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

Universidad del País Vasco
Euskal Herriko Unibertsitatea

The MAGNDATA database and how to properly report a magnetic structure

J. Manuel Perez-Mato
Facultad de Ciencia y Tecnología
Universidad del País Vasco, UPV-EHU
BILBAO, SPAIN

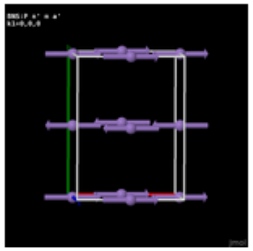
MAGNDATA: A Collection of magnetic structures with portable cif-type files

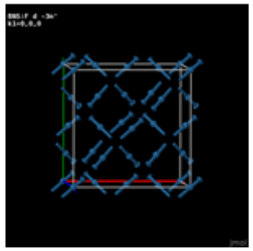
Element search (separate with space or comma): ⦿AND ○OR Search

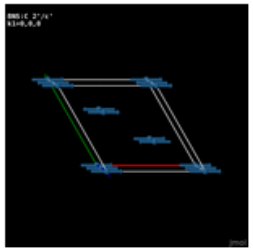
312 structures found

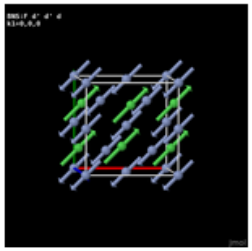
Update: by Nov 2024 it contains about 2200 structures

Zero propagation vector


0.1 $LaMnO_3$


0.2 $Cd_2Os_2O_7$


0.3 Ca_3LiOsO_6

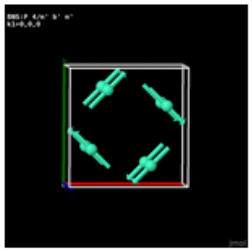

0.4 $NiCr_2O_4$

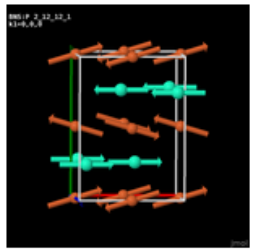

0.5 Cr_2S_3


0.6 $YMnO_3$


0.7 $ScMnO_3$


0.8 $ScMnO_3$


0.9 GdB_4


0.10 $DyFeO_3$

$Sr_2F_2Fe_2OS_2$ (MAGNDATA #2.2)

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)

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

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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

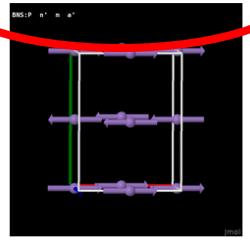
Element search (separate with space or comma): AND OR Search Advanced Search & Statistics

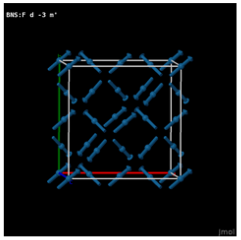
Enter the label of the structure: Submit

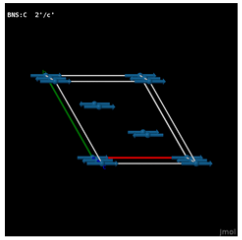
614 structures found

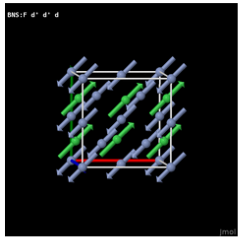
label 0.n

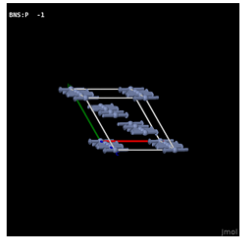
Zero propagation vector

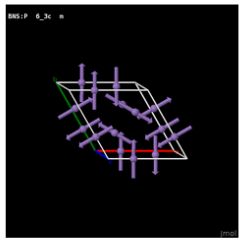

0.1 $LaMnO_3$

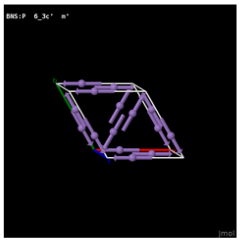

0.2 $Cd_2Os_2O_7$


0.3 Ca_3LiOsO_6

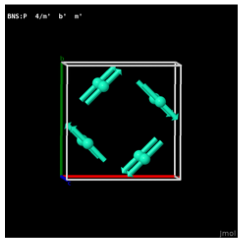

0.4 $NiCr_2O_4$

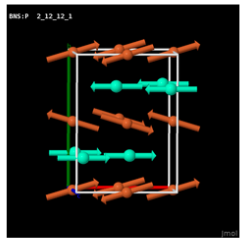

0.5 Cr_2S_3

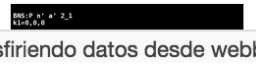

0.6 $YMnO_3$


0.7 $ScMnO_3$


0.8 $ScMnO_3$


0.9 GdB_4


0.10 $DyFeO_3$



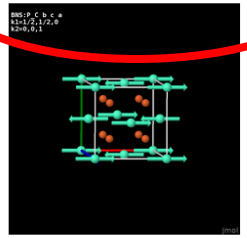
Transfiriendo datos desde webbdcrista1.ehu.es...

k=(0,0,0) → (no antitranslation)

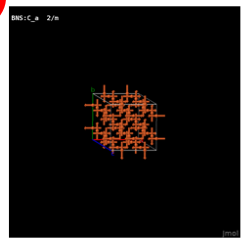
k=0 – structures (**Type I or III MSG symmetry**). The most interesting ones for magneto-structural properties! (magnetic point group without time reversal)

