Tutorial on the use of k-SUBGROUPSMAG and MAGMODELIZE of the Bilbao Crystallographic Server to explore possible models for a magnetic structure with known propagation vector(s).

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k-SUBGROUPSMAG is a freely available program in the Bilbao Crystallographic Server (www.cryst.ehu.es), which allows to explore online all possible magnetic symmetries which are consistent with one or more observed propagation vectors.

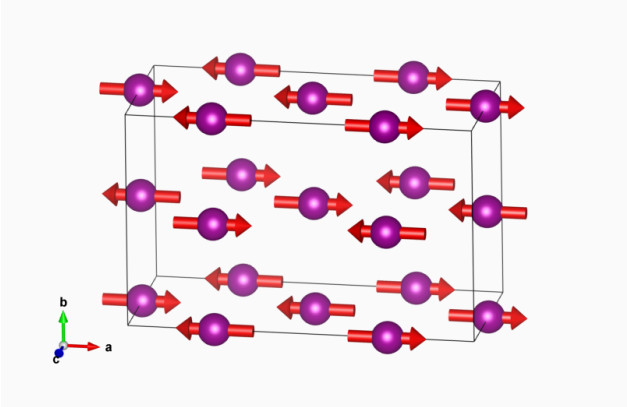
Introducing the space group of the paramagnetic phase (parent space group), the propagation vector(s), and the Wyckoff positions of the magnetic atoms, the program provides all possible symmetries of the magnetic structure, as subgroups of the parent gray group and shows their group-subgroup hierarchy. The conjugacy equivalent classes of subgroups can be obtained, and the irreps compatible with each symmetry are given.

The possible subgroups provided by the program can be filtered according to different criteria, in particular the condition that the subgroups should correspond to the action of an order parameter transforming according to one (or several) specific irreducible representation(s) of the parent space group.

Through a link with the program MAGMODELIZE, also in the Bilbao Crystallographic Server, if the parent paramagnetic structure is introduced, models of the magnetic structures which correspond to the set of possible symmetries chosen by the user among the list of subgroups provided by k-SUBGROUPSMAG can be constructed, visualized, and/or exported as magCIF files for further test, refinement or analysis. The link to MAGMODELIZE allows to determine the spin arrangements allowed for each chosen MSG, and defines its refinable parameters. A magCIF file can then be obtained for each of the alternative magnetic structures, which can then be refined in programs like JANA2006 [1] or FULLPROF [2], or they can be introduced in the program ISODISTORT [3] for mode analysis, or transformed with the structure editor STRCONVERT of the Bilbao Crystallographic Server. These magCIF files can also be used for 3D visualization with VESTA[4] or Jmol [5]. A direct link to the tool MVISUALIZE, also in the Bilbao Crystallographic Server, allows an inmediate visualization of each of the alternative models with JSmol.

In this tutorial a set of examples of the use of both programs can be found.

Example 1: Orthorhombic $HoMnO_3$ (see MAGNDATA #1.20)



Magnetic structure of $HoMnO_3$ (only Mn atoms) according to (Muñoz, A. et al., *Inorg. Chem.* (2001) **40** 1020 - 1028), with magnetic space group (MSG) P_bmn2_1(-**b**,**a**,**c**;1/8,1/4,0) (magndata #1.20).

This example in also used in the tutorial for the program MAXMAGN. Here one can see the additional possibilities that k-SUBGROUPSMAG provides.

The paramagnetic structure of $HoMnO_3$ can be summarized as (Muñoz, A. et al., *Inorg. Chem.* (2001) **40** 1020 - 1028):

Space group: Pnma (#62)
Lattice parameters:
5.83536 7.36060 5.25722

Asymmetric unit:
Ho1 - 0.08390 0.25000 0.98250
Mn1 - 0.00000 0.00000 0.50000
O1 - 0.46220 0.25000 0.11130
O2 - 0.32810 0.05340 0.70130

and the observed propagation vector is (½,0,0).

a) In the first input pages of k-SUBGROUPSMAG, introduce the parent space group, the propagation vector and the Wyckoff position (4b) of the magnetic atom Mn. Obtain (clicking on "submit" at the botton of the main page) the graph of all magnetic subgroups (conjugate classes) consistent with the observed propagation vector, and check that, apart from the monoclinic k-maximal subgroups, there is only a third possible centrosymmetric symmetry, namely a subgroup of type P_s-1, which a common subgroup of the two centrosymmetric monoclinic groups of maximal symmetry (Figure 1).

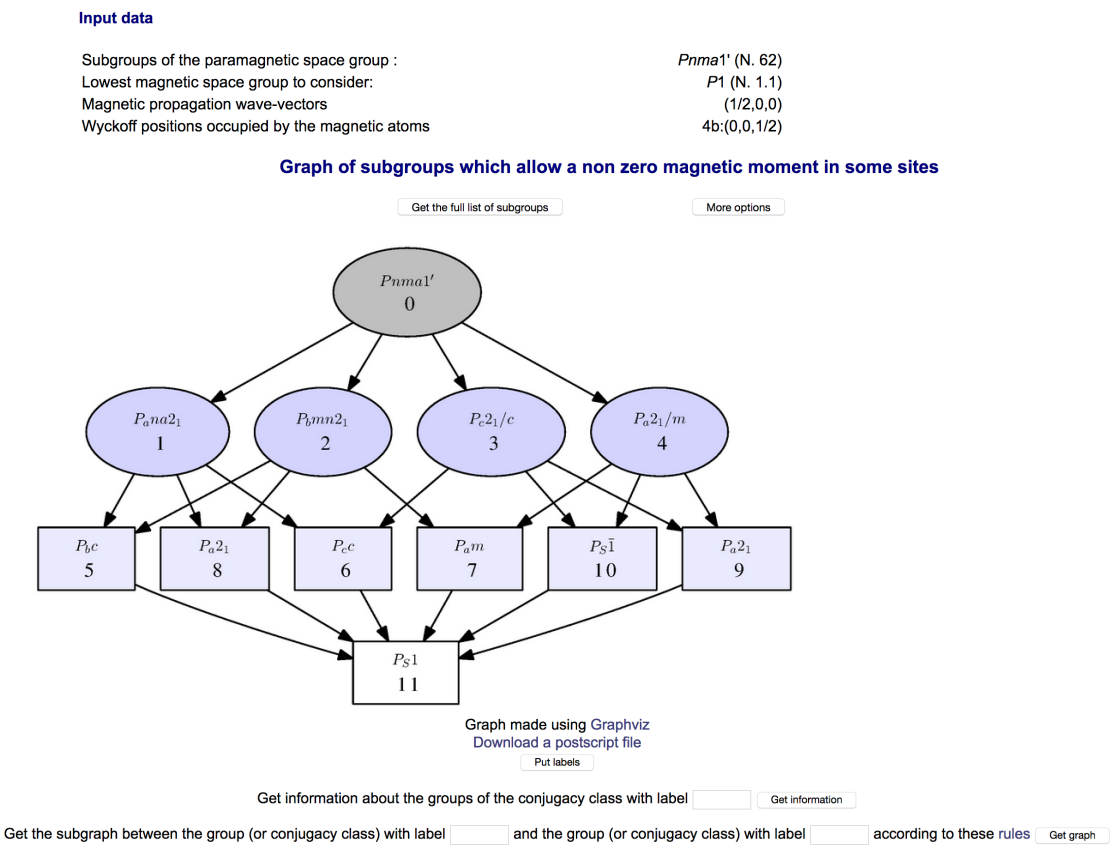


Figure 1. Output page of k-SUBGROUPSMAG showing the group-subgroup hierarchy of all possible magnetic symmetries of a magnetic ordering for a paramagnetic structure with space group *Pnma* and a propagation vector (1/2 0 0) (the condition of the magnetic site to be *4b*, does not produce any further restriction on the possible subgroups) . Only the BNS label of the corresponding group type is indicated. The k-maximal magnetic groups are highlighted with elliptical frames. Only one subgroup per conjugate class is shown. Except for the two monoclinic k-maximal subgroups and its common subgroup P_S*-1*, all other possible symmetries are polar and allow an induced electric polarization.

The numbers below the label of each conjugate class allows to identify the conjugacy class in the listing provided by the program (Figure 2). These numbers can be removed to obtain a tidier figure. The ouput page includes several menus to manipulate the graph, restricting its extent, etc...

The transformation (**P**,**p**) given for each subgroup in the list, where **P** is a 3x3 matrix and **p** = (p_1, p_2, p_3) a column vector, indicates in each case a choice of unit cell and origin, for which the subgroup adquires the standard setting of the corresponding magnetic space group (MSG) given by the MSG label, i.e. the symmetry operations of the subgroup would take when described using this unit cell and origin, the form used for this MSG in the listings taken as standard. The transformation (**P**,**p**) is defined with respect to the unit cell ($\mathbf{a}_p$,$\mathbf{b}_p$,$\mathbf{c}_p$) and origin $\mathbf{O}_p$ of the parent space group, in the following form:

$$(\mathbf{a}^s,\mathbf{b}^s,\mathbf{c}^s)= (\mathbf{a}_p,\mathbf{b}_p,\mathbf{c}_p).\mathbf{P} \quad , \quad \mathbf{O}^s = \mathbf{O}_p + p_1\,\mathbf{a}_p + p_2\,\mathbf{b}_p + p_3\,\mathbf{c}_p$$

where ($\mathbf{a}^s$,$\mathbf{b}^s$,$\mathbf{c}^s$) and $\mathbf{O}^s$ are the unit cell vectors and origin of a standard setting of the MSG.

N	Group Symbol	Transformation matrix	Group-Subgroup index	Other members of the Conjugacy Class	irreps	Magnetic structure models (MAGMODELIZE)
1	P_ana2_1 (No. 33.149)	$\begin{pmatrix} 2 & 0 & 0 & 1/4 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps	☐
2	P_bmn2_1 (No. 31.129)	$\begin{pmatrix} 0 & 2 & 0 & 1/4 \\ -1 & 0 & 0 & 1/4 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps	☐
3	P_c2_1/c (No. 14.82)	$\begin{pmatrix} 0 & 0 & -2 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps	☐
4	P_a2_1/m (No. 11.55)	$\begin{pmatrix} 2 & 0 & 0 & 1/2 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps	☐
5	P_bc (No. 7.29)	$\begin{pmatrix} 0 & 2 & 0 & 1/4 \\ -1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	8=2x4	Conjugacy Class	Get irreps	☐
6	P_cc (No. 7.28)	$\begin{pmatrix} 0 & 0 & -2 & 0 \\ 0 & 1 & 0 & 1/4 \\ 1 & 0 & 0 & 0 \end{pmatrix}$	8=2x4	Conjugacy Class	Get irreps	☐
7	P_am (No. 6.21)	$\begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1/4 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	8=2x4	Conjugacy Class	Get irreps	☐
8	P_a2_1 (No. 4.10)	$\begin{pmatrix} 2 & 0 & 0 & 1/4 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$	8=2x4	Conjugacy Class	Get irreps	☐
9	P_a2_1 (No. 4.10)	$\begin{pmatrix} 2 & 0 & 0 & 1/2 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	8=2x4	Conjugacy Class	Get irreps	☐
10	$P_S\bar{1}$ (No. 2.7)	$\begin{pmatrix} 0 & 0 & -2 & 1/2 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}$	8=2x4	Conjugacy Class	Get irreps	☐
11	P_S1 (No. 1.3)	$\begin{pmatrix} 0 & 0 & -2 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}$	16=2x8	Conjugacy Class	Get irreps	☐

Figure 2. List provided by k-SUBGROUPSMAG of all possible magnetic symmetries of a magnetic ordering for a paramagnetic structure with space group *Pnma* and a propagation vector (1/2 0 0) (the condition of the magnetic site to be *4b*, does not produce any further restriction on the possible subgroups). Only the BNS label of the corresponding group type is indicated. The k-maximal magnetic groups are highlighted with elliptical frames. Only one subgroup per conjugate class is shown. By clicking on the button "conjugacy class" a list of all distinct subgroups belonging to the conjugacy class is shown. The button "Get irreps" is a direct link to the program Get_mirreps, which allows to obtain all the irreps of the parent space group that are compatible with the listed subgroup of the gray parent group. The last column allows to choose those symmetries that one wants to transmit to MAGMODELIZE for further analysis of the corresponding magnetic structure models.

b) Check the button "more options" on the page with the list or with the graph of the possible subgroups (conjugacy classes). This gives the possibility to further filter the possible magnetic symmetries with the condition of allowing a non-zero magnetic moment of all magnetic sites (Figure 3) (The subgroups can be further limited to those allowing a collinear spin arrangement, which in the present case does not mean any additional restriction). One can see in Figure 3, that all possible symmetries allowing magnetic order of all Mn sites are polar.

c) Notice that in Figure 3 there are two distinct conjugacy classes of the same type P_a2_1. Although the MSG label is the same for both classes because the groups are of the same type, they are quite different as subgroups of *Pnma1'*. The binary axis of the *Pnma* group that is maintained in one or the other case are different. Go to the list of subgroups of Figure 3, and from the transformation to the standard setting given there, conclude that in one case the binary axis is along **c**, and in the

other case along **b**, in the *Pnma* setting. This can also be checked, clicking on the option that provides the subgroups within the conjugacy class, and clicking further on the listing of the symmetry operations in matrix format.

