The magnetic section of the Bilbao Crystallographic Server – 1st-Tutorial

J. Manuel Perez-Mato and Luis Elcoro
Dept. Física de la Materia Condensada, Facultad de Ciencia y Tecnología, Universidad del Pais Vasco (UPV/EHU), Apdo. 644, 48080 Bilbao

This first tutorial includes practical introductory examples for the following programs:

MGENPOS : Section2
IDENTIFY MAGNETIC GROUP : Section 3
MWYCKPOS: Section 4
MPOINT: Section 5
MTENSOR: Section 6

For other programs of the magnetic section see the 2nd and 3rd tutorials

1. Introduction

Below you can see a screenshot showing the databases, tools and programs that are available online at the Bilbao Crystallographic Server (www.cryst.ehu.es) in its second section entitled: "Magnetic Symmetry and Applications".

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

In this initial tutorial, we shall first become familiar with the databases and tools in this section (MGENPOS, MWYCKPOS, IDENTIFY MAGNETIC GROUP, MPOINT) which are purely informative about magnetic space groups (Shubnikov groups) and magnetic point groups. This will help us to get deeper into the mathematical structure of magnetic symmetry groups, and their consequences on the physical properties. We shall explore then the features of the program MTENSOR, which allows to know the symmetry adapted form of any kind of crystal tensor property for any magnetic point-group symmetry.

Further information on some of these programs and the theory behind can be found in [1] and [2].

2. MGENPOS: General Positions of Magnetic Space Groups

This tool is a database of the 1651 different possible magnetic space groups (MSGs), also called Shubnikov groups. It lists for any chosen MSG the set of symmetry operations defining the group. These symmetry operations are also called the "general positions of the group", as they represent for a general position with arbitrary magnetic moment: (x,y,z; mx,my,mz), all the positions (and magnetic moments) that are symmetry related (apart from those related by the lattice translations). The list of general positions or symmetry operations of the MSGs are given in the setting, which was first provided in computer readable form by the ISOTROPY webpage [3], and we take as the "*standard setting*" of the MSGs.

The symmetry operations describing the symmetry group of any commensurate magnetic structure can always be put, by choosing an appropriate unit cell and origin, in the standard form of one MSG (and only one!) of the 1651 MSGs, as listed here (see below the tool IDENTIFY MAGNETIC GROUP).

MGENPOS can list the operations of any MSG in either the BNS or the OG setting (this latter coinciding with the one used in Litvin's ebook [4]) , but for the moment in this tutorial we will restrict ourselves to the BNS setting. We leave some additional considerations about the OG setting for a more advanced tutorial.

Any desired MSG can be introduced in MGENPOS by means of its BNS numerical label, but the desired MSG can also be decided by first choosing its mathematically underlying space group:

2a) Click on the button "choose it". We then get a list of the 230 ordinary space groups. Click on one of them, say *Pcca* (N. 54). You will then obtain a listing of all possible MSGs derived in the BNS approach from the space group *Pcca* (N. 54), in the following form (disregard the second listing corresponding to the OG description):

The magnetic space groups derived from the Fedorov space group: Pcca (#54)

Listed with respect to the BNS setting:

