Instructions for the preparation of a magCIF file of a (published) commensurate magnetic structure, for uploading in the database MAGNDATA at the Bilbao Crystallographic Server.

In order to upload a commensurate magnetic structure in MAGNDATA only two files are required . One is a pdf file of the published article where this magnetic structure was reported, and the other one must be a magCIF file with the necessary information on the magnetic structure.

We call a magCIF file a CIF file, which uses the so-called magCIF extension for the description magnetic structures. In the Bilbao crystallographic server such type of files are given the extension ".mcif ", to be distinguished from CIF files of ordinary non-magnetic structures with the extension ".cif".

The magCIF file to be introduced in MAGNDATA must fulfill some specific requirements and these instructions explain in detail how to prepare it to be fully adapted for MAGNDATA.

We distinguish three cases for the starting situation:

Case 1: *You already have an initial magCIF file of the magnetic structure with its magnetic space group (MSG) identified.*

Case 2: *You have a magCIF file of the magnetic structure, but with no symmetry and listing ALL atomic positions and magnetic moments within the unit cell.*

Case 3: *You do NOT have yet a magCIF file of any kind but you have a model of the magnetic structure using some specific parameterization.*

Case 1. You already have an initial magCIF file of the magnetic structure with its magnetic space group identified.

*You are supposed to have already a magCIF file of the magnetic structure provided by the refinement program used or produced by any other means (see cases 2 and 3), where the magnetic space group of the structure is defined and it is used for the description. If you do not have such starting magCIF file, please go to **Case 2 or Case 3** below.*

Some of the most popular refinement programs, like FullProf, Jana2016/Jana2020 or GSAS-II, can produce a magCIF file of the magnetic structure being refined with a consistent use of its magnetic space group (MSG). We will consider that either one of these programs has been used, or that by any other means (see Cases 2 and 3 below) you have prepared such type of file.

Please note that depending on the procedure followed in the refinement, the magCIF file provided by the refinement program may only include the magnetic atoms. However, the knowledge of a magnetic structure is incomplete if it does not include the positions, at least approximate, of the NON-MAGNETIC atoms (i.e. the corresponding set of non-equivalent sites under the given MSG). Therefore

MAGNDATA only accepts files with ALL atoms. This means that the magCIF file must also include the non magnetic ones. In the case that your original magCIF only includes the magnetic atoms, the positions of the non-magnetic atoms will have to be added in the file either manually or by any other means. If the refinement was done in such a way that the positions of the non-magnetic atoms were not needed, probably the simplest way to obtain a magCIF file with all atoms is to repeat the refinement, but this time including in the starting model the non-magnetic atoms with all their positional parameters fixed according to some model coming from the knowledge of the non-magnetic structure, and then proceed with the refinement program in the same form as was done originally. Although the positions of the non-magnetic atoms will be irrelevant in the refinement, the program will then keep track of them and in principle they will be present in the final magCIF file provided by the program. Alternatively, if the nuclear structure was refined separately under a space group symmetry (usually the space group of the paramagnetic phase) in a "two phase" refinement process, a possible way to obtain a single magCIF file with all atoms included is to repeat the refinement as a single phase with all atoms, but adding manually the constraints (additional to those resulting from the MSG) that the assumed space group may imply for the atomic positions. The derivation and manual addition of these additional constraints may be avoided, if the starting atomic positions come from the final result of the "two phase" refinement and are maintained fixed in the single phase refinement.

Even if the non-magnetic atoms were not needed in the refinement, in practically all cases their positions are known, at least approximately, taken if necessary from the structure in the paramagnetic phase. In many cases this knowledge may come from a source different than the publication reporting the magnetic structure, and this is the reason why as you will see below, the magCIF file adapted for MAGNDATA includes some local tags (not present in the official magCIF dictionary) to indicate the source, temperature, etc, corresponding to this additional information about the non-magnetic atoms, which is not from the publication reporting the magnetic structure.

