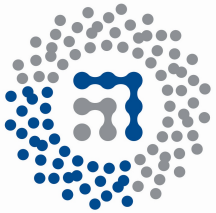


ZTF-FCT
Zientzia eta Teknologia Fakultatea
Facultad de Ciencia y Tecnología

eman ta zabal zazu

Universidad del País Vasco
Euskal Herriko Unibertsitatea

MAGNDATA: a database of magnetic structures under the magnetic CIF format

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

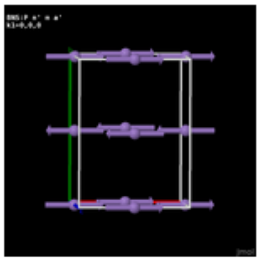
MAGNDATA: A Collection of magnetic structures with portable cif-type files

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

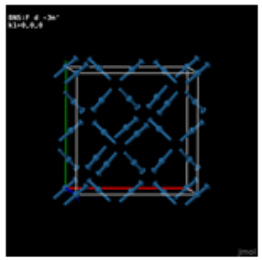
312 structures found

Update: by Jan. 2023 it contains more than 2000 structures

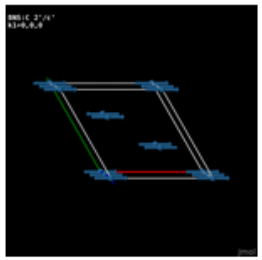
Zero propagation vector



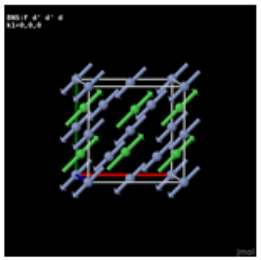
0.1 $LaMnO_3$



0.2 $Cd_2Os_2O_7$



0.3 Ca_3LiOsO_6



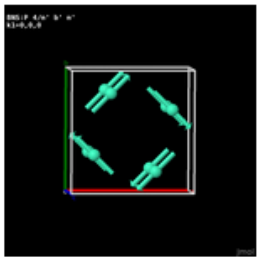
0.4 $NiCr_2O_4$

0.5 Cr_2S_3

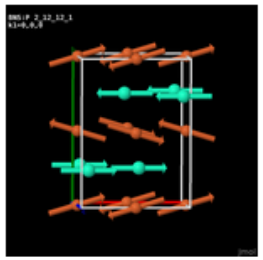
0.6 $YMnO_3$

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 collaborative work

- ***Bilbao:*** **Samuel V. Gallego, J.M. 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

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

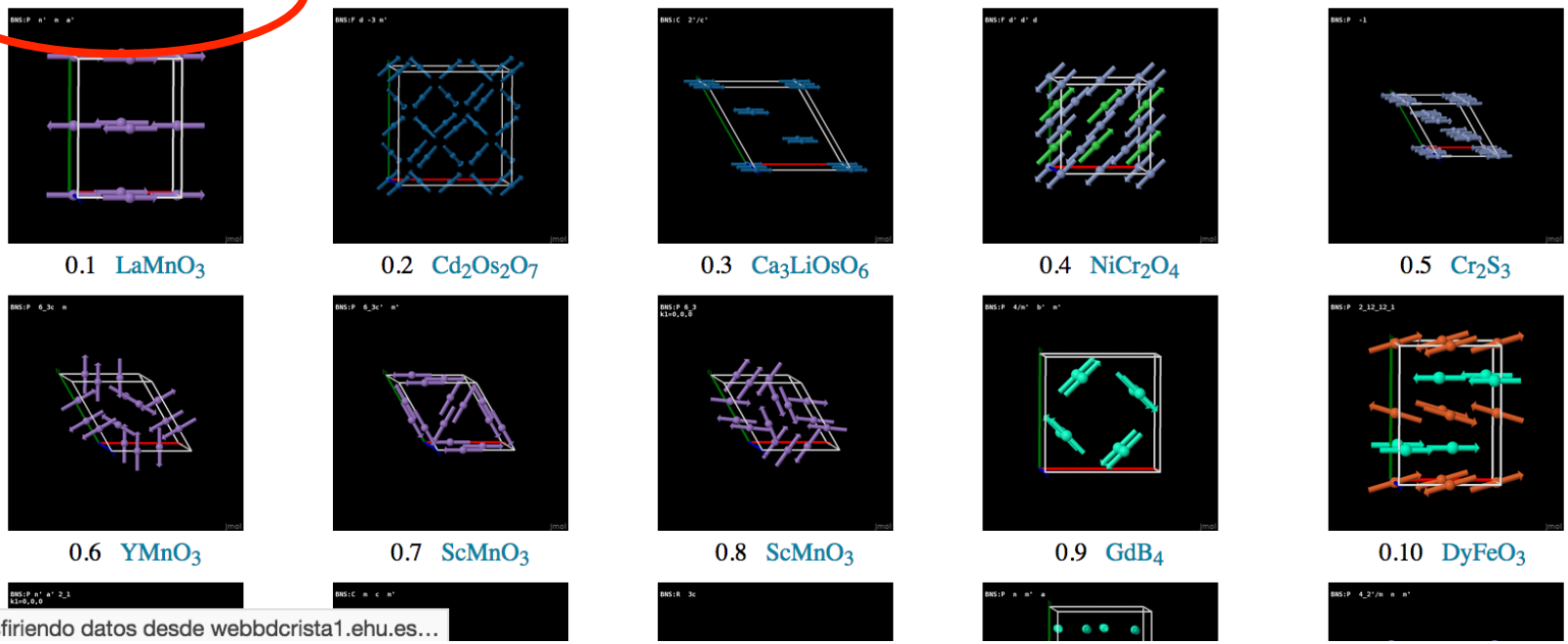
Element search (separate with space or comma): AND OR Search Advanced Search & Statistics

Enter the label of the structure: Submit

614 structures found

label 0.n

Zero propagation vector



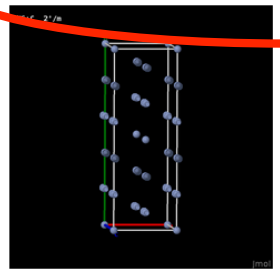
Transfiriendo datos desde webbdcrista1.ehu.es...

k=(0,0,0) → (no antitranslation)

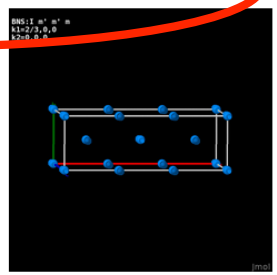
k=0 – structures (**Type I or III MSG symmetry**). The most interesting ones for magneto-structural properties! (magnetic point group without time reversal)

label 1.0.n

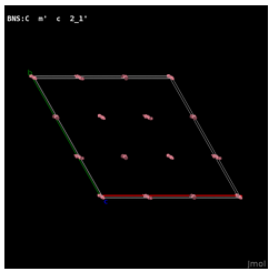
Non-zero propagation vector (Type III)



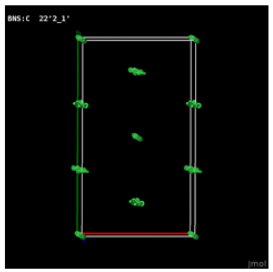
1.0.1 Ag_2CrO_2



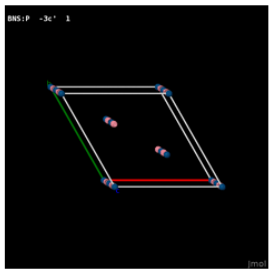
1.0.2 $URu_{0.96}Rh_{0.04}Si_2$



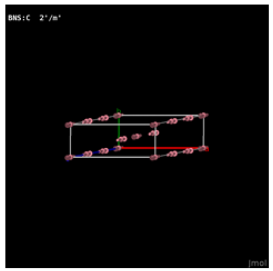
1.0.3 $CsCoBr_3$



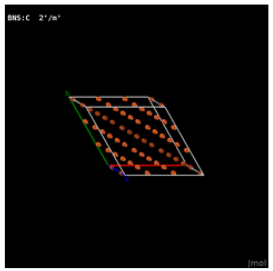
1.0.4 $CsNiCl_3$



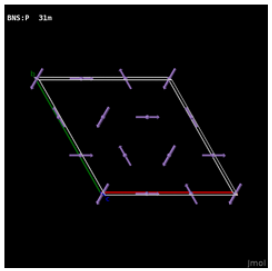
1.0.5 Sr_3CoIrO_6



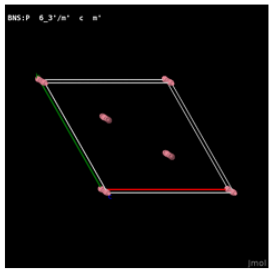
1.0.6 CoV_2O_6



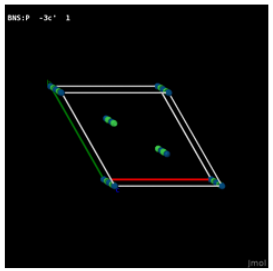
1.0.7 $LuFe_2O_4$



1.0.8 $Ba_3MnNb_2O_9$



1.0.9 $CsCoCl_3$



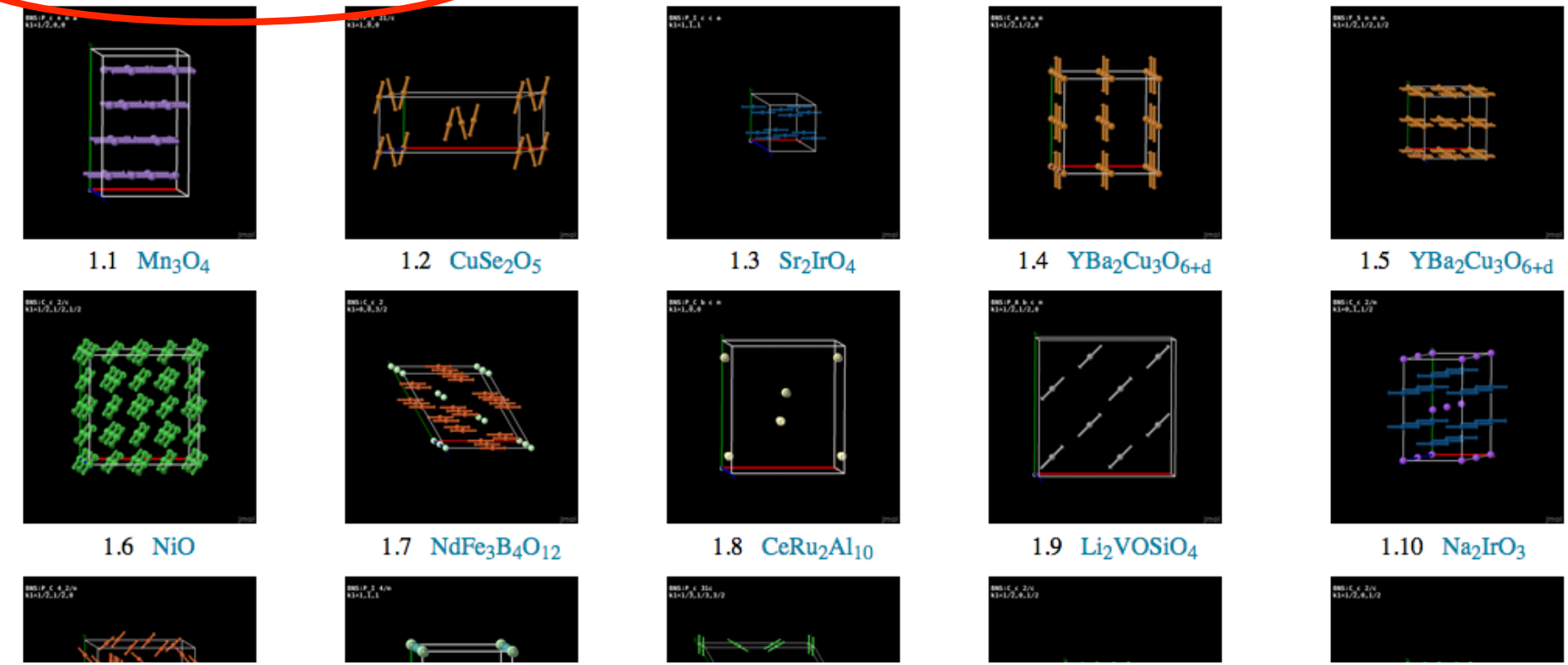
1.0.10 Sr_3NiIrO_6

k≠(0,0,0) BUT no antitranslation (n*k*=*H* with n-odd)