labels 2.n and 3.n

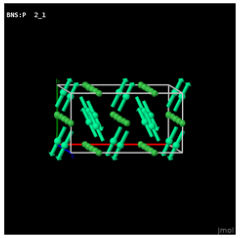
Two propagation vectors



2.1 $EuFe_2As_2$

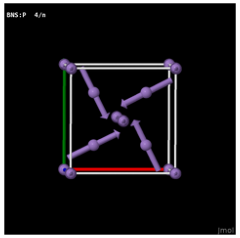


2.2 $Sr_2F_2Fe_2OS_2$

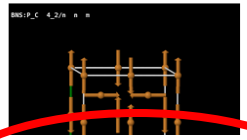


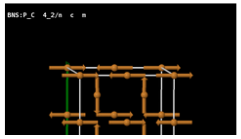
2.3 $HoNiO_3$

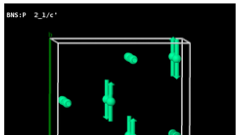
2.4 $Eu(Fe_{0.82}Co_{0.18})As_2$

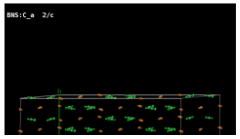


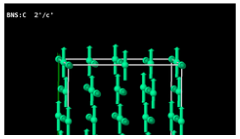
2.5 Mn_3CuN



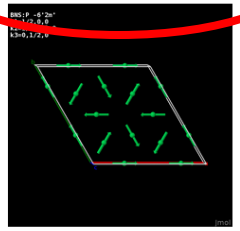




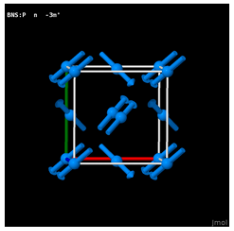




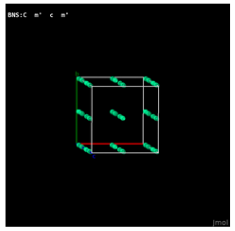
Three propagation vectors



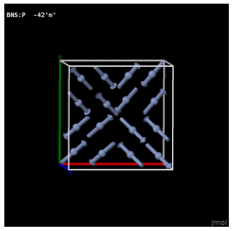
3.1 TmAgGe



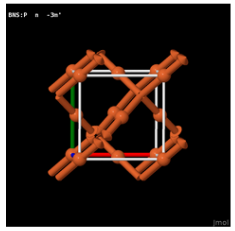
3.2 UO_2



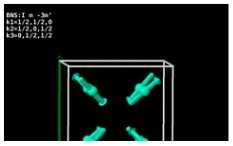
3.3 Ho_2RhIn_8

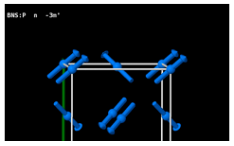


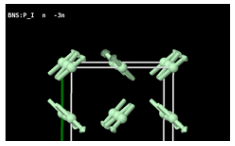
3.4 $MgCr_2O_4$

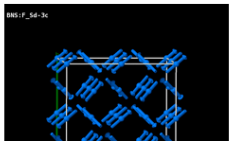


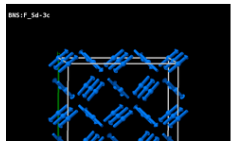
3.5 $Fe_{0.7}Mn_{0.3}$







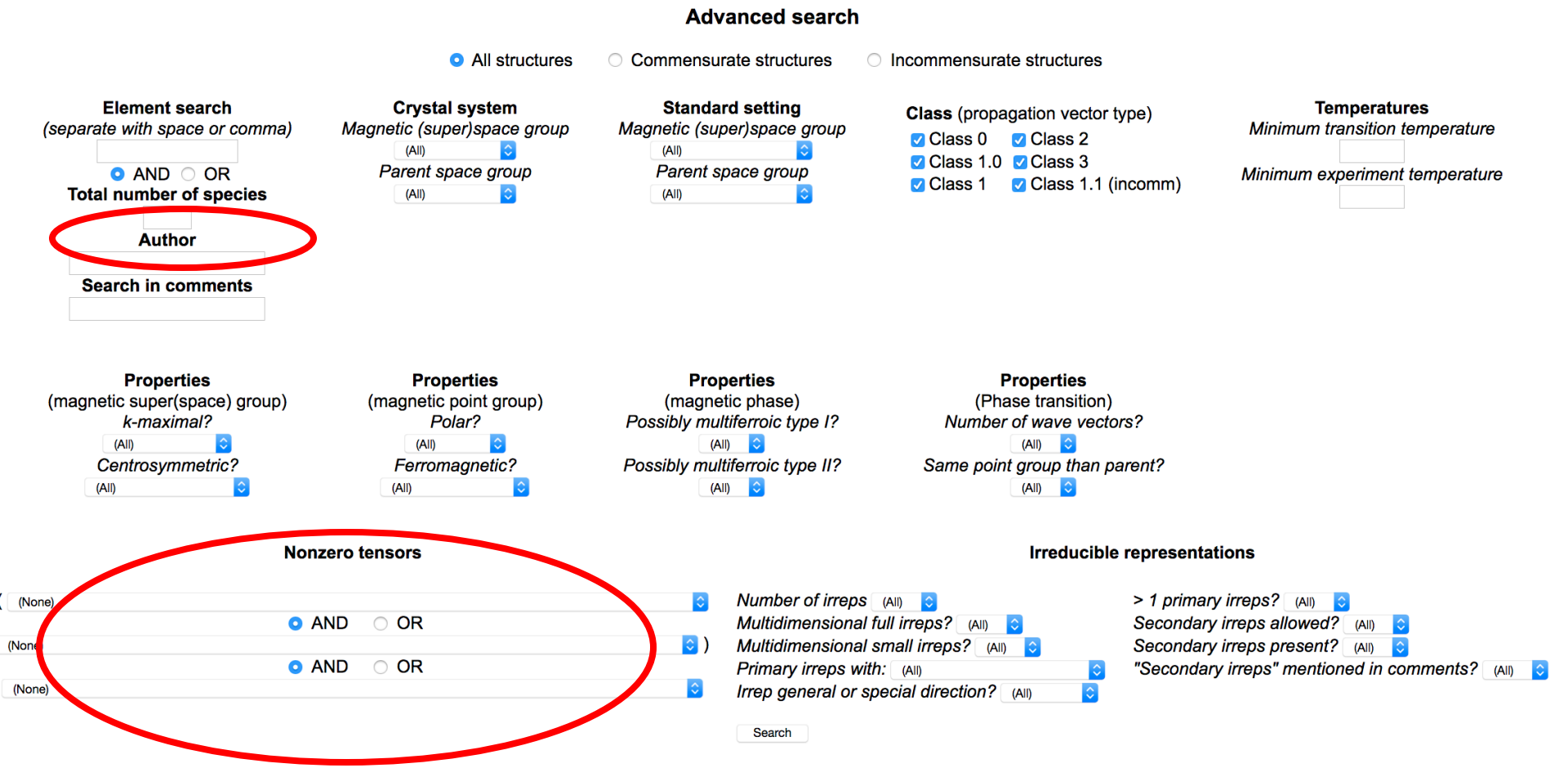




2k and ≥3k structures

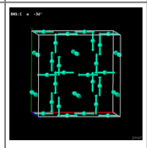
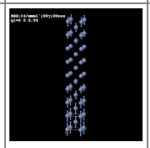
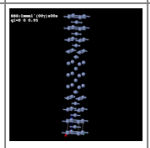
All types of MSG symmetries (with and without antitranslations)