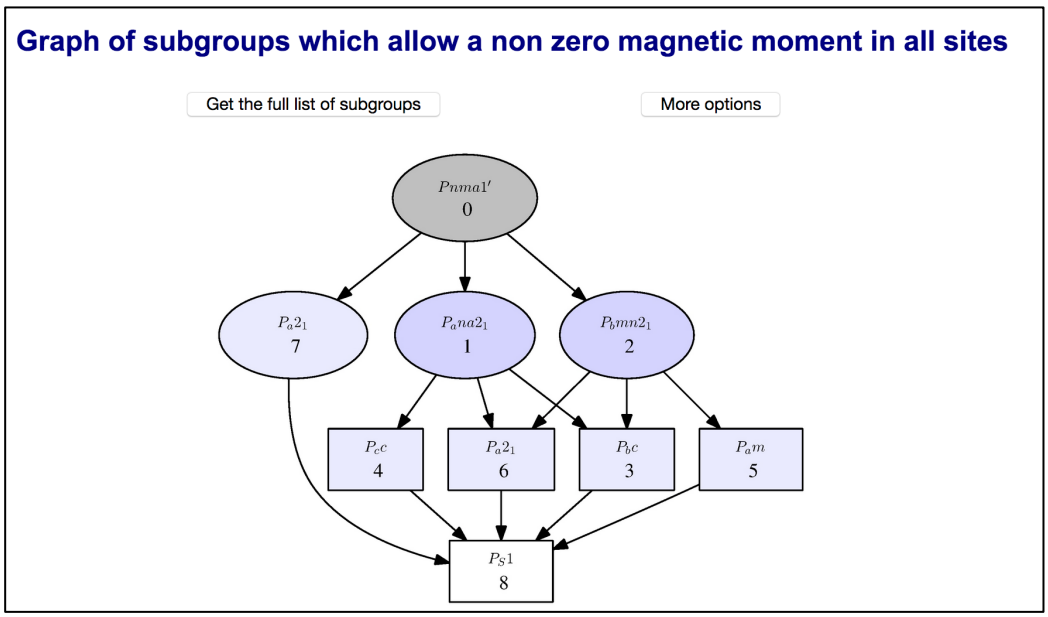
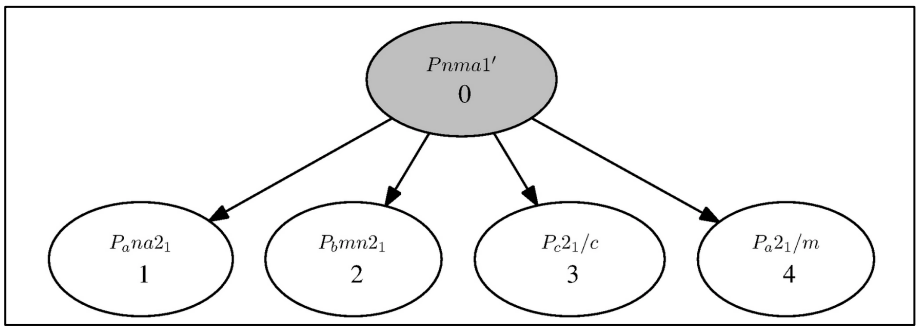
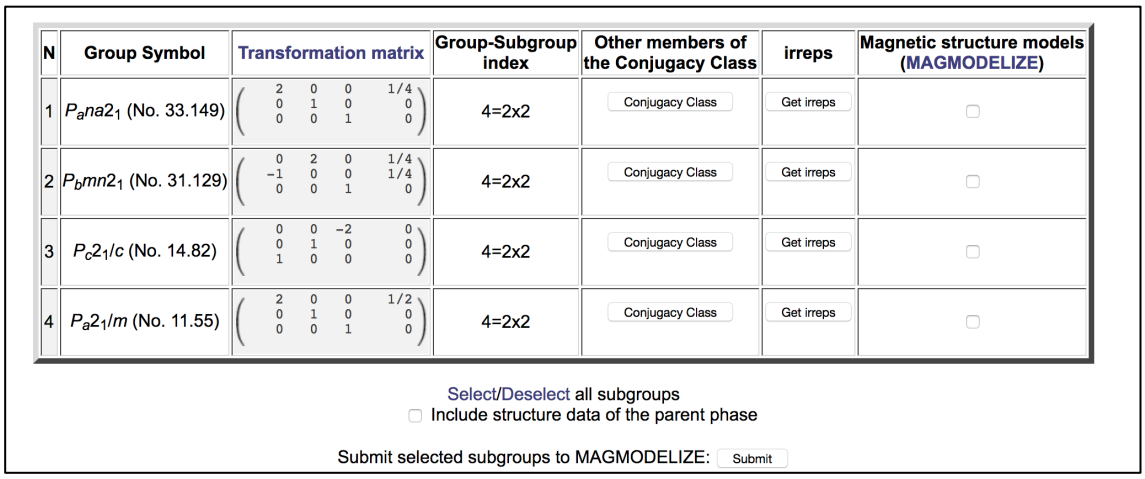


Figure 3: Graph of all possible subgroups (conjugacy classes) of the parent gray group *Pnma1'* allowing a non-zero magnetic moment at all sites described by the 4b Wyckoff position of the parent space group *Pnma*.

d) Go back to the main menu and check the option "Only maximal subgroups". This will produce a list and/or graph of only the k-maximal subgroups (Figure 4).





N	Group Symbol	Transformation matrix	Group-Subgroup index	Other members of the Conjugacy Class	irreps	Magnetic structure models (MAGMODELIZE)
1	P_ana2_1 (No. 33.149)	$\begin{pmatrix} 2 & 0 & 0 & 1/4 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps	☐
2	P_bmn2_1 (No. 31.129)	$\begin{pmatrix} 0 & 2 & 0 & 1/4 \\ -1 & 0 & 0 & 1/4 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps	☐
3	P_c2_1/c (No. 14.82)	$\begin{pmatrix} 0 & 0 & -2 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps	☐
4	P_a2_1/m (No. 11.55)	$\begin{pmatrix} 2 & 0 & 0 & 1/2 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps	☐

Select/Deselect all subgroups
☐ Include structure data of the parent phase

Submit selected subgroups to MAGMODELIZE: Submit

Figure 4. Graph and list of the k-maximal symmetries for the parent space group *Pnma* and k=(1/2,0,0). In this case, the condition of the magnetic site being *4b* does not restrict further the list.

This is a similar result to the one provided by the first ouput of MAXMAGN (see tutorial of this program). By checking on the last column of the list for all subgroups, and using the option at the bottom of the subgroup list, one can transmit the subgroups to MAGMODELIZE, which can then do a job similar to MAXMAGN for these symmetries, and initial magCIF files for the corresponding magnetic structure models can be created.

At this point, you may switch to the tutorial of MAXMAGN entitled: "***The magnetic structure of $HoMnO_3$. Tutorial example on the use of MAXMAGN and other tools of the Bilbao Crystallographic Server for the analysis of magnetic structures***" that you can download at the webpage of this program and follow the same steps indicated there using instead MAGMODELIZE. Thus, k-SUBGROUPSMAG combined with MAGMODELIZE somehow supersedes MAXMAGN, as the combination of these two programs can do what MAXMAGN does, but they are not restricted to maximal symmetries and to a single propagation vector. In addition, using these new programs one can filter further the possible subgroups and the resulting possible magnetic structures using representation analysis (see following steps). However, one should be aware that MAXMAGN, being a much simpler program, is more robust. Furthermore, it has been massively tested during the development of the MAGNDATA database, and its debugging is therefore much more complete.

e) Go back to the main input page of k-SUBGROUPSMAG, uncheck the "only maximal subgroup" option and come back to the default choice (the first one). In the option "choose irreps" click on "representations". The program provides then an output page with the irrep decompositions of the magnetic representation for the Wyckoff site 4b (Figure 5).

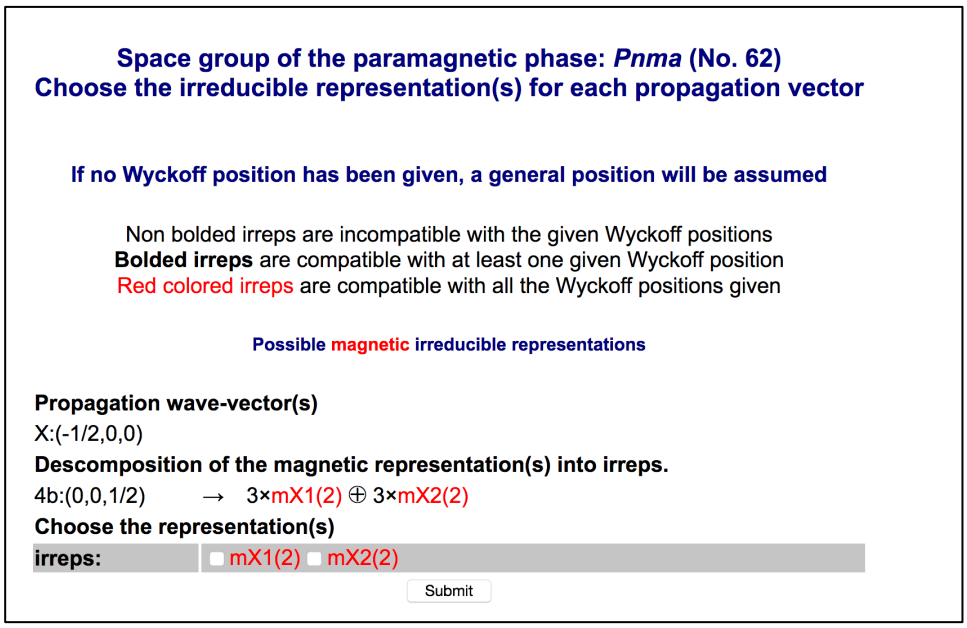


Figure 5. Irrep decomposition of the magnetic representation for the site *4b* of *Pnma*, as given by k-SUBGROUPSMAG. Irrep labels are those used by the ISOTROPY[3] webpage. In parenthesis, after the irrep label the dimension of the full irrep is indicated. As in this case the irrep star has only one

arm, this dimension coincides with that of the small irrep. The output shows that the total number of spin degrees of freedom (12) decomposes into 6 degrees for the irrep mX1 and 6 for the irrep mX2.
The irrep labels in Figure 5 are those also used in the ISOTROPY[3] webpage, and one can always inspect the actual irreps by going to the programs in the section "Representations and Applications" of the Bilbao Crystallographic Server, taking into account that the symbol *m* in the irrep label only indicates that the irrep is odd for time reversal.

Figure 5 shows that if the magnetic structure is assumed to originate from the condensation of an order parameter transforming according to a single irrep, two different irreps for the order parameter are possible.

f) On the mode decomposition output page (Figure 5) check the irrep mX1 and submit. The program them provides as list and/or graph the possible subgroups than can result from a magnetic ordering complying with the transformation properties of irrep mX1 (Figure 6).

