

Computational analysis tools for magnetic structures in the Bilbao Crystallographic Server

E.S. Tasci,^{a*} L. Elcoro,^b J. M. Perez-Mato,^c G. de la Flor,^d G. Madariaga^b and M. I. Aroyo^b

^aDepartment of Physics Engineering, Hacettepe University Ankara, Türkiye, ^bDepartamento de Física, Facultad de Ciencia y Tecnología, Universidad del País Vasco UPV/EHU, Apartado 644, Bilbao, Spain, ^cFacultad de Ciencia y Tecnología, Universidad del País Vasco UPV/EHU, Apartado 644, Bilbao, Spain, and ^dInstitute of Applied Geosciences, Karlsruhe Institute of Technology, Karlsruhe, Germany. *Correspondence e-mail: emre.tasci@hacettepe.edu.tr

Received 17 October 2024

Accepted 10 January 2025

Edited by V. Garlea, Oak Ridge National Laboratory, USA

This article is part of a focused issue on Magnetic Structures.

Keywords: magnetic structures; symmetry; computational tools.

Magnetic symmetry plays a critical part in the description of magnetic structures and their relations to their paramagnetic parent phases as well as to other magnetic structures through phase transitions. Here, we present the symmetry-based computational tools developed by the Bilbao Crystallographic Server for the analysis of magnetic structures, and their relations are illustrated through worked-out cases from the literature.

1. Introduction

The increasing number of computational and experimental research activities in the field of magnetic structures in recent years has created the need for specialized computational tools incorporating group theory. Litvin's definitive work on magnetic point and space groups (Litvin, 2013; Litvin, 2016) and Stokes and Campbell's computer-readable listing of the magnetic space groups (Stokes *et al.*, 2010) enabled the automated processing and application of invariance symmetry to magnetic structures. Based on these developments, at the Bilbao Crystallographic Server (<https://www.cryst.ehu.es>) (Aroyo *et al.*, 2006a; Aroyo *et al.*, 2006b; Aroyo *et al.*, 2011) (hereafter referred to as BCS), we have extended our portfolio in recent years to offer a variety of tools for the analysis of magnetic structures.

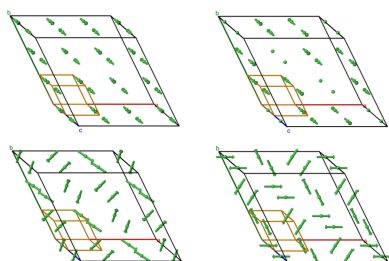
These tools are freely available from the BCS, under the 'Magnetic Symmetry and Applications' section. The 17 programs in this section can be grouped under three main types:

(1) Retrieval tools that act mainly as interfaces to databases containing tabulated information (*MGENPOS*, *MWYCKPOS*, *MKVEC*, *MPOINT*, *MAGNEXT*, *MAGNETIC REP*).

(2) Tools that perform basic operations (*IDENTIFY MAGNETIC GROUP*, *BNS2OG*, *mCIF2PCR*, *MVISUALIZE*).

(3) Tools with multiple options to deal with specific structures and/or symmetries (*MAXMAGN*, *k-SUBGROUPSMAG*, *MAGMODELIZE*, *STRCONVERT*, *MAGNDATA*, *MTENSOR*, *Get_mirreps*).

Some of the mentioned tools require selecting a specific magnetic space group as input. The magnetic space groups (MSGs) can be specified directly by their serial number as defined in *Magnetic Space Groups* by Litvin (2016) and *Table of Magnetic Space Groups* by Stokes and Campbell (Stokes *et al.*, 2010), either in Belov–Neronova–Smirnova (BNS) or



Opechowski–Guccione (OG) setting. Alternatively, the user can select the MSG type among the complete list of MSGs in two steps. First, the list of the 230 space groups is presented and once a root space group type has been chosen, two lists of MSGs are presented. One list includes the MSGs derived from the chosen space group according to the BNS classification and the other list shows the derived groups according to the OG classification. In both lists the symbols of the groups in both settings, along with the recently developed unified UNI notation (Campbell *et al.*, 2022) are included. [As the UNI notation uses the same indexing as BNS, only the label differs. This notation has been introduced into most of the tools and full integration is still in progress.]

Among these settings, the server follows the BNS notation, while providing support and conversion to and from the OG notation. Although standard setting¹ is presumed for the input in general, many of the tools allow the users to work in a non-conventional setting by defining a transformation from the user's basis to one where the MSG acquires its standard setting.

2. Retrieval tools

These tools return tabulated information based on the input data.

2.1. MGENPOS

MGENPOS (Gallego *et al.*, 2012; Perez-Mato *et al.*, 2015) lists the general positions, or in other terms the symmetry operators (apart from those related by the lattice translations) of the given MSG. The result containing the list of the symmetry operators are presented in the coordinate triplets (*x,y,z*), matrix-column representation, geometric interpretation and Seitz symbol (Glazer *et al.*, 2014) formats². The operators with time inversion are highlighted in red and listed after the operators without time inversion. The output page also includes an option to switch the BNS or OG settings, along with the transformation matrices relating both settings. For detailed information on the transformations of coordinate systems, refer to Section 1.5 of ITA (Aroyo, 2016). A sample of the output page is presented in Fig. 1.

The output page also includes direct links to the Wyckoff positions (*MWYCKPOS*) and systematic absences for non-

¹ For space groups with more than one description in *International Tables for Crystallography* Vol. A (hereafter referred to as ITA) (Aroyo, 2016), the following settings are chosen as standard: for monoclinic groups: unique axis *b* setting, cell choice 1; for rhombohedral groups: hexagonal axes setting; and for the centrosymmetric groups listed with respect to two origins in ITA: origin choice 2 (origin at the inversion center).

² (i) The list of coordinate triplets (*x,y,z*) reproduces the data from the general position blocks of the magnetic space-group tables found in Litvin's work (Litvin, 2016). The coordinate triplets may also be interpreted as shorthand descriptions of the matrix forms of the corresponding symmetry operations. (ii) For the matrix-column representations, the symmetry operations of the space groups are described by (3 × 4) matrix-column pairs (**W,w**) with reference to a coordinate system consisting of an origin *O* and a basis (*a*₁, *a*₂, *a*₃). (iii) The geometric interpretation of the symmetry operations is given following the conventions in ITA (Aroyo, 2016) [including the symbol of the symmetry operation, its glide or screw component (if relevant), and the location of the related geometric element].

General Positions of the Group *P*_c4 (#75.4) [BNS setting]

75.4 *P*4₁′[*P*4] (UNI symbol)

To display the general positions in the OG setting, please follow this link: *P*_{2c}4 (#75.4.664) [Transformation matrix]

Translation lattice generators: (1|1,0,0), (1|0,1,0), (1|0,0,1), (1|0,0,0)

Black-and-white lattice generators: (1|1,0,0), (1|0,1,0), (1|0,0,1), (1′|0,0,1/2)

N	Standard/Default Setting			
	(<i>x,y,z</i>) form	Matrix form	Geom. interp.	Seitz notation
1	<i>x</i> , <i>y</i> , <i>z</i> , +1 <i>m_x</i> , <i>m_y</i> , <i>m_z</i>	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	1±1	{1 0}
2	− <i>y</i> , <i>x</i> , <i>z</i> , +1 − <i>m_y</i> , <i>m_x</i> , <i>m_z</i>	$\begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	4 ⁺ 0,0, <i>z</i> ±1	{4 ⁺ ₀₀₁ 0}
3	<i>y</i> , − <i>x</i> , <i>z</i> , +1 <i>m_y</i> , − <i>m_x</i> , <i>m_z</i>	$\begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	4 [−] 0,0, <i>z</i> ±1	{4 [−] ₀₀₁ 0}
4	− <i>x</i> , − <i>y</i> , <i>z</i> , +1 − <i>m_x</i> , − <i>m_y</i> , <i>m_z</i>	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	2 0,0, <i>z</i> ±1	{2 ₀₀₁ 0}
5	<i>x</i> , <i>y</i> , <i>z</i> +1/2, −1 − <i>m_x</i> , − <i>m_y</i> , − <i>m_z</i>	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1/2 \end{pmatrix}$	1 (0,0,1/2)±1	{1′ 0 0 1/2}
6	− <i>y</i> , <i>x</i> , <i>z</i> +1/2, −1 <i>m_y</i> , − <i>m_x</i> , − <i>m_z</i>	$\begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1/2 \end{pmatrix}$	4 ⁺ (0,0,1/2) 0,0, <i>z</i> ±1	{4 ⁺ ₀₀₁ 0 0 1/2}
7	<i>y</i> , − <i>x</i> , <i>z</i> +1/2, −1 − <i>m_y</i> , <i>m_x</i> , − <i>m_z</i>	$\begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1/2 \end{pmatrix}$	4 [−] (0,0,1/2) 0,0, <i>z</i> ±1	{4 [−] ₀₀₁ 0 0 1/2}
8	− <i>x</i> , − <i>y</i> , <i>z</i> +1/2, −1 <i>m_x</i> , <i>m_y</i> , − <i>m_z</i>	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 1/2 \end{pmatrix}$	2 (0,0,1/2) 0,0, <i>z</i> ±1	{2′ ₀₀₁ 0 0 1/2}

Go to the list of the Wyckoff Positions of the Group *P*_c4 (#75.4)
Go to the Systematic Absences for the Group *P*_c4 (#75.4)

Figure 1
Output of *MGENPOS* for the MSG *P*_c4 (No. 75.4) in the BNS setting.

polarized neutron magnetic diffraction (*MAGNEXT*) related to the chosen MSG.