The steps to transform your magCIF file into one fully adapted for uploading in MAGNDATA are the following:

1) Upload your starting magCIF file in the program MVISUALIZE of the Bilbao crystallographic server. The program will then produce using Jmol a graphical representation of the structure, where you can check that the structure is being correctly described. If the graphic representation of the structure does not appear, your file is probably defective.

2) Then, on the left of the page, you can find the text: "*Download complete mcif file (including all tags needed for submission to MAGNDATA)*". Click on this text and the program will produce a new magCIF file that you have to download. Save the file using the extension ".mcif". This new file includes the necessary information present the original input file, while deleting all unnecessary one, and it also includes additional items, which have to be completed by hand, as explained in the next steps.

3) Open with a text editor the downloaded new magCIF file and complete manually the unfilled items according to the instructions given in the next consecutive steps, **where we follow their order in the file, using an example as illustration**.

Most of the items to be filled in the following steps are obligatory. Those that are optional and can be skipped and left unedited in the downloaded file, will be indicated in the corresponding step with the term: "[Optional]" in red.

4) Complete information on the compound composition:

```
_chemical_name_systematic
;
;
_chemical_name_common            ?
_chemical_formula_moiety         ?
_chemical_formula_structural      ?
_chemical_formula_analytical       ?
_chemical_formula_iupac          ?
_chemical_formula_sum            "Dy Mn2 O5"
_chemical_formula_weight          ?
_chemical_melting_point          ?
_chemical_compound_source         ?
_chemical_absolute_configuration     ?
```

Fill the tag "_chemical_formula_sum" with the chemical composition (between quotes) of the compound, substituting the default interrogation symbol present in the original file. Parenthesis should not be used, but each atomic species with their multiplicity and separated by a space, with the whole expression between quotes. The other tags can be left empty. But, if desired, they can be filled following the definitions and rules of the general CIF format. Definitions and examples of these items can be found at:

https://www.iucr.org/resources/cif/dictionaries/search

5) Complete the bibliographic information of the publication where the magnetic structure was reported.

```
_citation_journal_abbrev      "J. Phys. C: Solid State Phys."
_citation_journal_volume       14
_citation_page_first          1671
_citation_page_last           1683
_citation_article_id            .
_citation_year                1981
_citation_DOI                 10.1088/0022-3719/14/11/027
```

The magnetic structure must have been published in a scientific journal and the bibliographic data of the publication must be given in this set of tags. Substitute the default interrogation signs by the appropriate information, as

in the example above. Only a word or a string is expected in each row. If several words are to be included in a row, like in the journal abbreviation, then the full string of words should be written between quotes. Use as quotes either " " or ' '.

The tag "_citation_article_id " must be filled in the case that the journal, like for instance Phys. Rev B, uses some numerical index to classify the articles, and the page numbers are not relevant. In the case of a journal where articles are classified by their page numbers, the tag "_citation_article_id" should be filled with a dot: . , which indicates that this item is irrelevant. Reversely, if the tag "_citation_article_id " is used, then the tags for the page numbers are irrelevant and should be filled with a dot. The DOI index of the publication in the last row is very important and should be filled in any case. All these rules mean that no interrogation symbol should be left in any of the lines, once they are completed.

6) Authors:

```
loop_
_citation_author_name
"C. Wilkinson"
"F. Sinclair"
"P. Gardner"
"J.B. Forsyth"
"B.M.R. Wanklyn"
```

Write one by one **in separate rows**, and in quotes, ALL the authors of the publication. Use preferably only initials for the first names. Avoid special characters and all kind of accents, tildes, etc. , as they are not supported by the database.

7) Source of the data on the atomic positions:

```
_atomic_positions_source_database_code_ICSD     18308
_atomic_positions_source_other                      .
```

In many cases the positional structure, either from the non-magnetic atoms, or from all atoms, has been taken from other sources and has NOT been refined in the publication reporting the magnetic structure. In these cases, these atomic positions come from another source, **which must be indicated here,** either with its entry code in the ICSD database, if it exists, or with a bibliographic reference IN QUOTES of the article where this structure was reported.