Also of **Type I or III MSG symmetry**. The most interesting ones for magneto-structural properties! (magnetic point group without time reversal)

label 1.n

Non-zero propagation vector (Type IV)



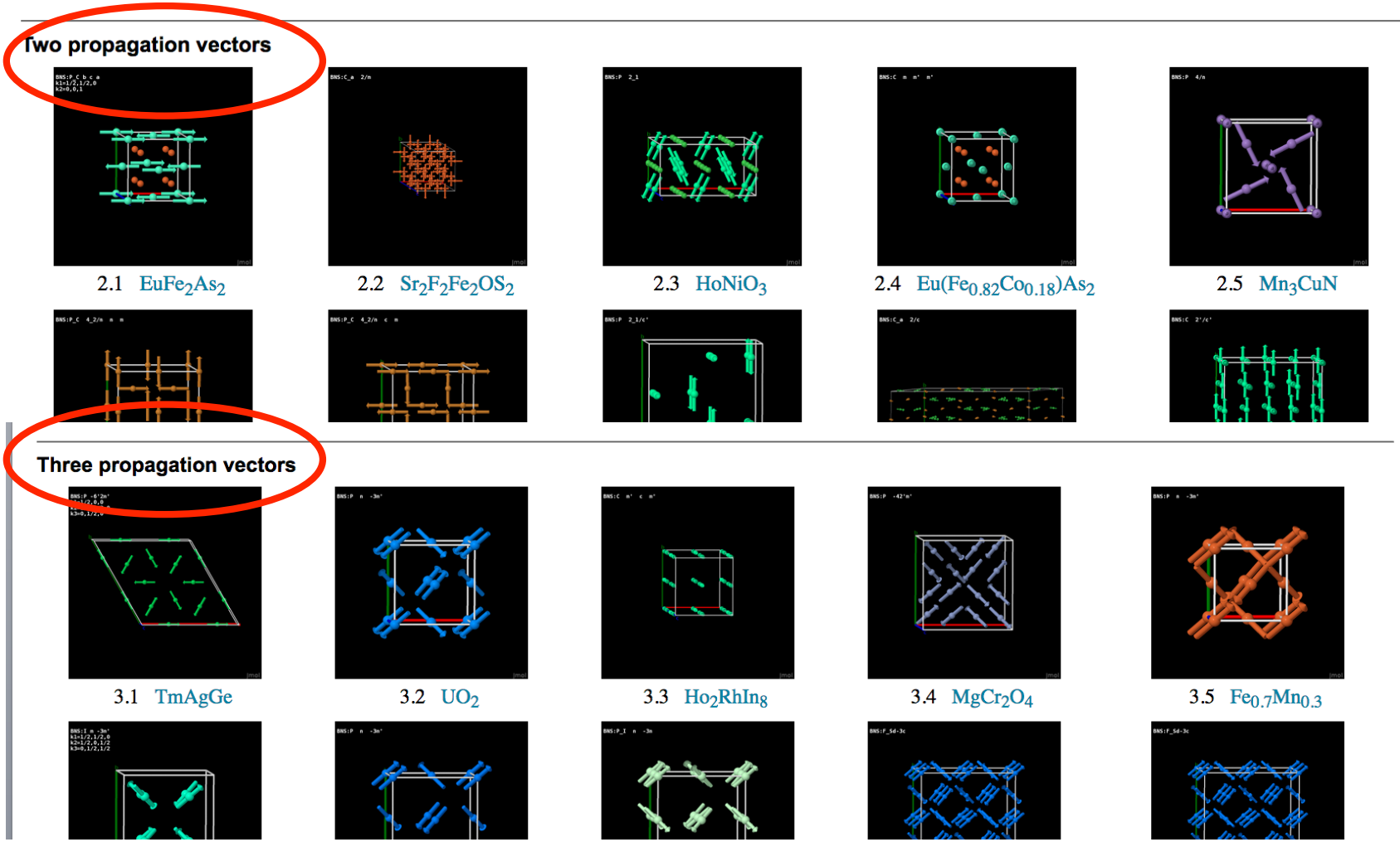
1.1 Mn_3O_4 1.2 $CuSe_2O_5$ 1.3 Sr_2IrO_4 1.4 $YBa_2Cu_3O_{6+d}$ 1.5 $YBa_2Cu_3O_{6+d}$

1.6 NiO 1.7 $NdFe_3B_4O_{12}$ 1.8 $CeRu_2Al_{10}$ 1.9 Li_2VOSiO_4 1.10 Na_2IrO_3

k≠(0,0,0) with antitranslations (nk**=H** with n-even)

Type IV MSG symmetry. Magnetic point group includes time reversal as those of non-magnetic structures: symmetry restrictions on linear tensor properties similar to non-magnetic structures.

labels 2.n and 3.n

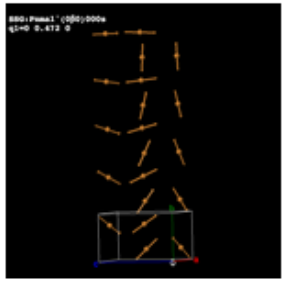


2k and ≥3k structures

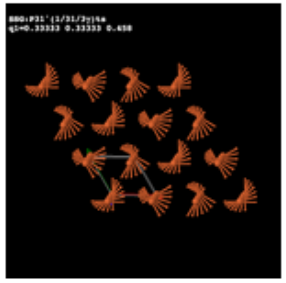
All types of MSG symmetries (with and without antitranslations)