2.2. MWYCKPOS

The program *MWYCKPOS* (Gallego *et al.*, 2012; Perez-Mato *et al.*, 2015) lists the Wyckoff positions for a designated MSG. The Wyckoff-position block starts with the general position at the top, followed downwards by the various special Wyckoff positions with decreasing multiplicity and increasing site symmetry. Similar to the *MGENPOS* tool, one can directly access the symmetry operators (*MGENPOS*) and systematic absences (*MAGNEXT*) for the given MSG from the result page.

The output of the program for the MSG *P*_{cn}ma (No. 62.452) is presented in Fig. 2. The elements of the Wyckoff positions along with their allowed and restricted magnetic moment forms are listed in detail.

2.3. MKVEC

MKVEC (Elcoro *et al.*, 2021; Xu *et al.*, 2020) lists the **k** vectors of the input MSG along with their labels, stars and little co-groups. The program also lists the coordinates, symbol and the site-symmetry group of the given **k** vector in the standard setting of the unitary subgroup of the MSG. The unitary subgroup is the type I magnetic group which contains all the symmetry operations of the MSG not combined with

Wyckoff Positions of the Group $P_{c2}nma$ (#62.452) [BNS setting]

62.452 $Pnma.1'$ [$Pbma$] (UNI symbol)

To display the Wyckoff positions in the OG setting, please follow this link: $P_{2ab}bc'm$ (#57.11.468)

Multiplicity	Wyckoff letter	Coordinates	
		$(0,0,0) + (0,0,1/2) +$	
16	e	$(x,y,z m_x, m_y, m_z)$	$(x+1/2, -y+1/2, -z+1/2 m_x, -m_y, -m_z)$
		$(-x, y+1/2, -z -m_x, m_y, -m_z)$	$(-x+1/2, -y, z+1/2 -m_x, -m_y, m_z)$
		$(-x, -y, -z m_x, m_y, m_z)$	$(-x+1/2, y+1/2, z+1/2 m_x, -m_y, -m_z)$
		$(x, -y+1/2, z -m_x, m_y, -m_z)$	$(x+1/2, y, -z+1/2 -m_x, -m_y, m_z)$
8	d	$(x, 1/4, z 0, m_y, 0)$	$(x+1/2, 1/4, -z+1/2 0, -m_y, 0)$
		$(-x, 3/4, -z 0, m_y, 0)$	$(-x+1/2, 3/4, z+1/2 0, -m_y, 0)$
8	c	$(1/4, 0, z m_x, m_y, 0)$	$(3/4, 1/2, -z+1/2 m_x, -m_y, 0)$
		$(3/4, 0, -z m_x, m_y, 0)$	$(1/4, 1/2, z+1/2 m_x, -m_y, 0)$
8	b	$(0, 0, 0 m_x, m_y, m_z)$	$(1/2, 1/2, 1/2 m_x, -m_y, -m_z)$
		$(0, 1/2, 0 -m_x, m_y, -m_z)$	$(1/2, 0, 1/2 -m_x, -m_y, m_z)$
8	a	$(0, 0, 3/4 0, 0, 0)$	$(1/2, 1/2, 3/4 0, 0, 0)$
		$(0, 1/2, 1/4 0, 0, 0)$	$(1/2, 0, 1/4 0, 0, 0)$

Site Symmetries of the Wyckoff Positions

WP	Representative	Site symmetry
8a	$(0, 0, 3/4 0, 0, 0)$	$-1'$
8b	$(0, 0, 0 m_x, m_y, m_z)$	-1
8c	$(1/4, 0, z m_x, m_y, 0)$	$.2'$
8d	$(x, 1/4, z 0, m_y, 0)$	$.m$
16e	$(x, y, z m_x, m_y, m_z)$	1

List the original elements of the orbits
List all the elements of the orbits

Go to the list of the Symmetry Operators of the Group $P_{c2}nma$ (#62.452)
Go to the Systematic absences for the Group $P_{c2}nma$ (#62.452)

Figure 2
Output of *MWYCKPOS* for the MSG $P_{c2}nma$ (No. 62.452) in the BNS setting.

time reversal. In a separate list, it also lists additional $\mathbf{k}$ vectors that are particular cases of the $\mathbf{k}$ vectors in the main list (each $\mathbf{k}$ vector in this list has the same site-symmetry group as the corresponding $\mathbf{k}$ vector in the main list) but that are not particular cases in other MSGs of the same Bravais class. Detailed information is available in the supplementary section of Elcoro *et al.* (2021).

2.4. *MPOINT*

MPOINT lists the symmetry operations of the requested point group. In addition to the symmetry operations, some properties of the point group such as centrosymmetry, polarity and its compatibility with ferromagnetism are summarized. Following the listing of the symmetry operations, an option to list the subgroups along with checking various properties' compatibilities with this magnetic point group (via the *MTENSOR* tool, see Section 4.6) is provided.

2.5. *MAGNEXT*

By default, *MAGNEXT* (Gallego *et al.*, 2012; Perez-Mato *et al.*, 2015) lists the systematic absences or extinction rules for a specified MSG. It also provides the symmetry-forced form of the magnetic structure factor for every type of reflection, so that additional systematic absences can be inferred, depending on the specific orientation of the spins. Apart from the stan-

dard settings, the program also has an additional interface to work with any setting, identified through the symmetry operations' representations in the sought setting. *MAGNEXT* can be used to perform a search the other way around as well: by directly specifying the systematic absences (which can be further filtered via seeking compatibility with a given non-MSG or a crystal class), it returns the list of MSGs compatible with the defined absences.

In addition, the program also supports $(3+1)$ magnetic superspace groups (defined through a set of generators and the indication of the type of propagation vector).

2.6. *MAGNETIC REP*

For a given space group and the specified propagation vector(s), the program decomposes the magnetic representations associated with any Wyckoff position into irreducible representations (irreps). A detailed treatment on the usage of irreducible representations for MSGs can be found in Perez-Mato *et al.* (2015).

3. Tools that perform basic operations

These tools are characterized by their simple input and they undertake basic yet important operations.

3.1. *IDENTIFY MAGNETIC GROUP*

Given a set of generators of an MSG in the $(x, y, z, \pm 1)$ format (either in BNS or OG setting), this tool identifies the corresponding MSG type. As there are an infinite number of different settings that can represent an MSG, the power of this tool comes in the further derivation of the transformation matrix $(\mathbf{P}, \mathbf{p})$ that relates the given setting to that of the standard setting. This program is used in the background by many other more complex programs of this section.

3.2. *BNS2OG*

Given a set of generators of an MSG in an arbitrary basis in the BNS or OG setting, this program identifies the group and gives the set of symmetry operations in a 'reasonable' basis for the description of the magnetic group in the other setting (OG when the set operations are given in the BNS setting and vice versa). It tries to keep the description in the second setting as close as possible to the one given in the first setting, *i.e.* it tries to keep the $\mathbf{a}$, $\mathbf{b}$ and $\mathbf{c}$ basis vectors parallel to the original ones, or it tries to keep a relation between both basis similar to the relation between the two basis of the standard BNS and OG settings.

Furthermore, *BNS2OG* also gives an alternative second description of the group in the OG setting for which the sets of translations and anti-translations of the magnetic moments are defined by a wavevector such that a lattice translation $\mathbf{t}$ is kept as a pure translation if $\mathbf{k} \cdot \mathbf{t} = n$, $n \in \mathbb{Z}$ while it is an anti-translation when $\mathbf{k} \cdot \mathbf{t} = n + \frac{1}{2}$, $n \in \mathbb{Z}$ (here $\mathbf{k}$ is a wavevector which satisfies $2\mathbf{k} = \mathbf{K}$, with $\mathbf{K}$ being a reciprocal lattice vector).