- #54.337 Pcca [OG: Pcca #54.1.428] *Type I (Fedorov)*
- #54.338 Pcca1' [OG: Pcca1' #54.2.429] *Type II (grey group)*
- #54.339 Pc'ca [OG: Pc'ca #54.3.430] *Type III (translationgleiche)*
- #54.340 Pcc'a [OG: Pcc'a #54.4.431] *Type III (translationgleiche)*
- #54.341 Pcca' [OG: Pcca' #54.5.432] *Type III (translationgleiche)*
- #54.342 Pc'c'a [OG: Pc'c'a #54.6.433] *Type III (translationgleiche)*
- #54.343 Pcc'a' [OG: Pcc'a' #54.7.434] *Type III (translationgleiche)*
- #54.344 Pc'ca' [OG: Pc'ca' #54.8.435] *Type III (translationgleiche)*
- #54.345 Pc'c'a' [OG: Pc'c'a' #54.9.436] *Type III (translationgleiche)*
- #54.346 $P_a$cca [OG: P_{2a}ccm' #49.10.373] *Type IV (klassengleiche)*
- #54.347 $P_b$cca [OG: P_{2b}cca #54.10.437] *Type IV (klassengleiche)*
- #54.348 $P_c$cca [OG: P_{2c}m'm'a #51.18.404] *Type IV (klassengleiche)*
- #54.349 $P_A$cca [OG: C_Pm'ca #64.11.538] *Type IV (klassengleiche)*
- #54.350 $P_B$cca [OG: C_Pm'ma #67.13.589] *Type IV (klassengleiche)*
- #54.351 $P_C$cca [OG: C_Pc'ca #68.9.602] *Type IV (klassengleiche)*
- #54.352 $P_I$cca [OG: I_Pb'ca #73.7.649] *Type IV (klassengleiche)*

The BNS numerical labels of all the listed MSGs include the number 54 showing their relation with the ordinary space group *Pcca* (N. 54). For each group the type of MSG is indicated at the end of the line. In between the corresponding labelling used for the same group in the OG description is also shown.

2b) Click on one MSG of type IV, say 54.352 $P_{I}cca$, and click next on "standard/default setting". The list of the symmetry operations of the MSG appears. It has 16 operations and we show below a partial view:

General Positions of the Group $P_{I}cca$ (#54.352) [BNS setting]

To display the general positions in the OG setting, please follow this link: $I_Pb'ca$ (#73.7.649) [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'|1/2,1/2,1/2)

N	Standard/Default Setting			
	(x,y,z) form	Matrix form	Geom. interp.	Seitz notation
1	x, y, z, +1 m_x,m_y,m_z	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	1 +1	{ 1 | 0 }
2	x+1/2, -y, -z+1/2, +1 $m_x,-m_y,-m_z$	$\begin{pmatrix} 1 & 0 & 0 & 1/2 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 1/2 \end{pmatrix}$	2 (1/2,0,0) x,0,1/4 +1	{ 2_{100} | 1/2 0 1/2 }
3	-x, y, -z+1/2, +1 $-m_x,m_y,-m_z$	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 1/2 \end{pmatrix}$	2 0,y,1/4 +1	{ 2_{010} | 0 0 1/2 }
4	-x+1/2, -y, z, +1 $-m_x,-m_y,m_z$	$\begin{pmatrix} -1 & 0 & 0 & 1/2 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	2 1/4,0,z +1	{ 2_{001} | 1/2 0 0 }
5	-x, -y, -z, +1 m_x,m_y,m_z	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \end{pmatrix}$	-1 0,0,0 +1	{ -1 | 0 }
6	-x+1/2, y, z+1/2, +1 $m_x,-m_y,-m_z$	$\begin{pmatrix} -1 & 0 & 0 & 1/2 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1/2 \end{pmatrix}$	c 1/4,y,z +1	{ m_{100} | 1/2 0 1/2 }
7	x, -y, z+1/2, +1	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}$	c x,0,z +1	{ m_{010} | 0 0 1/2 }

The heading lists a set of lattice generators, showing in this case that the lattice is primitive (The P from the label). A set of generators of the black & white lattice, i.e. the lattice formed by both translations and "antitranlations" (translations plus time reversal) is also listed. Being a MSG of type IV, this list includes one antitranslation, which in this case is a body centered antitranslation (this corresponds to the "I" subindex in the MSG label).

The symmetry operations are listed in four different formats in four consecutive columns: i) as a transformed (x, y, z) position in relative coordinates with respect to the lattice unit cell, and the corresponding transformation of the associated magnetic moment (m_x, m_y, m_z); ii) as a 3x3 transformation matrix and a column vector indicating the rotation or roto-inversion plus translation of a general point (x, y, z) expressed in unit cell relative coordinates; iii) a geometrical interpretation of the operation using the symbols proposed in the International Tables for Crystallography; and iv) in a Seitz notation extended to magnetic group operations. The operations that include time reversal are distinguished by either a "-1" index, instead of "+1", or by the addition of a "prime" on the symbol of the operation. They are also listed in red, instead of black. For our purposes it is sufficient to understand and consider the last column where the operations are given Seitz notation.