INCOMMENSURATE STRUCTURES

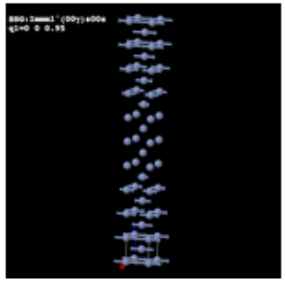
One propagation vector



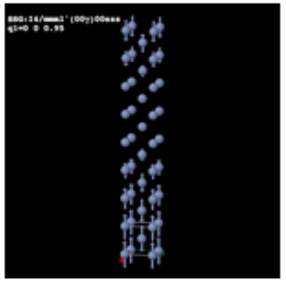
1.1.1 Cs_2CuCl_4



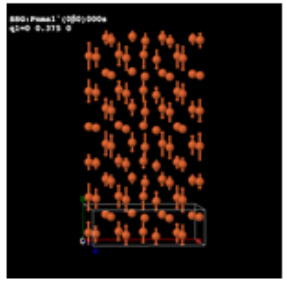
1.1.2 $RbFe(MoO_4)_2$



1.1.3 Cr

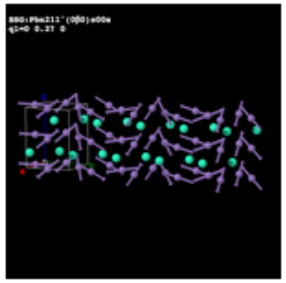


1.1.4 Cr

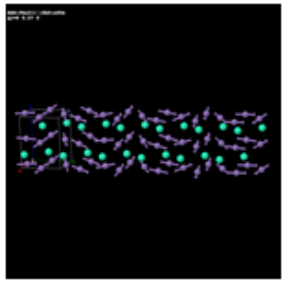


1.1.5 $CaFe_4As_3$

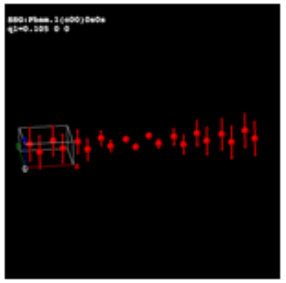
1.1.6 $TbMnO_3$



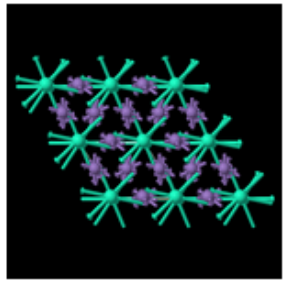
1.1.7 $TbMnO_3$



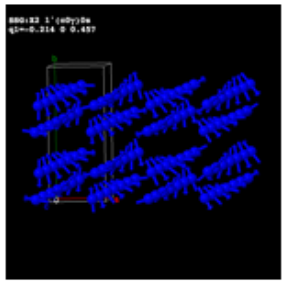
1.1.8 $TbMnO_3$



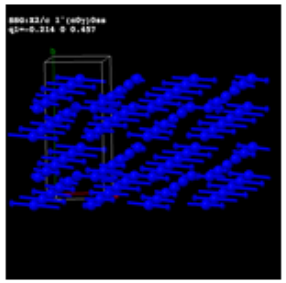
1.1.9 Ce_2Pd_2Sn



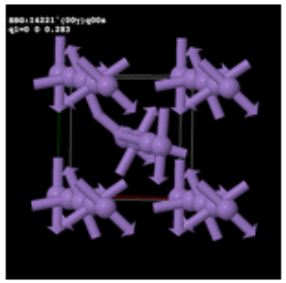
1.1.10 $DyMn_6Ge_6$



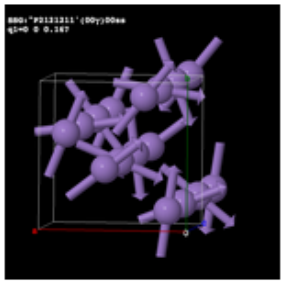
1.1.11 $MnWO_4$



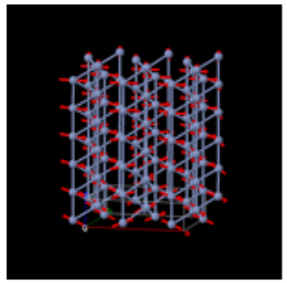
1.1.12 $MnWO_4$



1.1.13 $MnAu_2$

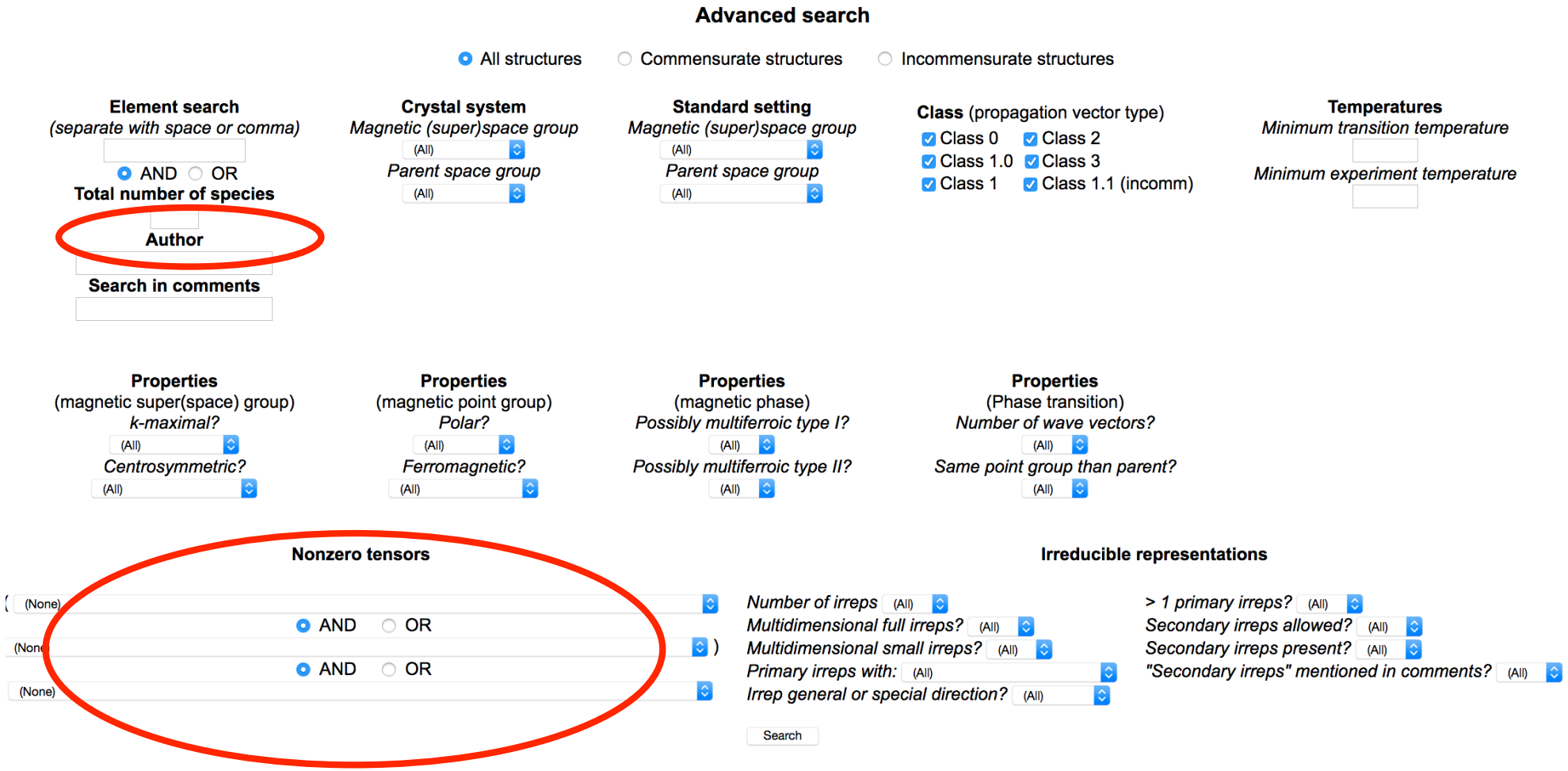


1.1.14 MnGe



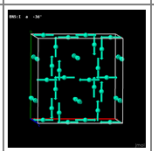
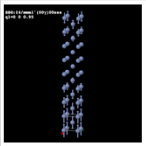
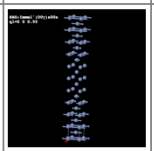
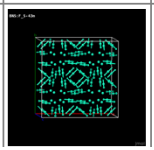
1.1.15 $CaCr_2O_4$

Search optional filters

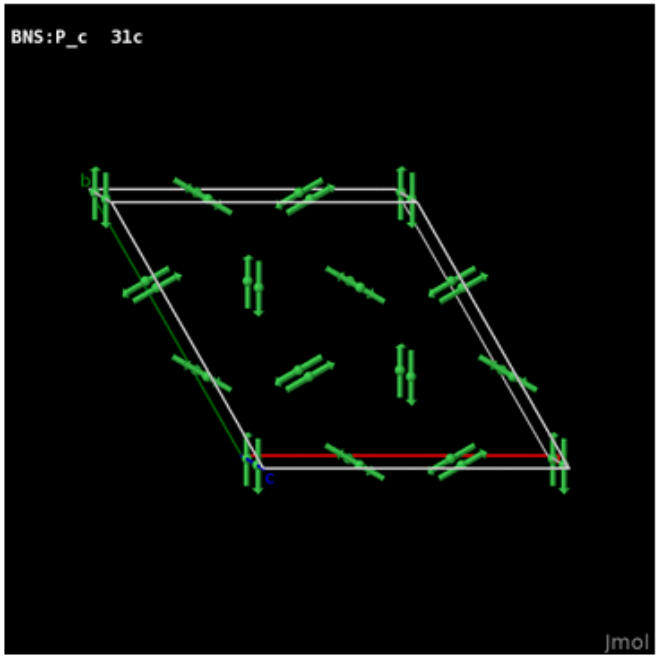


ordering according to parent space group

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

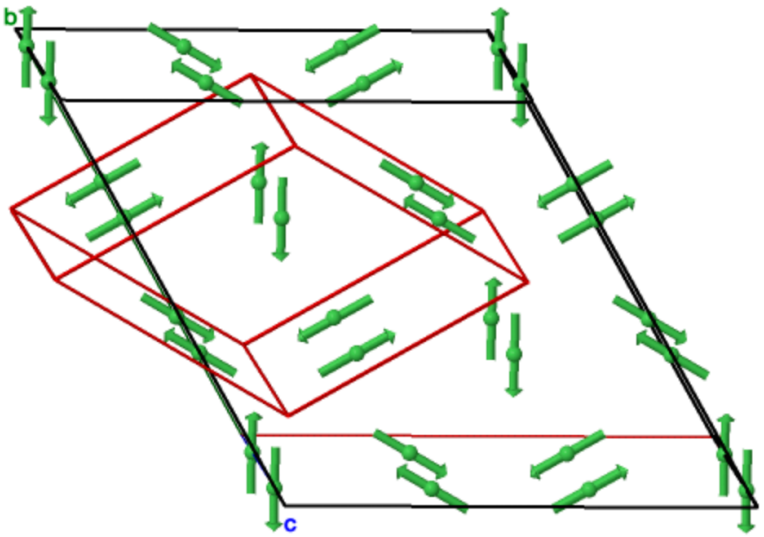
MAGNDATA Structure Viewer: 3D Visualization of magnetic structures with Jmol

$Ba_3Nb_2NiO_9$ (#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

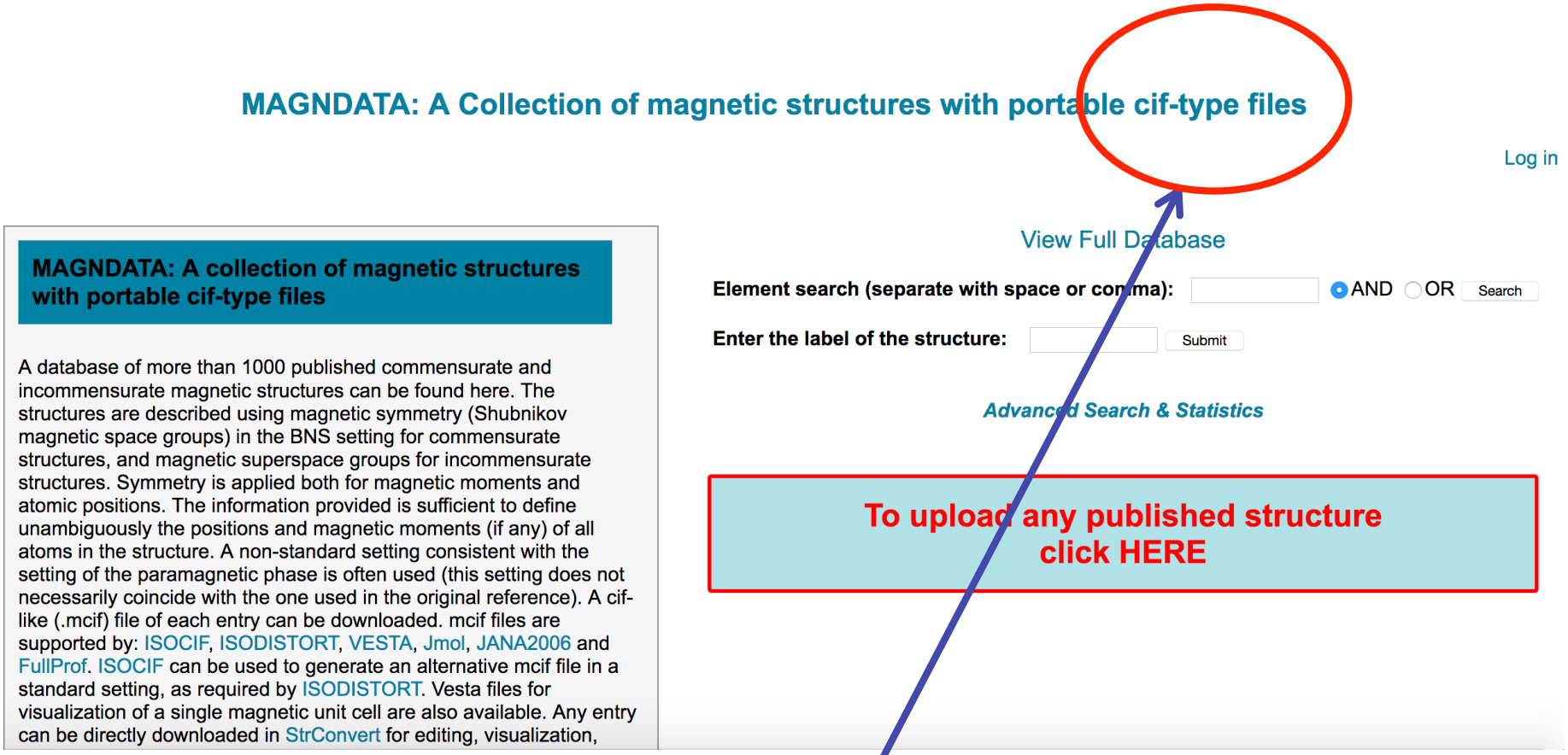
White
Toggle Quality
Center

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
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_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
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_cell_angle_gamma               120.0000