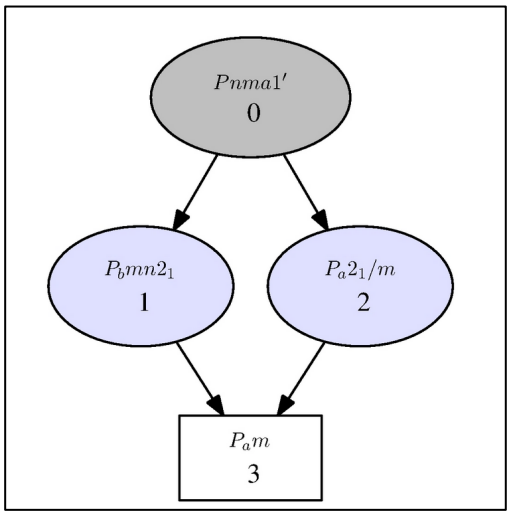
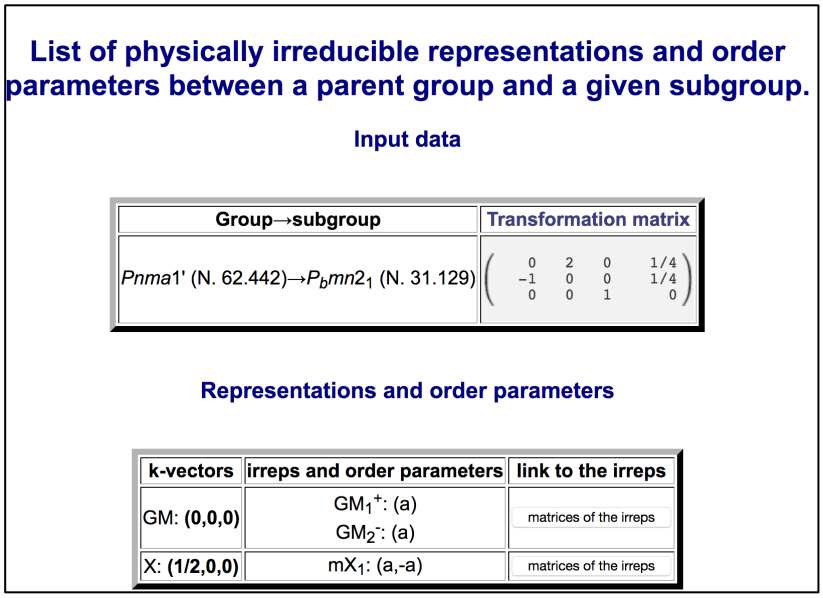


Figure 6. Possible MSGs that can result from a magnetic ordering according to the irrep mX1 (k=(1/2,0,0)) *of Pnma1'*.

g) On the list of subgroups corresponding to irrep mX1, and for the subgroups P_bmn2_1 and P_am, click on the button "Get_irreps". The output (Figure 7) shows that mX1 is the only magnetic irrep allowed for these symmetries, so that no secondary spin degrees of freedom corresponding to additional irreps compatible with the MSG exist for these symmetries. In the MSG P_bmn2_1 , after the irrep label mX1, the necessary direction of the order parameter within the 2-dim irrep space is indicated as (a,-a). This means that each pair of spin basis functions transforming according to the irrep mX1 must combine in a particular form, forming a single basis function complying with this specific MSG. This implies that the number of spin degrees of freedom in this MSG is only 3, instead of the 6 in an arbitrary combination of the mX1 basis functions. This latter happens in the lower irrep kernel P_am, where the order parameter is allowed an arbitrary direction: (a,b).



List of physically irreducible representations and order parameters between a parent group and a given subgroup.

Input data

Group→subgroup	Transformation matrix
*Pnma*1' (N. 62.442)→P_bmn2_1 (N. 31.129)	$\begin{pmatrix} 0 & 2 & 0 & 1/4 \\ -1 & 0 & 0 & 1/4 \\ 0 & 0 & 1 & 0 \end{pmatrix}$

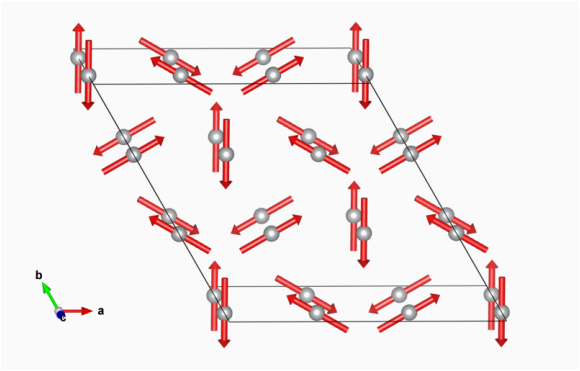
Representations and order parameters

k-vectors	irreps and order parameters	link to the irreps
GM: **(0,0,0)**	GM_1^+: (a) GM_2^-: (a)	matrices of the irreps
X: **(1/2,0,0)**	mX_1: (a,-a)	matrices of the irreps

Figure 7. Output of the option "Get_irreps" showing all the irreps (magnetic and non-magnetic that are compatible with a specific subgroup of *Pnma1'* of type P_bmn2_1. The transformation to the standard setting, indicated in the output, fully defines the subgroup which is being considered.

g) Come back to the mode decomposition and check instead the irrep mX2 to obtain the possible magnetic symetries for this alternative irrep.

Example 2: $Ba_3Nb_2NiO_9$ (magndata #1.13)
[Hwang, J. et al., *Phys. Rev. Lett.* (2012) 109, 257205]
(file: Ba3Nb2NiO9_parent.cif)



Magnetic structure of $Ba_3Nb_2NiO_9$ (only Ni atoms), according to (Hwang, J. et al., *Phys. Rev. Lett.* (2012) 109, 257205), with MSG P_c31c (2/3**a**+1/3**b**, -1/3**a**+1/3**b**, **c**;1/9,2/9,0) (magndata #1.13).

The paramagnetic structure of $Ba_3Nb_2NiO_9$ can be summarized as (Lufaso, Chem. Mat. 16, 2148 (2004) and Hwang, J. et al., *Phys. Rev. Lett.* (2012) 109, 257205):

Space group: P-3m1 (N. 164)

Lattice parameters: 5.7550, 5.7550, 7.0656 90 90 120

Asymmetric unit:

Ba1 0.33333 0.66667 0.66380
Ba2 0.00000 0.00000 0.00000
Ni1 0.00000 0.00000 0.50000
Nb2 0.33333 0.66667 0.17700
O1 0.50000 0.00000 0.00000
O2 0.16978 0.33960 0.32623

(The small occupancy mixing reported in the older reference is neglected)

Magnetic atom: Ni
Observed propagation vector: (1/3,1/3,1/2)

We will use k-SUBGROUPSMAG and MAGMODELIZE to explore the possible magnetic orderings compatible with the observed propagation vector. The exploration is done in a hierarchical way starting with those orderings having as much symmetry as possible. The restriction to a single irrep can also be included.

a) Open the main page of k-SUBGROUPSMAG, introduce the number of the space group of the paramagnetic phase and the propagation vector, and submit with the rest of options in their default values. A list of 25 possible MSGs are obtained. The Ni atom lies on a special position, and some of the listed

symmetries may be then irrelevant because they force a zero magnetic moment on the position of all Ni atoms.

b) Go back to the main menu and clicking on "Wyckoff" introduce the Wyckoff position occupied by the Ni atoms. This will filter the list of MSGs, only leaving those that allow non-zero magnetic moments at least for some of the Ni atoms. The list of possible MSGs now reduces to 17, and some of the maximal MSGs are of quite low symmetry (Figure 8)

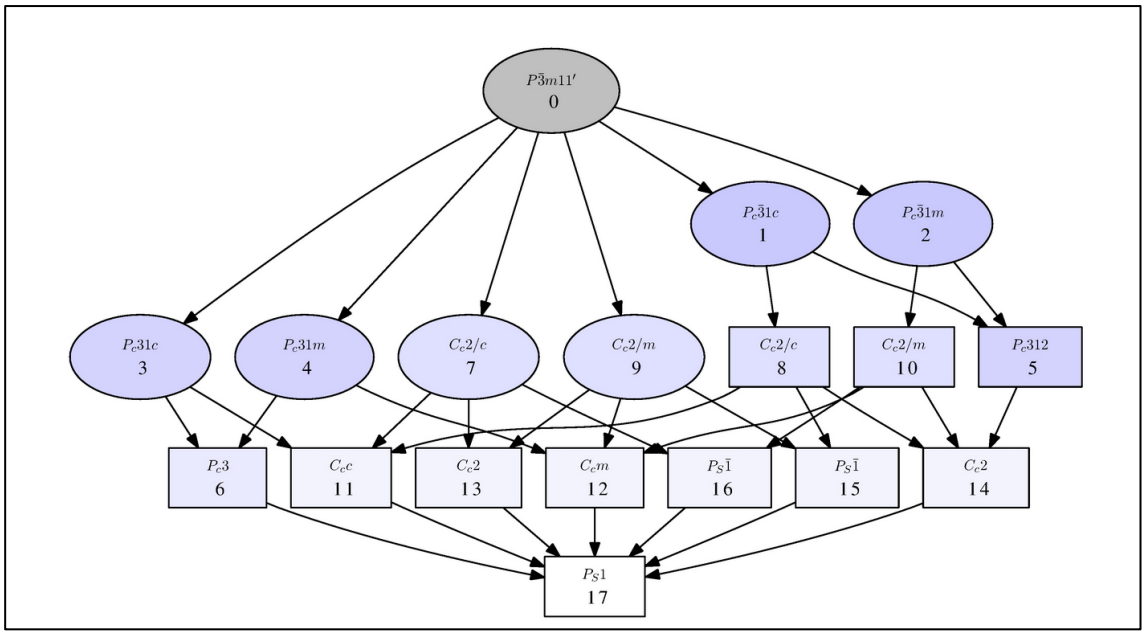
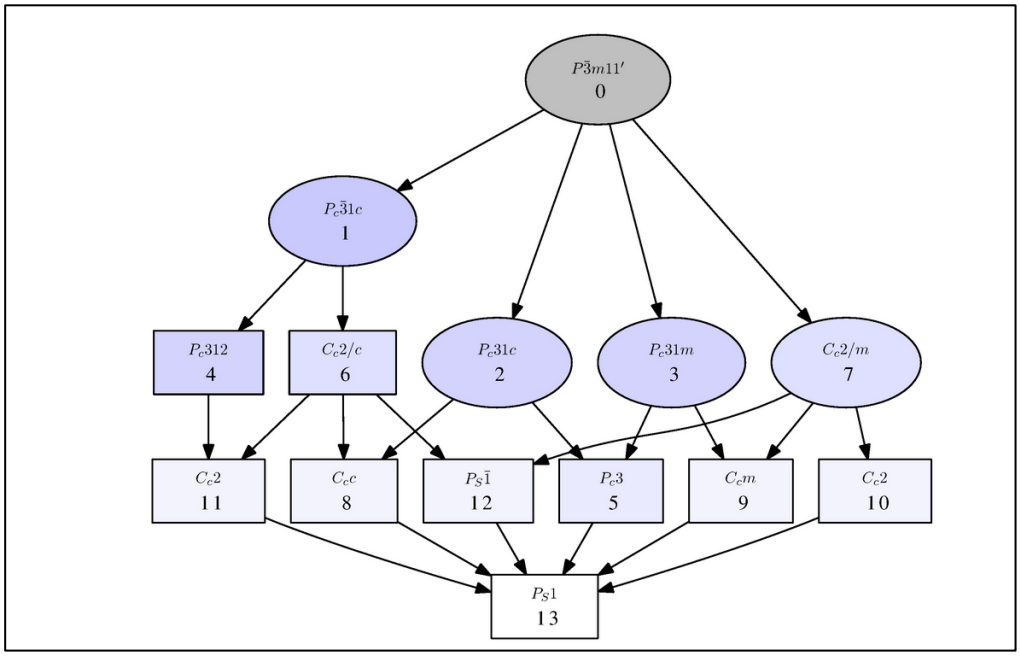


Figure 8. Possible MSGs that can be realized in a structure with parent space group *P-3m1* and propagation vector (1/3,1/3,1/2), if the magnetic atom is at the Wyckoff position *1b*.

c) Press the button "more options" and filter further the posible subgroups on condition that they allow non-zero magnetic moments at all Ni sites. The number of possible symmetries is then further reduced to 13 (Figure 9) . The subgroup conjugacy classes numbered 1, 2, 3 and 7 are maximal on these conditions and therefore the first candidates to explore in an eventual fit of experimental diffraction data. The structure reported for $Ba_3Nb_2NiO_9$ corresponds to one of these four MSGs, namely *P_c31c*, which is polar. In fact, two of these four possible maximal symmetries are polar along the trigonal axis, and therefore correspond to a magnetic phase bound to have some magnetically induced electric polarization (type II multiferroic).



N	Group Symbol	Transformation matrix	Group-Subgroup index	Other members of the Conjugacy Class	irreps	Magnetic structure models (MAGMODELIZE)
1	$P_c\bar{3}1c$ (No. 163.84)	$\begin{pmatrix} 1 & 1 & 0 & 0 \\ -1 & 2 & 0 & 1 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	6=6x1	Conjugacy Class	Get irreps	☐
2	P_c31c (No. 159.64)	$\begin{pmatrix} 1 & 1 & 0 & -2/3 \\ -1 & 2 & 0 & -1/3 \\ 0 & 0 & 2 & 0 \end{pmatrix}$	12=6x2	Conjugacy Class	Get irreps	☐
3	P_c31m (No. 157.56)	$\begin{pmatrix} 1 & 1 & 0 & -2/3 \\ -1 & 2 & 0 & -1/3 \\ 0 & 0 & 2 & 0 \end{pmatrix}$	12=6x2	Conjugacy Class	Get irreps	☐
4	P_c312 (No. 149.24)	$\begin{pmatrix} 1 & 1 & 0 & 0 \\ -1 & 2 & 0 & 0 \\ 0 & 0 & 2 & 0 \end{pmatrix}$	12=6x2	Conjugacy Class	Get irreps	☐
5	P_c3 (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_c2/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_c2/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_cc (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_cm (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_c2 (No. 5.16)	$\begin{pmatrix} 2 & 0 & 0 & 0 \\ 1 & 3 & 0 & 0 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	36=6x6	Conjugacy Class	Get irreps	☐
11	C_c2 (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	$P_S\bar{1}$ (No. 2.7)	$\begin{pmatrix} 2 & -1 & 0 & -1/2 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	36=6x6	Conjugacy Class	Get irreps	☐
13	P_S1 (No. 1.3)	$\begin{pmatrix} 2 & -1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 2 & 0 \end{pmatrix}$	72=6x12	Conjugacy Class	Get irreps	☐

Figure 9. Possible MSGs that can be realized in a structure with parent space group *P-3m1* and propagation vector (1/3,1/3,1/2), if the magnetic atom is at the Wyckoff position *1b*, and on the additional condition that all magnetic atoms should be allowed to have non-zero magnetic moments. These are therefore the MSGs that allow a complete magnetic ordering of all magnetic atoms.