The list includes 16 symmetry operations divided into 8 which do not include time reversal and 8 that are generated by multiplying these initial 8 operations by the body centered antitranslation {1'| ½ ½ ½ }:

8	x+1/2, y, -z, +1 $-m_x,-m_y,m_z$	(1 0 0 1/2 ; 0 1 0 0 ; 0 0 −1 0)	a x,y,0 +1	{ m_{001} | 1/2 0 0 }
9	x+1/2, y+1/2, z+1/2, -1 $-m_x,-m_y,-m_z$	(1 0 0 1/2 ; 0 1 0 1/2 ; 0 0 1 1/2)'	t (1/2,1/2,1/2) -1	{ 1' | 1/2 1/2 1/2 }
10	x, -y+1/2, -z, -1 $-m_x,m_y,m_z$	(1 0 0 0 ; 0 −1 0 1/2 ; 0 0 −1 0)'	2 x,1/4,0 -1	{ $2'_{100}$ | 0 1/2 0 }
11	-x+1/2, y+1/2, -z, -1 $m_x,-m_y,m_z$	(−1 0 0 1/2 ; 0 1 0 1/2 ; 0 0 −1 0)'	2 (0,1/2,0) 1/4,y,0 -1	{ $2'_{010}$ | 1/2 1/2 0 }
12	-x, -y+1/2, z+1/2, -1 $m_x,m_y,-m_z$	(−1 0 0 0 ; 0 −1 0 1/2 ; 0 0 1 1/2)'	2 (0,0,1/2) 0,1/4,z -1	{ $2'_{001}$ | 0 1/2 1/2 }
13	-x+1/2, -y+1/2, -z+1/2, -1 $-m_x,-m_y,-m_z$	(−1 0 0 1/2 ; 0 −1 0 1/2 ; 0 0 −1 1/2)'	-1 1/4,1/4,1/4 -1	{ -1' | 1/2 1/2 1/2 }
14	-x, y+1/2, z, -1 $-m_x,m_y,m_z$	(−1 0 0 0 ; 0 1 0 1/2 ; 0 0 1 0)'	b 0,y,z -1	{ m'_{100} | 0 1/2 0 }
15	x+1/2, -y+1/2, z, -1 $m_x,-m_y,m_z$	(1 0 0 1/2 ; 0 −1 0 1/2 ; 0 0 1 0)'	a x,1/4,z -1	{ m'_{010} | 1/2 1/2 0 }
16	x, y+1/2, -z+1/2, -1 $m_x,m_y,-m_z$	(1 0 0 0 ; 0 1 0 1/2 ; 0 0 −1 1/2)'	b x,y,1/4 -1	{ m'_{001} | 0 1/2 1/2 }

Go to the list of the Wyckoff Positions of the Group P_Icca (#54.352)
Go to the Systematic Absences for the Group P_Icca (#54.352)

This is the typical layout of the symmetry operations of a type IV MSG: a set of operations that define an ordinary space group F without time reversal, plus the same set of operations, but multiplied by an antitranslation, such that all operations in this second set include time reversal. The total set G then can be expressed as:

$$G = F + \{1'|\ t\}\ F$$

In our case the ordinary space group F is the number 54, Pcca. All type IV MSGs in the initial list have therefore the same set of "black" symmetry operations in the list given by MGENPOS, as all of them have *Pcca* as the group F in the above decomposition. You can check this fact by looking at the list given by the program for any other MSG **of type IV**, and see that the set of black operations, i.e. operations without time reversal coincide with those obtained previously for 54.352.