Search optional filters

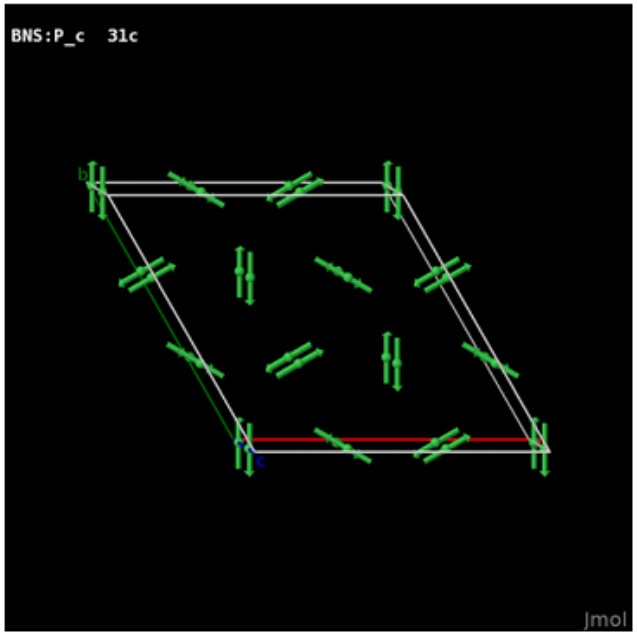


ordering according to parent space group

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

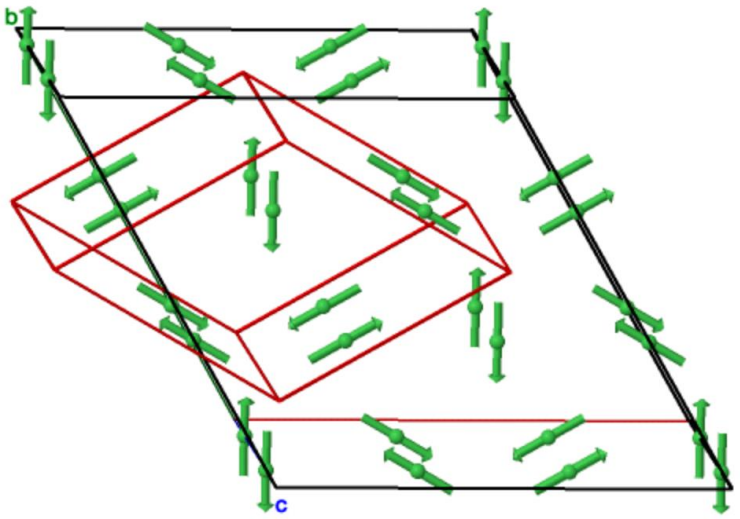
MAGNDATA Structure Viewer: 3D Visualization of magnetic structures with Jmol

$Ba_3Nb_2NiO_9$ (#1.13)