Alternatively, in the case that the nuclear or positional structure has also been determined and reported in the same publication reporting the magnetic structure, and this positional structure is already an entry in the ICSD database as an ordinary structure, the ICSD tag here should be filled with its corresponding entry code in the database.

In all other cases, i.e. if the positional structure is reported in the same publication reporting the magnetic structure, but it is not yet in the ICSD, then these two tags are irrelevant and should be filled with a dot.

8) Report the temperatures relevant for the information about the positional structure, which is present in the file, in the case that these temperatures are different from the temperature at which the magnetic moments were determined:

```
_temperature_position_structure        300
_temperature_atom_positions             .
_temperature_non-magn_atom_positions    .
_temperature_cell_parameters            .
```

If both atomic positions and unit cell parameters of your magnetic structure have values determined at the same temperature than the magnetic moments, you can skip this step, leaving these four tags with dots, which indicate that they are irrelevant.

If on the contrary, some of the structural values in the file come from an experiment at a different temperature either reported in the same publication or from some other source, substitute then the dot of the relevant tag(s) by the appropriate temperature value (in K), according to the following rules:

i) If the whole positional structure, including the unit cell, comes from a determination at a different temperature than the one of the experiment determining the magnetic moments, indicate this temperature in the first row (_temperature_position_structure), and fill the other three rows with dots as irrelevant.

ii) If the positional structure, **with the exception of the unit cell**, comes from a determination at a different temperature than the one of the experiment determining the magnetic moments, indicate this temperature in the second row (_temperature_atom_positions). Then fill the other rows with dots, as irrelevant, except the last one (_temperature_cell_parameters), which should be filled with the temperature at which the unit cell parameters were determined, if different from that of the magnetic moments (otherwise, it should also remain with a dot).

iii) If ONLY the positions of the **non-magnetic** atoms come from a determination at a different temperature than that of the experiment for the magnetic moments and the rest of the structural parameters, then fill the third tag (_temperature_non-magn_atom_positions) with that temperature, and fill with dots the other three tags, as irrelevant.

iv) If **only the unit cel**l comes from a determination at a different temperature, while the rest of the positional parameters correspond to the temperature at which the magnetic moments where determined, then fill the fourth tag (temperature_cell_parameters) with that temperature, while fill the other three tags with dots, as irrelevant.

5

9) Transition and experiment temperatures:

_transition_temperature   8.4
_experiment_temperature   4.2

The first tag should be completed with the temperature (in K) below which the system transforms into the phase being reported. In the case of a system with several magnetic phases, this temperature is that of the transition that is closer and above the temperature of the experiment. If this transition temperature is not known, then this tag should be left with the interrogation symbol "?". The second tag must be filled with the temperature (in K) corresponding to the experimental data used for the determination of the magnetic moments.

10) Information on the possible irreducible representations (irreps) that may be active in the structure **[Optional]**:

loop_
_irrep_id
_irrep_dimension
_irrep_small_dimension
_irrep_direction_type
_irrep_action
_irrep_modes_number
_irrep_presence
? ? ? ? ? ? ?

The filling of this loop is optional and can be skipped, i.e. left with the default interrogation symbols. But do not delete it, it will then be edited by us.

This loop deals with the irreps that are relevant in the reported magnetic sructure. Each row corresponds to one irrep and contains the following seven items :

1) Irrep label (in the CDML notation, i.e. the common notation used by the Bilbao server, the ISOTROPY webpage, Jana, etc.).
2) dimension of the full irrep
3) dimension of the small irrep
4) In the case of multidimensional irreps: the word "special" or "general" depending if the irrep basis functions are restricted along a special symmetry direction within the irrep space or not. In the case of 1-dim irreps this tag is irrelevant and should filled with a dot.
5) Indication with "primary" or "secondary" if this irrep can be considered as a primary or a secondary irrep in the observed magnetic structure, i.e. if the associated irrep distortion participates in the observed symmetry break or not.
6) Number of degrees of freedom associated with the irrep, i.e. number of irrep spin basis functions corresponding to this irrep (taking into account the additional additional restrictions in the case that these basis functions have to comply with a special direction within the irrep space).
7) In the case of the secondary irreps, indication with "yes" or "no" if the reported magnetic arrangement has a contribution associated with this

secondary irrep. In the case of primary irreps, this tag is irrelevant because by definition a primary irrep must be involved in the observed magnetic ordering, and therefore this item should then be filled with a dot.

