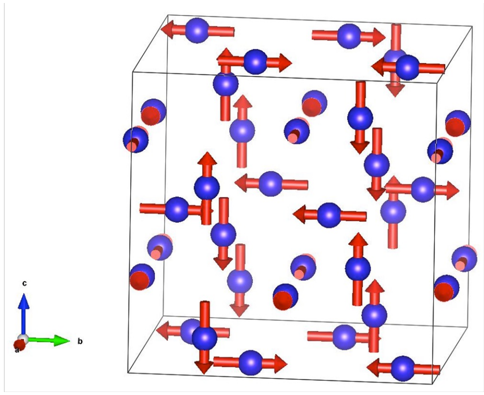
$\mathbf{k_2}$ = (0,1,0)

$\mathbf{k_3}$ = (0,0,1)

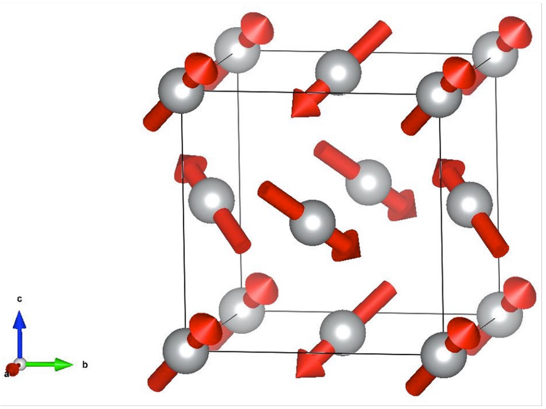
multiaxial structures that are single k:



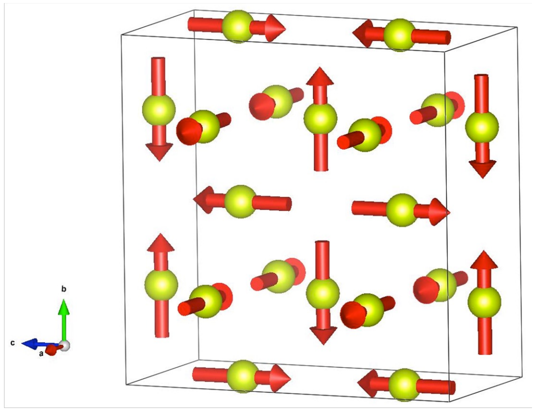
$Mn_3Cu_{0.5}Ge_{0.5}N$ (#0.74)
R-3m (#166.97)
k = (0, 0, 0)



$Dy_3Al_5O_{12}$ (#0.127)
Ia-3d’ (#230.148)
k = (0, 0, 0)

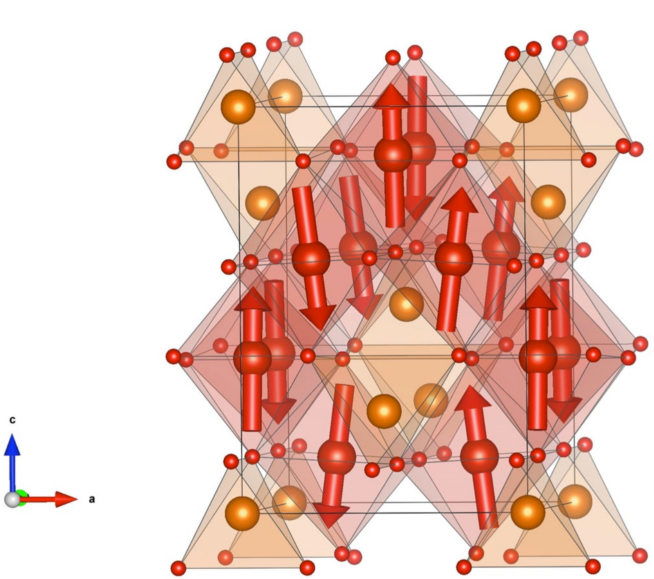


NiS_2 (#0.150)
Pa-3 (#205.33)
k = (0, 0, 0)

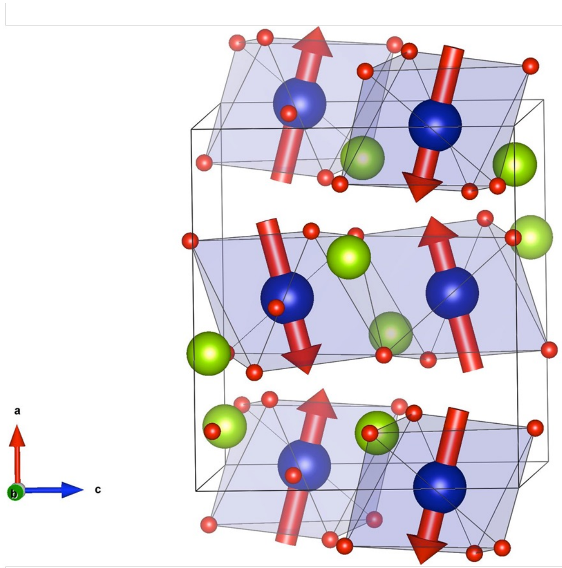


Ce_3NIn (#1.152)
P_C-4b2 (#117.305)
k = (0, 1/2, 1/2)

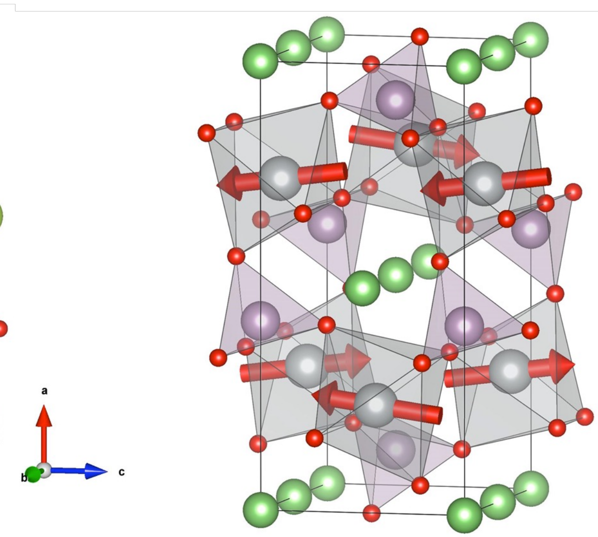
Spin canting vs. collinearity :



MgV_2O_4 (#1.138)
Parent group: *I-4m21’*
C_A222_1 ($\mathbf{a}_p+\mathbf{b}_p$,$-\mathbf{a}_p+\mathbf{b}_p$,$\mathbf{c}_p$;1/4,1/4,0)



