OAK RIDGE National Laboratory

# Magnetic Symmetry: an overview of Representational Analysis and Magnetic Space groups

**Stuart Calder**

**Neutron Scattering Division**
**Oak Ridge National Laboratory**

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U.S. DEPARTMENT OF ENERGY

# Bilbao Crystallographic Server (http://www.cryst.ehu.es/)

FCT/ZTF

## bilbao crystallographic server

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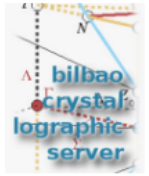



**Bilbao Crystallographic Server in forthcoming schools and workshops**

**News:**

- **New Article in Acta Cryst. A** 05/2019: Gallego *et al.* "Automatic calculation of symmetry-adapted tensors in magnetic and non-magnetic materials: a new tool of the Bilbao Crystallographic Server." *Acta Cryst.* (2019) **A75**, 438-447.
- **New Article in Nature** 03/2019: Vergniory *et al.* "A complete catalogue of high-quality topological materials" *Nature* (2019). **566**, 480-485.
- **Updated versions of TENSOR and MTENSOR** 03/2019: The programs give the general expression of tensor properties for a given point group and magnetic point group, respectively..
- **New option in COMPSTRU** 08/2018: The program provides the visual comparison of structures.
- **New program: Check Topological Mat** 08/2018: Given the electronic bands calculated from the structural parameters, the program checks if a given material is topological or not.

Tutorials
Material used in workshops and schools
Archive

### Space-group symmetry

#### Magnetic Symmetry and Applications

| | |
|---|---|
| MGENPOS | General Positions of Magnetic Space Groups |
| MWYCKPOS | Wyckoff Positions of Magnetic Space Groups |
| MNORMALIZER | Normalizers 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 transportable 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 |

### Group-Subgroup Relations of Space Groups

### Representations and Applications

### Solid State Theory Applications

### Structure Utilities

### Subperiodic Groups: Layer, Rod and Frieze Groups

### Structure Databases

### Raman and Hyper-Raman scattering

### Point-group symmetry

**Quick access to some tables**

Space Groups
Plane Groups
Layer Groups
Rod Groups
Frieze Groups
2D Point Groups
3D Point Groups
Magnetic Space Groups

# Bilboa Crystallographic Server (http://www.cryst.ehu.es/)

MAGNDATA → Collection of Magnetic Structures

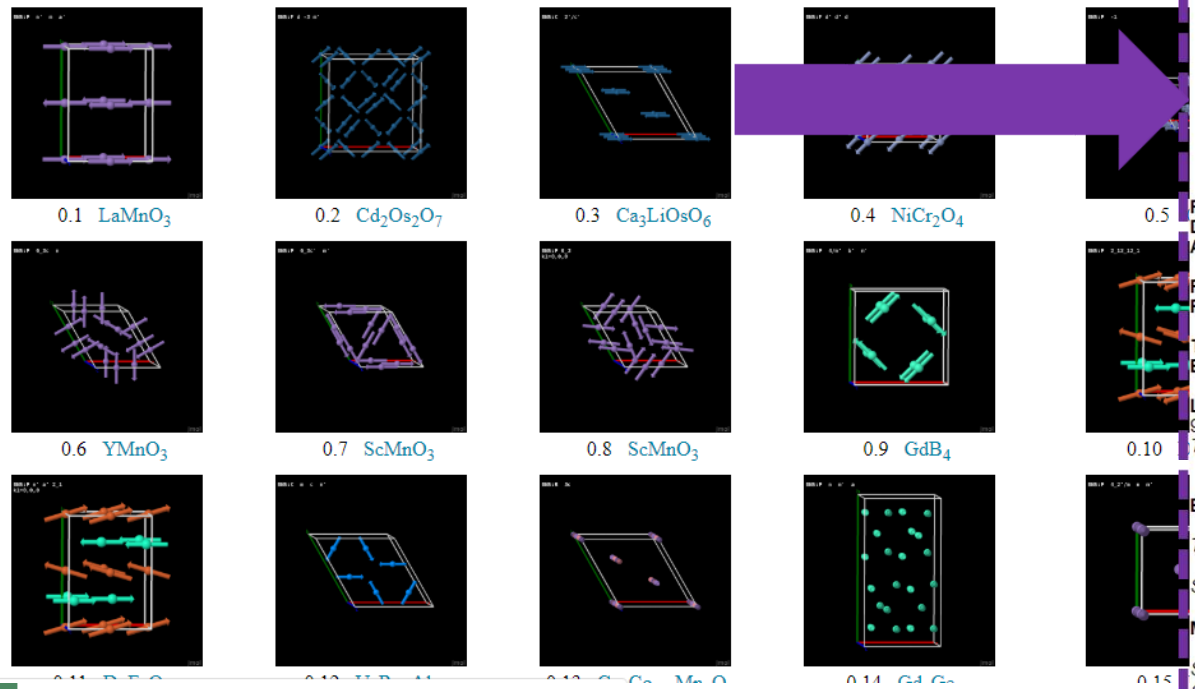
## MAGNDATA: A Collection of magnetic structures with portable cif-type files