Linking the output shown in Figure 9 with MAGMODELIZE one can obtain the magnetic structure model corresponding to these four maximal symmetries.

The transformation (**P**,**p**) listed for each subgroup, where **P** is a 3x3 matrix and **p** = (p_1, p_2, p_3) a column vector, indicates in each case a choice of unit cell and origin, for which the subgroup adquires the standard setting of the corresponding magnetic space group (MSG) given by the MSG label, i.e. the symmetry operations of the subgroup would take when described using this unit cell and origin, the form used for this MSG in the listings taken as standard. The transformation (**P**,**p**) is defined with respect to the unit cell ($\mathbf{a}_p$,$\mathbf{b}_p$,$\mathbf{c}_p$) and origin $\mathbf{O}_p$ of the parent space group, in the following form:

$$(\mathbf{a}^s,\mathbf{b}^s,\mathbf{c}^s)= (\mathbf{a}_p,\mathbf{b}_p,\mathbf{c}_p).\mathbf{P} \quad , \quad \mathbf{O}^s = \mathbf{O}_p + p_1\,\mathbf{a}_p + p_2\,\mathbf{b}_p + p_3\,\mathbf{c}_p$$

where ($\mathbf{a}^s$,$\mathbf{b}^s$,$\mathbf{c}^s$) and $\mathbf{O}^s$ are the unit cell vectors and origin of a standard setting of the MSG.

d) In the last column of the list reproduced in Figure 9, check the mentioned subgroups numbered 1 ,2 ,3 and 7; at the bottom of the page , check "include structure data of the parent phase", and submit to MAGMODELIZE. A first page appears to introduce the structure of the paramagnetic phase. Submit the cif file of Ba3Nb2NiO9_parent.cif or introduce by hand the parent structure that is described at the beginning of this example. In the next page, check the Ni atom as the only magnetic atom. The resulting output page (Figure 10) lists the subgroups that have been anayzed and is similar to the first output page of MAXMAGN, with similar capabilities.

N	Group (BNS)	Transformation matrix	General positions	Properties	Magnetic structure
1	P_c-31c (#163.84) Go to a subgroup	$\begin{pmatrix} 1 & 1 & 0 & 0 \\ -1 & 2 & 0 & 1 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
2	P_c31c (#159.64) Go to a subgroup	$\begin{pmatrix} 1 & 1 & 0 & 7/3 \\ -1 & 2 & 0 & 8/3 \\ 0 & 0 & 2 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
3	P_c31m (#157.56) Go to a subgroup	$\begin{pmatrix} 1 & 1 & 0 & 7/3 \\ -1 & 2 & 0 & 8/3 \\ 0 & 0 & 2 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
4	C_c2/m (#12.63) Go to a subgroup	$\begin{pmatrix} 2 & 0 & 0 & 0 \\ 1 & 3 & 0 & 5/2 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show

Figure 10. Output page of MAGMODELIZE for the four subgroups of maximal symmetry that were transmitted from k-SUBGROUPSMAG.

e) Construct the magnetic structures corresponding to the second subgroup on the list reproduced in Fig. 9, namely the one of type *P_c31c* by clicking on the last column. The resulting output page (Figure 11) shows that the Ni site remains unsplit, with a single symmetry-independent atom.

Magnetic Structure

Selected magnetic space group: 2- P_c31c (#159.64)

Setting parent-like (**3a, 3b, 2c** ; 0, 0, 0)

Parent space group 164 (*P*-3*m*1)

Lattice parameters: a=17.26500, b=17.26500, c=14.13120, alpha=90.00, beta=90.00, gamma=120.00

[Go to setting standard (**a-b, a+2b, 2c** ; 7/3, 8/3, 0)]
[Go to an alternative setting]

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

Atomic positions, Wyckoff positions and Magnetic Moments

2	Ba2 Ba 0.00000 0.00000 0.00000	(1/3,0,0 | $-m_y,-2m_y,m_z$) (1/3,0,1/2 | $m_y,2m_y,-m_z$) (1/3,1/3,0 | $-m_y,m_y,m_z$) (1/3,1/3,1/2 | $m_y,-m_y,-m_z$) (1/3,2/3,0 | $2m_y,m_y,m_z$) (1/3,2/3,1/2 | $-2m_y,-m_y,-m_z$) (2/3,0,0 | $-m_y,m_y,m_z$) (2/3,0,1/2 | $m_y,-m_y,-m_z$) (2/3,1/3,0 | $2m_y,m_y,m_z$) (2/3,1/3,1/2 | $-2m_y,-m_y,-m_z$) (2/3,2/3,0 | $-m_y,-2m_y,m_z$) (2/3,2/3,1/2 | $m_y,2m_y,-m_z$)	18	-	-
3	Ni1 Ni 0.00000 0.00000 0.25000	(0,0,1/4 | $2m_y,m_y,m_z$) (0,0,3/4 | $-2m_y,-m_y,-m_z$) (0,1/3,1/4 | $-m_y,-2m_y,m_z$) (0,1/3,3/4 | $m_y,2m_y,-m_z$) (0,2/3,1/4 | $-m_y,m_y,m_z$) (0,2/3,3/4 | $m_y,-m_y,-m_z$) (1/3,0,1/4 | $-m_y,-2m_y,m_z$) (1/3,0,3/4 | $m_y,2m_y,-m_z$) (1/3,1/3,1/4 | $-m_y,m_y,m_z$) (1/3,1/3,3/4 | $m_y,-m_y,-m_z$) (1/3,2/3,1/4 | $2m_y,m_y,m_z$) (1/3,2/3,3/4 | $-2m_y,-m_y,-m_z$) (2/3,0,1/4 | $-m_y,m_y,m_z$) (2/3,0,3/4 | $m_y,-m_y,-m_z$) (2/3,1/3,1/4 | $2m_y,m_y,m_z$) (2/3,1/3,3/4 | $-2m_y,-m_y,-m_z$) (2/3,2/3,1/4 | $-m_y,-2m_y,m_z$) (2/3,2/3,3/4 | $m_y,2m_y,-m_z$)	18	**($2M_y,M_y,M_z$)**	M_y = 0.00000 M_z = 0.00000

Figure 11. Partial view of the output of MAGMODELIZE describing the magnetic structure under the subgroup of type P_c31c listed in Figure 10, as obtained when clicking in the column "Magnetic structure". The table indicates the positions and moments which correspond to all atoms that are symmetry related with the one listed as representative in the asymmetric unit (all described in the parent-like setting mentioned in the text). The number of symmetry related atoms within the used unit cell (multiplicity) is given in the fourth column. The fifth column indicates the symmetry restrictions on the value of the components of the magnetic moment for the representative magnetic atom listed in the second colum (if any), while the last column on the right allows to introduce specific values for the symmetry-free moment components.

The unit cell and origin used by default (what we call "parent-like" setting) is indicated at the heading of the list reproduced in Figure 11, giving its relation with respect to the parent unit cell. This setting (generally non-standard) keeps the origin and also the unit cell orientation of the parent/paramagnetic phase, but if necessary, multiplies the cell parameters to produce a supercell consistent with the periodicity kept by the propagation vector. At the heading of the list one can also find the transformation from the parent unit cell and origin to the standard setting of the MSG, and one can change the description to this setting, or to any consistent arbitrary basis chosen by the user. The output includes a list of the atoms of an asymmetric unit (second column), the corresponding orbit of symmetry related atoms within the defined unit cell (third column), the number of atoms of each orbit (fourth column), the symmetry constraints on the magnetic moments for the representative magnetic atoms in the asymmetric unit (fifth column), and a window to introduce a value to the free components of the magnetic moments (sixth column). One can see in this output, reproduced partially in Figure 11, that the Ni spins have only two free parameters, with the spin

direction on the xy plane of the independent Ni atom being symmetry dictated, and an additional free z component. Let us assume for the moment that the z spin component is zero, and write only a non-zero arbitrary value of 1 for the m_y component.

f) Click on "Export data to MCIF file/Visualize". A magCIF file of the model is then created, which is shown on a non-editable window. Save the magCIF file by clicking on the link "bcs_file.mcif". Inspect the text of the magCIF file and locate the place where the transformation to the standard setting from the one used in the file is indicated. Check that this transformation is:

(1/3**a**-1/3**b**, 1/3**a**+2/3**b**, **c**; 7/9, 8/9, 0)

Compare with the transformation to standard given in the output page obtained in step e) (see Figure 11). Why are they different?

g) Click on the button "submit to MVISUALIZE" to visualize the structure online with JSmol, using the MVISUALIZE tool. On the webpage that appears, use the button "toggle parent cell" to visualize simultaneously the parent unit cell, and the one that is being used in the description of the magCIF file. (Figure 12).

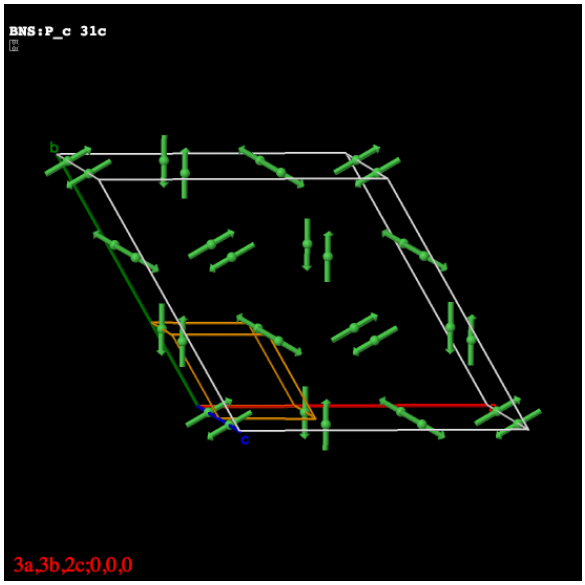


Figure 12. Representation of the magnetic structure with symmetry P_c31c as obtained with MVISUALIZE, and showing both the parent unit cell and the one of the parent-like setting used.

Use the button "toggle standard" to visualize the standard unit cell proposed by the transformation indicated in the magCIF file. (Figure 13).

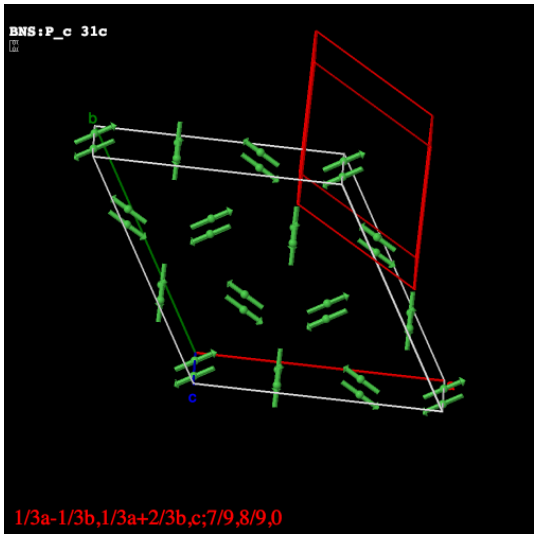


Figure 13. Representation of the magnetic structure with symmetry P_c31c as obtained with MVISUALIZE, and showing both the standard unit cell indicated in the magCIF file and the one of the parent-like setting used.

In the button-menu entitled "select cell", select "standard cell" to visualize the structure using the standard unit cell proposed in the magCIF file (Figure 14). Explore the explicit control, editing, and export buttons that the page offers. An addition window to introduce any Jmol command is also available. In addition, by right-clicking on the symbol JSmol of the graphic window, a menu is open, and in particular a Jmol console can be opened to control the graphic window.