3.3. *mCIF2PCR*

mCIF2PCR is an auxiliary tool that converts an mCIF file³ describing any magnetic structure into the .pcr format that can be used as input for the *FullProf* program (Rodríguez-Carvajal, 1993). This program (*mCIF2PCR*), designed by J. Rodríguez-Carvajal, actually belongs to the *FullProf* suite (Rodríguez-Carvajal, 2001) and is included in the 'Magnetic Symmetry and Applications' section of the BCS to facilitate the communication between the two platforms.

3.4. *MVISUALIZE*

MVISUALIZE (Perez-Mato *et al.*, 2015; Gallego *et al.*, 2016b) is a highly customized interface to *Jmol* (Hanson, 2010a; Hanson, 2010b) for visualizing a given magnetic structure, introduced in the form of an mCIF file. It contains many options to refine the 3D visualization to one's need. The image can be exported to various image formats as well as to 3D model formats. A screenshot of the program is presented in Fig. 3. *MVISUALIZE* is either linked to or directly incorporated by most of the magnetic tools of the BCS. If the input mcif file includes the corresponding information, using this tool one can visualize the relation between the unit cell being used and the parent unit cell associated with the paramagnetic phase. The structure can also be shown using a unit cell, for which its MSG is in its standard setting.

This tool can also be used to prepare a new mcif file that contains all the necessary information required for a submission to the MAGNDATA database.

4. Tools with multiple options to deal with specific structures and/or symmetries

These tools employ tabulated data and/or do real time calculations based on specific cases provided by the user.

4.1. *MAXMAGN*

MAXMAGN (Perez-Mato *et al.*, 2015) provides the maximal magnetic subgroups of the gray magnetic group associated with the space group of a given paramagnetic phase (parent space group), which are compatible with the defined propagation vector **k**.

The MSGs of the non-magnetic parent structure and the magnetic structure are related through a group-subgroup relation, always defined by the accompanying transformation matrix⁴. The transformation matrix relating the standard settings of the two groups is in general necessary to unambiguously identify the relation, as inclusion of solely the space group type symbol can correspond to many different subgroups with the same symbol.

³ An mCIF file is a data file based on the CIF format, adhering to the magCIF standard (as defined by the Magnetic CIF dictionary (https://www.iucr.org/resources/cif/dictionaries/cif_mag), developed by the IUCr to accommodate magnetic structure data.

⁴ For the definition and properties of the transformation matrix, refer to Section 1.2. of *International Tables for Crystallography* Vol. A1 (Wondratschek & Müller, 2011).

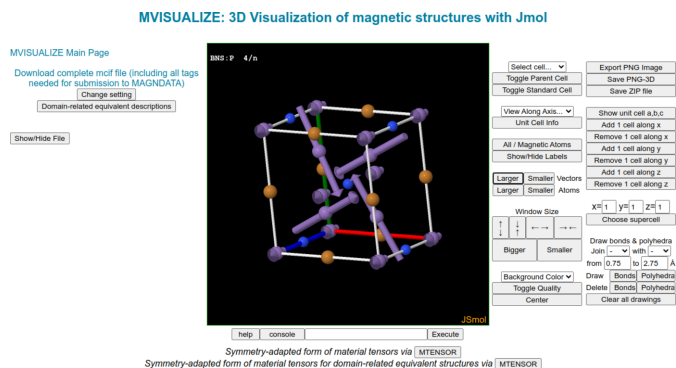


Figure 3

Interface of *MVISUALIZE*. [The visualized structure is Mn_3CuN (Fruchart & Bertaut, 1978) with MSG $P4/n$ (No. 85.59). It is available from the MAGNDATA database with the assigned label: 2.5].

The maximal subgroups listed by the program can be considered the most probable candidates for the MSG of a magnetic structure with this propagation vector. About 70% of the published single-**k** magnetic structures have one of the maximal symmetries that this program provides. If a parent structure is introduced, the program indicates which of the listed maximal subgroups allow non-zero magnetic moment at the magnetic sites. The program can construct a magnetic structure model under each of the listed symmetries, which can be visualized via the *MVISUALIZE* tool, and can be exported in the mcif format. The basis used for the magnetic subgroup is the one of the parent space group, if the magnetic group keeps its lattice. Otherwise, for convenience, a supercell that maintains the parent main crystallographic axes is used, and the resulting setting of the magnetic group is called parent-like. These mcif files can be used as starting models for the different symmetries to be considered in the refinement of experimental data.

4.2. *k-SUBGROUPSMAG*

The *k-SUBGROUPSMAG* (Perez-Mato *et al.*, 2015) tool is one of the most powerful tools on the magnetic section of the BCS, providing all the possible magnetic subgroups of the gray magnetic group associated with a paramagnetic phase that are compatible with various adjustable criteria such as the observed propagation vector(s), Wyckoff positions occupied by the magnetic atoms, groups compatible with specific magnetic irrep(s), centrosymmetric or non-centrosymmetric groups, polar or non-polar groups, *etc.* The search can also be restricted within a specified parameter of depth like the lowest space/point group/crystal system to consider or to include only the maximal subgroups. The results are presented as a list or a graph.

If a parent structure is supplied, general models for the magnetic structures corresponding to any of the listed possible magnetic subgroups can be constructed (internally via *MAGMODELIZE*) and downloaded as mcif files (as single

files or with the option of an automatic generation and collection within a single zip archive file).

Similarly as in *MAXMAGN*, this set of mcif files can be used as the starting point for a systematic exploration of all these alternative models with different magnetic symmetries, using a refinement program.

4.3. MAGMODELIZE

MAGMODELIZE can be used to explore the properties of a given MSG derived from the symmetry of a parent paramagnetic phase, and to construct the corresponding magnetic structure model. To use the program, one must identify the (paramagnetic) space group of the parent structure and the group-subgroup transformation matrix defining the subgroup associated with the magnetic structure. Afterwards, the derived magnetic subgroup's properties (general positions, systematic absences and tensor properties) are displayed in the basis of the parent space group or a closely related one, as described in the *MAXMAGN* section.

Even though it can work without a structure at hand, the most relevant use of *MAGMODELIZE* (Perez-Mato *et al.*, 2015) requires a CIF file of a paramagnetic structure and the definition of a magnetic subgroup of the gray group of the paramagnetic phase. The magnetic subgroup must be introduced using its BNS symbol and the transformation matrix⁵. With this option, the output of the program is a magnetic structure under the input MSG that can be exported to .mcif file format and/or visualized through *MVISUALIZE*. As in the case of *k-SUBGROUPSMAG*, this magnetic structure can be used to compare, refine or further explore an observed structure.

4.4. STRCONVERT

This tool can be used for the manipulation of magnetic structures. It supports several formats including CIF, mCIF, *VESTA* (Momma & Izumi, 2011) and *VASP* (Kresse & Furthmüller, 1996) formats, along with native format of the BCS⁶. The structure on which the program operates can be imported, or if needed can be defined from scratch.

Upon introducing the structure, the user is presented with the properties of the structure such as its MSG number, unit-cell parameters, symmetry operators, atomic positions, site occupancies and magnetic moment components as shown in Fig. 4. These values are presented as input forms that can be edited accordingly. The program also provides options for adding or removing atomic sites, removing the magnetic and/or symmetry information, reducing the symmetry to *P1* and exporting the structure data in various formats. It presents a concise summary of the structure including the atomic positions and magnetic moments for a quick overview. If the

⁵ If not readily known, a valid transformation matrix for the group-subgroup pair can be obtained via *k-SUBGROUPSMAG*, for instance.

⁶ The native format used in the BCS is composed of the space group's ITA classification id, unit-cell parameters, number of sites in the asymmetric unit cell and occupied sites' information (species, label, Wyckoff symbol and position). An example of this format can be found for the $\text{Ba}_3\text{Nb}_2\text{NiO}_9$ structure in Section 5.1.

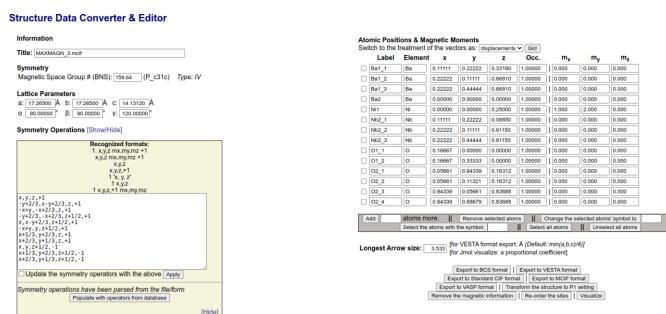


Figure 4
Sample interface of *STRCONVERT* (edited for clarity).

symmetry of the structure is triclinic (as it is usual in the output provided by *DFT* packages), it also offers an option to deduce the symmetry via the *FINDSYM* program (Stokes & Hatch, 2005).