For our example, this part becomes:

```
loop_
_irrep_id
_irrep_dimension
_irrep_small_dimension
_irrep_direction_type
_irrep_action
_irrep_modes_number
_irrep_presence
mX2 2 2 special primary 1 .
```

(The tools Get_mirreps and MAGNETIC REP. in the Bilbao crystallographic server (www.cryst.ehu.es) can be useful to obtain the information to be included in this loop. Get_mirreps provides the irreps in CDML notation that can be involved in your structure, and in the case that several irreps are listed, then MAGNETIC REP can be used to check if some of them can be discarded because they are not present in the decomposition of the magnetic representation for the sites occupied by the magnetic atoms.)

(Another very efficient tool to obtain the irrep decomposition of the magnetic structure is ISODISTORT (method 4) in the ISOTROPY Software Suite (https://stokes.byu.edu/iso/isotropy.php). As input only the CIF file of the parent structure and a magCIF file of the magnetic structure are needed. The program however requires that the magCIF file describes the magnetic structure in the standard setting of its magnetic space group (MSG). Therefore, in the very common case that the magCIF file, which you have, describes the magnetic structure in a non-standard setting of the MSG, then you should first use ISOCIF, also in the ISOTROPY webpage, to obtain a new magCIF file with the MSG in its the standard setting.)

11) Comments related with the experiment or with the features of the magnetic structure.

```
_exptl_crystal_magnetic_properties_details
;
NSD
Positional structure from a room temperature determination
See #1.76 for a different model of the same structure, having the same symmetry, but
quite different magnetic moments.
;
```

You can include here, between the two semicolons ";", any relevant comments concerning the experiment. It is obligatory in particular to indicate the technique used: NSD (neutron single crystal diffraction), NPD (neutron powder diffraction), etc. It is also important to mention if the atomic positions come from this experiment or from another one at a different temperature.

Any kind of extraordinary circumstance concerning the experiment can also be mentioned here. If for instance, the magnetic structure was determined at non-ambient pressure or under some field, it should be mentioned here indicating the value of the pressure or the field.

Among other things that can also be included: brief information on other magnetic phases if they exist for the same compound, comments on other published models of the same magnetic structure, if they exist; observed or expected properties of the phase: Ferrimagnetic, Ferromagnetic, linear magnetoelectric, etc.

These comments are all ***optional EXCEPT*** ***those referring to the employed technique and any exceptional condition of the experiment (pressure, field), if existing. In any case, they will be further edited according to our unifying criteria for MAGNDATA.***

12) Comments related with the symmetry of the structure and its consequences **[Optional]**:

> _active_magnetic_irreps_details
> ;
> 1k magnetic structure
> k-maximal magnetic symmetry
> 2-dim irrep along a special direction as primary
> magnetic order breaks the symmetry into a polar group with polarity along b in the parent setting
> magnetically induced ferroelectricity to be expected along b in the parent setting (multiferroic of type II)
> ;

You can include here, between the two semicolons ";", any relevant comments concerning the symmetry of the structure and its consequences. In particular it is recommended to indicate if the structure is a 1k, 2k, 3k, etc. magnetic structure, and in the case that you know it, if the symmetry is "k-maximal", i.e. it is one of the maximal ones for the relevant propagation vector(s).

In any case, this set of comments will be further edited according to our unifying criteria for MAGNDATA.