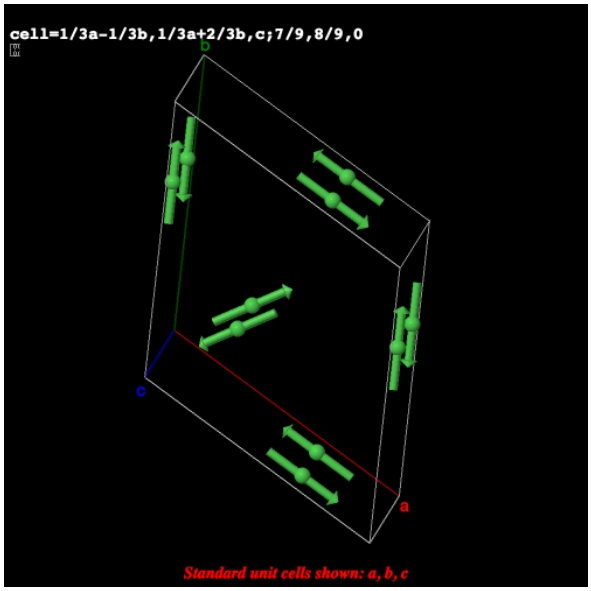


Figure 14. Representation of the magnetic structure with symmetry P_c31c as obtained with MVISUALIZE, using the standard unit cell indicated in the magCIF file.

h) Do analogous steps to e), f) and g) for the other three subgroups in the list of Figure 9 to obtain magCIF files of the corresponding magnetic structures and visualize them either with Jmol or with VESTA. (Figure 15)

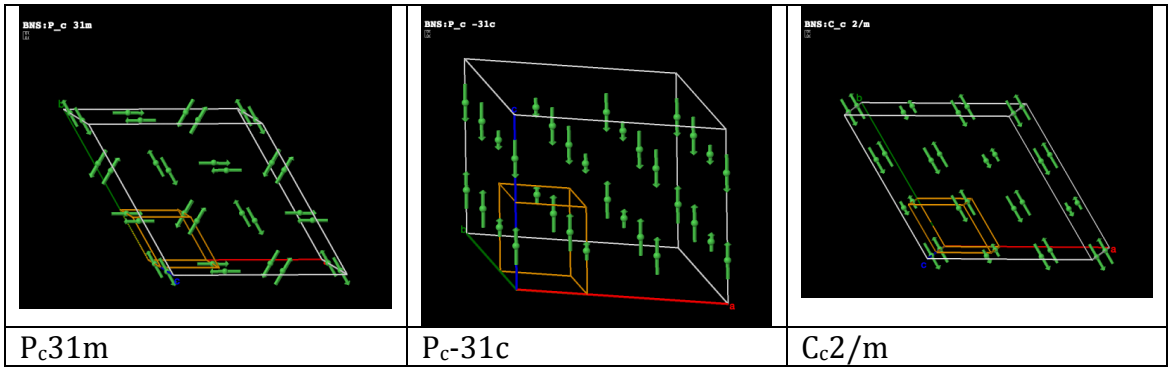


Figure 15. Scheme of the magnetic structures with the indicated maximal symmetries listed in Figure 9, as obtained with MVISUALIZE using the corresponding magCIF files created with MAGMODELIZE. For the case of P_c-*31c* and C_c*2/m*, the Ni site splits into two symmetry independent sites, each with a single free parameter, and they have been given arbitrary different values to distinguish the two sites. In the case of P_c*31m*, the single Ni site has only one free parameter, with no z spin component allowed.

Up to now we have only made use of the condition that the MSG describing the symmetry of the magnetic structure should be a subgroup of the gray group *P-3m11'*, and be consistent with the observation of (1/3,1/3,1/2) as single propagation vector. But k-SUBGROUPSMAG can also introduce the additional filter that the symmetry break should be the result of a spin arrangement according to one (or more) specific irrep(s).

i) Go back to the main input page of k-SUBGROUPSMAG and in the option "choose irreps" click on "representations". The program provides then an output page with the irrep decomposition of the magnetic representation for the Wyckoff site *1b* (Figure 16).

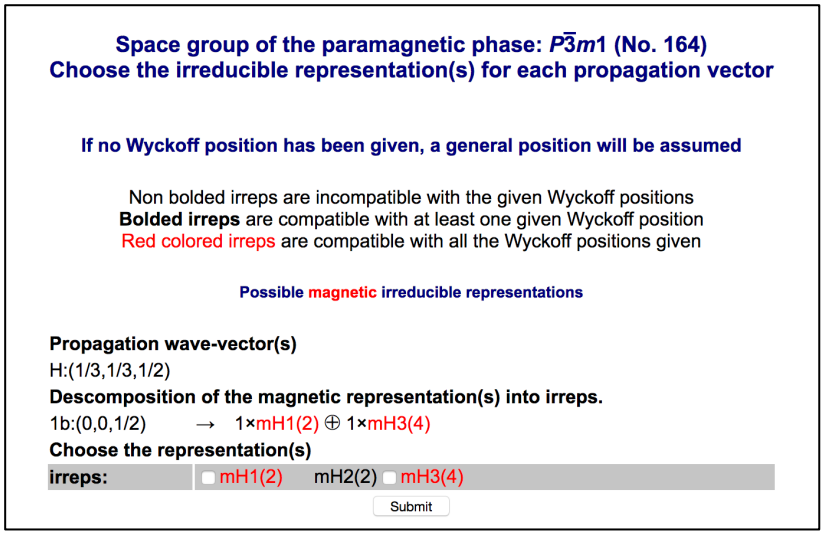


Figure 16. Irrep decomposition of the magnetic representation for the propagation vector (1/3,1/3,1/2) and the site *1b*, as given by k-SUBGROUPSMAG. The number in parenthesis after each irrep indicates the dimension of the full irrep, which in this case is twice the dimension of the small irrep (the star of **k** includes ***k*** and –***k***).

The irrep labels in the output are those also used in the ISOTROPY[3] webpage, and one can always inspect the actual irreps by going to the programs in the section "Representations and Applications" of the Bilbao Crystallographic Server, taking into account that the symbol *m* in the irrep label only indicates that the irrep is odd for time reversal. One can see from Figure 16 that there are two possible irreps for the magnetic ordering.

j) Check irrep mH1 and submit to include this condition in the input. Submit the new input page. The list and graph of possible MSGs for this irrep can then be obtained (Figures 17).

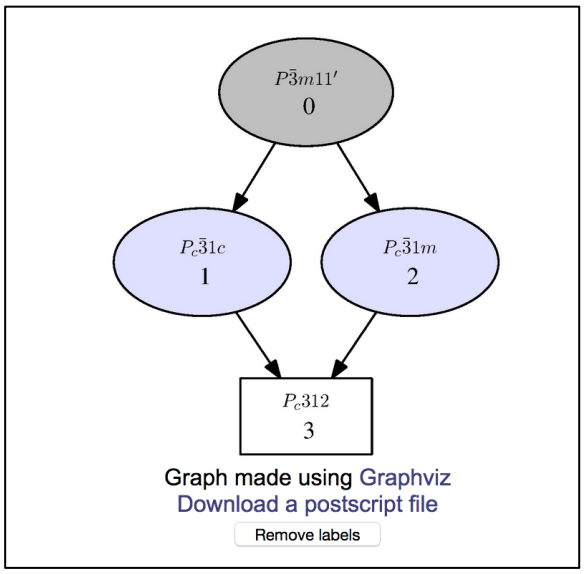


Figure 17. Graph of the possible MSGs that can be realized by a magnetic ordering according to the 2-dim irrep mH1.

The two epikernels of mH1, of type P_c*-31c* and P_c*-31m*, shown in Figure 17 are two of the six k-maximal subgroups that were already obtained above in step b) and shown in Figure 8. The second one, P_c*-31m*, forces a cero magnetic moment at some of the Ni sites, as can be checked using the button "more options" in the page showing the graph or the list. This is the reason why this subgroup disappeared in step c) and is not present in Figure 9.

A word of caution is obliged here: magnetic structures with some fraction of the magnetic sites having zero average magnetic moments are not very common, and therefore one may consider them less probable to be realized, but there is no reason to discard them completely, and magnetic structures of this type are also reported (see for instance the structure of $Gd_2Ti_2O_7$ (magndata #1.56)).

k) Come back to the output page with the irrep decomposition and check irrep mH3, instead of mH1, and submit to include this condition in the input. Submit the new input page. The list and graph of possible MSGs that can be realized by a magnetic ordering according to this irrep can then be obtained (Figures 18).

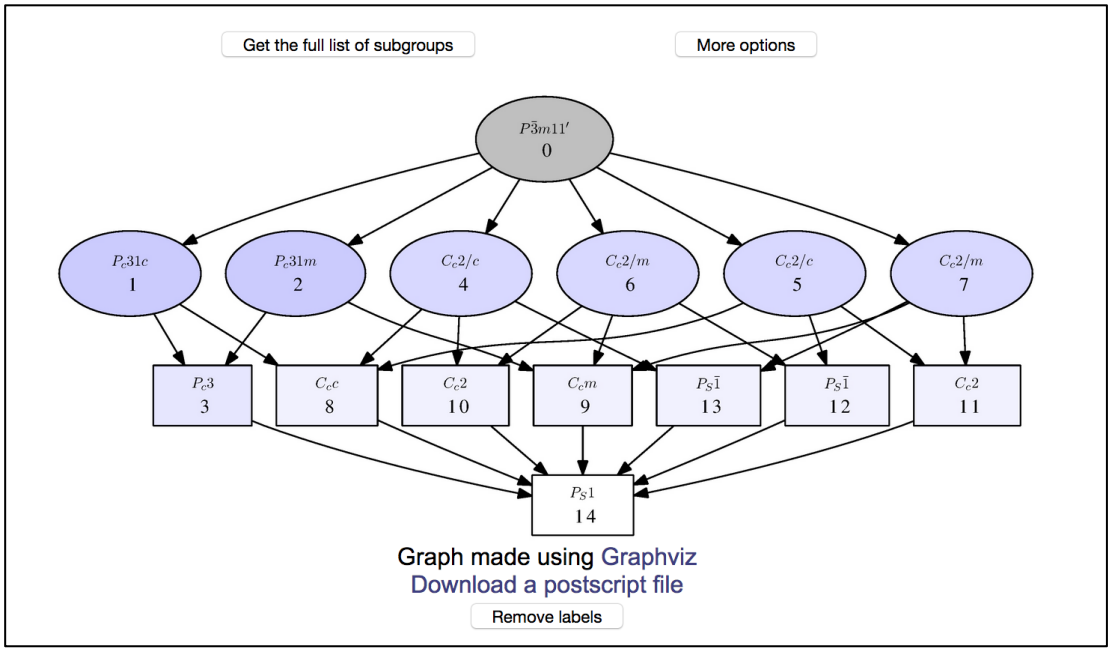


Figure 18. Graph of the possible MSGs that can be realized by a magnetic ordering according to the 4-dim irrep mH3.

The large dimension of this irrep makes the number of possible distinct magnetic symmetries also quite large, namely fourteen, with 13 distinct irrep epikernels, from which six are maximal. Some of these maximal subgroups split the *1b* site, with some of the resulting split sites being symmetry forced to have zero spin. These groups can be filtered and droped out using the first option that appears clicking the "more options" button. (Figure 19) The number of possible MSGs reduces then to 11, and the number of maximal epikernels to 4. Three of these maximal epikernels can be identified with the remaining three k-maximal MSGs obtained in step c) and Figure 9. The fourth maximal epikernel, of type *C_c2/c*, is not k-maximal. This means that there is a MSG consistent with the propagation vector, allowing magnetic order at all Ni sites, which is a supergroup of this group of type C_c2/c. This supergroup can be easily seen on Figure 8: it is the subgroup *P_c-31c*, which has been discussed in step j).

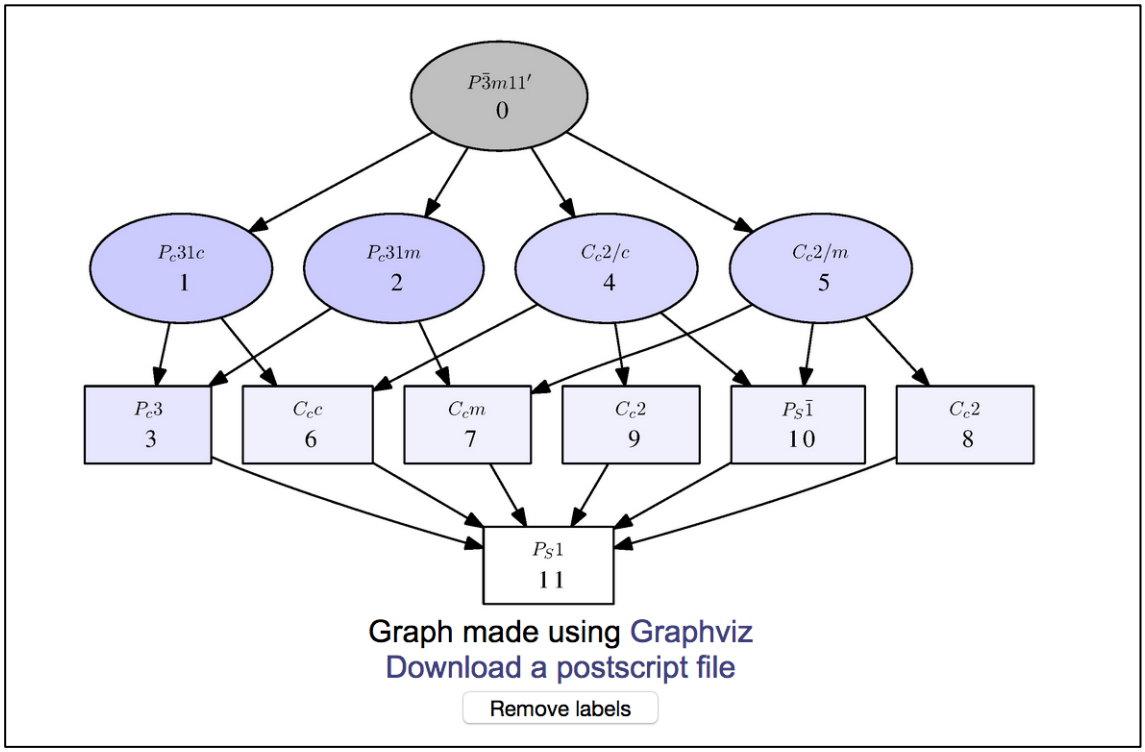


Figure 19. Graph of the possible MSGs that can be realized by a magnetic ordering according to the 4-dim irrep mH3, with the additional restriction that the MSG should allow non-zero magnetic moments at all sites derived from the Wyckoff positions *1b* of the parent space group P-3m1.

l) Check the link "Get_irreps" for subgroup of type C_c2/c in the listing of subgroups corresponding to Figure 18. The resulting output (Figure 20) shows that not only irrep mH3, but also the irrep mH1 is also compatible with this symmetry.