4.5. MAGNDATA

MAGNDATA is a database of magnetic structures (Gallego *et al.*, 2016a; Gallego *et al.*, 2016b) and currently holds more than 2000 entries on published magnetic structures. The structures are described crystallographically under their MSG, reducing the information on the atomic positions and magnetic moments to an asymmetric unit with respect to this MSG. Additional information about its relation with its paramagnetic phase, like propagation vector(s), relevant irreps, *etc.* can also be found.

Each entry includes direct links to some of the programs listed here, so that they can be applied to this specific structure in a straightforward manner. The data can be exported to .mcif and *VESTA* formats, and can be directly visualized via the integrated *Jmol* program (Hanson, 2010a; Hanson, 2010b).

4.6. MTENSOR

MTENSOR (Gallego *et al.*, 2019) lists the symmetry-adapted form of tensor properties for a given magnetic point group. Although macroscopic crystal tensor properties of magnetic structures only depend on the magnetic point group of the system, the program allows the input of a full MSG as well, because then it considers the point group with the orientation associated with the standard setting of the space group, which in general, may not be the standard setting for the point group⁷. Around 170 distinct crystal tensors are collected under the equilibrium, optical, non-linear optical susceptibility and transport classes. The user can also get the symmetry constraints for a tensor not included in the list. The tensor must be defined through its Jahn symbol (Jahn, 1949).

MTENSOR can also be used in a more generic form by listing the symmetry-adapted form of a chosen tensor for all magnetic point groups.

⁷ As a side note, all type IV MSGs have gray point group symmetry and correspondingly, the symmetry restrictions on their tensor properties do not differ from those of a paramagnetic structure with the same magnetic point group.

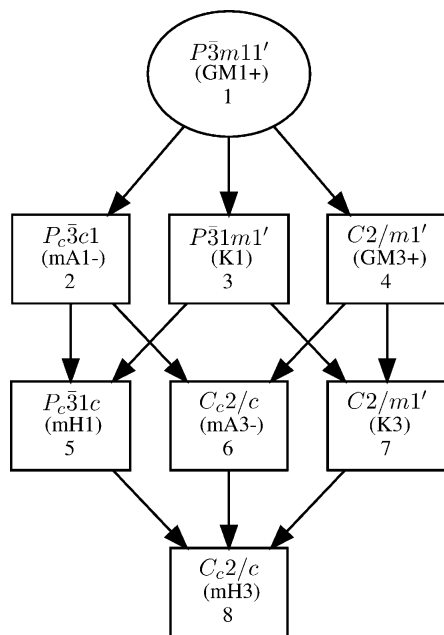


Figure 5

Get_mirreps graph of isotropy subgroups for the magnetic gray group $P3m1'$ (No. 164.86) and its subgroup $Cc2/c$ (No. 15.90), with their standard settings related by the transformation ($2a + b, 3b, 2c; 0, -1/2, 1/2$). The graph indicates for each subgroup the compatible irrep. The graph may include subgroups that are not reachable by a single irrep and therefore are not one of the listed isotropy subgroups.

4.7. *Get_mirreps*

By specifying a parent space group and one of its magnetic subgroups of the associated parent magnetic gray group (identified through the relating transformation matrix), *Get_mirreps* lists the magnetic and non-magnetic physically irreducible representations that are symmetry-allowed in a phase transition between the given groups, becoming compatible with the specified magnetic subgroup. The output lists the irreps of the parent space group corresponding to degrees of freedom that are allowed in the low-symmetry group after the symmetry breaking phase transition (the prefix 'm' in the label of an irrep indicates that it is a magnetic irrep, *i.e.* odd for time reversal). The information for each irrep is completed with the so-called order parameter direction, indicating any necessary subspace restriction within the irrep space. Additionally, the program determines the list and graph (subgroup-tree) of isotropy subgroups (group number and transformation matrix) that the parent structure would transform to, due to the distortions according to each of the irreps listed. By definition, all of these subgroups must be supergroups of the input subgroup, or this subgroup itself. A sample graph from *Get_mirreps* is shown in Fig. 5 depicting the full group-subgroup scheme relating the gray magnetic group corresponding to a parent paramagnetic space group $P3m1$ (No. 164) and its magnetic subgroup $Cc2/c$ (No. 15.90) related with the ($2a + b, 3b, 2c; 0, -1/2, 1/2$) transformation matrix. The graph may include subgroups that are not reachable by a single irrep and therefore are not one of the listed isotropy subgroups.

5. Case studies

To demonstrate the usage of the tools, we analyze the following three cases in detail via their direct application:

5.1. Symmetry identification of the magnetic phase of $Ba_3Nb_2NiO_9$

The paramagnetic structure of $Ba_3Nb_2NiO_9$ can be summarized as (Lufaso, 2004; Hwang *et al.*, 2012):

```
# Ba3Nb2NiO9 // P-3m1
164
5.7550 5.7550 7.0656 90.000 90.000 120.000
6
Ba 1 2d 0.33333 0.66667 0.66380
Ba 2 1a 0.00000 0.00000 0.00000
Ni 1 1b 0.00000 0.00000 0.50000
Nb 1 2d 0.33333 0.66667 0.17700
O 1 3e 0.50000 0.00000 0.00000
O 2 6i 0.16978 0.33960 0.32623
```

with the magnetic atom identified as Ni and the propagation vector observed via neutron diffraction pattern to be $(1/3, 1/3, 1/2)$. The small occupancy mixing reported in Lufaso (2004) is neglected.

Just introducing the number of the space group of the paramagnetic structure and the propagation wavevector, *k-SUBGROUPSMAG* gives the list and graph of the compatible magnetic groups. However, the list of subgroups can be further refined by providing the Wyckoff position of the magnetic atom (1b in our example) in the input: setting the rest of options offered by the input page to their default values⁸. The resulting list of compatible subgroups is presented in Fig. 6. The corresponding graph depicting the hierarchy between the conjugacy classes in a group-subgroup tree is drawn by the program as in Fig. 7. Looking at this graph, we can identify the *k-maximal subgroups* under the given conditions as those that belong to the conjugacy classes 1, 2, 3 and 7.

Even though one can continue to use *k-SUBGROUPSMAG* to explore systematically all possible magnetic symmetries for the system, and construct the corresponding models to be checked as mcif files, we will proceed with *MAXMAGN*, due to the fact that, as mentioned in the description of the tool above, many of the published single-*k* magnetic structures belong to the maximal symmetries listed by *MAXMAGN*.

Submitting the parent space group type, the propagation vector and the (optional) structure data of the paramagnetic phase (hence specifying the occupied magnetic sites) results in the list presented in Fig. 8. The figure shows the maximal subgroups of the gray group of the paramagnetic phase compatible with the specified *k* vector with two different background colors. Those magnetic groups with white back-

⁸ For this case, the default options result in the search to be extended all the way down to $P1.1$ and limiting the space groups to those allowing a non-zero magnetic moment in all sites of the specified Wyckoff positions. This criterium can be changed with the 'More options' button, for example, to include also those subgroups that allow non-zero magnetic moments at some of the sites, not necessarily all, in which case 4 subgroups will be listed in addition.