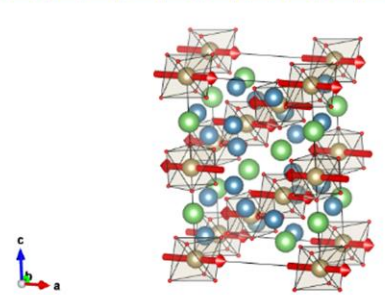
**Element search (separate with space or comma):** AND OR Search Advanced Search & Statistics

**Enter the label of the structure:** Submit

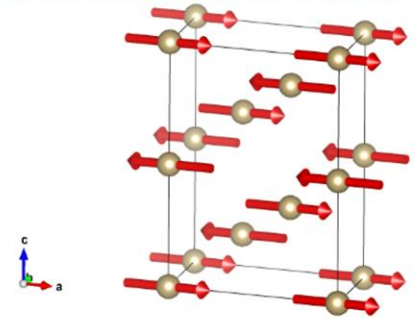
624 structures found

**Zero propagation vector**



*Magnetic structure with all atoms*



*Magnetic structure with only magnetic atoms*

**Reference:** S. Calder, M. D. Lumsden, V. O. Garlea, J. W. Kim, Y. G. Shi, H. L. Feng, K. Yamaura, A. D. Christianson et al., *PHYSICAL REVIEW B* (2012) **86** 054403
**DOI:** 10.1103/PhysRevB.86.054403
**Atomic positions from:** same reference

**Parent space group** (paramagnetic phase): R-3c (#167)
**Propagation vector:** k1 (0, 0, 0)

**Transition Temperature:** 117.1 K
**Experiment Temperature:** 4 K

**Lattice parameters of the magnetic unit cell:**
9.2570 9.2570 10.7630 90.0000 90.0000 120.0000
*Transformation from parent structure:* (**a**,**b**,**c**;0,0,0)
*[View matrix form]*

**BNS Magnetic Space Group:** C2'/c' (#15.89) (non-standard)
*[View symmetry operations]*
*Transformation to a standard setting:* (-**a**/3-2**b**/3-2**c**/3,-**a**,**a**/3+2**b**/3-**c**/3;0,1/2,0)
*[View matrix form]*
*Systematic absences for this Magnetic Space Group via* MAGNEXT

**Magnetic Point Group:** 2'/m' (5.5.16)
*[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*

# Bilboa Crystallographic Server (http://www.cryst.ehu.es/)

- Input space group, k-vector

**Maximal magnetic space groups for the parent space group 136 ($P4_2/mnm$) and the propagation vector k = (0, 0, 0)**

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

| N | Group (BNS) | Transformation matrix | General positions | Properties | Magnetic structure |
|---|---|---|---|---|---|
| 1 | $P4_2/m'n'm'$ (#136.503) Go to a subgroup | Alternatives (domain-related) | Show | Systematic absences MAGNEXT Tensor properties MTENSOR | Show |
| 2 | $P4_2/m'nm'$ (#136.502) Go to a subgroup | Alternatives (domain-related) | Show | Systematic absences MAGNEXT Tensor properties MTENSOR | Show |
| 3 | $P4_2/mn'm'$ (#136.501) Go to a subgroup | Alternatives (domain-related) | Show | Systematic absences MAGNEXT Tensor properties MTENSOR | Show |
| 4 | $P4_2/m'n'm$ (#136.500) Go to a subgroup | Alternatives (domain-related) | Show | Systematic absences MAGNEXT Tensor properties MTENSOR | Show |
| 5 | $P4_2/mnm'$ (#136.499) Go to a subgroup | Alternatives (domain-related) | Show | Systematic absences MAGNEXT Tensor properties MTENSOR | Show |
| 6 | $P4_2/mn'm$ (#136.498) Go to a subgroup | Alternatives (domain-related) | Show | Systematic absences MAGNEXT Tensor properties MTENSOR | Show |
| 7 | $P4_2/m'nm$ (#136.497) Go to a subgroup | Alternatives (domain-related) | Show | Systematic absences MAGNEXT Tensor properties MTENSOR | Show |
| 8 | $P4_2/mnm$ (#136.495) Go to a subgroup | Alternatives (domain-related) | Show | Systematic absences MAGNEXT Tensor properties MTENSOR | Show |
| 9 | $Cmm'm'$ (#65.486) Go to a subgroup | Alternatives (domain-related) | Show | Systematic absences MAGNEXT Tensor properties MTENSOR | Show |
| 10 | $Cm'mm$ (#65.483) Go to a subgroup | Alternatives (domain-related) | Show | Systematic absences MAGNEXT Tensor properties MTENSOR | Show |
| 11 | $Pnn'm'$ (#58.398) Go to a subgroup | Alternatives (domain-related) | Show | Systematic absences MAGNEXT Tensor properties MTENSOR | Show |
| 12 | $Pn'nm$ (#58.395) Go to a subgroup | Alternatives (domain-related) | Show | Systematic absences MAGNEXT Tensor properties MTENSOR | Show |