13) Information about the parent space group (the space group of the paramagnetic phase):

> _parent_space_group.name_H-M_alt 'P b a m'
> _parent_space_group.IT_number   55
> _parent_space_group.transform_Pp_abc 'a,b,c;0,0,0'

These tags must be filled with the symbol of the space group of the paramagnetic phase, its number according to the International Tables for Crystallography, and the transformation to its standard setting. Every item should be in quotes if necessary (i.e. if it includes some space). Use as quotes either " " or ' '.

We consider as standard settings for the transformations those indicated in the Bilbao server, namely:

- *unique axis b (cell choice 1)* for space groups within the monoclinic system.
- *obverse triple hexagonal unit cell* for R space groups.
- *origin choice 2* - inversion center at (0,0,0) - for the centrosymmetric space groups for which there are two origin choices, within the orthorhombic, tetragonal and cubic systems.

For instance, taking another example, if the parent space group is Pbnm, i.e. the space group N. 62, Pnma, but described in a *non-standard* setting, then these three tags would be filled in the following form:

```
_parent_space_group.name_H-M_alt 'P  b  n m'
_parent_space_group.IT_number              62
_parent_space_group.transform_Pp_abc 'b,c,a;0,0,0'
```

If the parent space group is being considered in its standard setting, then the transformation to be indicated in the third tag is the identity: 'a,b,c;0,0,0'

14) Propagation vector(s) with respect to the parent space group:

```
loop_
_parent_propagation_vector.id
_parent_propagation_vector.kxkykz
k1  [1/2 0 0]
```

If more than one propagation is present in the structure, write them **in consecutive rows** using the same format, and with consecutive labels k1, k2, etc. The components of the propagation vector(s) are to be expressed as fractions to make patent that the vector is considered commensurate.

15) Basis transformations relating the unit cell of the magnetic structure with the parent unit cell and with the standard setting of the MSG of the structure:

```
_parent_space_group.child_transform_Pp_abc '2a,b,c;0,0,0'
_space_group_magn.transform_BNS_Pp_abc 'a,c,-b;7/8,0,0'
```

This part will already be filled if the tags were present and populated in the original magCIF file that you have introduced in MVISUALIZE. Otherwise, they will appear with interrogation symbols, which must be substituted by the appropriate transformations. The first item should be the transformation from the unit cell and origin of the paramagnetic structure, whose space group has been introduced in the step 13), to the unit cell and origin being used for the magnetic structure (see step 16). In the above example the unit cell of the magnetic structure has its cell parameter *a*

doubled with respect to the parent unit cell, while the remaining values, including the cell origin are the same.

The second item should be a transformation from the unit cell of the magnetic structure (see step 16), to one basis (unit cell and origin) where the MSG operations would have a form fully coincident with the one present in the listings of the MSG (in BNS notation), available in internet, which can be considered the standard BNS setting of this MSG. This transformation is in general not unique. If you do not know one, you can use the tool in the Bilbao crystallographic server: "IDENTIFY MAGNETIC GROUP". You only need to introduce the symmetry operations listed in the file and the program will identify the MSG type and provide a possible transformation into its standard setting.

16) Magnetic space group (MSG) in BNS notation, and unit cell:

```
_space_group_magn.number_BNS            29.104
_space_group_magn.name_BNS          "P_a  c  a  2_1"
_space_group_magn.point_group_name      "mm21'"
_space_group_magn.point_group_number    "7.2.21"
_cell_length_a          14.58800
_cell_length_b          8.55510
_cell_length_c          5.68750
_cell_angle_alpha          90.00
_cell_angle_beta          90.00
_cell_angle_gamma          90.00
```

As in the previous step, this part will be already filled, if the information in your original magCIF file was complete. No change will then be required and you can go to the next step.

However, in some cases the initial input magCIF file may lack the information concerning the first two tags in this set (as they are not mandatory in the magCIF format). In this case, they will appear in our file with interrogation symbols, and must then be filled with the numerical index and the BNS symbol of the MSG type corresponding to the symmetry operations that are listed in the file.