Input data

Subgroups of the paramagnetic space group :
Lowest magnetic space group to consider:
Magnetic propagation wave-vectors
Wyckoff positions occupied by the magnetic atoms

$P\bar{3}m1'$ (N. 164)
P1 (N. 1.1)
(1/3, 1/3, 1/2)
1b(0,0,1/2)

List of subgroups which allow a non zero magnetic moment in all sites

Get the subgroup-graph

More options

N	Group Symbol	Transformation matrix	Group-Subgroup Index	Other members of the Conjugacy Class	irreps	Magnetic structure models (MAGMODELIZE)
1	$P\bar{3}1c$ (No. 163.84)	$\begin{pmatrix} 2 & -1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	6=6x1	Conjugacy Class	Get irreps	☐
2	$P\bar{3}1c$ (No. 159.64)	$\begin{pmatrix} 2 & -1 & 0 & -2/3 \\ 1 & 1 & 0 & -1/3 \\ 0 & 0 & 2 & 0 \end{pmatrix}$	12=6x2	Conjugacy Class	Get irreps	☐
3	$P\bar{3}1m$ (No. 157.56)	$\begin{pmatrix} 2 & -1 & 0 & -2/3 \\ 1 & 1 & 0 & -1/3 \\ 0 & 0 & 2 & 0 \end{pmatrix}$	12=6x2	Conjugacy Class	Get irreps	☐
4	$P\bar{3}12$ (No. 149.24)	$\begin{pmatrix} 2 & -1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 2 & 0 \end{pmatrix}$	12=6x2	Conjugacy Class	Get irreps	☐
5	$P\bar{3}$ (No. 143.3)	$\begin{pmatrix} 2 & -1 & 0 & 1/3 \\ 1 & 1 & 0 & -1/3 \\ 0 & 0 & 2 & 0 \end{pmatrix}$	24=6x4	Conjugacy Class	Get irreps	☐
6	C_2/c (No. 15.90)	$\begin{pmatrix} 2 & 0 & 0 & 0 \\ 1 & 3 & 0 & -1/2 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	18=6x3	Conjugacy Class	Get irreps	☐
7	C_2/m (No. 12.63)	$\begin{pmatrix} 2 & 0 & 0 & 0 \\ 1 & 3 & 0 & -1/2 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	18=6x3	Conjugacy Class	Get irreps	☐
8	C_2/c (No. 9.40)	$\begin{pmatrix} 2 & 0 & 0 & 1/5 \\ 1 & 3 & 0 & -2/5 \\ 0 & 0 & 2 & 0 \end{pmatrix}$	36=6x6	Conjugacy Class	Get irreps	☐
9	C_2/m (No. 8.35)	$\begin{pmatrix} 2 & 0 & 0 & 1/5 \\ 1 & 3 & 0 & -2/5 \\ 0 & 0 & 2 & 0 \end{pmatrix}$	36=6x6	Conjugacy Class	Get irreps	☐
10	C_2 (No. 5.16)	$\begin{pmatrix} 2 & 0 & 0 & 0 \\ 1 & 3 & 0 & -1/2 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	36=6x6	Conjugacy Class	Get irreps	☐
11	C_2 (No. 5.16)	$\begin{pmatrix} 2 & 0 & 0 & 0 \\ 1 & 3 & 0 & 0 \\ 0 & 0 & 2 & 0 \end{pmatrix}$	36=6x6	Conjugacy Class	Get irreps	☐
12	$P\bar{3}1$ (No. 2.7)	$\begin{pmatrix} 1 & 1 & 0 & -1/2 \\ -1 & 1 & 0 & 0 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	36=6x6	Conjugacy Class	Get irreps	☐
13	$P\bar{3}1$ (No. 1.3)	$\begin{pmatrix} 1 & 1 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 0 & 0 & 2 & 0 \end{pmatrix}$	72=6x12	Conjugacy Class	Get irreps	☐

Select/Deselect all subgroups

☒ Include structure data of the parent phase

Submit selected subgroups to MAGMODELIZE:

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

Figure 6

List of magnetic subgroups of the paramagnetic parent phase $P\bar{3}m1$ (No. 164) compatible with the $\mathbf{k} = (1/3, 1/3, 1/2)$ propagation vector with the magnetic site occupying the 1b Wyckoff position and having all sites to allow a non-zero magnetic moment, as calculated by *k-SUBGROUPSMAG*.

ground force zero magnetic moments at all sites derived from the Wyckoff position (1b) of the magnetic atom and they do not need to be considered in the analysis. Note that these subgroups are not included in the output of *k-SUBGROUPSMAG* because this tool removes the MSGs that does not allow magnetic moments on the specified magnetic sites, before the construction of the group-subgroup tree. Then, the MSG C_2/m , although being not maximal, becomes maximal under the given conditions (non-zero

Input data

Subgroups of the paramagnetic space group :
Lowest magnetic space group to consider:
Magnetic propagation wave-vectors
Wyckoff positions occupied by the magnetic atoms

$P\bar{3}m1'$ (N. 164)
P1 (N. 1.1)
(1/3, 1/3, 1/2)
1b(0,0,1/2)

Graph of subgroups which allow a non zero magnetic moment in all sites

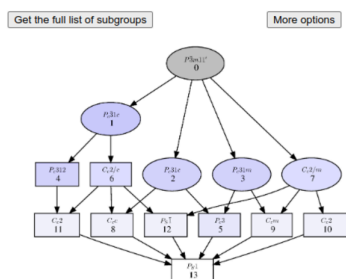


Figure 7

Output of *k-SUBGROUPSMAG* with the search conditions summarized at the top and below the graph showing the relations of the magnetic subgroups listed in Fig. 6.

Maximal magnetic space groups for the parent space group $P\bar{3}m1$ (No. 164) and the propagation vector $\mathbf{k} = (1/3, 1/3, 1/2)$

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

N	Group (BNS)	Transformation matrix	General positions	Properties	Magnetic structure
1	$P\bar{3}1c$ (#163.84) Go to a subgroup	$\begin{pmatrix} 2 & -1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNET Tensor properties MTENSOR	Show
2	$P\bar{3}1c$ (#163.84) Go to a subgroup	$\begin{pmatrix} 2 & -1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 2 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNET Tensor properties MTENSOR	Show
3	$P\bar{3}1m$ (#162.78) Go to a subgroup	$\begin{pmatrix} 2 & -1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 2 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNET Tensor properties MTENSOR	Show
4	$P\bar{3}1m$ (#162.78) Go to a subgroup	$\begin{pmatrix} 2 & -1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNET Tensor properties MTENSOR	Show
5	$P\bar{3}1c$ (#159.64) Go to a subgroup	$\begin{pmatrix} 2 & -1 & 0 & 8/3 \\ 1 & 1 & 0 & 7/3 \\ 0 & 0 & 2 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNET Tensor properties MTENSOR	Show
6	$P\bar{3}1m$ (#157.56) Go to a subgroup	$\begin{pmatrix} 2 & -1 & 0 & 8/3 \\ 1 & 1 & 0 & 7/3 \\ 0 & 0 & 2 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNET Tensor properties MTENSOR	Show

Figure 8

List obtained via *MAXMAGN* showing the maximal subgroups of the parent space group $P\bar{3}m1$ (No. 164) and propagation vector $\mathbf{k} = (1/3, 1/3, 1/2)$. Subgroups with white background are maximal subgroups but they force zero magnetic moments at all sites derived from the given Wyckoff position 1b.

magnetic moment at position 1b must be allowed), thus it is a $\mathbf{k}$ -maximal subgroup for this structure. Subgroups with dark-gray background allow non-zero magnetic moment at Wyckoff position 1b. There are two different classes of subgroups of the same type $P\bar{3}1c$ (No. 163.84) and $P\bar{3}1m$ (No. 162.78), but while one class allows non-zero magnetic moments at the specified site, the other does not.

Proceeding with the subgroups that allow non-zero magnetic moments, we can generate the magnetic structures from the parent structure by following the 'Show' button on the last column. Clicking on this button will carry the user to a model of the magnetic structure under this specific MSG, which includes the atomic coordinates of a representative atom of the orbit, the coordinates of the atomic positions of all the atoms in the orbit and the parametric form of their magnetic moments. The input boxes in the last column allows the user to assign values to the independent free components of the magnetic moment. A redacted version of the output is presented in Fig. 9 for the $P\bar{3}1c$ (No. 163.84) ($2\mathbf{a} + \mathbf{b}$, $-\mathbf{a} + \mathbf{b}$, $2\mathbf{c}$; 0, 0, 1/2) symmetry selected from the list in Fig. 8 (1st option). In the listing, it can also be seen that the Ni site of the parent structure has been split. Investigation of the allowed magnetic moments for the indicated site in the compatible maximal subgroups reveals that only $P\bar{3}1c$ (No. 159.64) ($2\mathbf{a} + \mathbf{b}$, $-\mathbf{a} + \mathbf{b}$, $2\mathbf{c}$; 8/3, 7/3, 0) and $P\bar{3}1m$ (No. 157.56) ($2\mathbf{a} + \mathbf{b}$, $-\mathbf{a} + \mathbf{b}$, $2\mathbf{c}$; 8/3, 7/3, 0) allow magnetic moment components along the x and y directions (with $P\bar{3}1c$ allowing a spin canting along z), while $P\bar{3}1c$ and $P\bar{3}1m$ (No. 162.78) ($2\mathbf{a} + \mathbf{b}$, $-\mathbf{a} + \mathbf{b}$, $2\mathbf{c}$; 0, 0, 0) support magnetic moments only along the z direction.