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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_
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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

```
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_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
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O2_4 O 0.94340 0.88680 0.83688 1

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_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)

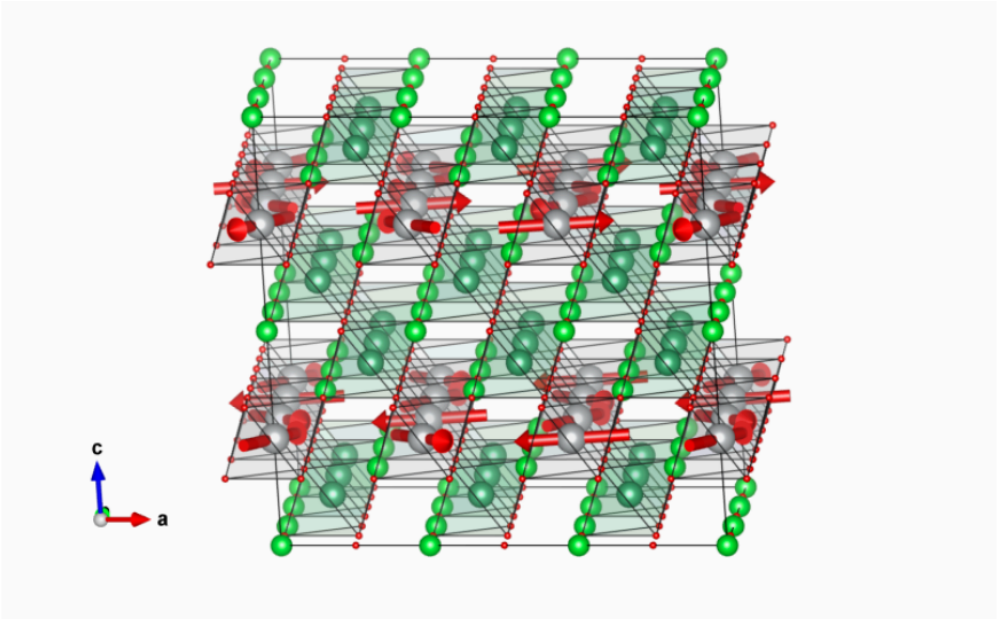
symmetry-independent magnetic moments

components

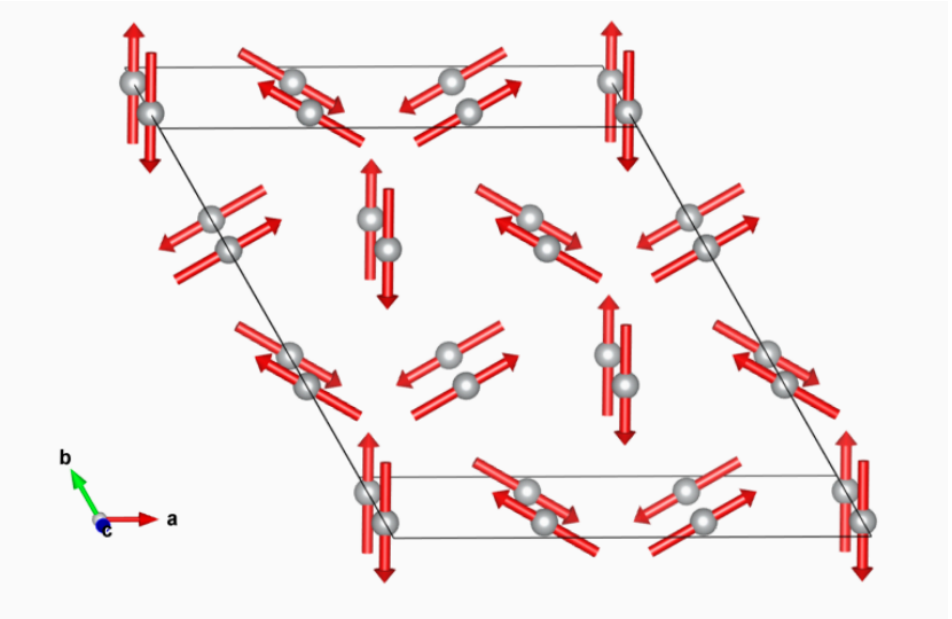
symmetry constraints

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

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

it includes a direct link to the reference (DOI)

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

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 uB*

[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

Comments:

- NPD
- 120-degrees magnetic ordering
- multiferroic with magnetic induced ferroelectricity along z.

Comments (symmetry):

- 1k magnetic structure
- k-maximal magnetic symmetry (from 4 possible)
- symmetry-allowed secondary irrep mA1- with k2=3k1=(0,0,1/2),
- corresponding to the z component of the Ni moments not observed.

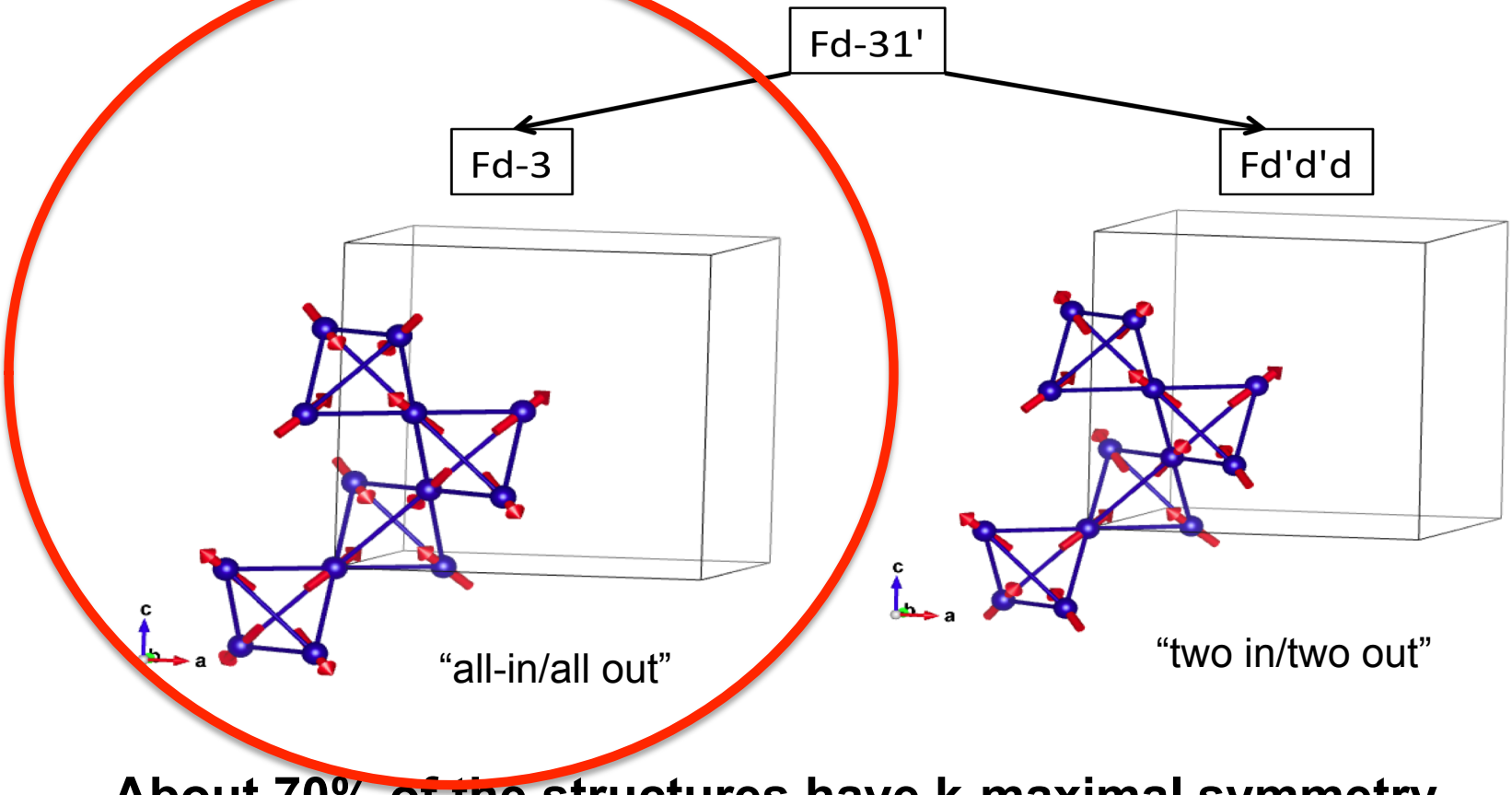
k-maximal symmetry

m_z is a third harmonic that can appear through coupling

$Na_3Co(CO_3)_2Cl$ (*magndata #0.70)*

space group: ***Fd-3*** magnetic ordering wih **k**=(0,0,0)

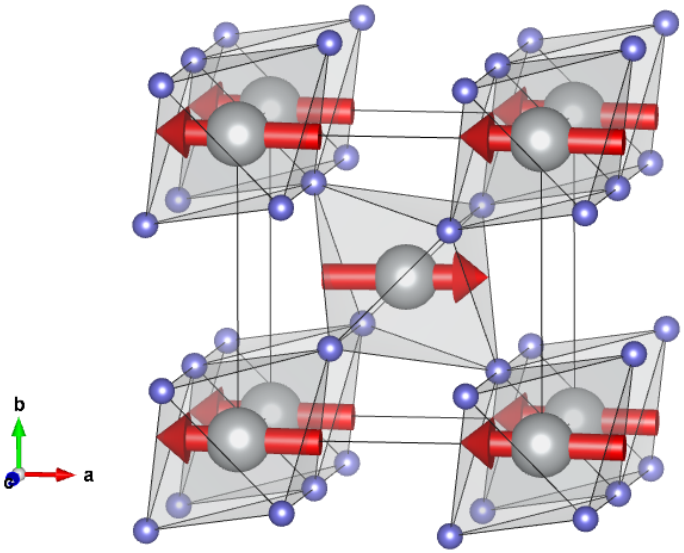
Possible maximal symmetries compatible with the observed propagation vector (k-maximal symmetries)



About 70% of the structures have k-maximal symmetry

NiF_2 magndata #0.36

"historical" weak ferromagnet



k=(0,0,0)

$P4_2/mnm1'$ → Pnn'm' (b,-a,c;0,0,0)

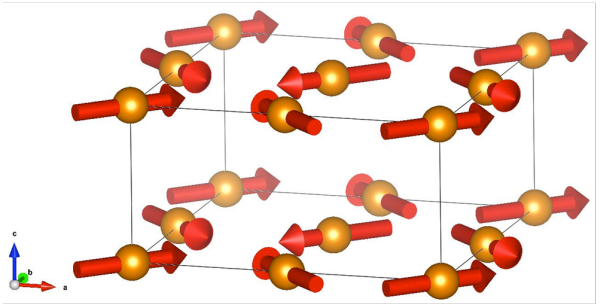
k-maximal symmetry **weak FM along y**

- 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