If you do not know the symbol and/or the numerical index of the MSG type that corresponds to the symmetry operations listed in your file (see step 17), you can use the tool in the Bilbao crystallographic server: "IDENTIFY MAGNETIC GROUP". You only need to introduce the symmetry operations listed in the file and the program will identify the MSG type and provide a possible transformation into its standard setting.

The third and fourth tags in this set are filled with information about the magnetic point group, which are calculated and have been added to the file by the program MVISUALIZE. Therefore, normally they will be filled. But if they are empty, it is **optional** to fill them manually or to leave them with an interrogation symbol. They are intended to indicate the magnetic point group of the structure with both its symbol and its numerical index (the

employed numerical indices can be found in the program MPOINT of the Bilbao crystallographic server).

The remaining tags in this set define the unit cell of the structure and will already be filled with the values given in the original magCIF file introduced in MVISUALIZE.

17) Symmetry operations defining the MSG of the structure in BNS setting:

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

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

This part will be already filled with the symmetry operations, which were present in the original magCIF file, and in principle it will not require any change.

18) Atomic coordinates of **ALL** the atoms in an asymmetric unit with respect to the MSG:

```
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Dy1_1 Dy 0.06937 0.17169 0.00000 1
Dy1_2 Dy 0.93063 0.82831 0.00000 1
Mn1 Mn 0.00000 0.50000 0.25480 1
Mn2_1 Mn 0.20595 0.35000 0.50000 1
Mn2_2 Mn 0.79405 0.65000 0.50000 1
O1 O 0.00000 0.00000 0.27410 1
O2_1 O 0.08235 0.44520 0.00000 1
O2_2 O 0.91765 0.55480 0.00000 1
O3_1 O 0.07685 0.43540 0.50000 1
O3_2 O 0.92315 0.56460 0.50000 1
O4_1 O 0.19755 0.20820 0.24140 1
O4_2 O 0.80245 0.79180 0.24140 1
```

This part will be already filled with the values present in the original magCIF file. Depending on the procedure followed in the refinement, the original file may have only the positions of the magnetic atoms. In this case the starting file must be modified to include the positions of the non-magnetic atoms or alternatively they can be added here. MAGNDATA only

accepts models with ALL atoms included (see comments at the beginning of these instructions on this matter).

Depending on the procedure followed to obtain the magCIF file introduced in MVISUALIZE, you may consider the atomic labels or even the atoms chosen as symmetry independent in the file far from being the most adequate, as they may have been produced by an automatic process of some program (see for instance the process followed in case 2). Here you can then change the atomic labels according to your criteria. You can also change the choice of a certain symmetry independent atom in the list, but in this case your choice will be limited to those atomic positions generated by the MSG from the one being listed.

If the atomic sites become split with respect to the paramagnetic structure, it is recommended that the atom labels keep track of this splitting, as in the example above, where for instance the atomic site Mn2 becomes split into two symmetry independent sites Mn2_1 and Mn2_2, or the atom O4 becomes split into O4_1 and O4_2, etc.

19) Magnetic moments (in Bohr magnetons) of the magnetic atoms in the asymmetric unit, whose positions are defined in the previous loop.

```
loop_
_atom_site_moment.label
_atom_site_moment.crystalaxis_x
_atom_site_moment.crystalaxis_y
_atom_site_moment.crystalaxis_z
_atom_site_moment.symmform
_atom_site_moment.magnitude
_atom_site_moment.spherical_azimuthal
_atom_site_moment.spherical_polar
Dy1_1 4.51(3) -8.02(1) 0.0 mx,my,0  ? ? ?
Dy1_2 -4.51(3) 8.02(1) 0.0 mx,my,0    ? ? ?
Mn1 -1.44(4) -1.35(1)  0.0 mx,my,mz ? ? ?
Mn2_1 2.10(4) 1.26(1) 0.0 mx,my,0   ? ? ?
Mn2_2 2.10(4) 1.26(1) 0.0 mx,my,0  ? ? ?
```