2c) Come back to the list of possible MSGs derived from the space group 54, and click on a group of type III, say 54.343 *Pcc'a'* :

General Positions of the Group *Pcc'a'* (#54.343)

For this space group, BNS and OG settings coincide.
Its label in the OG setting is given as: Pcc'a' (#54.7.434)

N	Standard/Default Setting			
	(x,y,z) form	Matrix form	Geom. interp.	Seitz notation
1	x, y, z, +1 m_x,m_y,m_z	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	1 +1	$\{ 1 \mid 0 \}$
2	x+1/2, -y, -z+1/2, +1 $m_x,-m_y,-m_z$	$\begin{pmatrix} 1 & 0 & 0 & 1/2 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 1/2 \end{pmatrix}$	2 (1/2,0,0) x,0,1/4 +1	$\{ 2_{100} \mid 1/2\ 0\ 1/2 \}$
3	-x, -y, -z, +1 m_x,m_y,m_z	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \end{pmatrix}$	-1 0,0,0 +1	$\{ -1 \mid 0 \}$
4	-x+1/2, y, z+1/2, +1 $m_x,-m_y,-m_z$	$\begin{pmatrix} -1 & 0 & 0 & 1/2 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1/2 \end{pmatrix}$	c 1/4,y,z +1	$\{ m_{100} \mid 1/2\ 0\ 1/2 \}$
5	-x, y, -z+1/2, -1 $m_x,-m_y,m_z$	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 1/2 \end{pmatrix}'$	2 0,y,1/4 -1	$\{ 2'_{010} \mid 0\ 0\ 1/2 \}$
6	-x+1/2, -y, z, -1 $m_x,m_y,-m_z$	$\begin{pmatrix} -1 & 0 & 0 & 1/2 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}'$	2 1/4,0,z -1	$\{ 2'_{001} \mid 1/2\ 0\ 0 \}$
7	x, -y, z+1/2, -1 $m_x,-m_y,m_z$	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 1/2 \end{pmatrix}'$	c x,0,z -1	$\{ m'_{010} \mid 0\ 0\ 1/2 \}$
8	x+1/2, y, -z, -1 $m_x,m_y,-m_z$	$\begin{pmatrix} 1 & 0 & 0 & 1/2 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \end{pmatrix}'$	a x,y,0 -1	$\{ m'_{001} \mid 1/2\ 0\ 0 \}$

Go to the list of the Wyckoff Positions of the Group *Pcc'a'* (#54.343)
Go to the Systematic Absences for the Group *Pcc'a'* (#54.343)

The lattice of type III MSGs trivially coincides with the one of the ordinary space group used in their labelling, and there are no antitranslations. Therefore the list heading does not include any information on the lattice generators, etc, as it happens with type IV MSGs. The list of operations does not include any antitranslation and the total set of operations is now reduced to 8. They correspond to the ordinary space group *Pcca*, but half of them include time reversal. The set of 4 "black" operations without time reversal generate a subgroup of *Pcca*. It is in fact a subgroup of type P2/c, with the monoclinic axis along a. Hence, being a type III MSG, this group can be described as:

$$G = F + \{R'|t\}\ F$$

where F is a subgroup of *Pcca*, and {R|t} (without time reversal) is an operation of the ordinary space group *Pcca,* not belonging to F.

We can check that F in this example is a group of type $P2_1/c$ using a tool in the Bilbao Crystallographic Server for ordinary space groups, which is outside its magnetic section, namely the program IDENTIFY GROUP in the first section: "Space Group Symmetry".

2d) Doing copy/paste, just take the "black" operations in the list deleting the "+1", to convert them in operations of an ordinary space group:

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

Paste this set of four operations in the input window of "IDENTIFY GROUP", and submit. The program will then identify the group as $P2_1/c$, but with the monoclinic axis along *a*, as it is shown in the transformation it proposes to pass to the standard setting of this space group. If we follow the same procedure, but including the 8 operations, disregarding the "-1" of the other 4 operations, what space group will be identified by the program, and which transformation to standard?