weak FM is explained by the MSG of the structure

Multi-k structures



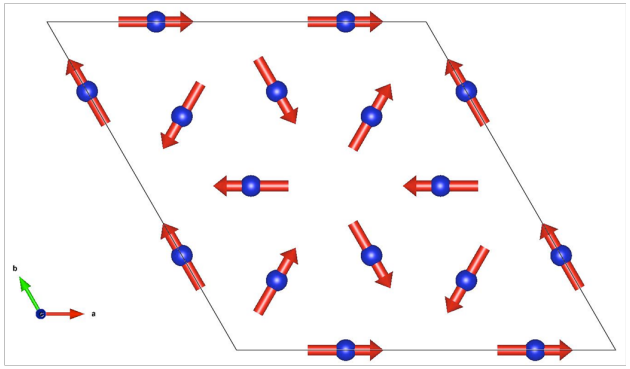
NdMg (#2.14)

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)

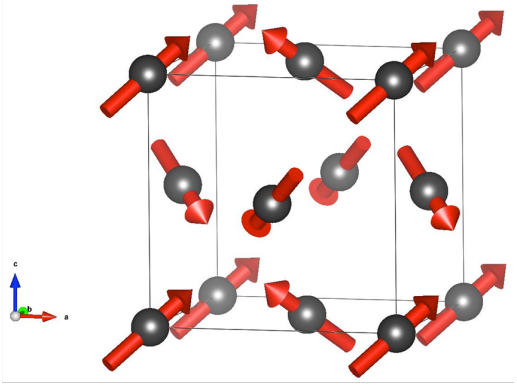
Parent: *P-62m1'*

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'*

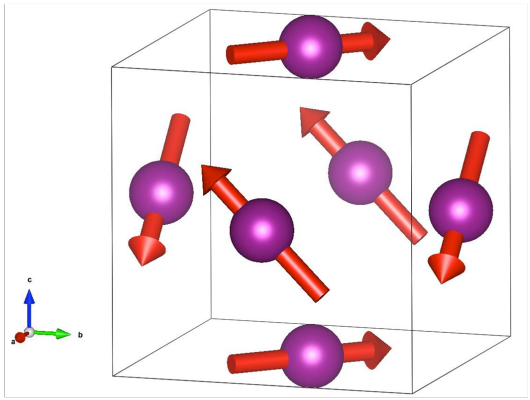
Pn-3m' ($\mathbf{a}_p, \mathbf{b}_p, \mathbf{c}_p$; 0,0,0)

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

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

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

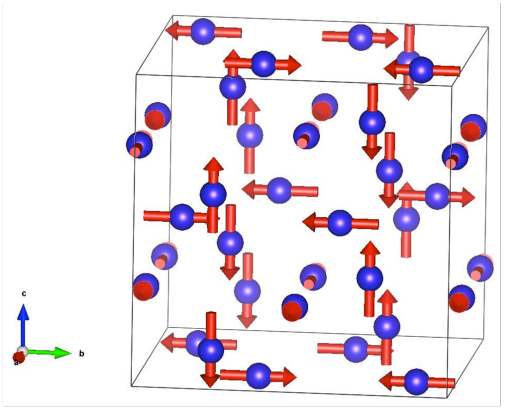
multiaxial structures that are single k:



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

R-3m (#166.97)

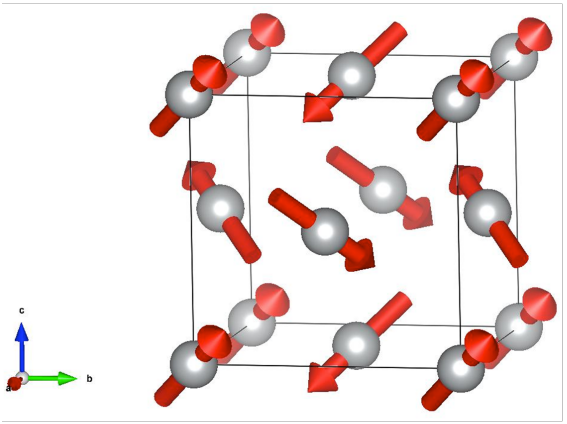
k = (0, 0, 0)



$Dy_3Al_5O_{12}$ (#0.127)

Ia-3d' (#230.148)

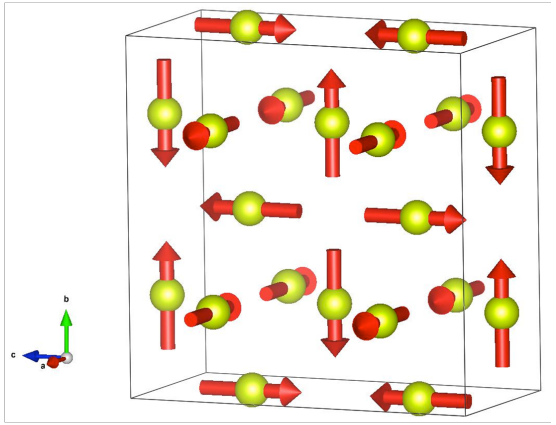
k = (0, 0, 0)



NiS_2 (#0.150)

Pa-3 (#205.33)

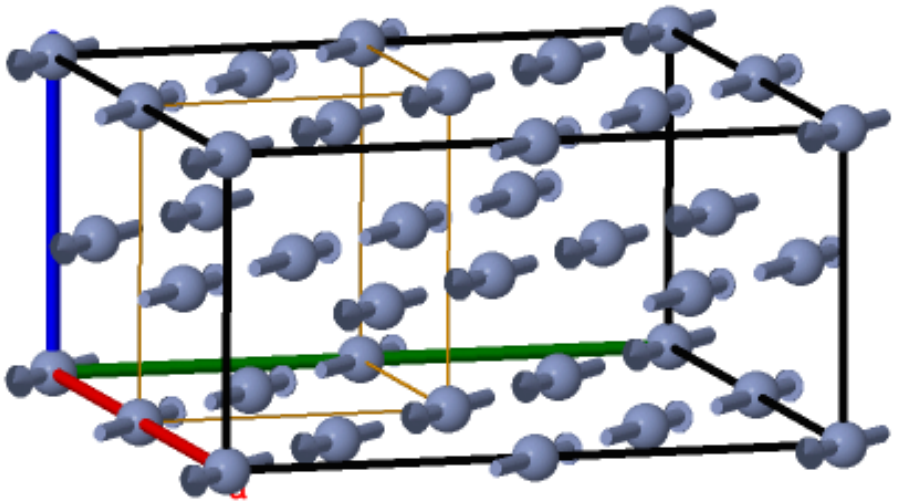
k = (0, 0, 0)



Ce_3NIn (#1.152)

P_C*-4b2* (#117.305)

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



CrN *Phys Rev (1960) 117 929*

Paramagnetic symmetry: **Fm-3m1'**

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

MSG: $P_a nma$

k-maximal symmetry

Magndata 1.28

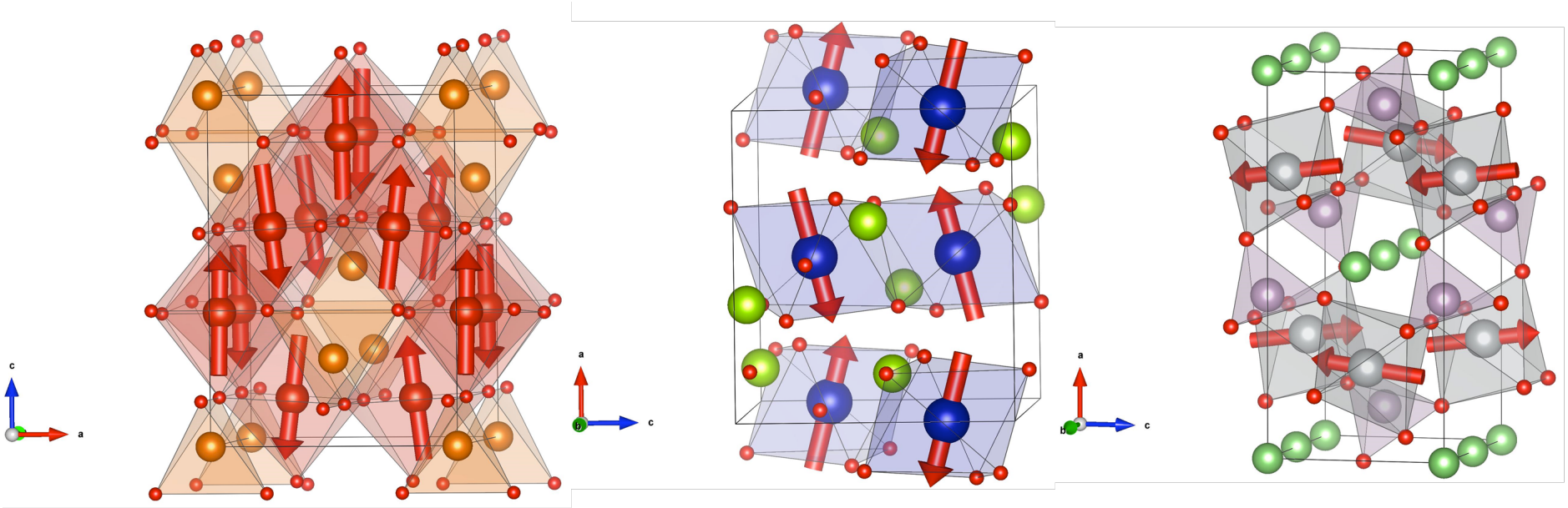
Label	Atom type	x	y	z	Symmetry constraints on M	M_x	M_y	M_z
Cr1	Cr	0.00000	0.00000	0.00000	$m_x,-m_x,0$	1.7	-1.7	0.0

colinear structure – "symmetry protected"

Atom	x	y	z	Symmetry constraints on M
1	0.00000	0.00000	0.00000	$m_x,-m_x,0$
2	0.50000	0.00000	0.00000	$-m_x,m_x,0$
3	0.00000	0.25000	0.50000	$m_x,-m_x,0$
4	0.75000	0.00000	0.50000	$-m_x,m_x,0$
5	0.50000	0.75000	0.50000	$m_x,-m_x,0$
6	0.25000	0.50000	0.50000	$-m_x,m_x,0$
7	0.25000	0.75000	0.00000	$m_x,-m_x,0$
8	0.25000	0.25000	0.00000	$-m_x,m_x,0$
9	0.75000	0.75000	0.00000	$-m_x,m_x,0$
10	0.25000	0.00000	0.50000	$m_x,-m_x,0$
11	0.00000	0.75000	0.50000	$-m_x,m_x,0$
12	0.75000	0.50000	0.50000	$m_x,-m_x,0$