MAGNDATA Main Page

Show/Hide File

BNS:P_c 31c



2/3a+1/3b,-1/3a+1/3b,c;1/9,2/9,0

JSmol

help | console | Execute

Working 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

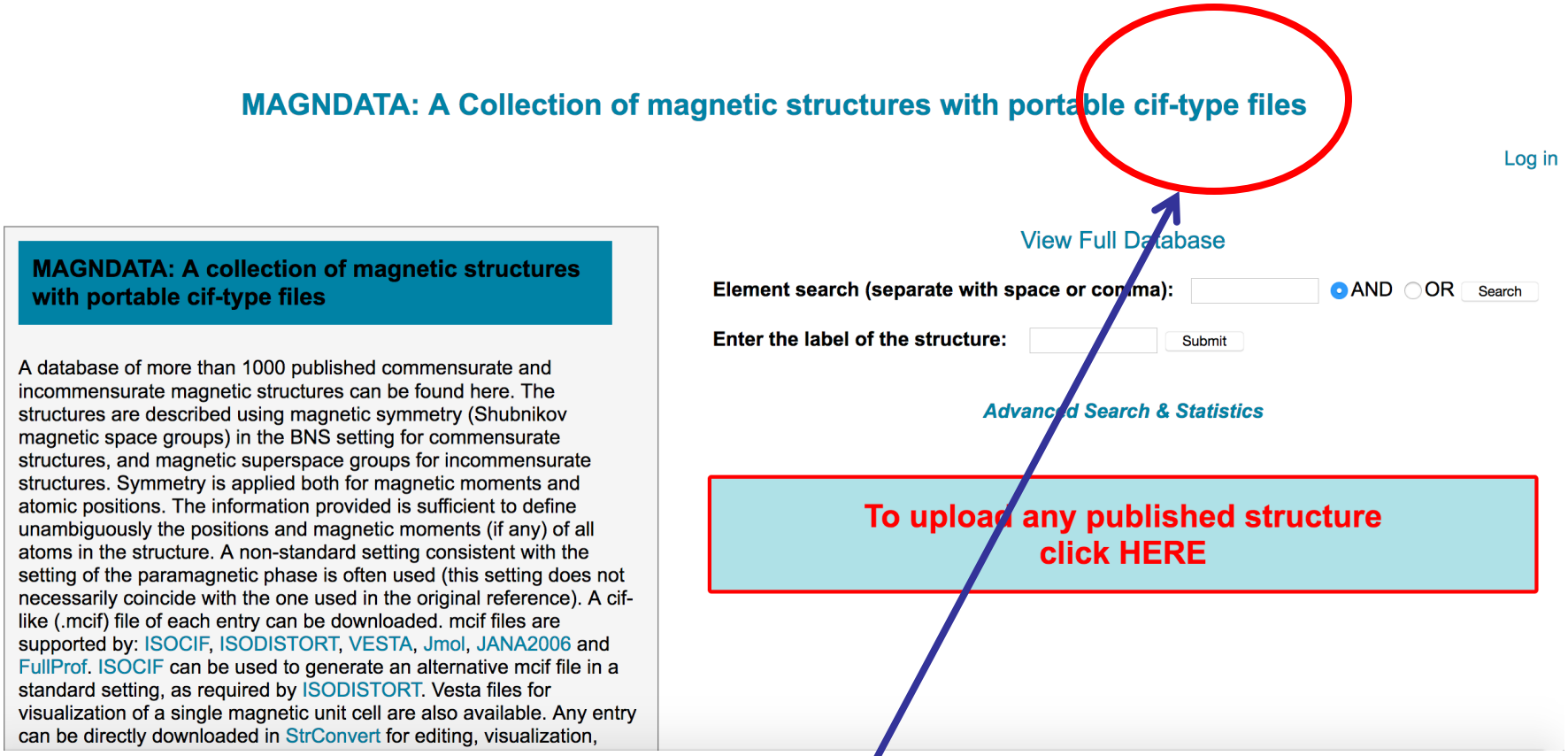
White
Toggle Quality
Center

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
Delete all drawings



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

```
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_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"
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_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_
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_space_group_symop_magn_operation.xyz
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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)

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]

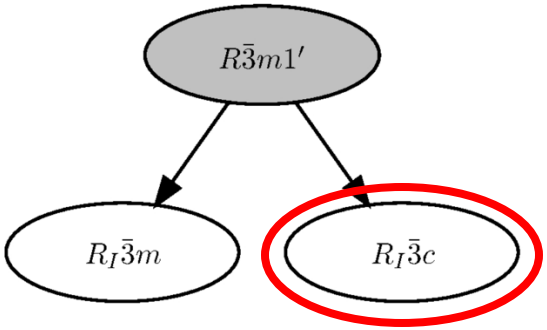
m_z is symmetry allowed, but zero

Active Irreps: *Irrep decomposition via* Get_mirreps

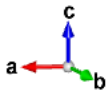
label	dim. full irrep	dim. small irrep	direction	action
mH3	4	2	special	primary

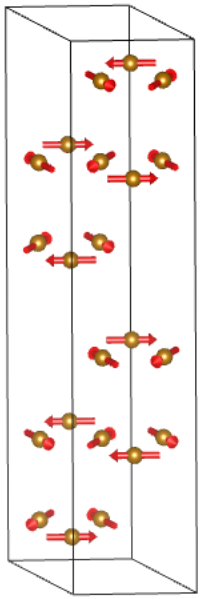
$KFe_3(OH)_6(SO_4)_2$

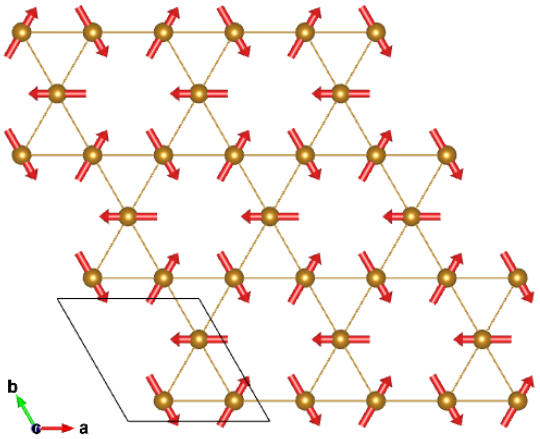
magndata 1.25



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





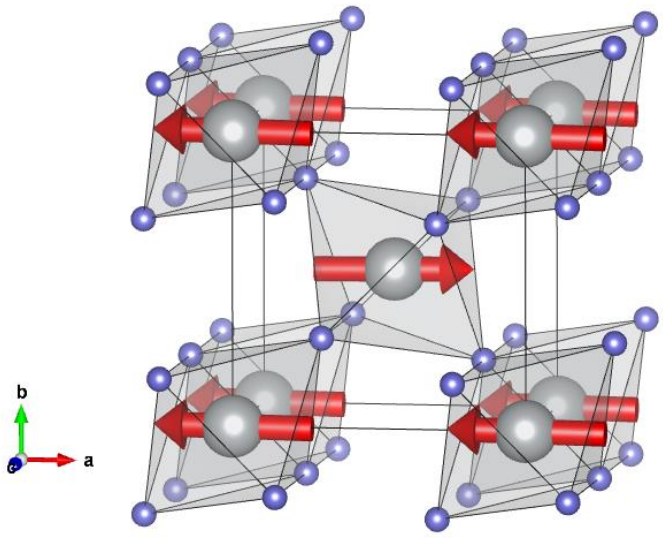


(about 70% of the structures have k-maximal symmetry)

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)**

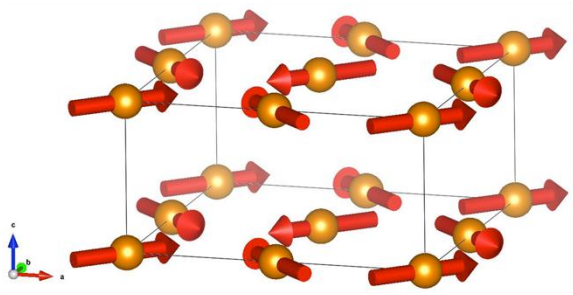
irrep mGM5 (2-dim), special direction

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

weak FM is explained by the MSG of the structure

FM component from a macroscopic measurement

Multi-k structures