**Magnetic Structure**

**Selected magnetic space group: 12- *Pn'nm* (#58.395)**

Setting of the parent group

Parent space group 136 ($P4_2/mnm$)

Lattice parameters: a=4.57100, b=4.57100, c=8.85300, alpha=90., beta=90., gamma=90.

[Go to setting standard (**a, b, c** ; 0, 0, 0)]
[Go to an alternative setting]

Export data to MCIF file/Visualize | Go to a subgroup

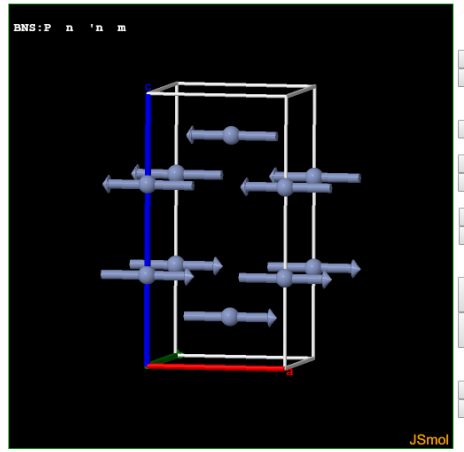
**Atomic positions, Wyckoff positions and Magnetic Moments**

| N | Atom | New WP | Multiplicity | Magnetic moment | Values of $M_x$, $M_y$, $M_z$ |
|---|---|---|---|---|---|
| 1 | W1 W 0.00000 0.00000 0.00000 | (0,0,0 \| 0,0,0) (1/2,1/2,1/2 \| 0,0,0) | 2 | - | - |
| 2 | Cr1 Cr 0.00000 0.00000 0.33300 | (0,0,z \| $m_x$,$m_y$,0) (1/2,1/2,z+1/2 \| -$m_x$,$m_y$,0) (1/2,1/2,-z+1/2 \| $m_x$,-$m_y$,0) (0,0,-z \| -$m_x$,-$m_y$,0) | 4 | ($M_x$,$M_y$,0) | $M_x$ = 1 $M_y$ = 0.00000 |
| 3 | O1 O 0.30800 0.30800 0.00000 | (x,x,0 \| 0,0,$m_z$) (-x,-x,0 \| 0,0,-$m_z$) (-x+1/2,x+1/2,1/2 \| 0,0,$m_z$) (x+1/2,-x+1/2,1/2 \| 0,0,-$m_z$) | 4 | - | - |
| 4 | O2 O 0.30800 0.30800 0.33300 | (x,x,z \| $m_x$,$m_y$,$m_z$) (-x,-x,z \| $m_x$,$m_y$,-$m_z$) (-x+1/2,x+1/2,z+1/2 \| -$m_x$,$m_y$,$m_z$) (x+1/2,-x+1/2,z+1/2 \| -$m_x$,$m_y$,-$m_z$) (-x+1/2,x+1/2,-z+1/2 \| $m_x$,-$m_y$,$m_z$) (x+1/2,-x+1/2,-z+1/2 \| $m_x$,-$m_y$,-$m_z$) (x,x,-z \| -$m_x$,-$m_y$,$m_z$) (-x,-x,-z \| -$m_x$,-$m_y$,-$m_z$) | 8 | - | - |