The MSG of a magnetic phase defines the symmetry constraints of all degrees of freedom of the structure, including the non-magnetic ones, as the atomic positions. But for non magnetic degrees of freedom the presence of time reversal or not in a symmetry operation is irrelevant, and the symmetry constraints can therefore be described by an ordinary space group, formed by all operations of the MSG disregarding the presence or not in them of time reversal. We shall call this ordinary space group, the *effective* space group of the MSG. In the case of the MSG Pcc'a', it is clear that this space group is Pcca, both groups having the same lattice. But what is the effective space group for the type IV MSG 54.352 P_Icca, which we have considered at the beginning? We shall obtain this effective space group using again "IDENTIFY GROUP"

2e) Come back to the listing of the MSG 54.352 P_Icca and copy/paste in the input window of "IDENTIFY GROUP" all the listed symmetry operations, disregarding the "-1" or "+1":

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

and submit. In fact, the program only needs as input a minimal set of generators, and therefore this list can be strongly shortened, if you make a appropriate choice of generators (only 4 generators are really needed). The program then identifies the effective space group:

Bilbao Crystallographic Server → IDENTIFY GROUP

The Space Group has been identified as *Ibca* (No. 73)

Transformation Matrix to the standard/default setting

$$\begin{pmatrix} 1 & 0 & 0 & 1/4 \\ 0 & 1 & 0 & 1/4 \\ 0 & 0 & 1 & 1/4 \end{pmatrix}$$

Check an alternative Transformation Matrix

Input generators

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

General positions of the Space Group *Ibca* in the given setting

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

1 x,y,z
2 -x,-y+1/2,z+1/2
3 -x+1/2,y+1/2,-z
4 x+1/2,-y,-z+1/2
5 -x+1/2,-y+1/2,-z+1/2
6 x+1/2,y,-z
7 x,-y,z+1/2
8 -x,y+1/2,z

The effective space group of P_Icca is therefore identified as *Ibca* (N. 73), with its standard origin shifted by (¼ ¼ ¼) with respect to the one being used in the standard setting of P_Icca. The effective space group is therefore not *Pcca* as in type III MSGs, but a different space group with a different lattice.

If we come back to the listing of operations of P_Icca, we can see on its heading that the alternative OG label for this MSG is $I_Pb'ca$ (73.7.649). This shows a nice general property of the OG labelling and description: the reference space group for the OG description and labelling of a MSG is in all cases the effective space group for the non-magnetic degrees of freedom. For type IV MSGs, this space group is in many cases different from the one considered by the BNS labelling, and also the reference lattice is different.

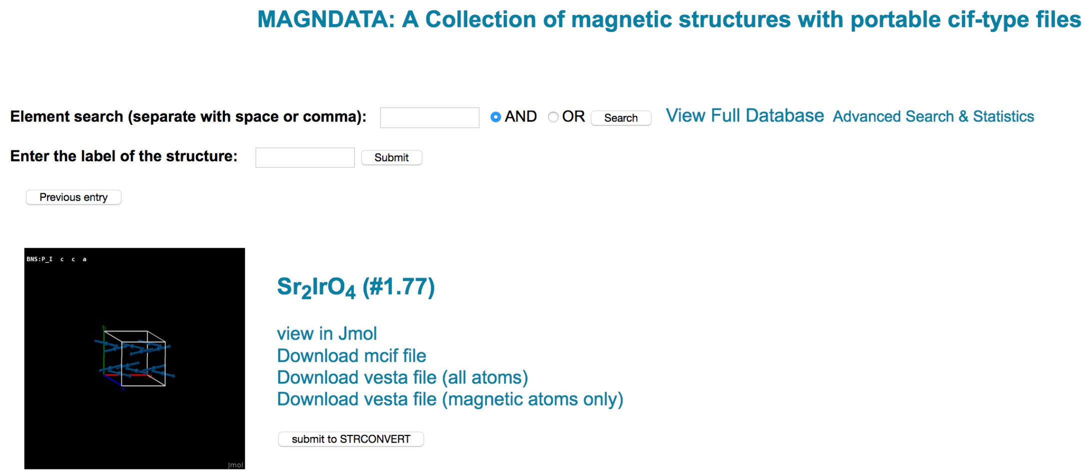
3. IDENTIFY MAGNETIC GROUP: Identification of a MSG from a set of generators in an arbitrary setting

Magnetic structures are usually described with the same origin and axes orientation as those used for its parent paramagnetic phase, which is taken as reference. In many cases, this means that the symmetry of the magnetic structure must be described by a MSG in a non-standard setting. In general, the transformation to a description with the MSG in its standard form requires a change of origin and a different choice of unit cell.