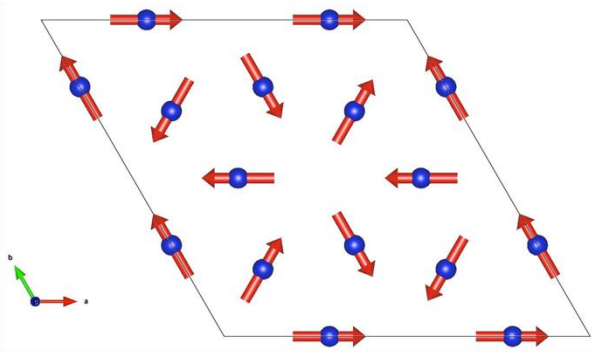
NdMg (#2.14)

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)

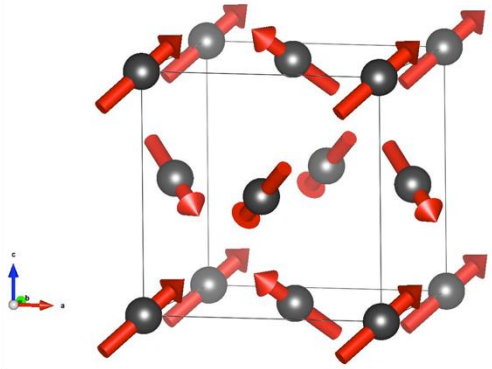
Parent: *P-62m1'*

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'*

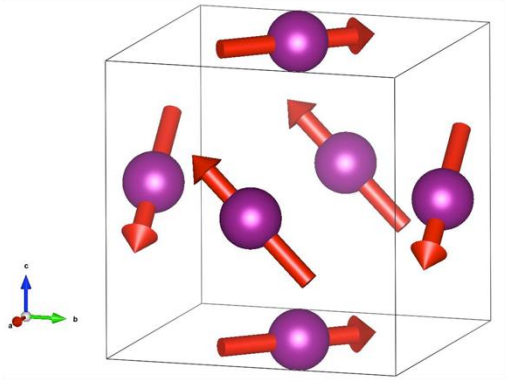
Pn-3m' ($\mathbf{a}_p, \mathbf{b}_p, \mathbf{c}_p$; 0,0,0)

$\mathbf{k}_1 = (1,0,0)$

$\mathbf{k}_2 = (0,1,0)$

$\mathbf{k}_3 = (0,0,1)$

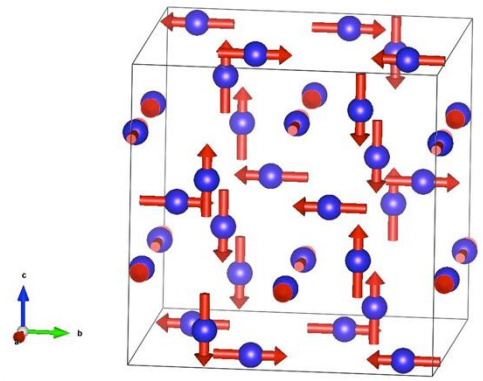
multiaxial structures that are single k:



$Mn_3Cu_{0.5}Ge_{0.5}N$ (#0.74)

R-3m (#166.97)

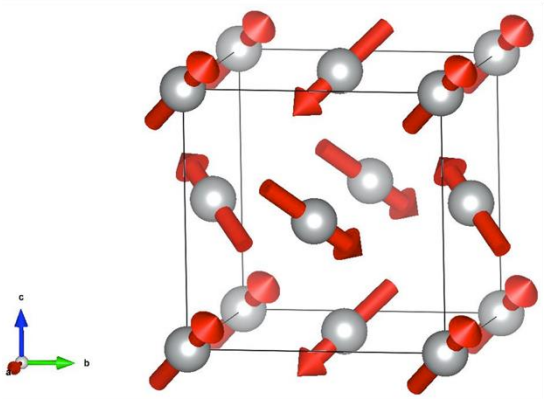
k = (0, 0, 0)



$Dy_3Al_5O_{12}$ (#0.127)

Ia-3d' (#230.148)

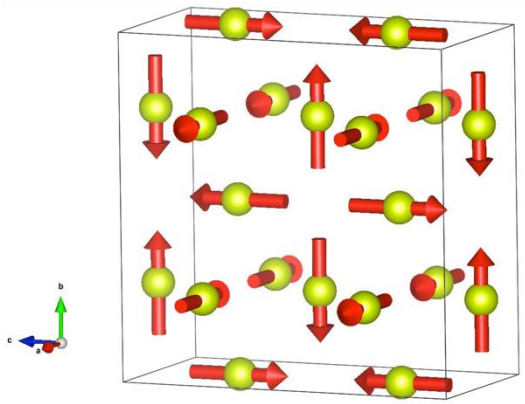
k = (0, 0, 0)



NiS_2 (#0.150)

Pa-3 (#205.33)

k = (0, 0, 0)

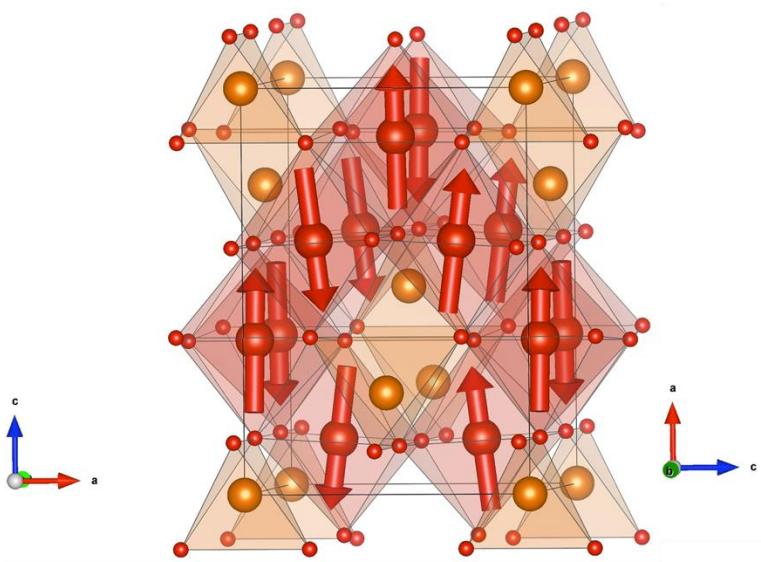


Ce_3NIn (#1.152)

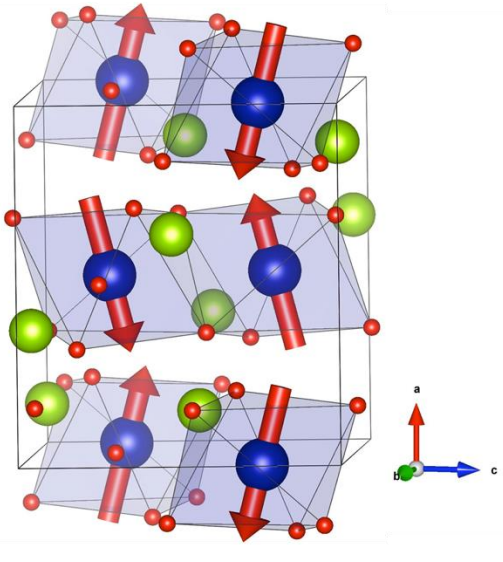
P_C*-4b2* (#117.305)

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

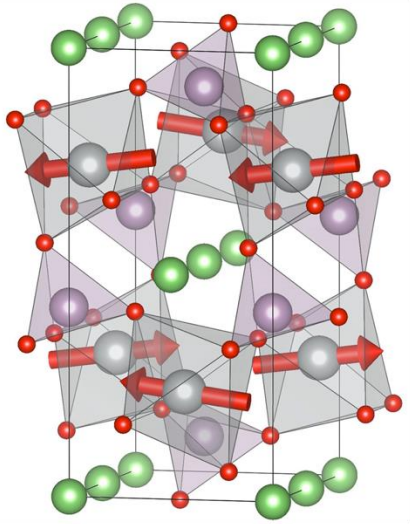
Spin canting vs. collinearity :



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)



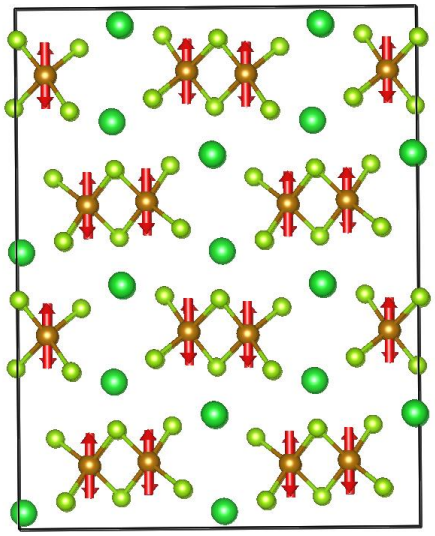
$LiNiPO_4$ (#0.88)
Parent group: *Pnma1'*
Pnm'a ($\mathbf{a}_p$,$\mathbf{b}_p$,$\mathbf{c}_p$;0,0,0)

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)

Parent space group: *Pnma*

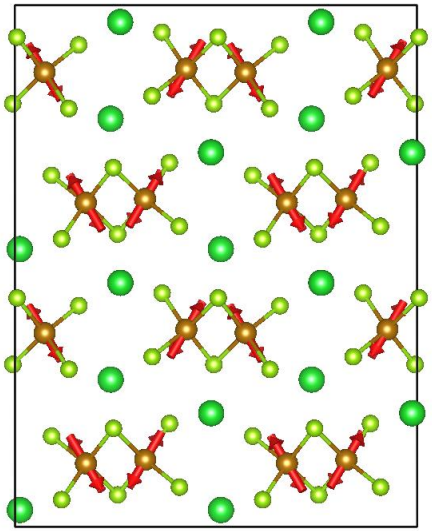
data: NPD

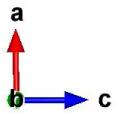


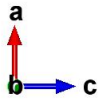
MSG: C_am

$Cm.1'_a[Pm]$

data: NSD







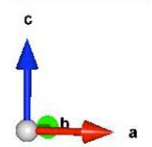
$BaFe_2Se_3$ #1.429

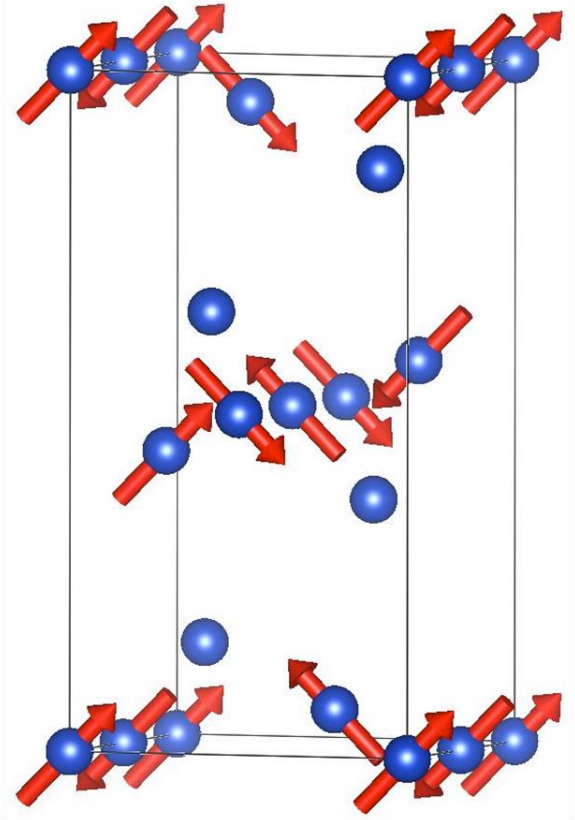
$BaFe_2Se_3$ #1.710

Label	Atom type	x	y	z	Multiplicity	Symmetry constrains 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