$CoSe_2O_5$ (#0.119)
Parent group: *Pbcn1’*
Pb’cn ($\mathbf{a}_p$,$\mathbf{b}_p$,$\mathbf{c}_p$;0,0,0)



$LiNiPO_4$ (#0.88)
Parent group: *Pnma1’*
Pnm’a ($\mathbf{a}_p$,$\mathbf{b}_p$,$\mathbf{c}_p$;0,0,0)

spin canting consistent with the MSG

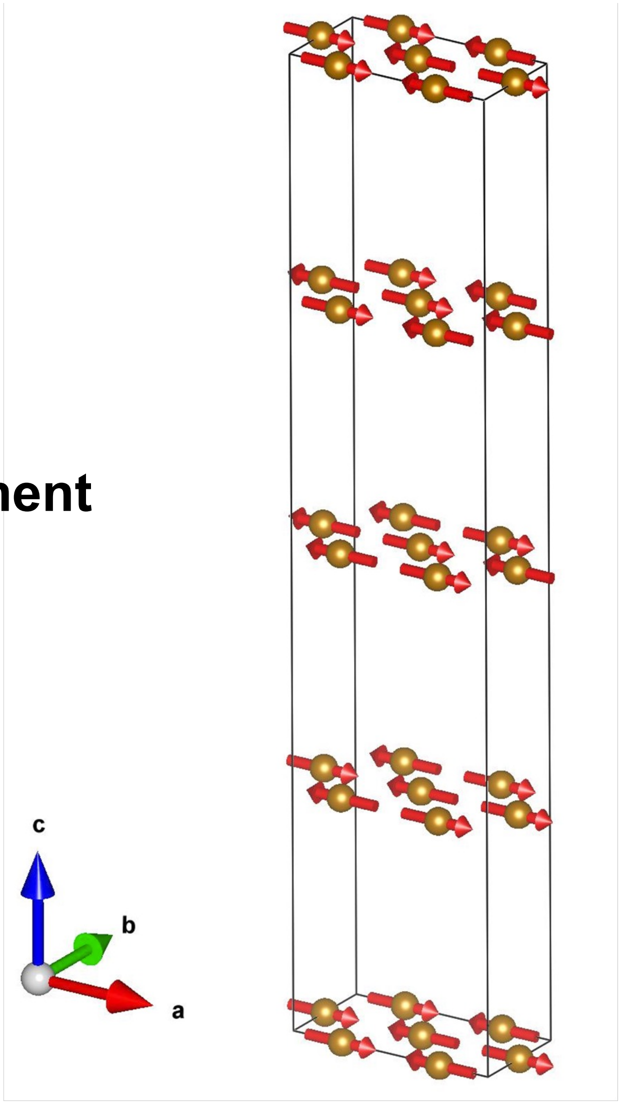
symmetry allowed spin canting is often observed
(specially with single crystal diffraction:
only 10% strict collinear structures are not forced by symmetry)

$La_2O_2Fe_2OSe_2$ (#1.58)

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

deceptive simplicity
of a collinear arrangement

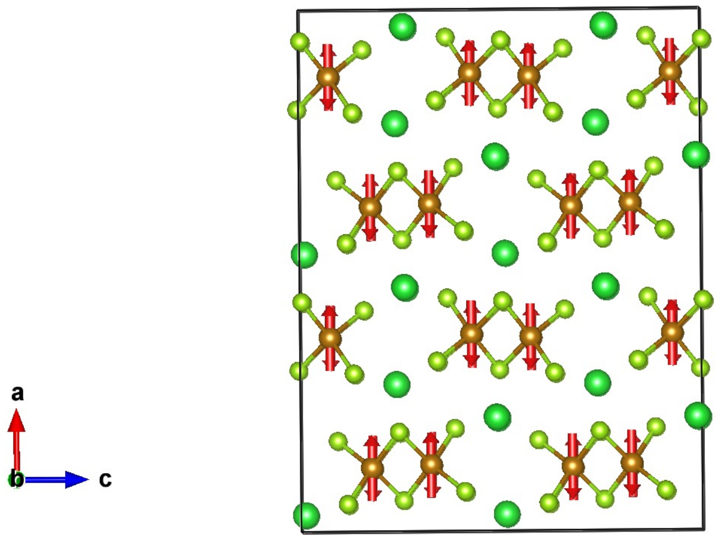
It requires 2 primary
Irreps !



$I4/mmm1' \rightarrow C_cc$ (**a**-**c**,**b**,**c**; 0,0,0) Polar symmetry !

Parent space group: *Pnma*

data: NPD

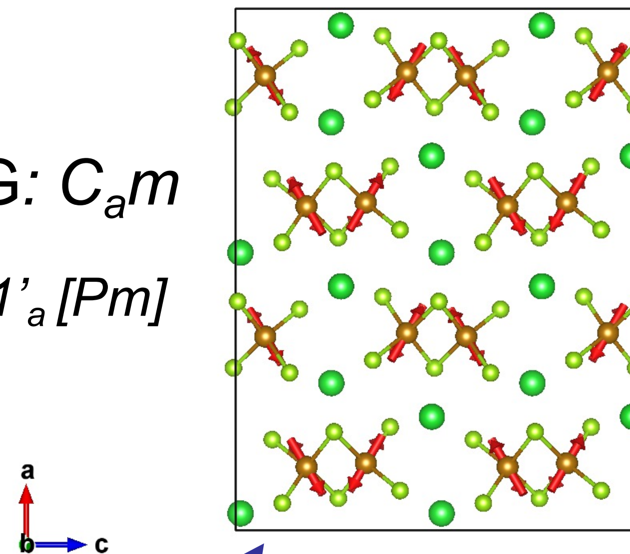


$BaFe_2Se_3$ #1.429

MSG: $C_a m$

Cm.1'$_a$ [Pm]