The magnetic structure is, by default, described for clarity using an origin and unit cell as similar as possible to those of the parent/paramagnetic structure, and in general they do not

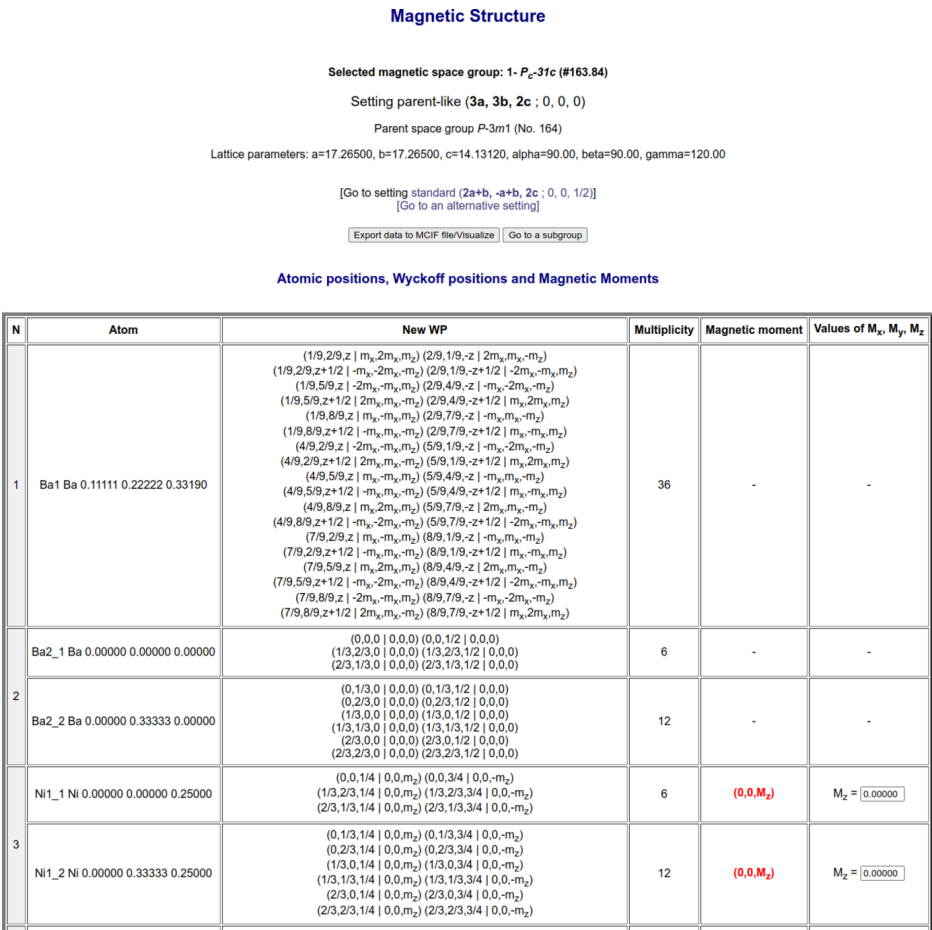


Figure 9
Output/input page of *MAXMAGN* with the description of a possible magnetic structure for $\text{Ba}_3\text{Nb}_2\text{NiO}_9$ under one of the possible MSGs listed in Fig. 8.

correspond to the standard setting of the MSG structure. This so-called ‘parent-like’ setting keeps the origin and also the unit-cell orientation of the parent/paramagnetic structure, but if necessary, multiplies the cell parameters to produce a

supercell consistent with the periodicity kept by the propagation vectors. If needed, one can switch to the description in the standard setting of the MSG by following the reported transformation matrix (or to an alternative setting which can

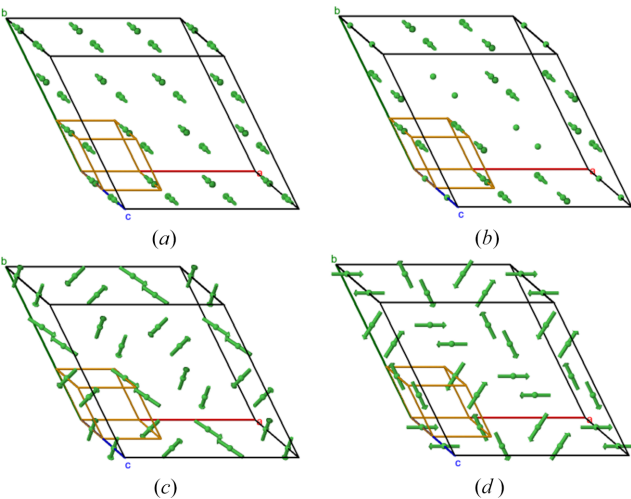


Figure 10
Visualization of the four possible symmetries [(a) $P_6\bar{3}1c$, (b) $P_6\bar{3}1m$, (c) $P_6\bar{3}1c$ and (d) $P_6\bar{3}1c$] of $\text{Ba}_3\text{Nb}_2\text{NiO}_9$ listed in Fig. 8 by *MVISUALIZE*. Only the magnetic sites are shown.

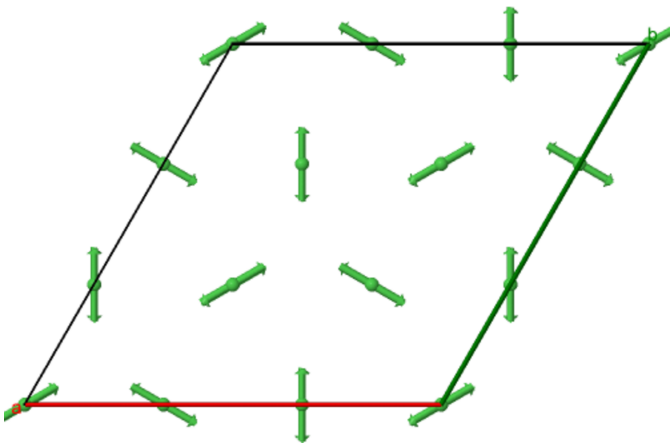


Figure 11
Representation of the magnetic structure of $\text{Ba}_3\text{Nb}_2\text{NiO}_9$ in the way reported by Hwang (2012), as obtained with *MAXMAGN*, which allows us to identify its MSG ($P_6\bar{3}1c$) and which of the six possible equivalent descriptions of the structure was considered in the report.

N	Coset representatives		Transformation matrix	Magnetic Structure
	(x,y,z) form	Seitz notation		
1	x,y,z,+1	{1 0}	$\begin{pmatrix} 2 & -1 & 0 & 8/3 \\ 1 & 1 & 0 & 7/3 \\ 0 & 0 & 2 & 0 \end{pmatrix}$	Show
2	x+1,y+1,z,+1	{1 110}	$\begin{pmatrix} 2 & -1 & 0 & 2/3 \\ 1 & 1 & 0 & 1/3 \\ 0 & 0 & 2 & 0 \end{pmatrix}$	Show
3	x,y+1,z,+1	{1 010}	$\begin{pmatrix} 2 & -1 & 0 & 8/3 \\ 1 & 1 & 0 & 1/3 \\ 0 & 0 & 2 & 0 \end{pmatrix}$	Show
4	y,x,-z,+1	{2 ₁₁₀ 0}	$\begin{pmatrix} 1 & 1 & 0 & 7/3 \\ 2 & -1 & 0 & 8/3 \\ 0 & 0 & -2 & 0 \end{pmatrix}$	Show
5	x-y,-y,-z,+1	{2 ₁₀₀ 0}	$\begin{pmatrix} 1 & -2 & 0 & 1/3 \\ -1 & -1 & 0 & 2/3 \\ 0 & 0 & -2 & 0 \end{pmatrix}$	Show
6	-x,-x+y,-z,+1	{2 ₀₁₀ 0}	$\begin{pmatrix} -2 & 1 & 0 & 1/3 \\ -1 & 2 & 0 & 8/3 \\ 0 & 0 & -2 & 0 \end{pmatrix}$	Show

Figure 12
Partial output of *MVISUALIZE* when using the option ‘domain-related equivalent descriptions’ for the magnetic structure constructed with *MAXMAGN* for Ba₃Nb₂NiO₉ under the subgroup *P*_c31c (No. 163.84) listed in Fig. 8. The six equivalent domain-related descriptions of the structure are listed, together with an operation that transforms it into the input one (the first one). The transformation matrix listed in the fourth column defines the subgroup of type *P*_c31c (No. 163.84), which is realized in each case. They are all conjugate subgroups and in this case they are all different, as a different transformation matrix is listed for each structure.

be defined by the user by the introduction of the relevant transformation matrix).