We shall see here a simple example of this quite general situation, using IDENTIFY MAGNETIC GROUP to identify the actual MSG describing the symmetry of a specific magnetic structure.

3a) Open MAGNDATA and search structures containing Sr and Ir using the corresponding element search option in the menu. From the list of structures appearing choose the entry #1.77 corresponding to Sr_2IrO_4.

This structure has a paramagnetic phase with space group *$I4_1/acd$* (N. 142), and its magnetic phase has a propagation vector **k** = (1,1,1). This means that the magnetic ordering breaks the *bcc* lattice centering of the paramagnetic structure but keeps the periodicity given by the tetragonal unit cell. The description of the magnetic structure is then done using the same unit cell.



3b) Among the options appearing at the head of the output for the entry #1.77, click on "download mcif file", and download or just open in your computer the file in magCIF format.

3c) Localize within the .mcif file the text, which defines the magnetic space group of the structure in the following form:

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

loop_
_space_group_symop_magn_centering.id
_space_group_symop_magn_centering.xyz
1 x,y,z,+1
2 x+1/2,y+1/2,z+1/2,-1
```

3d) Copy/paste these operations (or a minimal set that generates all of them) in the input window of IDENTIFY MAGNETIC GROUP and submit (in the default option: BNS setting). (the numerical labels of the operations have to be deleted to be an acceptable input format) Check that the program then identifies the MSG as P_Icca (54.352), i.e. the one we have discussed in the previous section. The output also shows a change of unit cell and origin to transform the symmetry operations to its standard setting. As this transformation is not the identity, it means that the MSG with the basis used is in a non-standard form, i.e. the operations do not coincide with those listed for this MSG in MGENPOS.

Note that the basis transformation to standard in the ouput of the program is given as a matrix with the transformed cell vectors as columns, such that the basis transformation to standard proposed by the program is (-**c**,**b**,**a**; 0,0,0):

The Magnetic Space Group has been identified as P_Icca (No. 54.352)
in the BNS setting

Transformation Matrix to the standard/default BNS setting

$$\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}$$

Check an alternative Transformation Matrix

General positions of the Magnetic Space Group P_Icca in the given BNS setting

Input generators

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

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

Notice that identification of the label of the MSG and its transformation to standard, unambiguously defines the symmetry of the phase, and the list of symmetry operations becomes redundant as these latter could be reconstructed from the standard listing of the MSG and the application of the inverse of the identified transformation.

The transformation to the standard setting of a MSG is in general not unique.

3e) Check for instance, using the corresponding option of the program, that a change of basis with an origin shift, such as (c,b,-a; 0 ,0,0) or (c,b,-a; ½ ,½,½) would also be appropriate to transform the MSG to its standard setting.

4. MWYCKPOS: Wyckoff positions of magnetic space groups

4a) Introduce the numerical label 54.352 correponding to the space group P_Icca, and submit for the standard setting. This program then provides a listing of all the possible Wyckoff positions for this MSG:

Wyckoff Positions of the Group P_Icca (#54.352) [BNS setting]

To display the Wyckoff positions in the OG setting, please follow this link: $I_Pb'ca$ (#73.7.649)