data: NSD

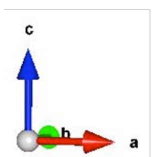


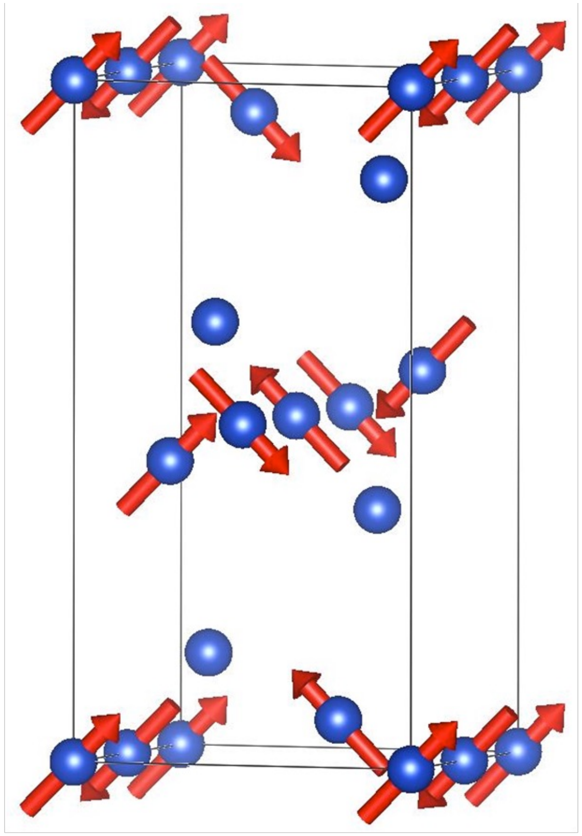
$BaFe_2Se_3$ #1.710

Label	Atom type	x	y	z	Multiplicity	Symmetry constraints on M	M_x	M_y	M_z	|M|
Fe1_1	Fe	0.24702	0.00074	0.17631	16	m_x,m_y,m_z	2.1	0.0	0.0	2.10
Fe1_2	Fe	0.00298	0.49926	0.42631	16	m_x,m_y,m_z	-2.1	0.0	0.0	2.10
Fe1_3	Fe	0.25298	0.25074	0.32369	16	m_x,m_y,m_z	-2.1	0.0	0.0	2.10
Fe1_4	Fe	0.49702	0.24926	0.07369	16	m_x,m_y,m_z	-2.1	0.0	0.0	2.10

different from zero when
better data is used. But same MSG

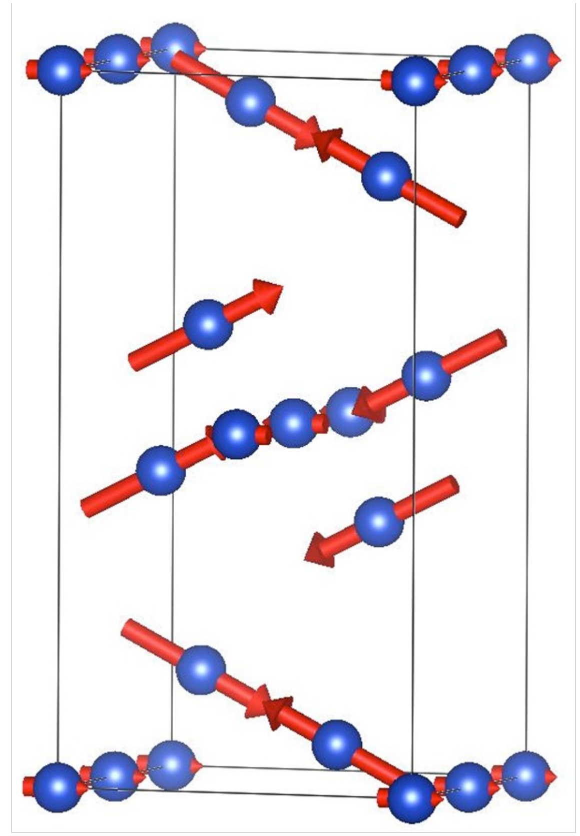
conflicting models:





$Cu_3Mo_2O_9$ (#0.129)

$P2_1'2_1'2_1$ ($\mathbf{a}_p$,-$\mathbf{c}_p$,$\mathbf{b}_p$;1/4,1/4,0)



$Cu_3Mo_2O_9$ (#0.130)

$Pm'c2_1'$ (-$\mathbf{b}_p$,-$\mathbf{c}_p$,$\mathbf{a}_p$;0,1/4,1/4)

Lattice parameters of the magnetic unit cell:
17.2650 17.2650 14.1312 90.0000 90.0000 120.0000
Transformation from parent structure: (3**a**,3**b**,2**c**;0,0,0)
[View matrix form]

#1.13

BNS Magnetic Space Group: P_c31c (#159.64) (non-standard)
[View symmetry operations]
Transformation to a standard setting: (2/3**a**+1/3**b**,-1/3**a**+1/3**b**,**c**;1/9,2/9,0)
[View matrix form]
Systematic absences for this Magnetic Space Group via MAGNEXT

Magnetic Point Group: 3m1' (19.2.69)
[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 μB*

[Show only magnetic atoms]
[Show all the atoms]

Use MVISUALIZE to:
Go to standard | Change setting | Domain-related equivalent descriptions

Label	Atom type	x	y	z	Multiplicity	Symmetry constraints on M	M_x	M_y	M_z	|M|
Ni1	**Ni**	**0.00000**	**0.00000**	**0.25000**	**18**	m_x,2m_x,m_z	**0.85**	**1.7**	**0.0**	**1.47**

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

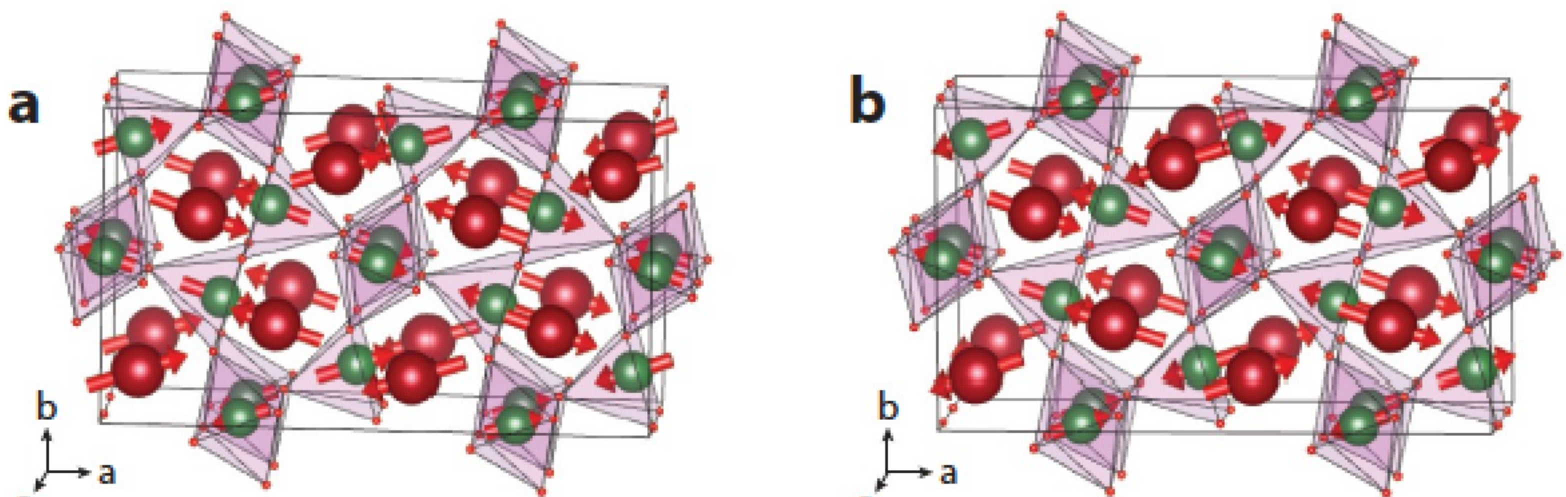
Active Irreps:

Irrep decomposition via Get_mirreps

label	dim. full irrep	dim. small irrep	direction	action
mH3	4	2	special	primary

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

Gd_2MnO_5 (magndata 1.54)

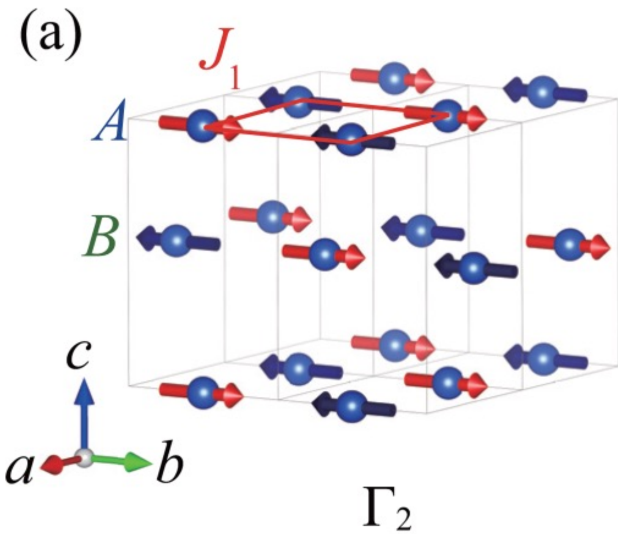


$P_a ca2_1$ (**a**, **c**, –**b**; –1/8, 0, 0) $P_a ca2_1$ (**a**, **c**, –**b**; 1/8, 0, 0)

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

Using MVISUALIZE…..

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

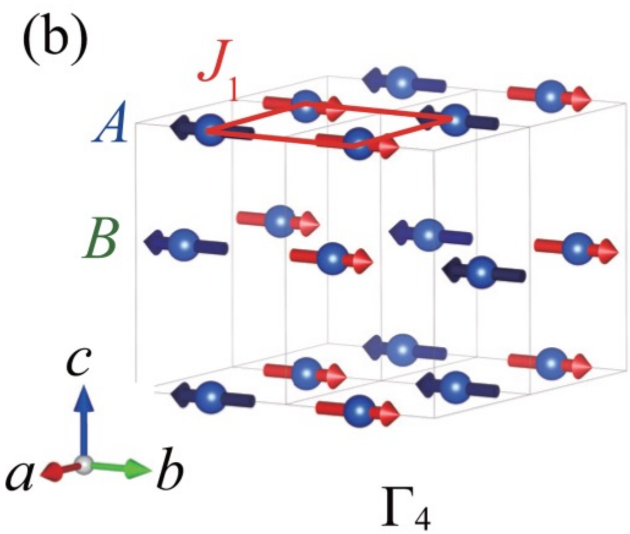


$SrLaCuSbO_6$ (MAGNDATA #1.674)

Phys. Rev. B (2022) **k**=(½ ½ 0)

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

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



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

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

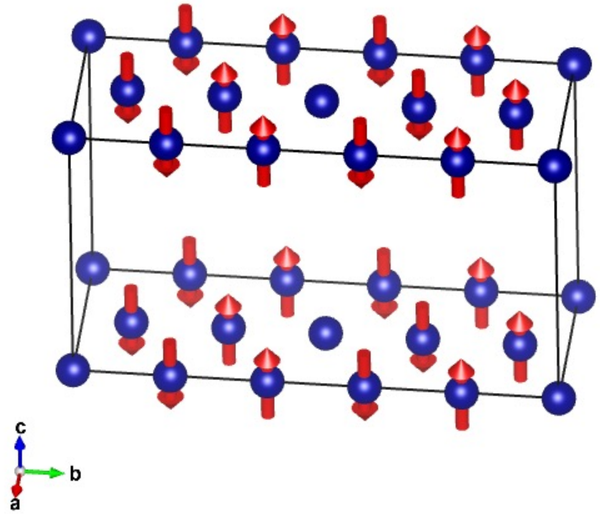
Some “dubious” structures:

1.0.1 Ag_2CrO_2

k=(1/5,1/5,0)

P-3m11’ -> C2’/m

trigonal **->** monoclinic
k-maximal symmetry



reported weak FM inconsistent with the symmetry.

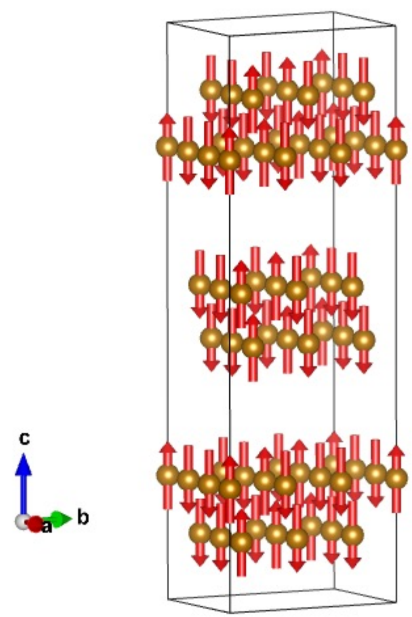
Equality of moments requires existence of reflections correponding to a 3**k** spin wave, and they were not observed.

1.0.7 $LuFe_2O_4$

k=(1/3,1/3,0)

R-3m1’ -> C2’/m’

trigonal **->** monoclinic
k-maximal symmetry



Claimed to be multiferroic, but Inconsistent with symmetry and structure

“Concomitant” structural transitions:

About 60% of the collected structures allow structural distortions forbidden in the paramagnetic phase

In most cases, these possible induced structural distortions are weak and remain unobserved.

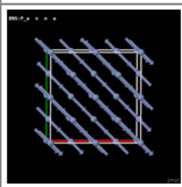
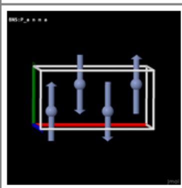
But for a few tens of structures a so-called concomitant or simultaneous structural phase transition is reported

In a majority of cases, the structural transition can be explained as a magnetostructural effect due to the magnetic symmetry break and a single phase transition exists.