This part will already be filled with the values of the magnetic moment components along the crystallographic axes and their symmetry constraints, if they were present in the original magCIF file. But the corresponding total moment magnitudes and the optional alternative description of the moments with spherical coordinates will be with interrogation symbols. It is then **obligatory** to fill manually the moment magnitudes, while the angles in spherical coordinates can remain with interrogations. The spherical angles are intended for models where refinement of the moments was done in spherical coordinates (see next step) :

```
loop_
_atom_site_moment.label
_atom_site_moment.crystalaxis_x
_atom_site_moment.crystalaxis_y
_atom_site_moment.crystalaxis_z
_atom_site_moment.symmform
_atom_site_moment.magnitude
```

```
_atom_site_moment.spherical_azimuthal
_atom_site_moment.spherical_polar
Dy1_1 4.51(3) -8.02(1) 0.0 mx,my,0   9.20 ? ?
Dy1_2 -4.51(3) 8.02(1) 0.0 mx,my,0   9.20 ? ?
Mn1 -1.44(4) -1.35(1)  0.0 mx,my,mz 1.97 ? ?
Mn2_1 2.10(4) 1.26(1) 0.0 mx,my,0    2.45 ? ?
Mn2_2 2.10(4) 1.26(1) 0.0 mx,my,0    2.45 ? ?
```

If you have changed the atomic labels in the previous loop, the corresponding labels in this loop should also be changed accordingly. Also, if you have changed the choice of some of the symmetry-independent atoms listed in the previous loop, their corresponding magnetic moments and their symmetry constraints, which can be different, should also be changed accordingly here.

In some cases, the fourth item in each row indicating the symmetry constraints on the moment components (tag: _atom-site_moment_symmform) may have not been present or filled in the original magCIF file that was introduced in MVISUALIZE. In this case it will have an interrogation symbol. If this is your case, fill manually the corresponding symmetry constraints for each atom, substituting the interrogation symbol. If the original magCIF file comes from a refinement program, this program must know these symmetry constraints even it has produced a magCIF file without them. This means that in general it must be possible to retrieve these symmetry constraints from the information available in other files used or created by the program during the refinement.

Do not confuse these symmetry constraints on the moments, coming from the MSG of the structure, with the restrictions that may have been introduced during the refinement to simplify the model or to lower the number of free parameters.

If you are not able to derive the symmetry constraints on the moments to be included in this loop, they can be left with an interrogation symbol. They will then be filled by us before introducing the structure in MAGNDATA.

20) If the refinement of the moments has been done in spherical coordinates, then the tags associated with the refined spherical angles can **also** be filled with the pertinent values. The final loop of the file then becomes (here a different example where the moment was refined in spherical coordinates is shown):

```
loop_
_atom_site_moment.label
_atom_site_moment.crystalaxis_x
_atom_site_moment.crystalaxis_y
_atom_site_moment.crystalaxis_z
_atom_site_moment.symmform
_atom_site_moment.magnitude
_atom_site_moment.spherical_azimuthal
_atom_site_moment.spherical_polar
Tb1   5.64  9.42  2.13  mx,my,mz 8.48(2)  84(2)  75(2)
```

The spherical coordinates of the moments in a magCIF file should be defined with respect to the following cartesian axes: x along the unit cell vector a, z along the vector c*, and the y axis completing a right-hand set. The azimuthal and polar angles are the angles denoted as φ and θ, respectively, in the usual notation for spherical coordinates.

It is important to note that even in the case that the moments have been refined in spherical coordinates, MAGNDATA requires to include also in the loop the corresponding values of the moment components along the crystallographic axes. Visualization programs like Vesta, Jmol, etc., or general programs in the ISOTROPY suite or in the Bilbao server, only support moment descriptions in terms of components. This is the reason why this components paramerization should always be present in the magCIF file, independently of the parameterization used in the refinement.

In the case that these obligatory moment components have been derived from the refined spherical coordinates, it is recommended that these component values are written in the file without errors and with enough digits, even if not significant, so that the resulting calculated moment magnitude is consistent with its refined value, which should also be filled in the file. Alternatively, these components derived from the refined spherical coordinates can be given with errors calculated with propagation error formulas, as done for instance by FullProf.