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

Site Symmetries of the Wyckoff Positions

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

Similarly as in the International Tables for Crystallography, the list includes por each possible special position the set of symmetry related ones, forming the so-called orbit of the Wyckoff position. Apart from the relative coordinates of the position, the information includes the components of a magnetic moment at this position, showing their symmetry constraints and relations within the orbit. Each Wyckoff orbit, defined in this form, can be interpreted as a set of spin basis modes compatible with the MSG.

The Wyckoff orbit corresponding to a general arbitrary position coincides with the list of symmetry operations or general positions, listed in MGENPOS.

The output also indicates the point group symmetry corresponding to each special position. Note, for instance the Wyckoff position 8b (¼, ¾, ¼) lies on a point with point group symmetry -1’, and this forbids the presence of a non-zero magnetic moment.

5. MPOINT: Magnetic Point Group Tables

Macroscopic crystal tensor properties of magnetic structures only depend on the magnetic point group of the system. This is just formed by the set of rotational and roto-inversion operations, with time reversal added or not, which are present in its MSG.

5a) Click on MPOINT to see all the possible magnetic point groups:

Magnetic Point Group Tables

The Magnetic Point Group tables contain:

- General properties of the group
- List of symmetry elements
- Table of magnetic point subgroups
- Material tensors for the point group

Choose a magnetic point group from the next table

1.1.1	1	1.2.2	11'	2.1.3	-1	2.2.4	-11'	2.3.5	-1'	3.1.6	2	3.2.7	21'	3.3.8	2'
4.1.9	m	4.2.10	m1'	4.3.11	m'	5.1.12	2/m	5.2.13	2/m1'	5.3.14	2'/m	5.4.15	2/m'	5.5.16	2'/m'
6.1.17	222	6.2.18	2221'	6.3.19	2'2'2	7.1.20	mm2	7.2.21	mm21'	7.3.22	m'm2'	7.4.23	m'm'2	8.1.24	mmm
8.2.25	mmm1'	8.3.26	m'mm	8.4.27	m'm'm	8.5.28	m'm'm'	9.1.29	4	9.2.30	41'	9.3.31	4'	10.1.32	-4
10.2.33	-41'	10.3.34	-4'	11.1.35	4/m	11.2.36	4/m1'	11.3.37	4'/m	11.4.38	4/m'	11.5.39	4'/m'	12.1.40	422
12.2.41	4221'	12.3.42	4'22'	12.4.43	42'2'	13.1.44	4mm	13.2.45	4mm1'	13.3.46	4'm'm	13.4.47	4m'm'	14.1.48	-42m
14.2.49	-42m1'	14.3.50	-4'2'm	14.4.51	-4'2m'	14.5.52	-42'm'	15.1.53	4/mmm	15.2.54	4/mmm1'	15.3.55	4/m'mm	15.4.56	4'/mm'm
15.5.57	4'/m'm'm	15.6.58	4/mm'm'	15.7.59	4/m'm'm'	16.1.60	3	16.2.61	31'	17.1.62	-3	17.2.63	-31'	17.3.64	-3'
18.1.65	32	18.2.66	321'	18.3.67	32'	19.1.68	3m	19.2.69	3m1'	19.3.70	3m'	20.1.71	-3m	20.2.72	-3m1'
20.3.73	-3'm	20.4.74	-3'm'	20.5.75	-3m'	21.1.76	6	21.2.77	61'	21.3.78	6'	22.1.79	-6	22.2.80	-61'
22.3.81	-6'	23.1.82	6/m	23.2.83	6/m1'	23.3.84	6'/m	23.4.85	6/m'	23.5.86	6'/m'	24.1.87	622	24.2.88	6221'
24.3.89	6'22'	24.4.90	62'2'	25.1.91	6mm	25.2.92	6mm1'	25.3.93	6'mm'	25.4.94	6m'm'	26.1.95	-6m2	26.2.96	-6m21'
26.3.97	-6'm'2	26.4.98	-6'm2'	26.5.99	-6m'2'	27.1.100	6/mmm	27.2.101	6/mmm1'	27.3.102	6/m'mm	27.4.103	6'/mmm'	27.5.104	6'/m'mm'
27.6.105	6/mm'm'	27.7.106	6/m'm'm'	28.1.107	23	28.2.108	231'	29.1.109	m-3	29.2.110	m-31'	29.3.111	m'-3'	30.1.112	432
30.2.113	4321'	30.3.114	4'32'	31.1.115	-43m	31.2.116	-43m1'	31.3.117	-4'3m'	32.1.118	m-3m	32.2.119	m-3m1'	32.3.120	m'-3'm
32.4.121	m-3m'	32.5.122	m'-3'm'												

There are 122 possible magnetic point groups.

5b) Choose the group *mmm1’* (8.2.25). You can see then that the group has 16 operations, and they are the 8 operations of the point group *mmm* plus another 8 operations obtained by “multiplying” this operation by time reversal. This can be expressed as:

mmm1’ = *mmm* + 1’ *mmm*