The produced magnetic structure model can be downloaded as an mcif file or visualized via *MVISUALIZE*. The visualizations of the models of the four magnetic structures from the list in Fig. 8 are presented in Fig. 10 (only the magnetic atoms are displayed). Here, it should be emphasized that we want to relate the theoretical model to that of the reported magnetic structure (Hwang *et al.*, 2012). Comparing the produced models to the reported structure (Fig. 11), it can be seen that the model shown in Fig. 10 for the MSG *P*_c31c looks very similar, but not the same. To proceed further, we use the ‘Alternatives (domain-related)’ button in the output page shown in Fig. 8 for the MSG corresponding to this structure. [This list can be accessed from *k-SUBGROUPSMAG*, *MAXMAGN* and *MVISUALIZE* (to access from *MVISUALIZE*, one must first save the structure in .mcif format and upload it to *MVISUALIZE*).] As the group–subgroup index for this subgroup is 12, there will be 12 different domain states, and therefore, six different forms (apart from the trivial global spin reversal) of describing the magnetic structure in the reference frame of the parent structure. By means of this optional button one obtains the list of six possible domain-

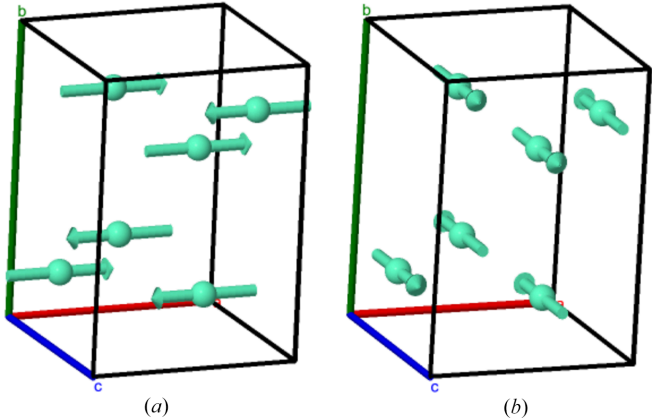


Figure 13
The two different models for the magnetic structure of EuZrO₃ having different MSGs: (a) *Pnm'a* (Avdeev *et al.*, 2014), (b) *Pn'm'a* (Saha *et al.*, 2016).

related equivalent structures (Fig. 12). For each structure a lost operation (coset representative) is given. This operation relates the domain-related structure of each row with the first one in the list, which is the one of the input .mcif file. The alternative descriptions of the structure can be retrieved via the ‘Show’ button. The resulting structure for the {1|010} operation is visualized in Fig. 11 and coincides with the published models of this magnetic structure. Thus, the MSG of the reported magnetic structure of Ba₃Nb₂NiO₉ (Hwang *et al.*, 2012) can be identified as *P*_c31c (No. 159.64) (which is included in the MAGNDATA database with the entry id No. 1.13).

It is worth noting that a commensurate magnetic structure model for any paramagnetic structure and any subgroup of the gray magnetic group associated with its space group can also be obtained via *MAGMODELIZE*. This program also works for subgroups that are not maximal.

5.2. Conflicting models

Two magnetic structure models have been reported for EuZrO₃ (Avdeev *et al.*, 2014; Saha *et al.*, 2016), and their MSGs can be identified as *Pnm'a* (No. 62.444) and *Pn'm'a'* (No. 62.449) with the parent space group of the compound being *Pnma*. These structures are included in MAGNDATA with entry ids No. 0.146 and No. 0.147, respectively. They are visualized side-by-side in Fig. 13.

Although it is the same collinear spin arrangement, the proposed easy axis is different. It may be experimentally difficult to unambiguously determine the direction of the easy axis, especially in pseudotetragonal structures such as this one, but the problem might be resolved via the investigation of the systematic absences. For this purpose, checking the systematic absences of the related MSG by *MAGNEXT* reveals that there will be absences along the (*h* 0 0) and (0 0 *l*) reflections for *odd* values of *h* and *l* for the MSG *Pnm'a*, whereas the absences will exist for the *even* values of *h* and *l* for the MSG *Pn'm'a'*.

The measurement of some physical properties of the material can also be helpful to elucidate among different possible magnetic groups. In our example one of these properties is the magnetoelectric effect α_{ij}^T which relates the applied electric field with the magnetization, $M_i = \alpha_{ij}^T E_j$. Entering the MSG information into *MTENSOR* and selecting the 'Magnetoelectric tensor α_{ij}^T (inverse effect)' from the list of predefined tensors, the program shows that, for the MSG $Pn'm'a'$, the induced magnetization is parallel to the applied electric field, whereas x and z directions are coupled for the MSG $Pnm'a$ [a magnetization along the x (z) direction will be induced when an electric field is applied along the z (x) direction].

If another specific property has been observed, an alternative comparison could also be done by specifying the tensor corresponding to that property and checking its components in all the point groups via the option 'Show symmetry-adapted tensors for all the magnetic point groups in standard setting'. In addition, as *MTENSOR* clearly highlights the non-zero tensors by shading the null tensors in the list with gray background, side by side comparison of the two lists belonging to the two different MSGs will directly yield the tensor properties that can be used to single-out the symmetry.

The Magnetic Space Group has been identified as P_c31c (No. 159.64) in the BNS setting

Transformation Matrix to the standard/default BNS setting

$$\begin{pmatrix} 1/3 & 1/3 & 0 & -1/9 \\ -1/3 & 2/3 & 0 & -2/9 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

Your Transformation Matrix is also valid.

Check an alternative Transformation Matrix

2/3	-1/3	0	8/9
1/3	1/3	0	7/9
0	0	1	0

Submit

Input generators

```
-x+y,-x+2/3,z,+1
-y+2/3,-
x+2/3,z+1/2,+1
x,x-y+2/3,z+1/2,+1
-x+y,y,z+1/2,+1
x,y,z,+1
x+1/3,y+2/3,z,+1
x+2/3,y+1/3,z,+1
x,y,z+1/2,-1
x+1/3,y+2/3,z+1/2,-1
x+2/3,y+1/3,z+1/2,-1
```

General positions of the Magnetic Space Group P_c31c in the given setting

(0,0,0),(1/3,2/3,0),(2/3,1/3,0)+

- 1 x,y,z,+1
- 2 -y+2/3,x-y+2/3,z,+1
- 3 -x+y,-x+2/3,z,+1
- 4 -x+y,y,z+1/2,+1
- 5 -y+2/3,-x+2/3,z+1/2,+1
- 6 x,x-y+2/3,z+1/2,+1
- 7 x,y,z+1/2,-1
- 8 -y+2/3,x-y+2/3,z+1/2,-1
- 9 -x+y,-x+2/3,z+1/2,-1
- 10 -x+y,y,z,-1
- 11 -y+2/3,-x+2/3,z,-1
- 12 x,x-y+2/3,z,-1

Figure 14

Result page of *IDENTIFY MAGNETIC GROUP* for the symmetry operations of the MSG P_c31c (No. 159.64) of the magnetic structure of $Ba_3Nb_2NiO_9$, described using a unit cell (3a, 3b, 2c) with respect to the parent unit cell (a, b, c) of its paramagnetic $P\bar{3}m1$ (No. 164) phase, and the same origin, as shown in Fig. 10, and corresponding to the fifth subgroup of $P\bar{3}m1.1'$ (No. 164.86) listed in Fig. 8. In addition to the identification of the MSG from the symmetry operators, the program also calculates the basis transformation matrix to the standard setting. The equivalency and hence the validity of the transformation matrix relating the parent unit cell and the current unit cell can be checked via the 'Check an alternative Transformation Matrix' option, as also shown in the figure.

5.3. Finding higher symmetries

STRCONVERT can be used to convert, modify or visualize magnetic structures. In addition to these operations, it can also be used to identify the symmetry of a structure defined in a triclinic MSG, which is usually the resulting structure in DFT calculations.

Let us take the magnetic structure of $Ba_3Nb_2NiO_9$ that we have identified in Section 5.1 as having the symmetry P_c31c (No. 159.64): suppose that the structure's lattice parameters, atomic positions and magnetic moments had been calculated in the triclinic MSG $P1.1$ (No. 1.1) (for demonstration purposes, one can obtain this low-symmetry structure by submitting the structure with P_c31c (No. 159.64) symmetry to *STRCONVERT* and afterwards clicking on the 'Transform the structure to P1 setting' button. This method is also applicable when one seeks a higher symmetry of a structure with a non-triclinic symmetry. After feeding this structure to *STRCONVERT*, due to it being triclinic, the additional option 'Find symmetry' will now be visible. Upon clicking on this button, its proper symmetry will be identified as P_c31c (No. 159.64) along with a basis transformation to the standard setting of this MSG. [This basis transformation which relates the unit cell and the origin used in the description of the structure should not be confused with the group-subgroup transformation matrix that relates the parent structure with a magnetic structure via group-subgroup relations.] The derived high-symmetry structure returned by the integrated *FINDSYM* program (Stokes & Hatch, 2005) will be by default represented in the standard setting of the MSG, but one can have it returned maintaining the origin and unit cell of the input file via the 'Keep the user's setting' option in the interface.