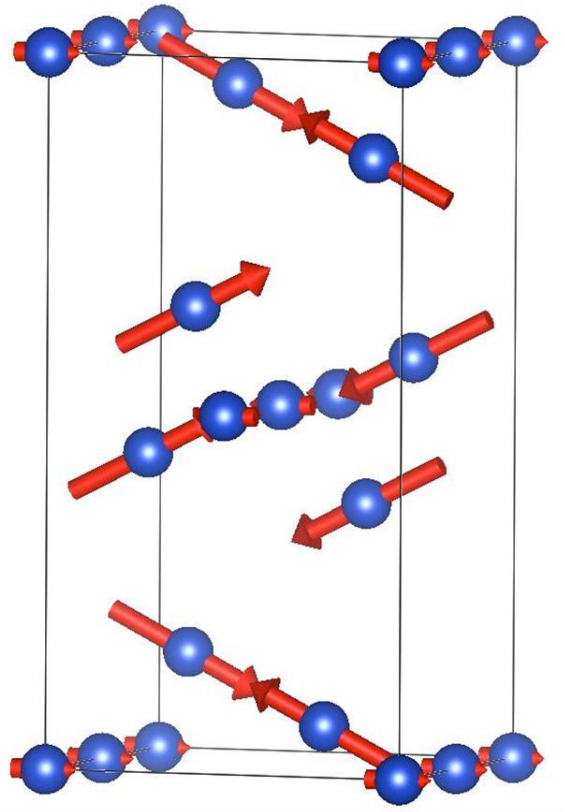
conflicting models:





$Cu_3Mo_2O_9$ (#0.129)

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

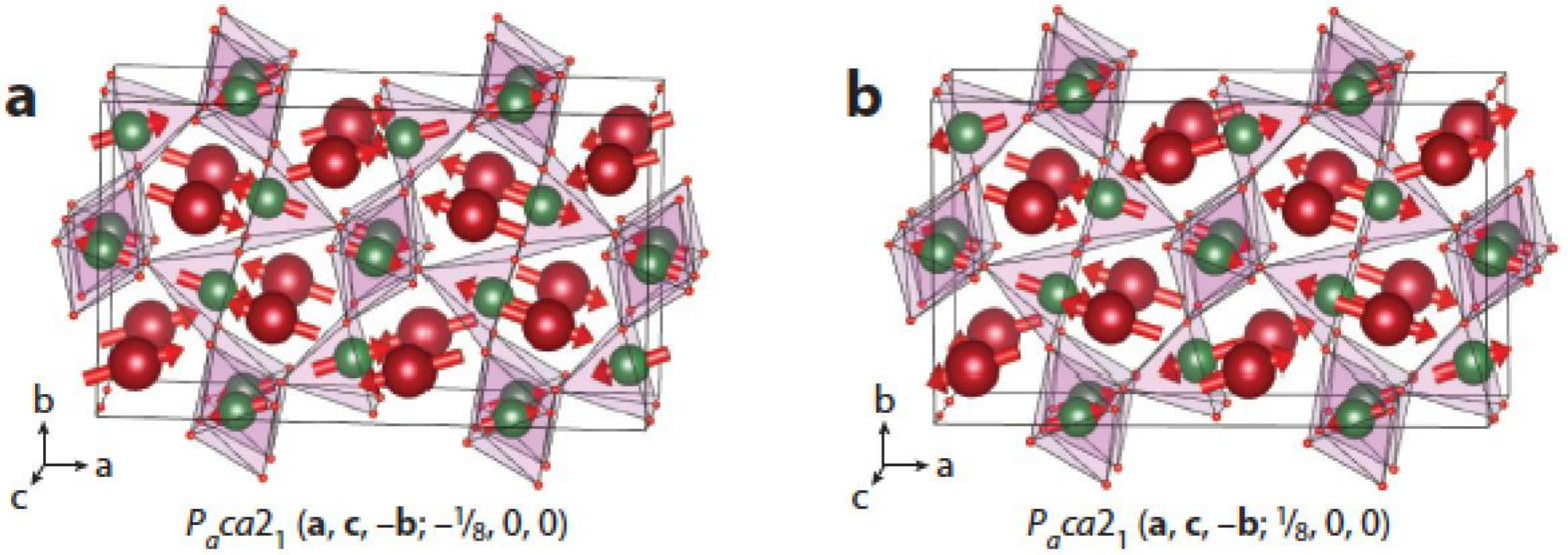


$Cu_3Mo_2O_9$ (#0.130)

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

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

Gd_2MnO_5 (magndata 1.54)



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

Using MVISUALIZE…..

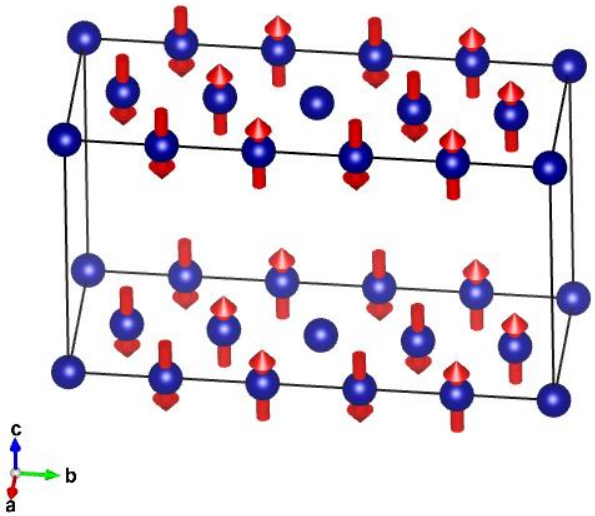
Some “dubious” structures:

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.

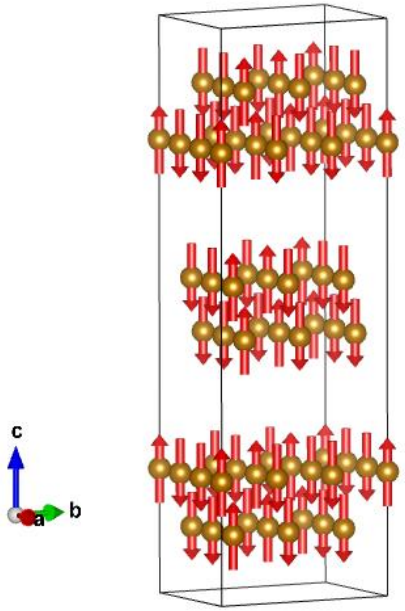
Equality of moments requires existence of reflections correponding to a 3**k** spin wave, and they were not observed.

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.

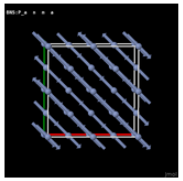
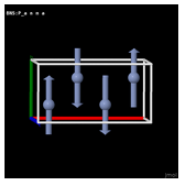
But for a few tens of structures a so-called concomitant or simultaneous structural phase transition is reported

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
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)
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)

year 1960

year 2022

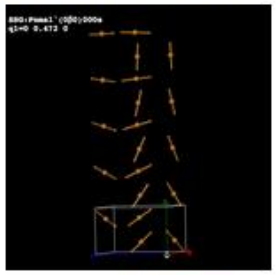
MSG OG symbol: $P_{2c}m'mn$ (59.9.486)

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

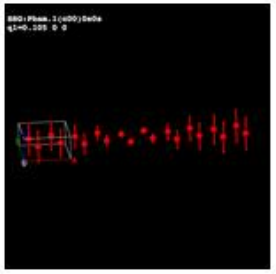
1.1.4 Cr

1.1.5 $CaFe_4As_3$

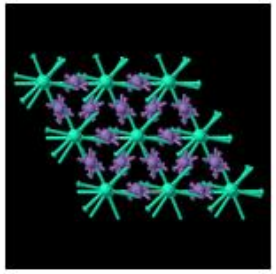
1.1.6 $TbMnO_3$

1.1.7 $TbMnO_3$

1.1.8 $TbMnO_3$



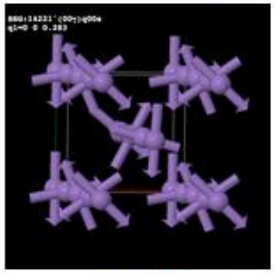
1.1.9 Ce_2Pd_2Sn



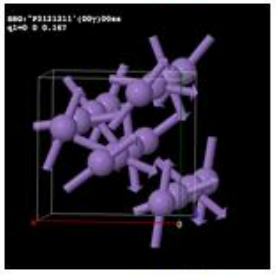
1.1.10 $DyMn_6Ge_6$

1.1.11 $MnWO_4$

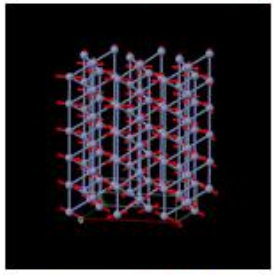
1.1.12 $MnWO_4$



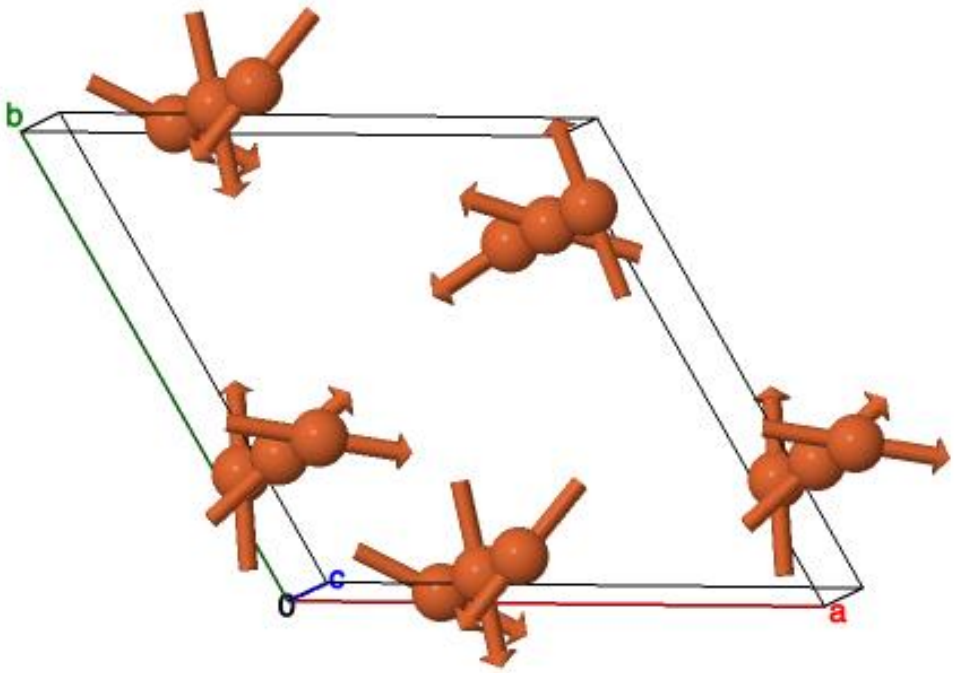
1.1.13 $MnAu_2$