List of physically irreducible representations and order parameters between a parent group and a given subgroup.

Input data

Group→subgroup	Transformation matrix
$P\bar{3}m11'$ (N. 164.86)→C_c2/c (N. 15.90)	$\begin{pmatrix} 2 & 0 & 0 & 0 \\ 1 & 3 & 0 & -1/2 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$

Representations and order parameters

k-vectors	irreps and order parameters	link to the irreps
GM: **(0,0,0)**	GM_1^+: (a) GM_3^+: (a,-($\sqrt{3}$ a))	matrices of the irreps
K: **(1/3,1/3,0)**	K_1: (a,$\sqrt{3}$ a) K_3: (a,0,$\sqrt{3}$ a,0)	matrices of the irreps
A: **(0,0,1/2)**	mA_1^-: (a) mA_3^-: (a,$\sqrt{3}$ a)	matrices of the irreps
H: **(1/3,1/3,1/2)**	mH_1: (a,-(a/$\sqrt{3}$)) mH_3: (a,0,-(a/$\sqrt{3}$),0)	matrices of the irreps

Figure 20. Output of the link "Get irreps" for the epikernel of mH3 of type C_c2/c.

As the magnetic representation of site *1b* decomposes in the form (Figure 16):

1 mH1 + 1 mH3

and the output reproduced in Figure 19 indicates a fixed direction within both irrep spaces, a spin arrangement complying with the subgroup C_c2/c, will have a single degree of freedom corresponding to each irrep. Figure 20 shows however that irreps for the wave vector A: (0,0,1/2), are also allowed. This wave vector is in fact associated to a third harmonic of the primary spin wave with propagation vector (1/3,1/3,1/2). These secondary irreps with label A can be the symmetry of additional degrees of freedom of the C_c2/c structure.

One can use the representations input option of k-SUBGROUPSMAG to derive the irrep decomposition of the magnetic representation for any wave vector. In this way, one can obtain that the decomposition for the wave vector A (0,0,1/2) is: 1 mA1- + 1 mA3-. Taking into account the output reproduced in Figure 20, this means that a structure according to the subgroup C_c2/c will have 4 free parameters, and these four degrees of freedom can be decomposed on 4 basis functions, one for each of the magnetic irreps listed in Figure 20. The primary spin basis function will correspond to the primary irrep mH3, but a refinement under this symmetry can explore the presence of the other three secondary magnetic degrees of freedom. The decomposition of the four degrees of freedom in terms of four spin basis functions, adapted to the four irreps can be done using ISODISTORT. This is not provided by k-SUBGROUPSMAG, which through MAGMODELIZE, only provides the magnetic structure model under this MSG with the four free parameters as spin components of the symmetry independent sites.

m) Submit to MAGMODELIZE the subgroup C_c2/c in the listing of subgroups reproduced in Figure 18, using the option at the bottom of the listing, and introducing when required the parent structure of $Ba_3Nb_2NiO_9$. One can see the four free parameters for the spins, as components of two split Ni sites (Figure 21). This is an example of the need of including both MSG and irreps constraints if one wants to refine the structure in a controlled way: if only the traditional method is employed and the refinement is restricted to the mH3 irrep, one will have four free parameters, and the symmetry of the spin arrangement to be refined is reduced to the minimal symmetry allowed by the irrep, i.e. the irrep kernel P_s1 (see Figure 19), while if the structure is refined under only the constraints of MSG C_c2/c, then again we have four free parameters to refine, but a set of arbitrary values of them combines in an uncontrolled way spin modes corresponding to the irreps mH3, mH1, mA1- and mA3-. If one wants to refine the structure under the condition that its symmetry is C_c2/c and in addition the magnetic ordering is restricted to the irrep mH3, and therefore with a single parameter to refine, then one needs to add to the symmetry constraints coming from the MSG the additional restrictions of the irrep mH3.

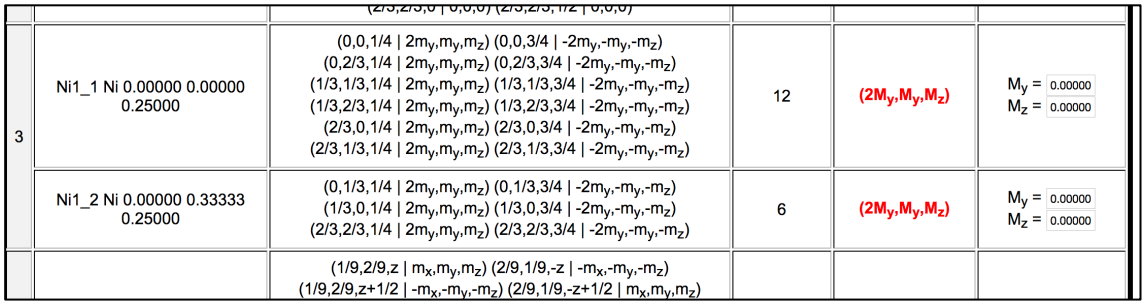
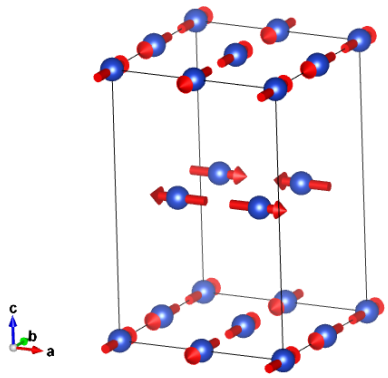


Figure 21. Partial view of the output of MAGMODELIZE for the epikernel of mH3 of type C_c2/c, as obtained when clicking in the column "Magnetic structure". One can see that the Ni atoms split into two independent sites and four free parameters exist. An arbitrary set of values for the four symmetry independent moment components implies however an uncontrolled combination of spin modes corresponding to four different irreps (see text).

Example 3: A multi-k structure. Nd_2CuO_4 (magndata #2.6)
[Skanthakumar, S. et al., *PHYSICAL REVIEW B* (1993) **47** 6173 - 6176]
(file: Nd_2CuO_4_parent.cif)



2**k**-magnetic structure of Nd_2CuO_4 (only Cu atoms), according to (Skanthakumar, S. et al., *PHYSICAL REVIEW B* (1993) 47, 6173 - 6176), with MSG P_C4_2/nnm (1/2**a**+1/2**b**, -1/2**a**+1/2**b**,**c**;0,0,0) (magndata #2.6).

The paramagnetic structure of $Ba_3Nb_2NiO_9$ can be summarized as (icsd 202885, Gopalakrishnan et al., Mat. Res. Bull. 24, 321-330 (1989)):

Space group: I4/mmm (N. 139)

Lattice parameters: 3.9385, 3.9385, 12.1465 90 90 90

Asymmetric unit:

Cu1 - 0.00000 0.00000 0.00000
Nd1 - 0.00000 0.00000 0.35150
O1 - 0.00000 0.50000 0.00000
O2 - 0.00000 0.50000 0.25000

This structure is reported to have a multi-k magnetic phase with two propagation vectors which are symmetry related by the parent symmetry:
k1= (1/2,1/2,0)
k2= (-1/2,1/2,0)

k-SUBGROUPSMAG combined with MAGMODELIZE can be used to explore and enumerate all possible multi-k magnetic structures for a set of observed propagation vectors. We will apply it here to this case.

a) Introduce in the input page of k-SUBGROUPSMAG the parent space group, the two wave vectors (click on the option "more wave vectors needed"), the Wyckoff position (2a) of the Cu atom, and submit. A list and graph of 18 possible MSGs are provided by the program, six of them maximal. (Figure 21)

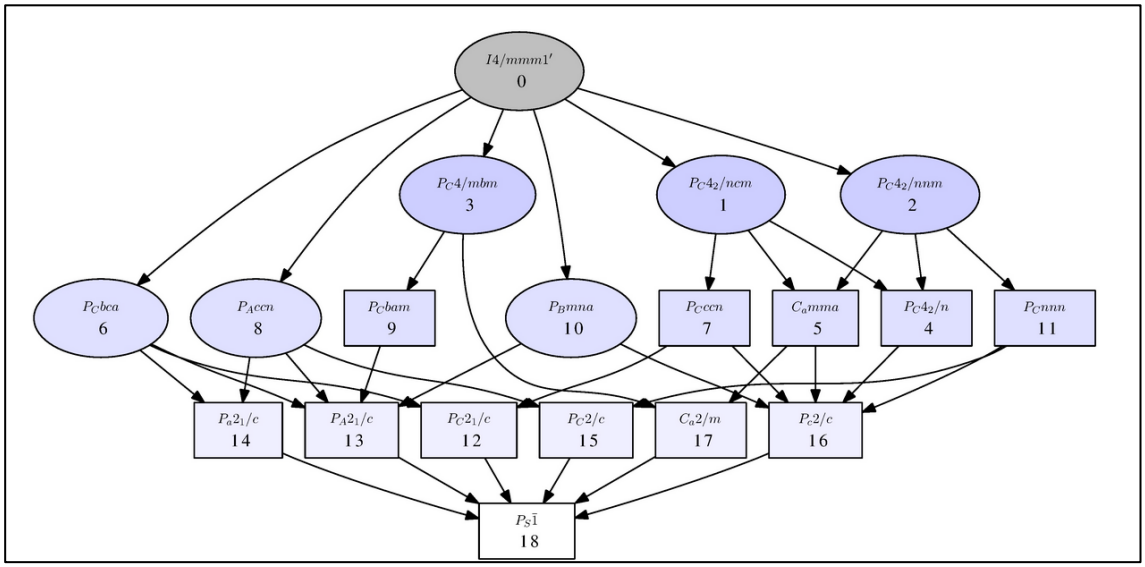


Figure 22. Possible MSGs that can be realized in a structure with parent space group *I4/mmm*, by a 2k magnetic ordering with propagation vectors (1/2,1/2,0) and (-1/2,1/2,0), and with the magnetic atom at the site 2a (0,0,0).

The transformation (**P**,**p**) listed for each subgroup, where **P** is a 3x3 matrix and **p** = (p_1, p_2, p_3) a column vector, indicates in each case a choice of unit cell and origin, for which the subgroup adquires the standard setting of the corresponding magnetic space group (MSG) given by the MSG label, i.e. the symmetry operations of the subgroup would take when described using this unit cell and origin, the form used for this MSG in the listings taken as standard. The transformation (**P**,**p**) is defined with respect to the unit cell ($\mathbf{a}_p$,$\mathbf{b}_p$,$\mathbf{c}_p$) and origin $\mathbf{O}_p$ of the parent space group, in the following form:

$$(\mathbf{a}^s,\mathbf{b}^s,\mathbf{c}^s)= (\mathbf{a}_p,\mathbf{b}_p,\mathbf{c}_p).\mathbf{P} \quad , \quad \mathbf{O}^s = \mathbf{O}_p + p_1\,\mathbf{a}_p + p_2\,\mathbf{b}_p + p_3\,\mathbf{c}_p$$

where ($\mathbf{a}^s$,$\mathbf{b}^s$,$\mathbf{c}^s$) and $\mathbf{O}^s$ are the unit cell vectors and origin of a standard setting of the MSG.

b) Go back to the input page and do the irrep decomposition for the site 2a.