**MVISUALIZE: 3D Visualization of magnetic structures with Jmol**

MVISUALIZE Main Page

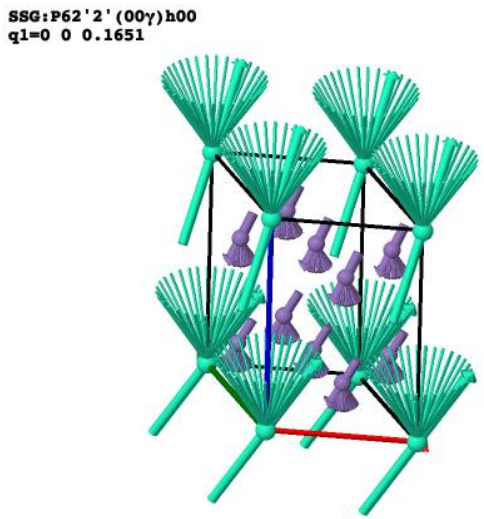
Show/Hide File

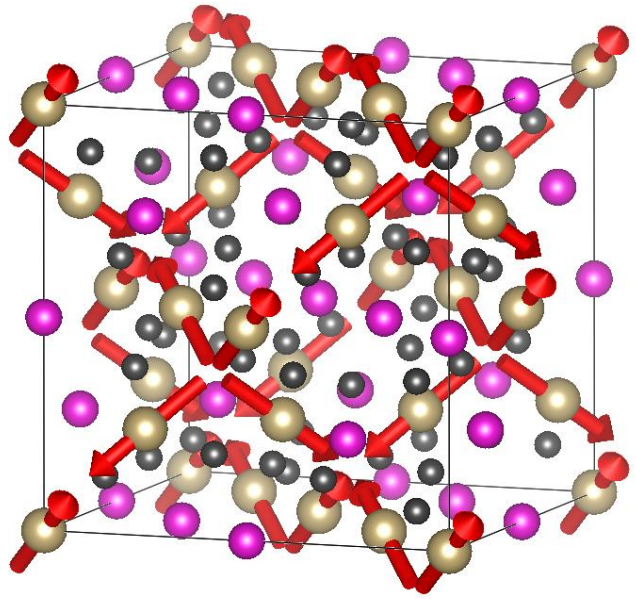


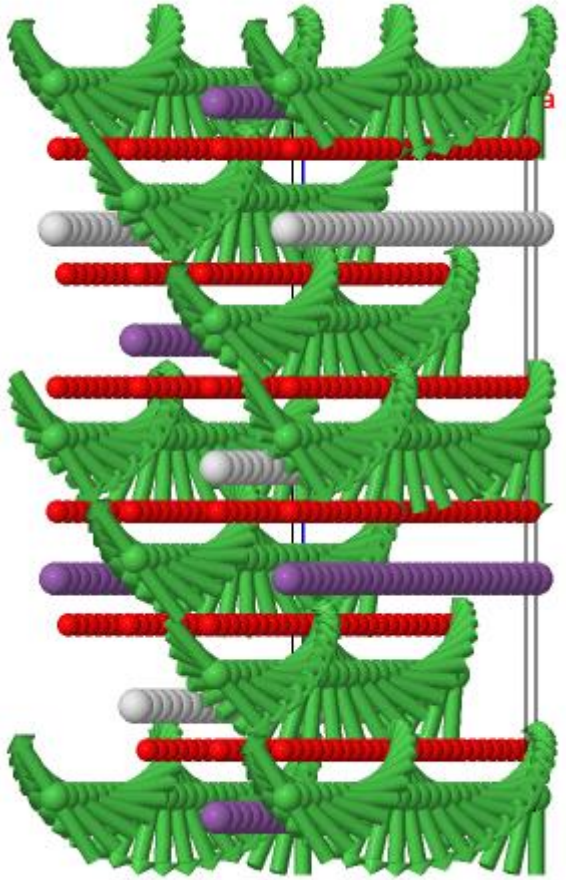

Select cell... | Export PNG Image
Toggle Parent Cell | Save PNG-3D
Toggle Standard Cell | Save ZIP file
View Along Axis... | Show unit cell a,b,c
Unit Cell Info | Add 1 cell along x
Remove 1 cell along x
All / Magnetic Atoms | Add 1 cell along y
Show/Hide Labels | Remove 1 cell along y
Larger | Smaller Vectors | Add 1 cell along z
Larger | Smaller Atoms | Remove 1 cell along z
Window Size | x=1 y=1 z=1 | Choose supercell
Bigger | Smaller | Draw bonds & polyhedra Join - with - from 0.75 to 2.75 Å
Background Color | Draw Bonds | Polyhedra
Toggle Quality | Delete Bonds | Polyhedra
Center | Clear all drawings
help | console | Execute

# mCIF file

- Magnetic structures are now standardized.
- Output from refinement software (Fullprof, TOPAS, GSAS(?) or generated from BCS, ISODISTORT).
- Read by most software
- Nice visualization with VESTA (commensurate and incommensurate)





# Examples

- Example3_Bilbao_SCalder/
  - Bilbao_Cr2WO6
  - Bilbao_Ho2BaNiO5
  - Bilbao_LaMnO3

- Lots of detailed examples on multiple programs on Bilbao Crystallographic Website → very powerful