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]

Magnetic Superspace Group: P3211'(00γ)000s

[View symmetry operations]

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]

MSSG

Magnetic point group

Magnetic Point Group: 321' (18.2.66)

[View symmetry operations]

Symmetry-adapted form of material tensors via MTENSOR

Average positions, magnetic moments and magnetic modulations 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]

Average positions and average moments, If any

Average atomic positions of symmetry independent atoms

Label	Atom type	x	y	z	Multiplicity
Fe1	**Fe**	**0.24964(4)**	**0**	**0.5**	**3**

Spin modulations

Magnetic moment modulation parameters of symmetry independent atoms

Wave vector 1

Atom	Magnetic moment Fourier Cos coeffs						Magnetic moment Fourier Sin coeffs					
	Symmetry constraints			Numerical values			Symmetry constraints			Numerical values		
	x	y	z	x	y	z	x	y	z	x	y	z
Fe1	$M_x$cos1	0	0	4	0.0	0.0	$M_x$sin1	$2M_x$sin1	$M_z$sin1	-2.31	-4.62	0.0

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

Magnetic moment modulation parameters of symmetry independent atoms

Wave vector 1

Atom	Magnetic moment Fourier Cos coeffs						Magnetic moment Fourier Sin coeffs					
	Symmetry constraints			Numerical values			Symmetry constraints			Numerical values		
	x	y	z	x	y	z	x	y	z	x	y	z
Fe1	$M_x$cos1	0	0	4	0.0	0.0	$M_x$sin1	$2M_x$sin1	$M_z$sin1	-2.31	-4.62	0.0

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

Average positions and magnetic moments of all atoms in unit cell, with magnetic moment relations explicitly given:

Set of atoms in the unit cell related by symmetry with the magnetic atom Fe1:

Average atomic positions

Atom	x	y	z
1	0.24964	0.00000	0.50000