The illustrative case of CrN:

Comment in entry (introduced in 2014!!): A Pnma distortion of the atomic positions is reported, but not fully defined. Not included here. The effective space group for atomic positions is not Pnma (62), as assumed in the reference, but Pmmn (59) (the family space group of the OG label of the MSG)….

Information table (2 entries found)

	N	Entry	Structure	Propagation vector(s)	Parent space group	Transformation from parent	Magnetic (super)space group	Magnetic point group
year 1960	1	1.28 CrN		1/2,1/2,0	Fm-3m (225) (standard)	(2**a**, 2**b**,**c**;0,0,0)	$P_a$nma (62.450) (1/2**a**+1/2**b**,-1/4**a**+1/4**b**,**c**;0,1/8,1/4)	mmm1' (8.2.25)
year 2022	2	1.678 CrN		1/2,1/2,0	Fm-3m (225) (standard)	(**a**+**b**,-1/2**a**+1/2**b**,**c**;1/2,3/4,1/4)	$P_a$nma (62.450) (standard)	mmm1' (8.2.25)

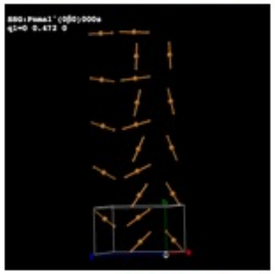
MSG OG symbol: $P_{2c}m'mn$ (59.9.486)

MSG Uni symbol: **62.450 *Pnma.1'$_a$[Pnmm]***

Comment in entry: The structure has a strong structural orthorhombic distortion according to the space group Pmmn, which is consistent with the MSG of the phase, and is concomitant with the magnetic transition….

INCOMMENSURATE STRUCTURES

One propagation vector

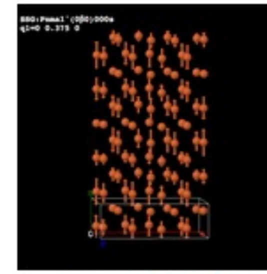


1.1.1 Cs_2CuCl_4

1.1.2 $RbFe(MoO_4)_2$

1.1.3 Cr

1.1.4 Cr

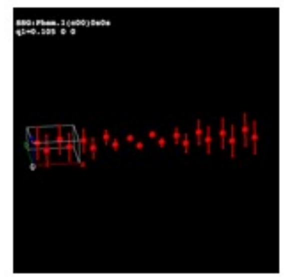


1.1.5 $CaFe_4As_3$

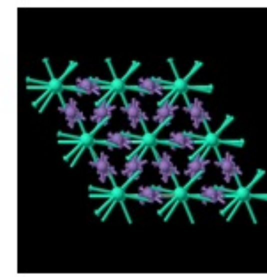
1.1.6 $TbMnO_3$

1.1.7 $TbMnO_3$

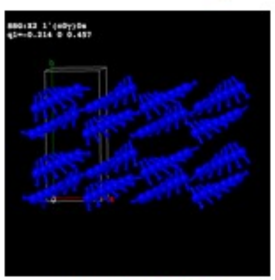
1.1.8 $TbMnO_3$



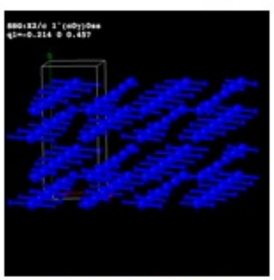
1.1.9 Ce_2Pd_2Sn



1.1.10 $DyMn_6Ge_6$

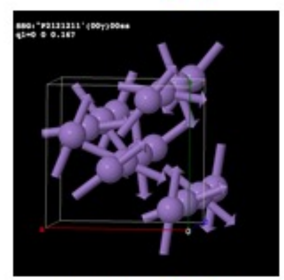


1.1.11 $MnWO_4$

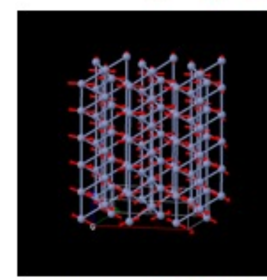


1.1.12 $MnWO_4$

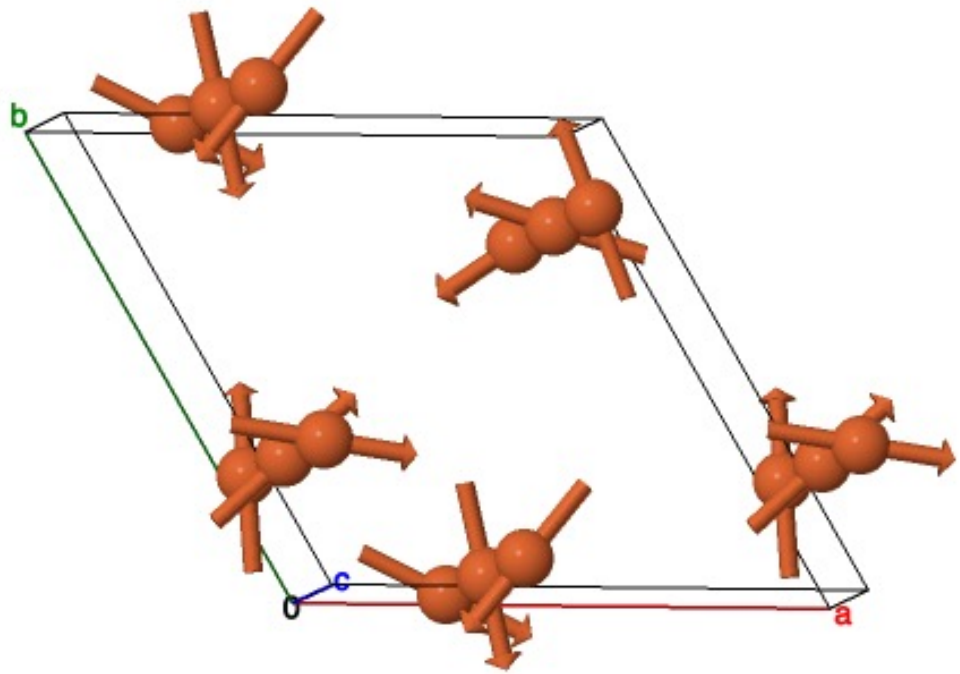
1.1.13 $MnAu_2$



1.1.14 MnGe



1.1.15 $CaCr_2O_4$



Symmetry described by a magnetic superspace group (MSSG)