Space group of the paramagnetic phase: *I4/mmm* (No. 139)
Choose the irreducible representation(s) for each propagation vector

If no Wyckoff position has been given, a general position will be assumed

Non bolded irreps are incompatible with the given Wyckoff positions
Bolded irreps are compatible with at least one given Wyckoff position
Red colored irreps are compatible with all the Wyckoff positions given

Possible magnetic irreducible representations

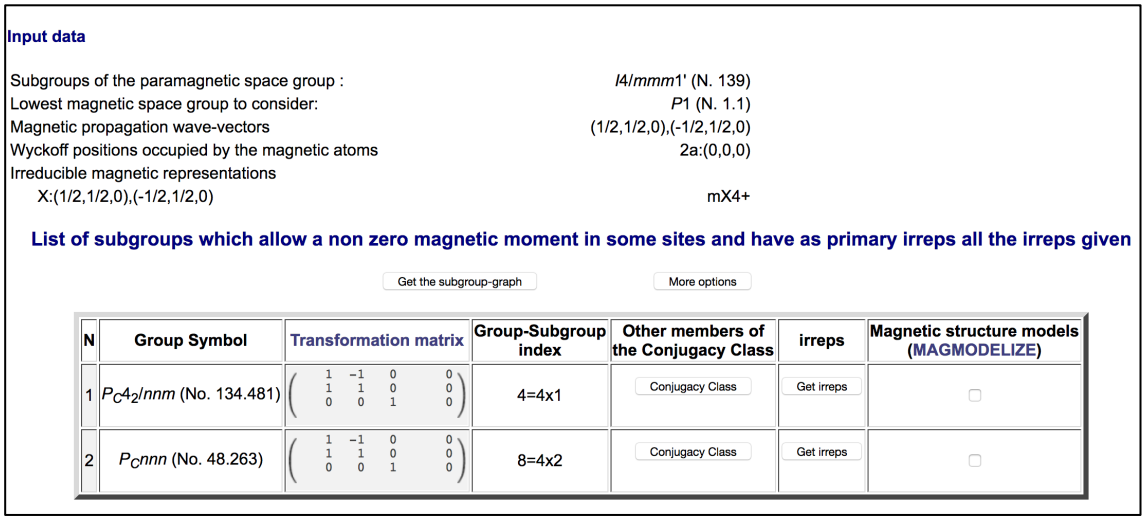
Propagation wave-vector(s)
X:(1/2,1/2,0),(-1/2,1/2,0)
Descomposition of the magnetic representation(s) into irreps.
2a:(0,0,0) → 1×mX2+(2) ⊕ 1×mX3+(2) ⊕ 1×mX4+(2)
Choose the representation(s)

irreps:	mX1+(2)	mX2+(2)	mX3+(2)	mX4+(2)	mX1-(2)	mX2-(2)	mX3-(2)	mX4-(2)
		☐	☐	☑				

Submit

Figure 23. Irrep decomposition of the magnetic representation for the site 2a for the wave vectors (1/2,1/2,0) and (-1/2,1/2,0). The parenthesis behind each irrep label indicates the dimension of the full irrep (the small irrep is 1-dim in all cases).

c) Choose the irrep mX4+ and submit. The program yields two possible MSGs (Figure 24) that are group-subgroup related, as can be seen by looking at the graph option.



Input data

Subgroups of the paramagnetic space group :	*I*4/*mmm*1' (N. 139)
Lowest magnetic space group to consider:	*P*1 (N. 1.1)
Magnetic propagation wave-vectors	(1/2,1/2,0),(-1/2,1/2,0)
Wyckoff positions occupied by the magnetic atoms	2a:(0,0,0)
Irreducible magnetic representations	
X:(1/2,1/2,0),(-1/2,1/2,0)	mX4+

List of subgroups which allow a non zero magnetic moment in some sites and have as primary irreps all the irreps given

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_C4_2/nnm (No. 134.481)	$\begin{pmatrix} 1 & -1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	4=4x1	Conjugacy Class	Get irreps	☐
2	P_Cnnn (No. 48.263)	$\begin{pmatrix} 1 & -1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	8=4x2	Conjugacy Class	Get irreps	☐

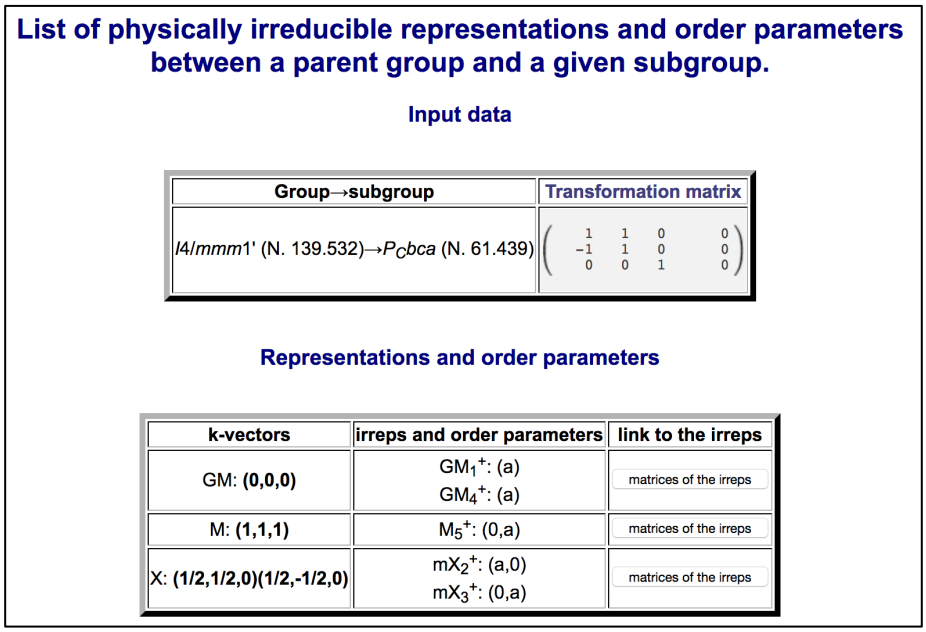
Figure 24. Possible MSGs for 2k-magnetic structures with the the indicated wave vectors, and with the magnetic ordering according to the irrep mX4+ of the parent space group *I4/mmm*.

d) Click on "Get irreps" for the two subgroups. The resulting output shows that while in the higher subgroup the direction within mX4+ is (a,-a), meaning that the two spin waves with different propagation vectors combine with equal amplitudes, in the lower group, the two spin waves have different amplitudes, with the irrep direction being represented by (a,b). The possible MSGs resulting from the presence of only one of the two spin waves, that is the directions (a,0) or (0,a), are not in the list; these are single k magnetic structures, and the program only lists the symmetries which correspond to spin arrangements where the two propagation vectors are involved, as requested in the input.

e) Come back to step c) and do a similar process for irreps mX3+ and mX2-. The program provides again a tetragonal MSG as maximal symmetry for each irrep. The three tetragonal MSGs, one per irrep, obtained in these steps, are the same as those obtained as k-maximal in a single go in a). But what type of spin arrangement corresponds to the other three maximal MSGs of orthorhombic symmetry that were obtained in step a)? This can be seen in the next steps.

f) Go back to the list of subgroups obtained in step a) and click on "Get irreps" for any of the three k-maximal orthorhombic MSGs. One can see (Figure 25) that these MSGs result from the superpositions of two spin waves with the two desired propagation vectors, but the spin wave for each propagation vector is associated with a different irrep. This type of orderings are in principle possible, but one can assume they are much less probable than the three orderings of

maximal symmetry which correspond to each of the three possible irreps, as single active irrep.



List of physically irreducible representations and order parameters between a parent group and a given subgroup.

Input data

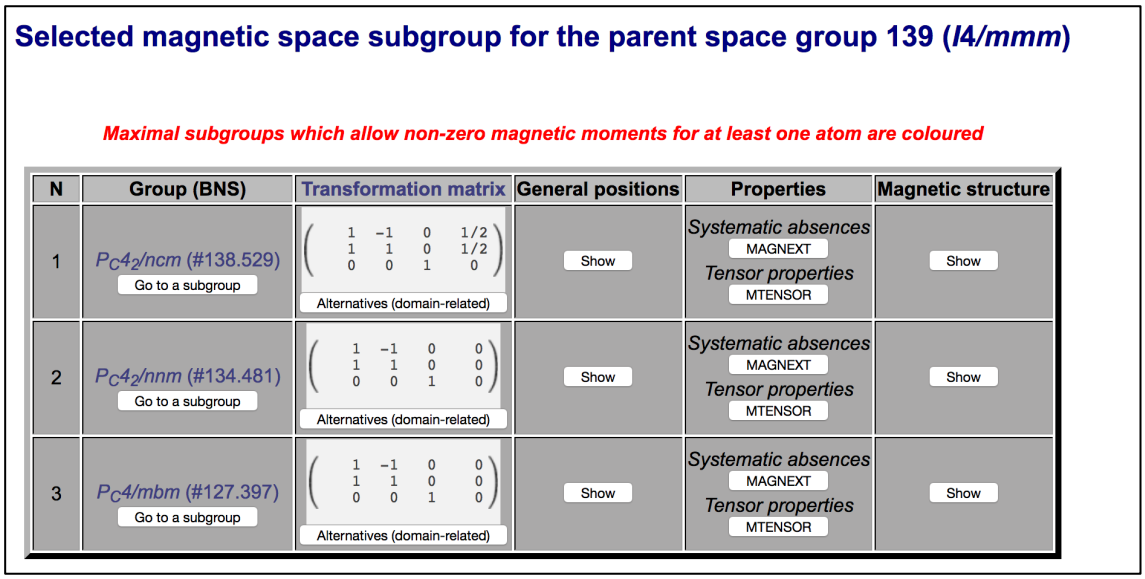
Group→subgroup	Transformation matrix
*I*4/*mmm*1' (N. 139.532)→$P_C bca$ (N. 61.439)	$\begin{pmatrix} 1 & 1 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$

Representations and order parameters

k-vectors	irreps and order parameters	link to the irreps
GM: **(0,0,0)**	GM_1^+: (a) GM_4^+: (a)	matrices of the irreps
M: **(1,1,1)**	M_5^+: (0,a)	matrices of the irreps
X: **(1/2,1/2,0)(1/2,-1/2,0)**	mX_2^+: (a,0) mX_3^+: (0,a)	matrices of the irreps

Figure 25. Irreps and OP directions compatible with the indicated subgroup of I4/mmm1', as obtained with "Get irreps" in the subgroup list.

g) Go back to the list of subgroups obtained in step a) and check in the last column the three tetragonal MSGs at the head of the list, check also "include structure data of the parent phase" at the bottom of the list and submit to MAGMODELIZE to construct the structure models consistent with these three symmetries. In the next page upload the cif file of the parent phase of Nd_2CuO_4 (Nd2CuO4_parent.cif). Choose Cu as magnetic and submit.



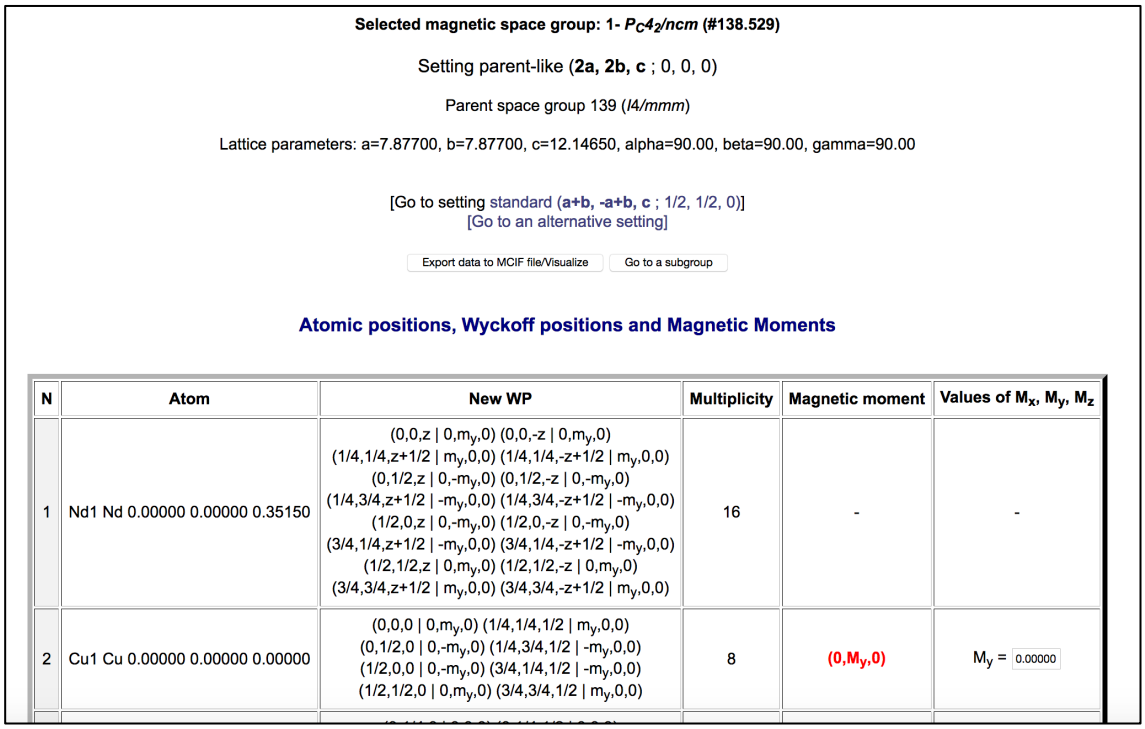
Selected magnetic space subgroup for the parent space group 139 (*I*4/*mmm*)

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_C4_2/ncm (#138.529) Go to a subgroup	$\begin{pmatrix} 1 & -1 & 0 & 1/2 \\ 1 & 1 & 0 & 1/2 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	*Systematic absences* MAGNEXT *Tensor properties* MTENSOR	Show
2	P_C4_2/nnm (#134.481) Go to a subgroup	$\begin{pmatrix} 1 & -1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	*Systematic absences* MAGNEXT *Tensor properties* MTENSOR	Show
3	P_C4/mbm (#127.397) Go to a subgroup	$\begin{pmatrix} 1 & -1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	*Systematic absences* MAGNEXT *Tensor properties* MTENSOR	Show

Figure 26. Output of MAGMODELIZE for the three chosen subgroups, with the different output options.

h) Click on the last column for the first MSG.