Check that these point group operations are indeed those that are present in the listing of MGENPOS for the MSG $P_I cca$ (considered in section 2), if the translations of the operations are disregarded. Thus, the magnetic point group associated with $P_I cca$ is the grey point group *mmm1’*, a group that includes time reversal, i.e. the same type of group as those of non-magnetically ordered systems: All type IV MSGs have grey 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.

5c) Go back and choose the group *m’m’m* (8.4.27). Check that this is the point group corresponding the MSG *Pcc’a’*, that we considered in section 2. Determine the transformation of basis required to make the point-group operations of the MSG fully equivalent to those of the point group *m’m’m* (it can be done by hand or you can use IDENTIFY GROUP by introducing the operations of *Pcc’a’* with the translations deleted.
In this example, the point group does not include the time reversal operation, and therefore, crystal tensor properties forbidden in the paramagnetic phase will be present.

6. MTENSOR: Symmetry adapted form of crystal tensors in magnetic phases

MTENSOR is a program that provides the symmetry adapted form of any type of crystal tensor. The desired property can be chosen among a list which specifies more than 100 distinct crystal tensors divided in four classes: equilibrium tensors, optical tensors, non-linear optical susceptibility tensors and transport tensors. In addition, using abstract generalized (so-called Jahn) symbols, which define the transformation properties of the tensor one can also get the symmetry-adapted form of any kind of tensor property for any magnetic point group, as long as its rank is not greater than 8.

6a) Open MTENSOR and choose the space group *Pcc'a'*. Although the symmetry constraints on a tensor only depend of the system magnetic point group, the program allows to introduce its full MSG, 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 group, as we have seen in the previous version.

6b) Choose among the equilibrium tensors: "Magnetization vector Mi", and check that this space group allows ferromagnetism along a.

6c) Come back and choose now the piezomagnetic tensor (direct effect):

Symmetry-adapted form of the Piezomagnetic tensor Λ_{ijk} (direct effect) for the magnetic space group *Pcc'a'* (#54.343)

Information about the selected tensor

- 3^{rd} rank Piezomagnetic tensor Λ_{ijk} (direct effect)
- Axial tensor which inverts under time-reversal symmetry operation
- Defining equation: $\mathbf{M_i=\Lambda_{ijk}\sigma_{jk}}$
- Relates Stress tensor σ_{ij} with Magnetization **M**
- Intrinsic symmetry symbol: **aeV[V^2]**
- Symmetrized indexes due to intrinsic symmetry:
  - $\Lambda_{ijk} = \Lambda_{ikj}$
- Abbreviated notation: $\Lambda_{ijk} \rightarrow \Lambda_{ij}$
  - $jk \rightarrow j$ if $j=k$, $jk \rightarrow 9-(j+k)$ if $j\neq k$

Table of tensor components

Λ_{ij}		j					
		1	2	3	4	5	6
i	1	Λ_{11}	Λ_{12}	Λ_{13}	0	0	0
	2	0	0	0	0	0	Λ_{26}
	3	0	0	0	0	Λ_{35}	0

Number of independent coefficients: 5

Note: semitransparent tensor components are identical or opposite to bold symbols due to the intrinsic symmetry of the tensor

Check that the ouput indicates that a shear xy can induce a magnetization along b, and a shear xz can induce a magnetization along c. Piezomagnetic effects are certainly forbidden in the paramagnetic phase. (The "a" in its Jahn symbol means that the tensor is odd for time reversal, and therefore it must be zero for any group that includes time reversal as symmetry operation, as it happens in all non-magnetically ordered structures)

6d) Verify with some trials that the symmetry-adapted form of any tensor is the same for the MSGs *Pmmm1'* and for *P$_I$cca.* Why?

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