$Ba_3NbFe_3Si_2O_{14}$ (#1.1.17)

P3211'(00γ)000s

Symmetry operations of the magnetic space group in the setting used:

N	(x,y,z)	Seitz notation
1	x1,x2,x3,x4,+1	{ 1 | 0 }
2	-x2,x1-x2,x3,x4,+1	{ 3^+_{001} | 0 }
3	-x1+x2,-x1,x3,x4,+1	{ 3^-_{001} | 0 }
4	x2,x1,-x3,-x4,+1	{ 2_{110} | 0 }
5	x1-x2,-x2,-x3,-x4,+1	{ 2_{100} | 0 }
6	-x1,-x1+x2,-x3,-x4,+1	{ 2_{010} | 0 }
(0,0,0,1/2)' + set		click here to show and hide

[Hide]

nature

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Massive surveys with the entries of MAGNDATA

nature > articles > article

Article | Published: 28 October 2020

High-throughput calculations of magnetic topological materials

Yuanfeng Xu, Luis Elcoro, Zhi-Da Song, Benjamin J. Wieder, M. G. Vergniory, Nicolas Regnault, Yulin Chen, Claudia Felser & B. Andrei Bernevig

Nature **586**, 702–707 (2020) | Cite this article

22k Accesses | **287** Citations | **105** Altmetric | Metrics

Abstract

The discoveries of intrinsically magnetic topological materials, including semimetals with a large anomalous Hall effect and axion insulators[1,2,3], have directed fundamental research in solid-state materials. Topological quantum chemistry[4] has enabled the understanding of and the search for paramagnetic topological materials[5,6]. Using magnetic topological indices

Screenshot

Recently three different groups from China report the identification of the spin space groups of the magnetic structures in MAGNDATA (relevant for their electronic band structure, if the SOC is negligible or weak)

PHYSICAL REVIEW X **14,** 031037 (2024)

Spin Space Groups: Full Classification and Applications

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[2] *Co-Innovation Center for New Energetic Materials, Southwest University of Science and Technology, Mianyang 621010, China*
[3] *Hefei National Laboratory, Hefei 230088, China*
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In this work, we exhaust all the spin space symmetries, which fully characterize collinear, noncollinear, and commensurate spiral as well as incommensurate spiral magnetism, etc., and investigate enriched features of electronic bands that respect these symmetries. We achieve this by systematically classifying the so-called spin space groups (SSGs)—joint symmetry groups of spatial and spin operations that leave the magnetic structure unchanged. Generally speaking, they are accurate (approximate) symmetries in systems where spin-orbit coupling (SOC) is negligible (finite but weaker than the energy scale of interest), but we also show that specific SSGs could remain valid even in the presence of strong SOC. In recent years, SSGs have played increasingly pivotal roles in various fields such as altermagnetism, topological electronic states, and topological magnon, etc. However, due to its complexity, a complete SSG classification has not been completed up to now. By representing the SSGs as $\mathrm{O}(N)$ representations, we—for the first time—obtain the complete classifications of 1421, 9542, and 56 512 distinct SSGs for collinear ($N = 1$), coplanar ($N = 2$), and noncoplanar ($N = 3$) magnetism, respectively. SSG not only fully characterizes the symmetry of spin degrees of freedom, but also gives rise to exotic electronic states, which, in general, form projective representations of magnetic space groups (MSGs). Surprisingly, electronic bands in SSGs exhibit features never seen in MSGs, such as (i) nonsymmorphic SSG Brillouin zone, where SSG operations behave as a glide or screw when acting on momentum, (ii) effective π flux, where translation operators anticommute with each other and yield duplicate bands, (iii) higher-dimensional representations unexplained by MSGs, and (iv) unconventional spin texture on a Fermi surface, which is completely determined by SSGs, independent of Hamiltonian details. To apply our theory, we identify the SSG for each of the 1595 published magnetic structures in the MAGNDATA database on the Bilbao Crystallographic Server. Material examples exhibiting the novel features (i)–(iv) are discussed with emphasis. We also investigate new types of SSG-protected topological electronic states that are unprecedented in MSGs. In particular, we propose a 3D $\mathbb{Z}_2$ topological insulator state with a fourfold degenerate Dirac point on the surface and a new scenario of anomalous $\mathbb{Z}_2$ helical states that appear on magnetic domain walls.

DOI: 10.1103/PhysRevX.14.031037

Subject Areas: Condensed Matter Physics, Magnetism, Topological Insulators

TABLE S2: Results of the space groups (SGs), magnetic space groups (MSGs) (with BNS number and OG number both listed), and spin-space groups (SSGs). We also give the label of materials in *MAGNDATA*[6, 76] from *Bilbao Crystallographic Server*.

Material	MAGNDATA label	SG	MSG (BNS)	MSG (OG)	SSG
$LaMnO_3$	0.1	$Pnma(62)$	62.448	62.8.509	62.1.2.5.L
$Cd_2Os_2O_7$	0.2	$Fd-3m(227)$	227.131	227.4.1631	227.1.24.2
Ca_3LiOsO_6	0.3	$R-3c(167)$	15.89	15.5.96	167.1.2.3.L
$NiCr_2O_4$	0.4	$I4_1/amd(141)$	70.530	70.4.619	141.1.1.1.L
Cr_2S_3	0.5	$R-3(148)$	2.4	2.1.4	148.1.1.1.L
$YMnO_3$	0.6	$P6_3cm(185)$	185.197	185.1.1429	185.1.12.1.P
$ScMnO_3$	0.7	$P6_3cm(185)$	185.201	185.5.1433	185.1.12.1.P
$ScMnO_3$	0.8	$P6_3cm(185)$	173.129	173.1.1360	185.1.12.1.P
GdB_4	0.9	$P4/mbm(127)$	127.395	127.9.1061	127.1.8.1.P
$DyFeO_3$	0.10	$Pnma(62)$	19.25	19.1.119	19.1.4.1.P
$DyFeO_3$	0.11	$Pnma(62)$	33.148	33.5.230	33.1.2.3.P
$U_3Ru_4Al_{12}$	0.12	$P6_3/mmc(194)$	63.461	63.5.515	63.1.4.9.P
$Ca_3Co_{2-x}Mn_xO_6$	0.13	$R-3c(167)$	161.69	161.1.1300	161.1.2.1.L
Gd_5Ge_4	0.14	$Pnma(62)$	62.444	62.4.505	62.1.2.3.L
MnF_2	0.15	$P4_2/mnm(136)$	136.499	136.5.1156	136.1.2.6.L
$EuTiO_3$	0.16	$I4/mcm(140)$	69.523	69.3.607	140.1.2.1.L
$FePO_4$	0.17	$Pnma(62)$	19.25	19.1.119	62.1.4.9.P
$BaMn_2As_2$	0.18	$I4/mmm(139)$	139.536	139.6.1184	139.1.2.2.L
$MnTiO_3$	0.19	$R-3(148)$	148.19	148.3.1249	148.1.2.1.L
$MnTe_2$	0.20	$Pa-3(205)$	205.33	205.1.1535	205.1.12.1
$PbNiO_3$	0.21	$R3c(161)$	161.69	161.1.1300	161.1.2.1.L
DyB_4	0.22	$P4/mbm(127)$	55.355	55.3.443	55.1.2.2.L
$Ca_3Mn_2O_7$	0.23	$Cmc2_1(36)$	36.174	36.3.251	36.1.2.3.L
$LiMnPO_4$	0.24	$Pnma(62)$	62.449	62.9.510	62.1.2.3.L
$NaOsO_3$	0.25	$Pnma(62)$	62.448	62.8.509	62.1.2.6.L