13	0.50000	0.25000	0.50000	$-m_x,m_x,0$
14	0.50000	0.50000	0.00000	$m_x,-m_x,0$
15	0.00000	0.50000	0.00000	$-m_x,m_x,0$
16	0.75000	0.25000	0.00000	$m_x,-m_x,0$

[Hide]

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

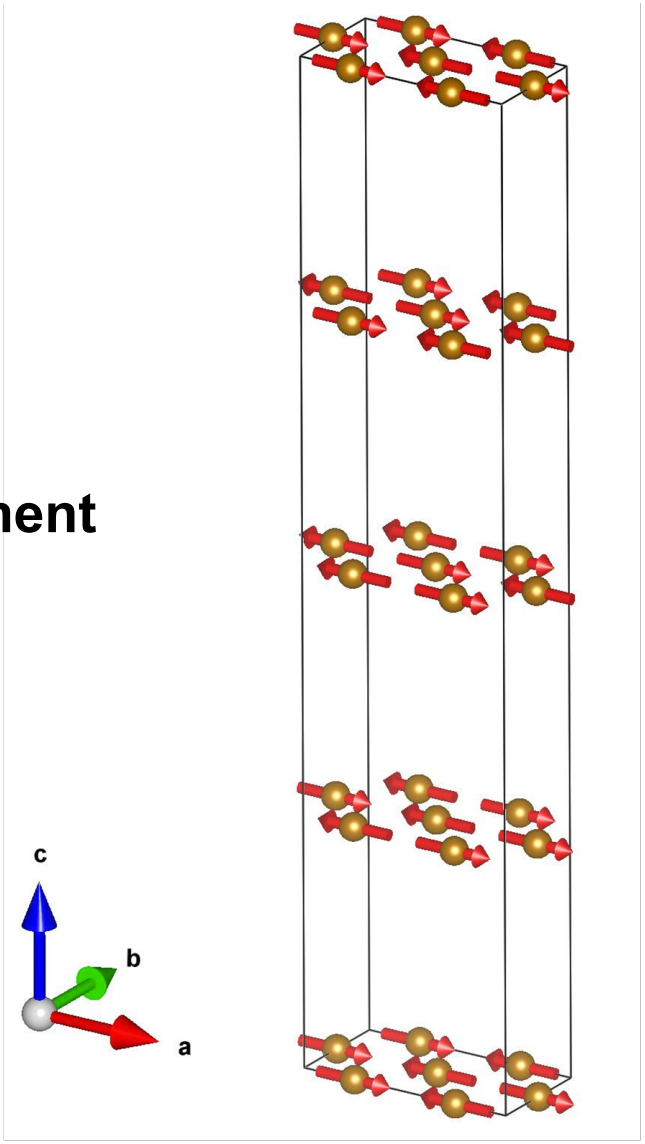
symmetry allowed spin canting is often observed
(specially with single crystal diffraction:
only 10% strict collinear structures are not forced by symmetry)

$La_2O_2Fe_2OSe_2$ (#1.58)

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

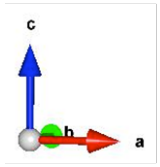
deceptive simplicity
of a collinear arrangement

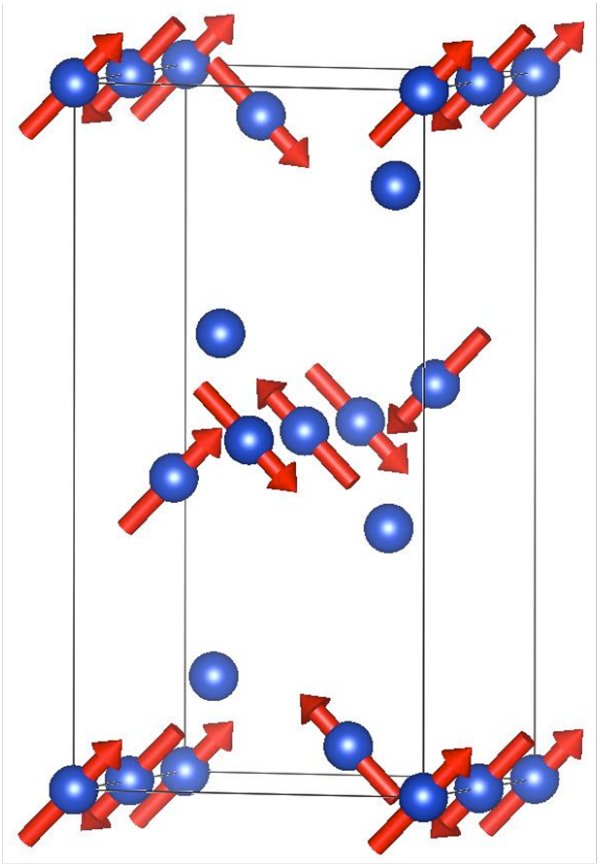
It requires 2 primary
Irreps !



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

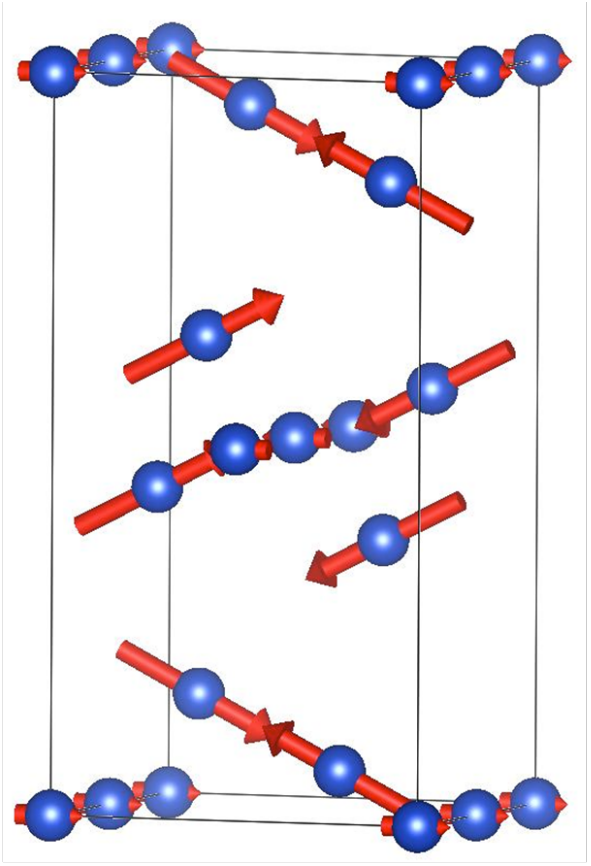
conflicting models:





$Cu_3Mo_2O_9$ (#0.129)

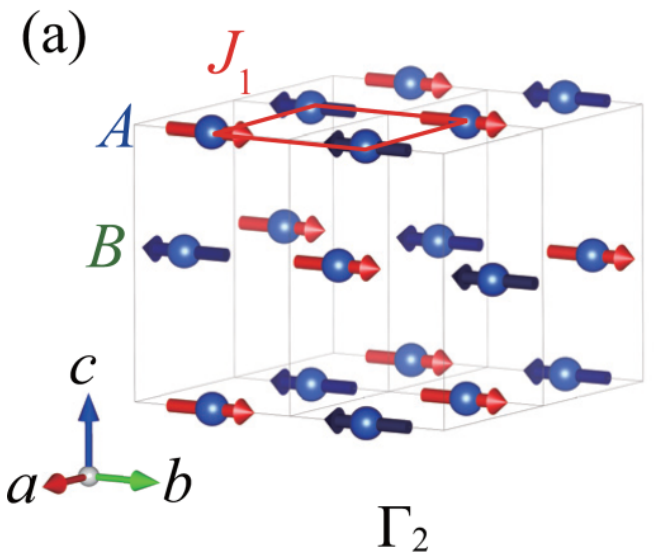
P2₁'2₁'2₁ (**a**$_p$,-**c**$_p$,**b**$_p$;1/4,1/4,0)

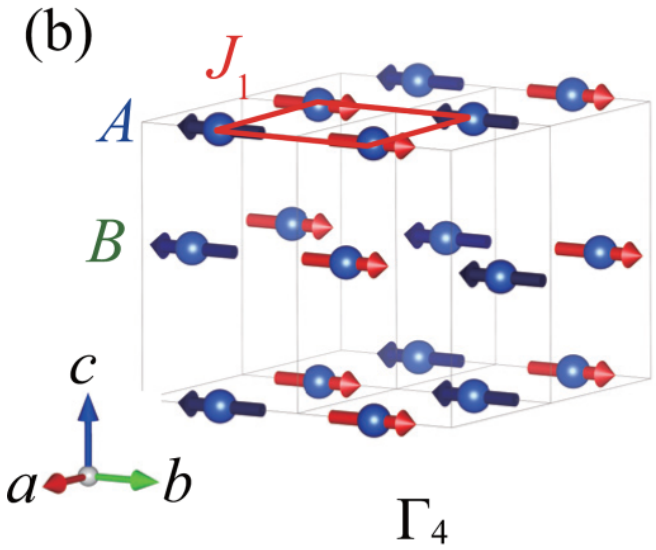


$Cu_3Mo_2O_9$ (#0.130)

Pm'c2₁' (-**b**$_p$,-**c**$_p$,**a**$_p$;0,1/4,1/4)

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

We do not have validation tools: being in MAGNDATA does not necessarily mean that structure is correct!

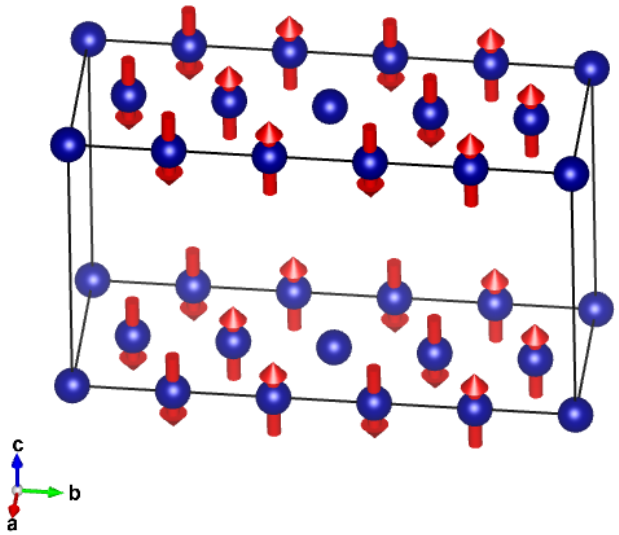
There are "dubious" structures:

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.

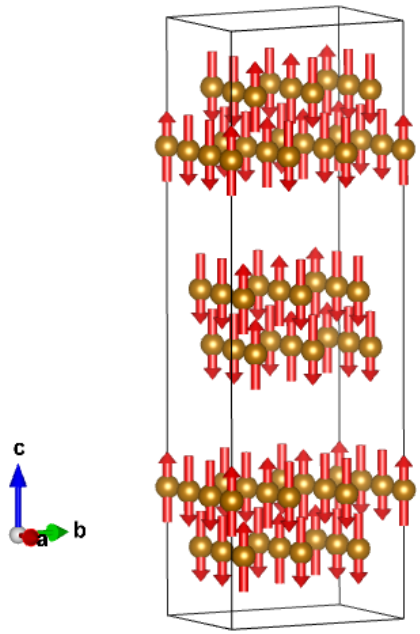
Equality of moments requires existence of reflections correponding to a 3**k** spin wave, and they were not observed.

1.0.7 $LuFe_2O_4$

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

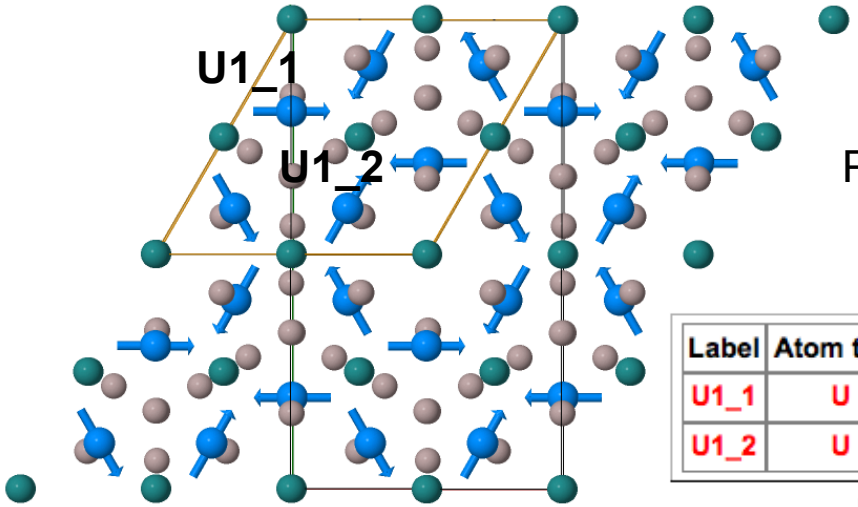
R-3m1' -> C2'/m'

trigonal -> monoclinic
k-maximal symmetry



Claimed to be multiferroic, but Inconsistent with symmetry and structure

Apparent (but false) symmetries: this specific "regular" arrangement does not have associated an hexagonal or trigonal symmetry



(Magndata 0.12)

$U_3Ru_4Al_{12}$ Magndata #0.12

Paramagnetic symmetry: $P6_3/mmc$ **k**=(0,0,0)

MSG: *Cmcm'*