We can further verify this fact via the symmetry operators contained in the *mcif* file produced by *MAXMAGN* in Section 5.1, which are:

```
-x+y,-x+2/3,z,+1
-y+2/3,-x+2/3,z+1/2,+1
x,x-y+2/3,z+1/2,+1
-x+y,y,z+1/2,+1
x,y,z,+1
x+1/3,y+2/3,z,+1
x+2/3,y+1/3,z,+1
x,y,z+1/2,-1
x+1/3,y+2/3,z+1/2,-1
x+2/3,y+1/3,z+1/2,-1
```

and the symmetry operators listed by *STRCONVERT* after the identification of the higher symmetry:

```
x,y,z,+1
-y,x-y,z,+1
-x+y,-x,z,+1
-x,-x+y,z+1/2,+1
x-y,-y,z+1/2,+1
y,x,z+1/2,+1
x,y,z+1/2,-1
```

Running the *IDENTIFY MAGNETIC GROUP* tool separately with these two lists of operations results in the same MSG, P_c31c (No. 159.64), as expected, yet, the first set is

accompanied by the transformation matrix $(1/3\mathbf{a} - 1/3\mathbf{b}, 1/3\mathbf{a} + 2/3\mathbf{b}, \mathbf{c}; -1/9, -2/9, 0)$ to the standard BNS setting (as reproduced in Fig. 14), while the second set is found to be already in the standard setting. The transformation to standard of the MSG provided by the program in the first case must be equivalent to the one that can be directly derived from the transformation to standard $(2\mathbf{a} + \mathbf{b}, -\mathbf{a} + \mathbf{b}, 2\mathbf{c}; 8/3, 7/3, 0)$, indicated in Fig. 8, when it is defined as subgroup of the gray paramagnetic group. As the parent-like basis used is $(3\mathbf{a}, 3\mathbf{b}, 2\mathbf{c}; 0, 0, 0)$, with respect to the parent unit cell, a valid transformation to standard setting of the MSG must be $(2/3\mathbf{a} + 1/3\mathbf{b}, -1/3\mathbf{a} + 1/3\mathbf{b}, \mathbf{c}; 8/9, 7/9, 0)$. This can be checked using the 'Check an alternative Transformation Matrix' button, as shown in Fig. 14.

6. Conclusion

The Bilbao Crystallographic Server hosts many interconnected tools to analyze magnetic structures and their relations via group theory. The applications can be used for purposes ranging from basic information retrieval like general positions, $\mathbf{k}$ vectors and irreducible representations, to much complex analysis such as identifying symmetries, listing allowed symmetry breaks, checking the existence and form of the physical properties present within the given states, or derivative operations such as systematically generating alternative magnetic structure models with different magnetic symmetries that are compatible with some given criteria.

Most of the tools within the server allow the user to input and output data in their preferred setting along with the option to convert these data to the standard setting that enables easy comparison and standardization.

As the programs support many commonly used formats and notations and also offer additional tools to convert one to the other, they provide high flexibility and transportability.

We have highlighted the usage of the tools hosted for different purposes using reported cases from the literature. Detailed tutorials on the usage and application of the tools with extended descriptions and step by step instructions are available on the tools' respective web pages.

Funding information

The following funding is acknowledged: Eusko Jaurlaritza (grant No. IT1458-22).

References

Aroyo, M. I. (2016). Editor. *International Tables for Crystallography, Volume A: Space-group symmetry*, 6th ed. Wiley.

- Aroyo, M. I., Kirov, A., Capillas, C., Perez-Mato, J. M. & Wondratschek, H. (2006a). *Acta Cryst. A* **62**, 115–128.
- Aroyo, M. I., Perez-Mato, J. M., Capillas, C., Kroumova, E., Ivantchev, S., Madariaga, G., Kirov, A. & Wondratschek, H. (2006b). *Z. Kristallogr. Cryst. Mater.* **221**, 15–27.
- Aroyo, M. I., Perez-Mato, J. M., Orobengoa, D., Tasci, E., de la Flor, G. & Kirov, A. (2011). *Bulg. Chem. Commun.* **43**, 183–197.
- Avdeev, M., Kennedy, B. J. & Kolodiazny, T. (2014). *J. Phys. Condens. Matter*, **26**, 095401.
- Campbell, B. J., Stokes, H. T., Perez-Mato, J. M. & Rodríguez-Carvajal, J. (2022). *Acta Cryst. A* **78**, 99–106.
- Elcoro, L., Wieder, B. J., Song, Z., Xu, Y., Bradlyn, B. & Bernevig, B. A. (2021). *Nat. Commun.* **12**, 5965.
- Fruchart, D. & Bertaut, E. (1978). *J. Phys. Soc. Jpn.* **44**, 781–791.
- Gallego, S. V., Etxebarria, J., Elcoro, L., Tasci, E. S. & Perez-Mato, J. M. (2019). *Acta Cryst. A* **75**, 438–447.
- Gallego, S. V., Perez-Mato, J. M., Elcoro, L., Tasci, E. S., Hanson, R. M., Aroyo, M. I. & Madariaga, G. (2016a). *J. Appl. Cryst.* **49**, 1941–1956.
- Gallego, S. V., Perez-Mato, J. M., Elcoro, L., Tasci, E. S., Hanson, R. M., Momma, K., Aroyo, M. I. & Madariaga, G. (2016b). *J. Appl. Cryst.* **49**, 1750–1776.
- Gallego, S. V., Tasci, E. S., de la Flor, G., Perez-Mato, J. M. & Aroyo, M. I. (2012). *J. Appl. Cryst.* **45**, 1236–1247.
- Glazer, A. M., Aroyo, M. I. & Authier, A. (2014). *Acta Cryst. A* **70**, 300–302.
- Hanson, R. M. (2010a). *Jmol: an open-source java viewer for chemical structures in 3d*. <https://www.jmol.org/>.
- Hanson, R. M. (2010b). *J. Appl. Cryst.* **43**, 1250–1260.
- Hwang, J., Choi, E. S., Ye, F., Dela Cruz, C. R., Xin, Y., Zhou, H. D. & Schlottmann, P. (2012). *Phys. Rev. Lett.* **109**, 257205.
- Jahn, H. A. (1949). *Acta Cryst.* **2**, 30–33.
- Kresse, G. & Furthmüller, J. (1996). *Phys. Rev. B*, **54**, 11169–11186.
- Litvin, D. B. (2013). *Magnetic Group Tables: 1-, 2- and 3-dimensional magnetic subperiodic groups and magnetic space groups*. International Union of Crystallography.
- Litvin, D. B. (2016). *Magnetic subperiodic groups and magnetic space groups*. In *International Tables for Crystallography, Vol. A, Space-group symmetry*, 2nd online ed., ch. 3.6, pp. 852–865, <https://doi.org/10.1107/97809553602060000934>.
- Lufaso, M. W. (2004). *Chem. Mater.* **16**, 2148–2156.
- Momma, K. & Izumi, F. (2011). *J. Appl. Cryst.* **44**, 1272–1276.
- Perez-Mato, J. M., Gallego, S. V., Tasci, E. S., Elcoro, L., de la Flor, G. & Aroyo, M. I. (2015). *Annu. Rev. Mater. Res.* **45**, 217–248.
- Rodríguez-Carvajal, J. (1993). *Physica B*, **192**, 55–69.
- Rodríguez-Carvajal, J. (2001). *FullProf suite*, <https://www.ill.eu/sites/fullprof/>.
- Saha, R., Sundaresan, A., Sanyal, M. K., Rao, C. N. R., Orlandi, F., Manuel, P. & Langridge, S. (2016). *Phys. Rev. B*, **93**, 014409.
- Stokes, H., Hatch, D. & Campbell, B. J. (2010). *Iso-Mag: tables of magnetic space groups, ISOTROPY Software Suite*, <https://iso.byu.edu>.
- Stokes, H. T. & Hatch, D. M. (2005). *J. Appl. Cryst.* **38**, 237–238.
- Wondratschek, H. & Müller, U. (2011). Editors. *International Tables for Crystallography, Vol A1, Symmetry relations between space groups*, 2nd ed. International Union of Crystallography.
- Xu, Y., Elcoro, L., Song, Z.-D., Wieder, B. J., Vergniory, M. G., Regnault, N., Chen, Y., Felser, C. & Bernevig, B. A. (2020). *Nature*, **586**, 702–707.