PHYSICAL REVIEW B **106**, 144402 (2022)

Editors' Suggestion

Ferroaxial moment induced by vortex spin texture

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(Received 16 June 2022; accepted 21 September 2022; published 4 October 2022)

We list the candidate materials to exhibit the ferro-axial moment under the magnetic orderings in Table V in accordance with MAGNDATA, the magnetic structures database [188, 189]. The materials hosting the vortex spin configurations in the hexagonal crystal struc-

TABLE V. Candidate materials to possess the ferro-axial moment under the magnetic orderings.

MPG	Materials
$6/m'$	$U_{14}Au_{51}$ [144]
6	$ScMnO_3$ [145], $Yb_{0.42}Sc_{0.58}FeO_3$ [146], $BaCoSiO_4$ [147]
$\bar{6}'$	$Cu_{0.82}Mn_{1.18}As$ [148], $Tb_{14}Ag_{51}$ [149]
$\bar{3}'$	$MgMnO_3$ [150], Yb_3Pt_4 [151]
3	Cu_2OSeO_3 [152], Mn_2FeMoO_6 [153]
$4/m'$	$(K,Rb)_yFe_{2-x}Se_2$ [154], $TlFe_{1.6}Se_2$ [155], $K_{0.8}Fe_{1.8}Se_2$ [156], NdB_4 [157]
4	Ce_5TeO_8 [158]
$\bar{4}'$	$CsCoF_4$ [159]
$2/m'$	$LiFePO_4$ [160], $(Co, Fe)_4Nb_2O_9$ [161–165], $ErGe_3$ [166], $CaMnGe$ [167], $KFeSe_2$ [168], $Fe_2Co_2Nb_2O_9$ [169]
2	$LiFeP_2O_7$ [170], $SrMn(VO_4)(OH)$ [171], $DyCrWO_6$ [172], $Ba_3MnSb_2O_9$ [173], $HoNiO_3$ [174]
m'	$MnTiO_3$ [175], $ScFeO_3$ [176], $GaFeO_3$ [177], Ce_2PdGe_3 [178], Mn_3O_4 [179]
$\bar{1}'$	$CaMnGe_2O_6$ [180], $MnPSe_3$ [181, 182], $BaNi_2P_2O_8$ [183], $YbMn_2Sb_2$ [184], $NaCrSi_2O_6$ [185], $CaMn_2Sb_2$ [186]
1	CuB_2O_4 [187]

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Classification of second harmonic generation effect in magnetically ordered materials

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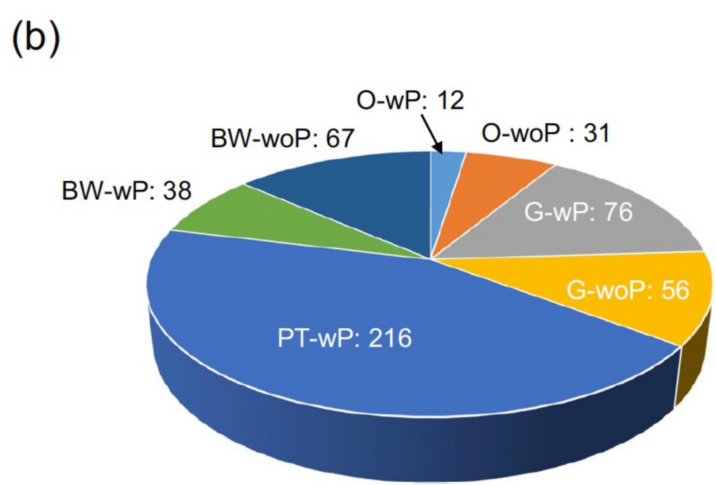

Fig. 3 Statistics on the SHG types in the MAGNDATA database. **a** Counting of materials with SHG and LMO effects in the 1432 magnetic structures (removing duplicate data). **b** Classification of the 496 magnetic structures with SHG effect. The detailed information of every material is presented in Supplementary Note 6.

points are not equivalent (as illustrated in the inset of Fig. 4g). Since its MSG is $P\overline{3}'m'1$, the corresponding SHG effect belongs to the PT-wP type. Its SHG tensor has only the odd part, and the SHG tensor is constrained by the 32 (D_3) symmetry. The calculated SHG coefficients are shown in Fig. 4h, which are consistent with our symmetry analysis. Indeed, the SHG effect in bilayer VBr_2 with A-type AFM magnetism reverses with the magnetic order, similar to that of bilayer CrI_3[25,61].

Example 2. SHG effect of $RMnO_3$ with various magnetic structures

The parent phase of $RMnO_3$ (R = Sc, Y, In, Dy, Ho, Er, Tm, Yb, and Lu) usually adopts the non-centrosymmetric structure with SG $P6_3cm$, as presented in Fig. 5a. The magnetism primarily arises from the Mn^{3+}, forming approximately equilateral triangles, as illustrated in the bottom panel of Fig. 5b. Below the Néel temperature, the strong super-exchange leads to 120° arrangement of the spins of Mn^{3+} in the basal plane, and small displacements of Mn^{3+} ions (occupy 6*c* positions, see Supplementary Table VIII) break the triangular frustration.

According to the MAGNDATA database and refs. [11,16,17,17,62–65],

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Editors' Suggestion

Symmetry analysis with spin crystallographic groups: Disentangling effects free of spin-orbit coupling in emergent electromagnetism

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IV. HIGH-THROUGHPUT SYMMETRY ANALYSIS OF SPIN GROUP SYMMETRY

The computational search for the spin space group allows us to identify physical properties free from the SOC effect [38,42]. We present symmetry analysis with dozens of observed spin configurations obtained from MAGNDATA [39,40]. We have performed the symmetry analysis of 1512 magnetic materials which have no site disorder. For the spin-structure dimension, 914 collinear, 403 coplanar, and 195 noncoplanar spin systems are studied. The magnetic materials are numbered by following the identification number provided in MAGNDATA such as Cr_2O_3 (No. 0.59).