Label	Atom type	x	y	z	Symmetry constraints on M	M_x	M_y	M_z
U1_1	U	0.60980	0.80490	0.25000	0,m_y,0	0.00000	-2.50000	0.00000
U1_2	U	0.19510	0.80490	0.25000	m_x,m_y,0	-2.50000	-2.50000	0.00000

label	dim. full irrep	dim. small irrep	direction	action	presence
mGM5-	2	2	special	primary	
mGM2-	1	1		secondary	yes

This magnetic order splits the U atoms into two types

This phase allows that the two U atoms have different non-related moments

The specific relation between the two U moments does NOT restrict the model to the primary irrep, but in fact it implies a very specific combination with the secondary irrep mode.

“Concomitant” structural transitions:

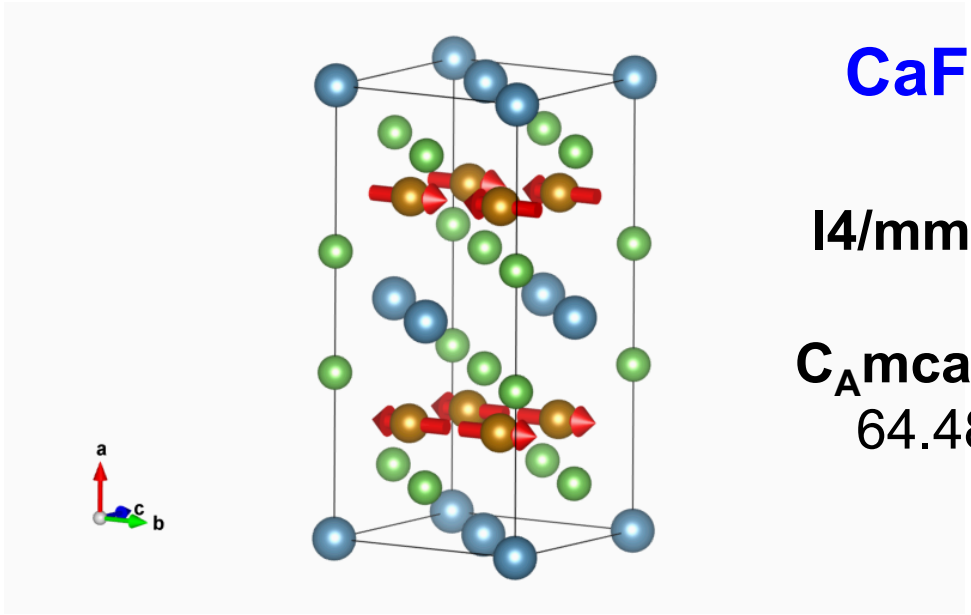
About 60% of the collected structures allow induced structural distortions forbidden in the paramagnetic phase

In most cases, these possible induced structural distortions are negligible 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.

“Concomitant” structural transition:



$CaFe_2As_2$ (magndata #1.52)

I4/mmm1’ → $C_A$mca (**c,a-b,a+b**;0,0,0)

$C_A$mca (BNS) = $F_C$mm’m’ (OG)
64.480 = 69.10.614

“Root” space group in BNS: **Cmce (64)**

“Root” space group in OG: **Fmmm (69)**

Expected “Concomitant” symmetry break for structural degrees of freedom:

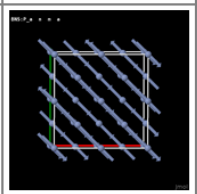
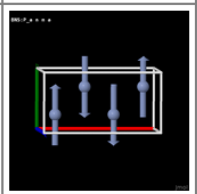
I4/mmm → Fmmm

a Fmmm structural distortion is reported

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 root space group of the OG label of the magnetic space group)….

Information table (2 entries found)

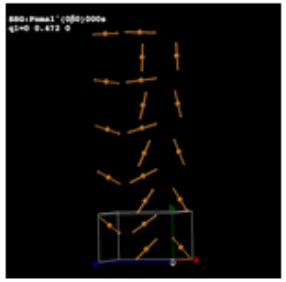
	N	Entry	Structure	Propagation vector(s)	Parent space group	Transformation from parent	Magnetic (super)space group	Magnetic point group
year 1960	1	1.28 CrN		1/2,1/2,0	Fm-3m (225) (standard)	(2**a**, 2**b**,**c**;0,0,0)	$P_a$nma (62.450) (1/2**a**+1/2**b**,-1/4**a**+1/4**b**,**c**;0,1/8,1/4)	mmm1' (8.2.25)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

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….