Selected magnetic space group: 1- P_C4_2/ncm (#138.529)

Setting parent-like (**2a, 2b, c** ; 0, 0, 0)

Parent space group 139 (*I4/mmm*)

Lattice parameters: a=7.87700, b=7.87700, c=12.14650, alpha=90.00, beta=90.00, gamma=90.00

[Go to setting standard (**a+b, -a+b, c** ; 1/2, 1/2, 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	Nd1 Nd 0.00000 0.00000 0.35150	(0,0,z | 0,m_y,0) (0,0,-z | 0,m_y,0) (1/4,1/4,z+1/2 | m_y,0,0) (1/4,1/4,-z+1/2 | m_y,0,0) (0,1/2,z | 0,-m_y,0) (0,1/2,-z | 0,-m_y,0) (1/4,3/4,z+1/2 | -m_y,0,0) (1/4,3/4,-z+1/2 | -m_y,0,0) (1/2,0,z | 0,-m_y,0) (1/2,0,-z | 0,-m_y,0) (3/4,1/4,z+1/2 | -m_y,0,0) (3/4,1/4,-z+1/2 | -m_y,0,0) (1/2,1/2,z | 0,m_y,0) (1/2,1/2,-z | 0,m_y,0) (3/4,3/4,z+1/2 | m_y,0,0) (3/4,3/4,-z+1/2 | m_y,0,0)	16	-	-
2	Cu1 Cu 0.00000 0.00000 0.00000	(0,0,0 | 0,m_y,0) (1/4,1/4,1/2 | m_y,0,0) (0,1/2,0 | 0,-m_y,0) (1/4,3/4,1/2 | -m_y,0,0) (1/2,0,0 | 0,-m_y,0) (3/4,1/4,1/2 | -m_y,0,0) (1/2,1/2,0 | 0,m_y,0) (3/4,3/4,1/2 | m_y,0,0)	8	(0,M_y,0)	M_y = 0.00000

Figure 27. Magnetic structure (partial view) under the constraints of the subgroup P_C4_2/ncm (a+b,-a+b,c; ½, ½, 0), as obtained when clicking in the column "Magnetic structure". The table indicates the positions and moments which correspond to all atoms that are symmetry related to the one listed as representative in the asymmetric unit, all described in the parent-like setting (see text). The number of symmetry related atoms within the used unit cell (multiplicity) is given in the fourth column. The fifth column indicates the symmetry restrictions on the value of the components of the magnetic moment for the representative magnetic atom listed in the second colum (if any), while the last column on the right allows to introduce specific values for the symmetry-free moment components.

The unit cell and origin used by default (what we call "parent-like" setting) is indicated at the heading of the list reproduced in Figure 27, giving its relation with respect to the parent unit cell. This setting (generally non-standard) keeps the origin and also the unit cell orientation of the parent/paramagnetic phase, but if necessary, multiplies the cell parameters to produce a supercell consistent with the periodicity kept by the propagation vector. At the heading of the list one can also find the transformation from the parent unit cell and origin to the standard setting of the MSG, and one can change the description to this setting, or to any consistent arbitrary basis chosen by the user. The output, which is partially reproduced in Figure 27, includes a list of the atoms of an asymmetric unit (second column), the corresponding orbit of symmetry related atoms within the defined unit cell (third column), the number of atoms of each orbit (fourth column), the symmetry constraints of the magnetic moments for the representative magnetic atoms in the asymmetric unit (fifth column), and a window to introduce a value to the free components of the magnetic moments (sixth column).

i) Introduce an arbitrary value, say 1, for the component m_y of Cu1 and click on "Export to MCIF file/Visualize" . A magCIF file of the model is then created, which is shown on a non-editable window. Save the magCIF file by clicking on the link "bcs_file.mcif". This magCIF file can then be visualized in a stand-alone version of VESTA or Jmol, or introduced for refinement in JANA2006 or FullProf.

j) Click on the button "submit to MVISUALIZE" to visualize the structure online with JSmol, using the MVISUALIZE tool.

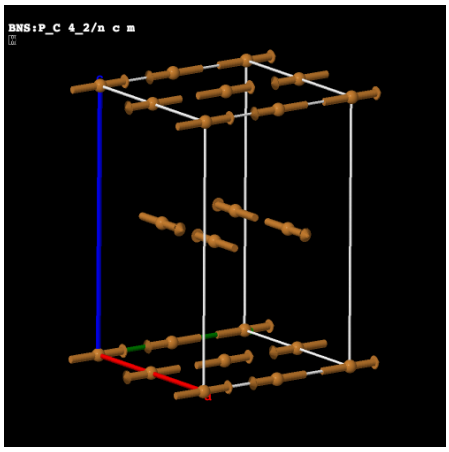


Figure 28. Scheme of the 2k magnetic structure of Nd_2CuO_4 (only Cu atoms), if the MSG were P_C4_2/ncm (a+b,-a+b,c; ½, ½, 0), as given by the visualization tool of MAGMODELIZE.

k) Come back to the list of 18 subgroups obtained in step a) and click on the conjugacy class button of the subgroup $P4_2/ncm$ (a+b,-a+b,c; ½, ½, 0) to see the set of subgroups within the conjugacy class.

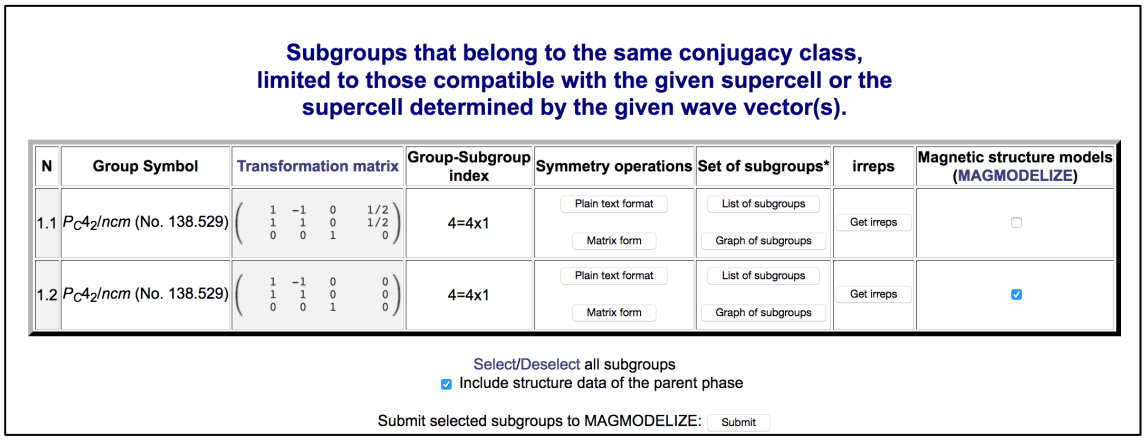


Figure 29. List of subgroups within the chosen conjugacy class

There are two different MSGs in the conjugacy class. They correspond to two domain-related equivalent spin arrangements.

l) Submit to MAGMODELIZE the second subgroup of the conjugacy class, and following the same steps as above, obtain the corresponding magnetic structure model. This spin arrangement is physically equivalent to the one obtained previously.

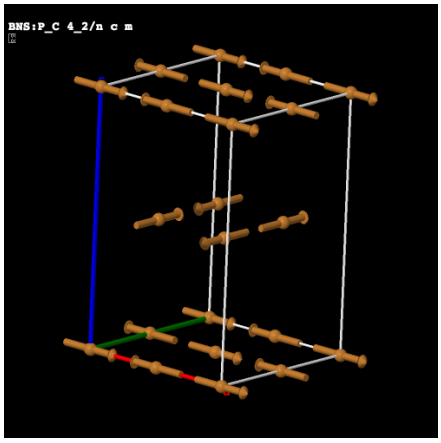
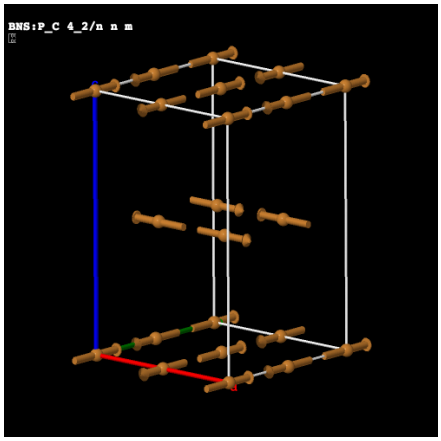


Figure 30. Scheme of the 2k magnetic structure (only Cu atoms) of Nd_2CuO_4 if the MSG were P_C4_2/ncm (a+b,-a+b,c; 0, 0, 0) (the second subgroup in the conjugacy class listed in Figure 29). This is physically equivalent to the one of Figure 28, and corresponds to a domain related configuration.

m) Go back to the list reproduced in Figure 26, and do similar steps for the two other MSGs in the list to obtain the corresponding magnetic structure models. (If a long time has passed since the creation of this list with MAGMODELIZE, you may have to repeat the process of creating this list, to avoid errors). Obtain magCIF files for each model and Figures similar to those shown below either with Jmol/MVISUALIZE or with VESTA.



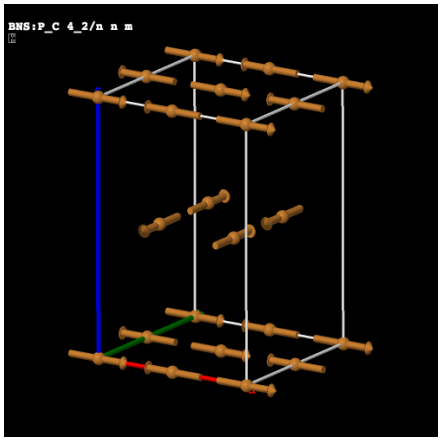


Figure 31. Scheme of the 2k magnetic structure (only Cu atoms) of Nd_2CuO_4 if its MSG were P_C4_2/nnm in its two equivalent domain-related configurations.

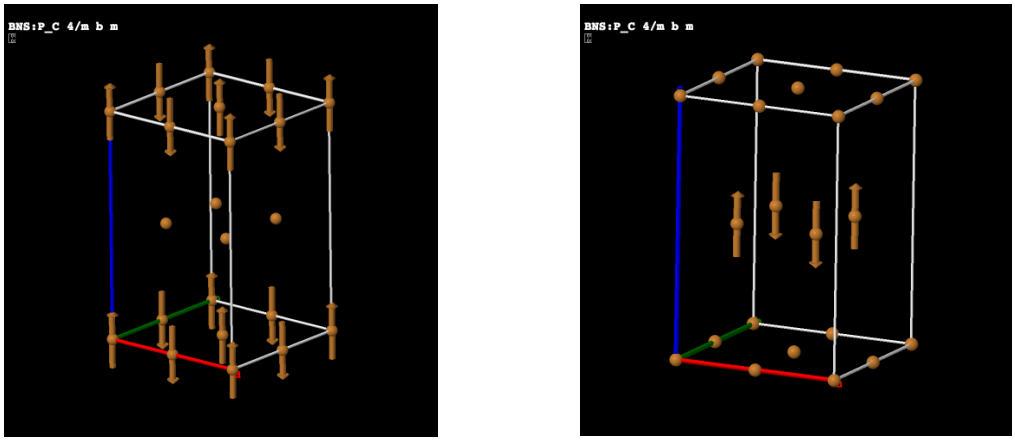


Figure 32. Scheme of the 2k magnetic structure (only Cu atoms) of Nd_2CuO_4 if its MSG were P_C4_2/mbm in its two equivalent domain-related configurations

REFERENCES

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