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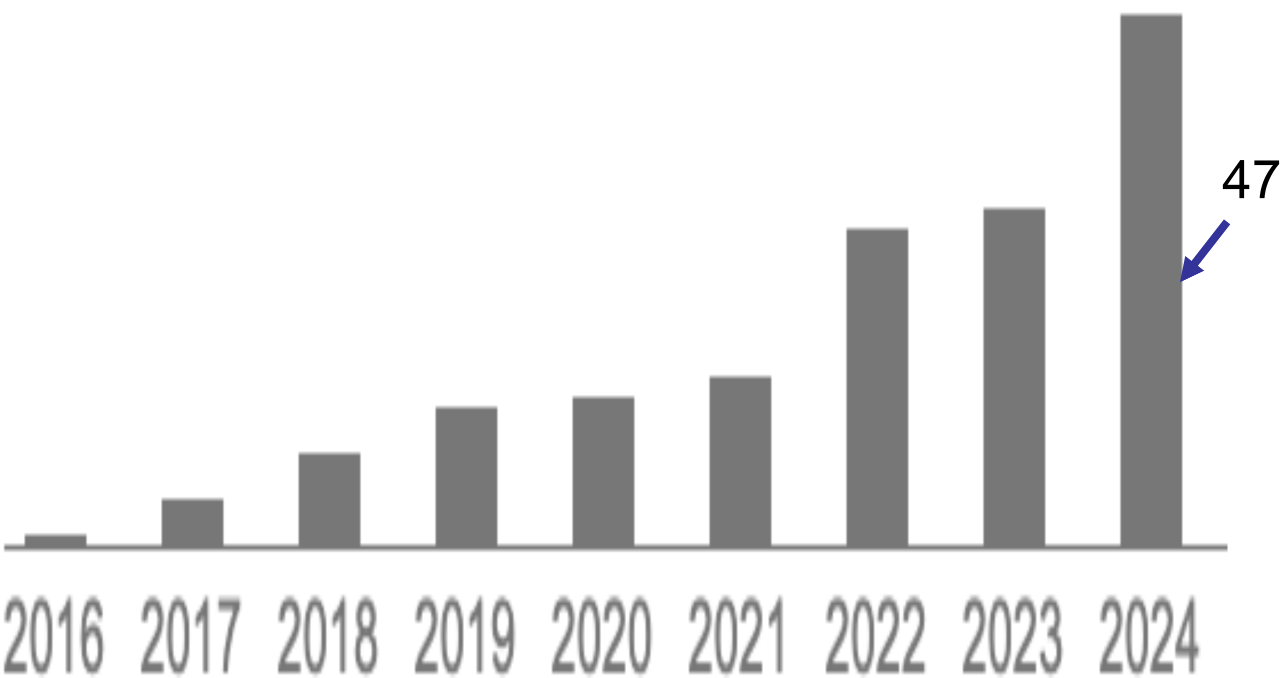
Unconventional magnons in collinear magnets dictated by spin space groups

Xiaobing Chen, Yuntian Liu, Pengfei Liu, Yutong Yu, Jun Ren, Jiayu Li, Ao Zhang & Qihang Liu

lines and charge-4 octuple points. On the basis of the MAGNDATA database[18], we identified 498 collinear magnets with unconventional magnons, among which more than 200 magnon band structures were obtained by using first-principles calculations and linear spin wave theory. In addition, we evaluated the influence of the spin–orbit-

Publications citing MAGNDATA (commensurate article)

(159 citations up to 2024)



In the long term MAGNDATA can only be kept updated, if the authors actively PARTICIPATE and directly SUBMIT their new published structures to the database in the form of magCIF files. This can be easily done following the instructions available in the webpage of the program

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

Log in

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

A database of more than 1000 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,

View Full Database

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

Enter the label of the structure: Submit

Advanced Search & Statistics

To upload any published structure click HERE

Submit your structure(s) if you wish that this database keeps updated!

MAGNDATA File Upload Page

Welcome to MAGNDATA File Upload Section. Any published commensurate magnetic structure that is not already present in MAGNDATA can be uploaded here.

- The upload can be performed not only by the authors of the publication reporting the structure, but also by anybody, thinking that this structure should be in this database.
- The uploaded files, if consistent, will be processed and transformed by the Bilbao Crystallographic Server team into a more complete form to be included in the database.
- Once the structure has been finally included in MAGNDATA, the uploader will be informed by e-mail. Also, in case we encounter any problems / have some questions & comments about the data, it is essential that we have your e-mail information.
- The necessary upload 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.

  To download the instructions on how to prepare a .mcif file of the magnetic structure that can be uploaded in MAGNDATA click here.

If you are using one of the mainstream refinement programs, it can produce already a mcif file of your model, which can be easily transformed for the submission following the instructions available online

Before proceeding to the file uploads, please provide your name, email and brief info *(info being optional)*. Once you have submitted these information, you'll be taken to the file submission page.

Your Name:
Your e-mail:

Brief info about the structure you are about to submit:

Proceed to File Uploads

Instructions for the preparation of a magCIF file of a (published) commensurate magnetic structure, for uploading in the database MAGNDATA at the Bilbao Crystallographic Server.

In order to upload a commensurate magnetic structure in MAGNDATA only two files are required . One is a pdf file of the published article where this magnetic structure was reported, and the other one must be a magCIF file with the necessary information on the magnetic structure.

We call a magCIF file a CIF file, which uses the so-called magCIF extension for the description magnetic structures. In the Bilbao crystallographic server such type of files are given the extension ".mcif ", to be distinguished from CIF files of ordinary non-magnetic structures with the extension ".cif".

The magCIF file to be introduced in MAGNDATA must fulfill some specific requirements and these instructions explain in detail how to prepare it to be fully adapted for MAGNDATA.

How to properly report a magnetic structure in publications and prepare a magCIF file for MAGNDATA?

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This article is part of a collection of articles in a focused issue on Magnetic Structures.[wording ok?]

Keywords: IUCr Commission on Magnetic Structures; magnetic structures; magnetic space groups; representation analysis; magnetic CIF; guidelines.

Guidelines for communicating commensurate magnetic structures. A report of the International Union of Crystallography Commission on Magnetic Structures

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