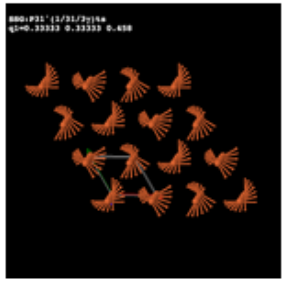
INCOMMENSURATE STRUCTURES

One propagation vector

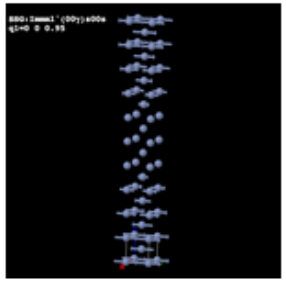
>140 entries



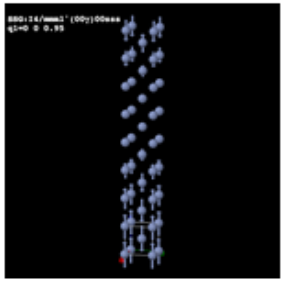
1.1.1 Cs_2CuCl_4



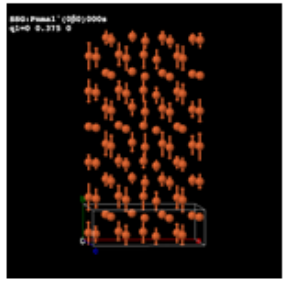
1.1.2 $RbFe(MoO_4)_2$



1.1.3 Cr

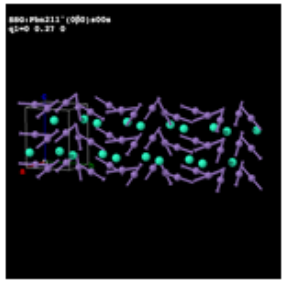


1.1.4 Cr

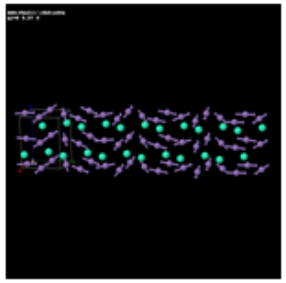


1.1.5 $CaFe_4As_3$

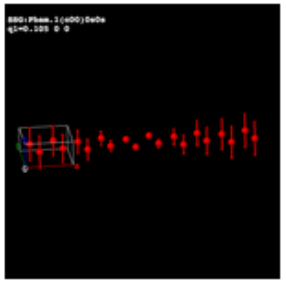
1.1.6 $TbMnO_3$



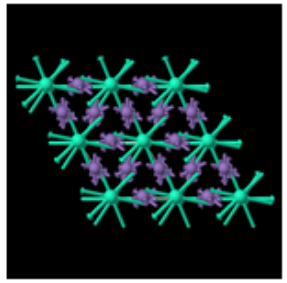
1.1.7 $TbMnO_3$



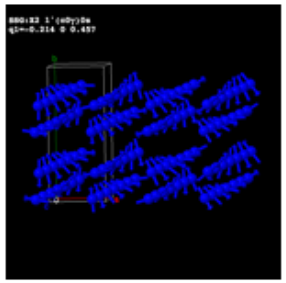
1.1.8 $TbMnO_3$



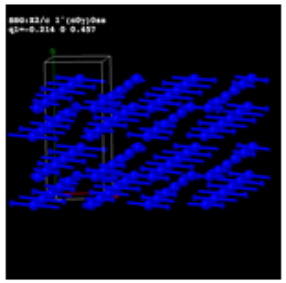
1.1.9 Ce_2Pd_2Sn



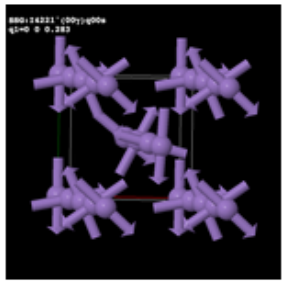
1.1.10 $DyMn_6Ge_6$



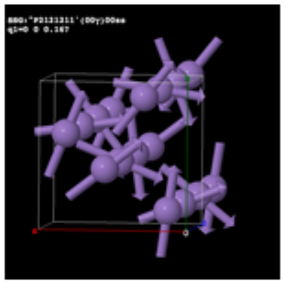
1.1.11 $MnWO_4$



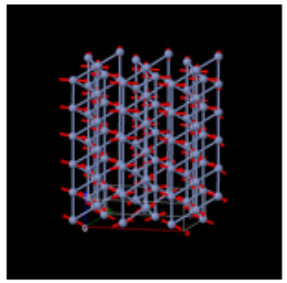
1.1.12 $MnWO_4$



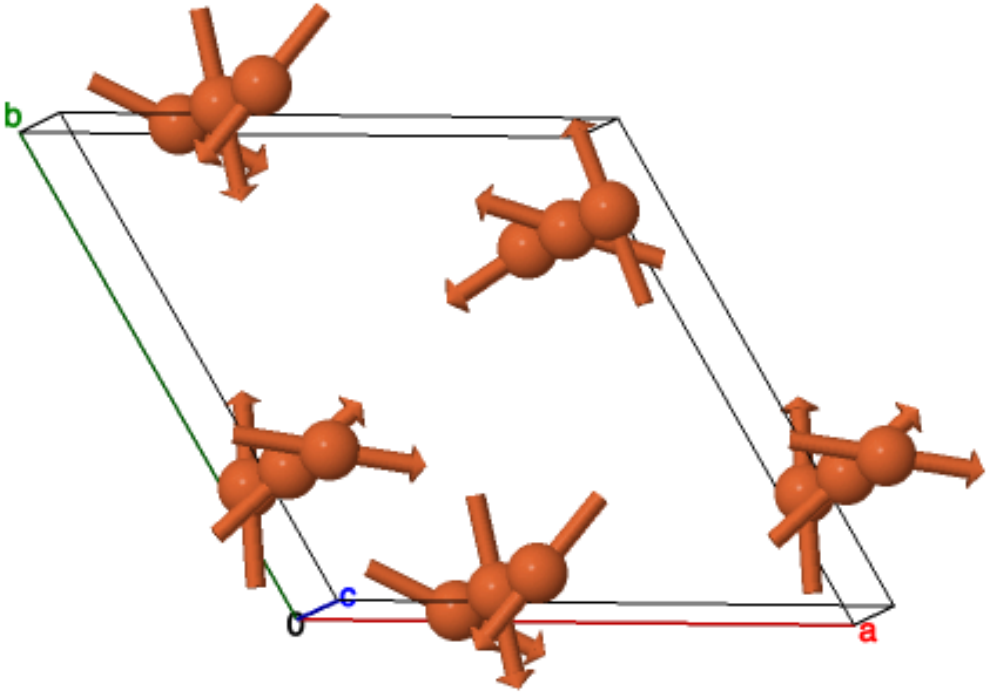
1.1.13 $MnAu_2$



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**	**2$M_x$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

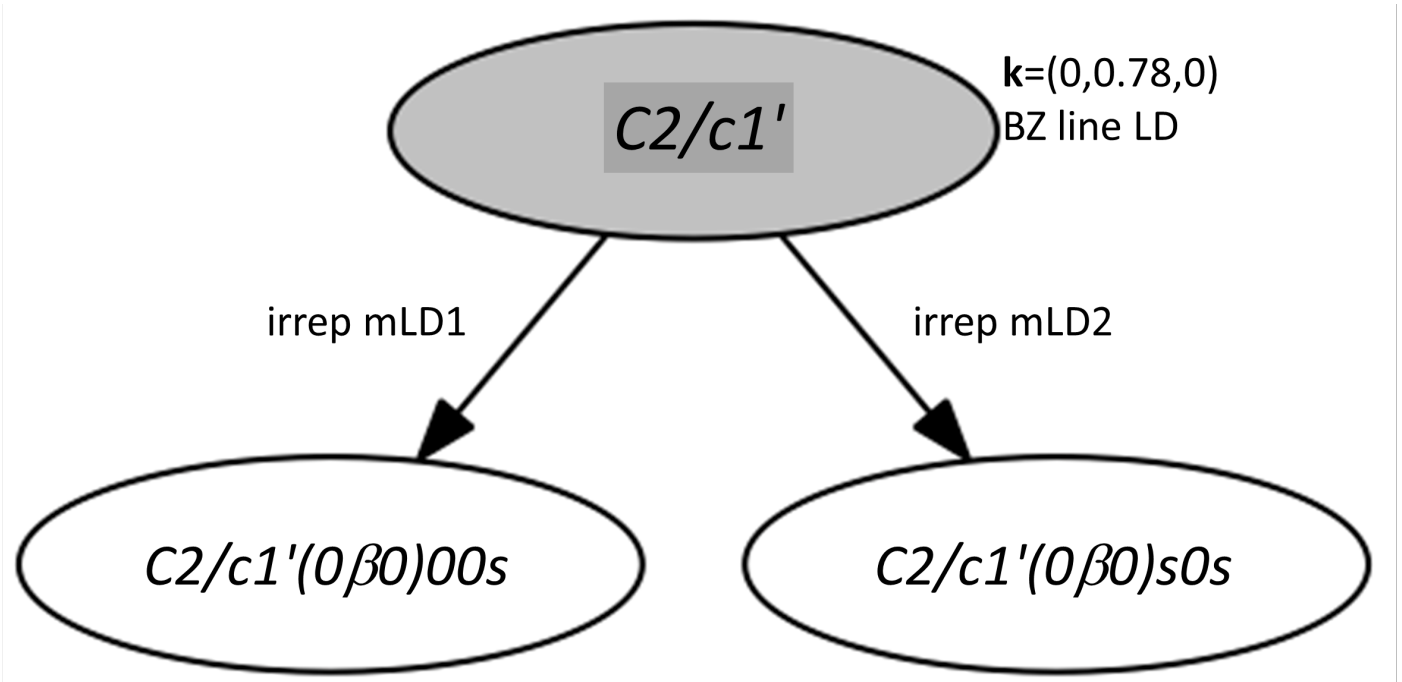
Wave vector 1

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

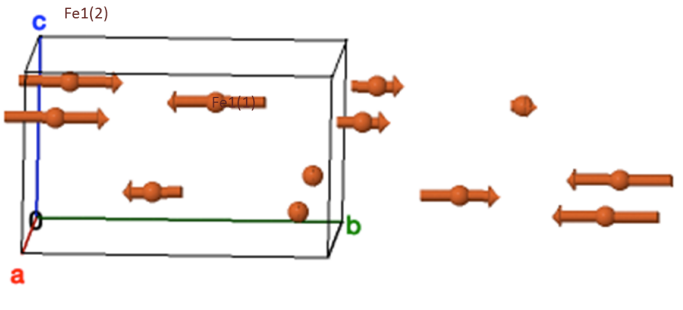
[Hide]

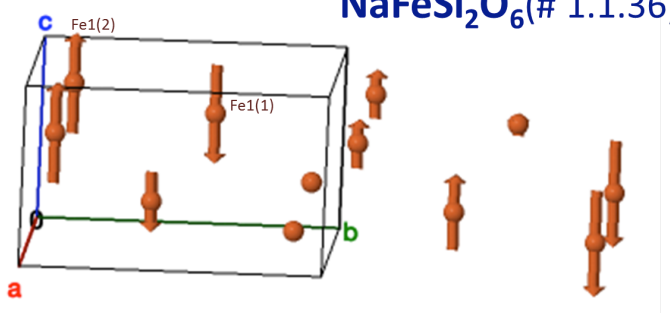
Possible MSSGs and the corresponding models have been derived using JANA2006 or ISODISTORT

for each irrep the possible MSSGs and models are derived:



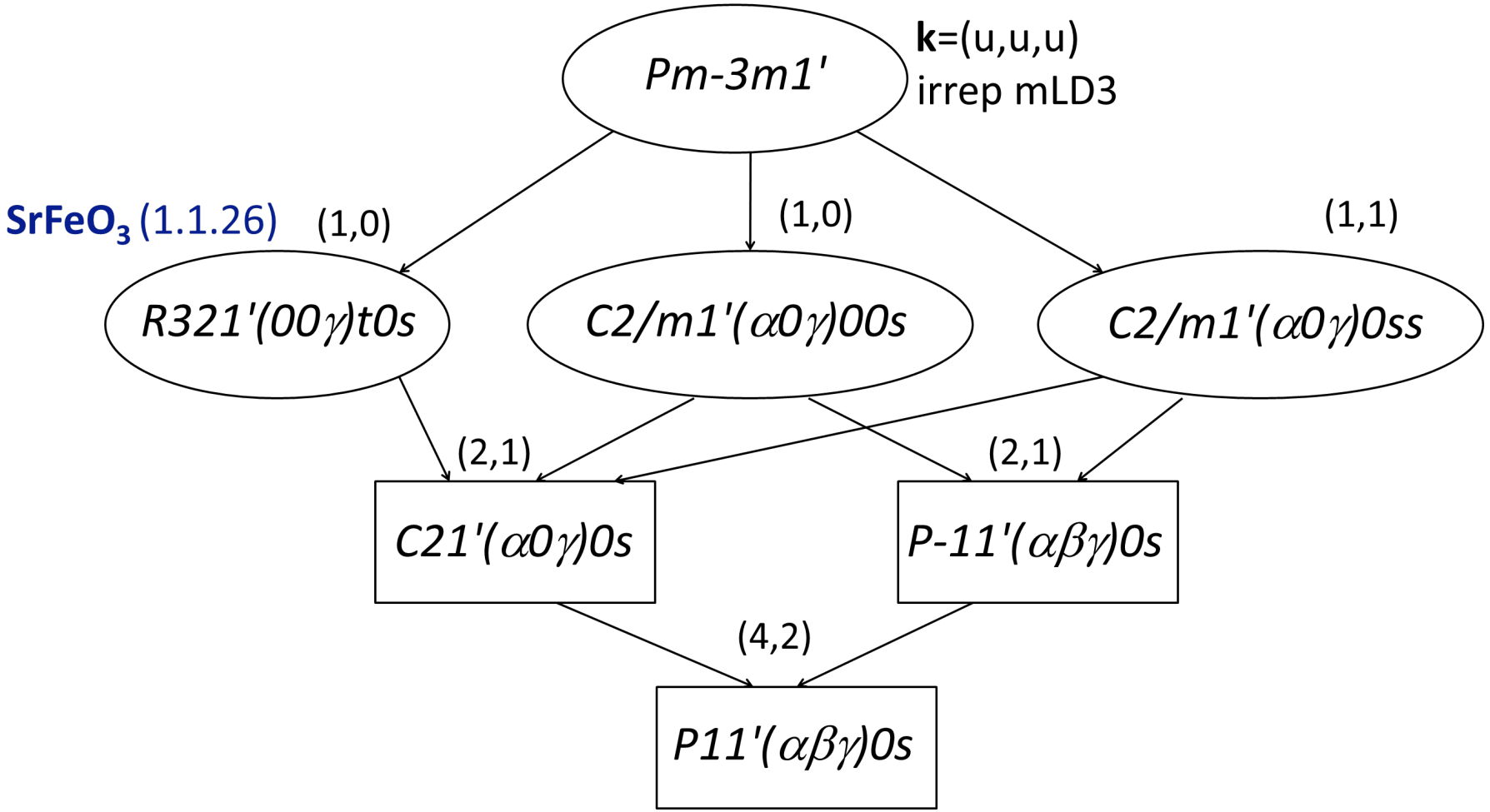
$NaFeSi_2O_6$(# 1.1.36)





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

for each irrep the possible MSSGs and models are derived:



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

Now you can help to complete the database and submit your structure(s) or any other published structure that is not yet in the collection

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.

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.

Tutorial on MAGNDATA:

Tutorial_magnetic_section_BCS_3
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