2	0.00000	0.24964	0.50000
3	0.75036	0.75036	0.50000

Relations between the spin modulations of all the atoms in the unit cell

Magnetic moment modulation parameters

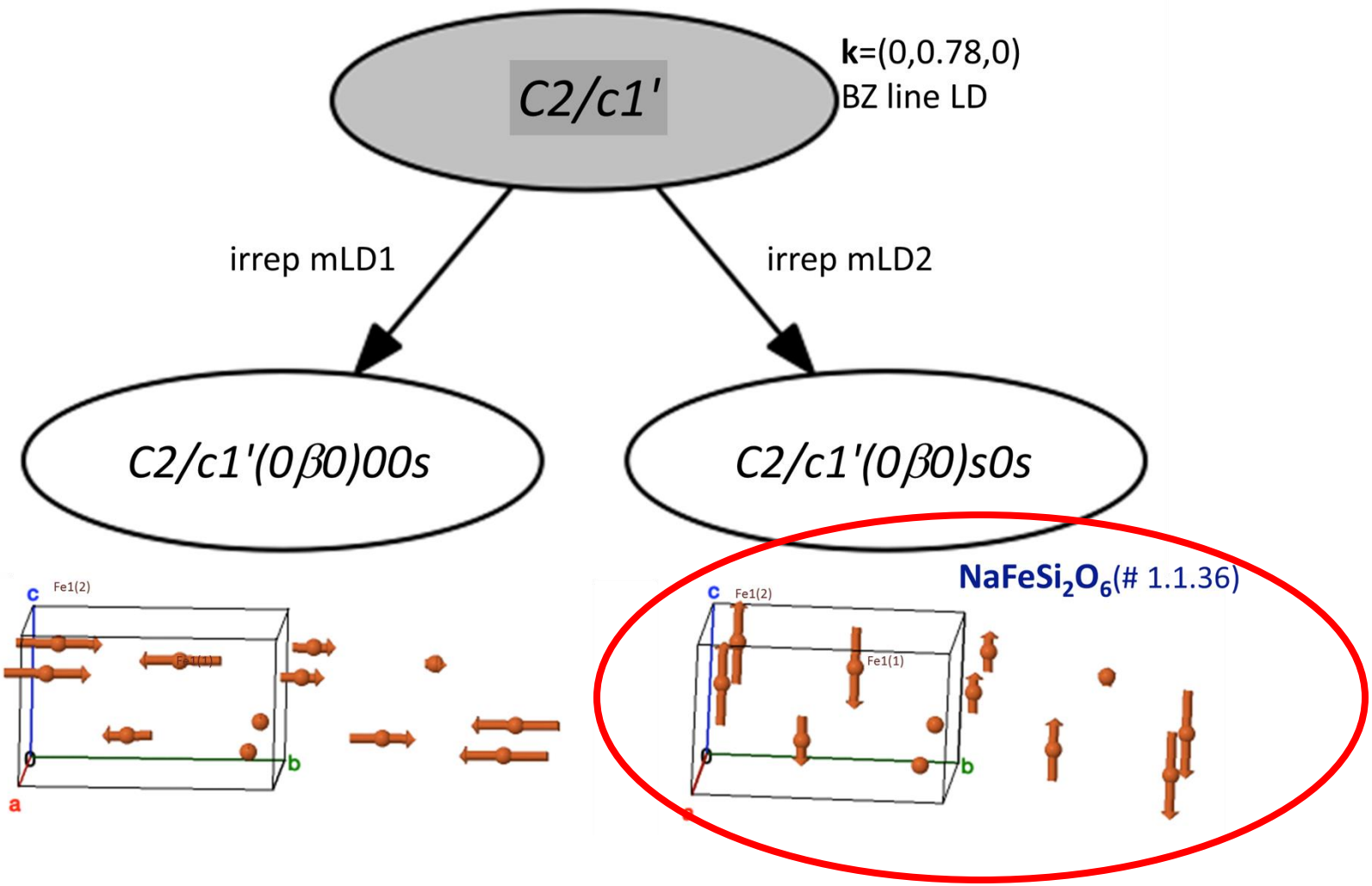
Wave vector 1

Atom	Magnetic moment Fourier Cos coeffs						Magnetic moment Fourier Sin coeffs					
	Symmetry constraints			Numerical values			Symmetry constraints			Numerical values		
	x	y	z	x	y	z	x	y	z	x	y	z
1	$M_x$cos1	0	0	4.00000	0.0	0.0	$M_x$sin1	$2M_x$sin1	$M_z$sin1	-2.31000	-4.62000	0.0
2	0	$M_x$cos1	0	0.0	4.00000	0.0	$-2M_x$sin1	$-M_x$sin1	$M_z$sin1	4.62000	2.31000	0.0
3	$-M_x$cos1	$-M_x$cos1	0	-4.00000	-4.00000	0.0	$M_x$sin1	$-M_x$sin1	$M_z$sin1	-2.31000	2.31000	0.0

[Hide]

Possible MSSGs and the corresponding models have been derived using JANA2006 or ISODISTORT

for each irrep the possible MSSGs and models are derived:



nature

Massive surveys with the entries of MAGNDATA

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

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

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*
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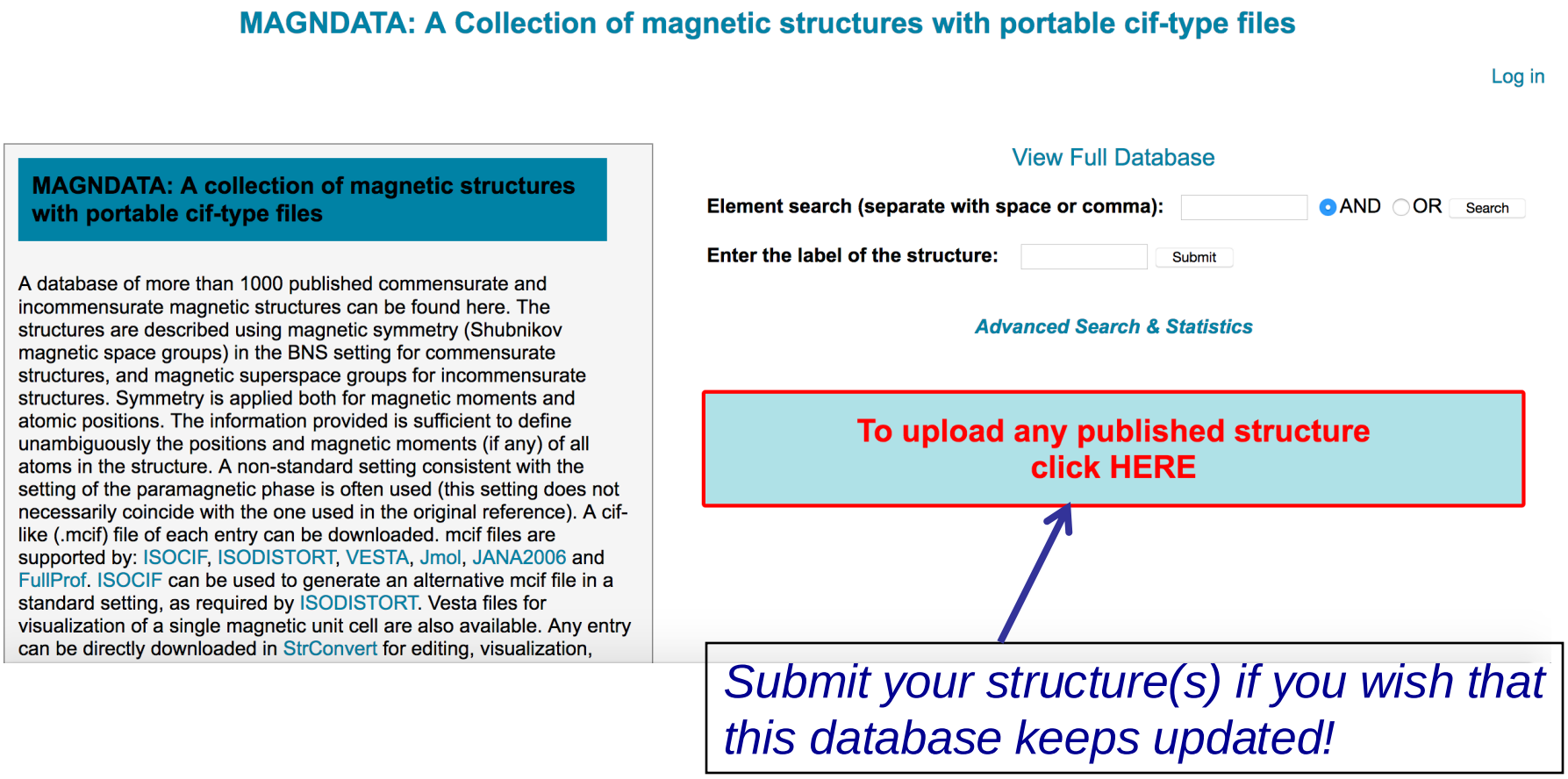
In this work, we exhaust all the spin space symmetries, which fully characterize collinear, noncollinear, and commensurate spiral as well as incommensurate spiral magnetism, etc., and investigate enriched features of electronic bands that respect these symmetries. We achieve this by systematically classifying 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 $O(N)$ 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

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 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.