21) Save the final edited file. You can now upload it in MVISUALIZE and check that the file is read without problem and a consistent graphical representation of the structure is produced.

In order to confirm that the format of file is not defective and complies with the CIF rules, you can also upload the file in ISOCIF in the ISOTROPY Software Suite (https://stokes.byu.edu/iso/isotropy.php) to check that this program also reads the file without problem and does not indicate any error.

The file is then ready to be submitted to MAGNDATA: just go to the upload page indicated in the first webpage of the program, where further instructions for the upload can be found.

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Case 2. You have a magCIF file of the magnetic structure, but with no symmetry and listing all atomic positions and magnetic moments within the unit cell.

*You are supposed in this case to have a magCIF file of the structure, but with no symmetry, except for the identity and the lattice periodicity. This means that the actual magnetic space group (MSG) of the structure is NOT used in the description and the file lists all atomic positions and magnetic moments in the unit cell. (If on the contrary you DO have a magCIF file with the magnetic space group identified and used, go directly to **case 1**).*

When magnetic symmetry groups are not used, independently of the method and parameterization used, some refinement programs can provide such primary simple magCIF files under the MSG P1, with all atomic positions and moments within the unit cell listed. Alternatively you may have obtained such type of magCIF file by other means (see for instance the instructions for case 3 below).

As we did for the case 1, it is important to stress that depending on the procedure followed in the refinement, the magCIF provided by the refinement programs will only include the magnetic atoms. However, the knowledge of a magnetic structure is incomplete if it does not include the positions, at least approximate, of the NON-MAGNETIC atoms. Therefore **MAGNDATA only accepts files with ALL atoms, including the non magnetic ones**.

In the case that your original magCIF file only includes the magnetic atoms, the positions of the non-magnetic atoms will have to be added either manually or by any other means. If the refinement was done in such a way that the positions of the non-magnetic atoms were not needed, probably the simplest way to obtain a magCIF file with all atoms is to repeat the refinement, but this time including in the starting model the non-magnetic atoms with all their positional parameters fixed according to some model coming from the knowledge of the non-magnetic structure, and then proceed with the refinement program in the same form as was done originally. Although the positions of the non-magnetic atoms will be irrelevant in the refinement, the program will then keep track of them and in principle they will be present in the final magCIF file provided by the program.

 (*If the refinement has been done using two distinct phases to model nuclear and magnetic scattering, then the refinement program will probably be able to generate two separate files: a CIF file for the nuclear structure, usually with the space group of the paramagnetic phase, and a magCIF file for the spin arrangement with no symmetry, in P1. In order to produce a single magCIF file with no symmetry with all atoms, one can then easily combine these two files using the online program ISOCIF on the ISOTROPY Software Suite (https://stokes.byu.edu/iso/isotropy.php). By means of this program the CIF file of the nuclear structure can be transformed into another CIF file where the symmetry has also been reduced down to P1, choosing the same unit cell as the one in the magCIF file. Note that if the propagation vector(s) of the magnetic structure contains fractional components (like 1/2,1/3 and so on) then the symmetry reduction of the nuclear structure, down to triclinic P1, has to be done with the appropriately enlarged unit cell, by choosing the appropriate lattice vectors*

of the structure to be two, three and so on times bigger than the original ones. In this way you will have the same unit cell for the nuclear and magnetic structures in the processed CIF and magCIF files. The atomic coordinates of the non-magnetic atoms in the new CIF file in P1 can then be copied and pasted into the magCIF file containing only the magnetic atoms. A similar procedure to obtain a single magCIF file with all atoms can also be applied in the case that the CIF file for the positional structure of the non-magnetic atoms is from a different source or a different refinement at a different phase, if they are considered also approximately valid for the magnetic phase. This combined single magCIF file can then be processed following the steps explained here for Case 2.)

Starting with the available magCIF file with no symmetry, one must create a new magCIF file, which is fully consistent with the MSG of the structure, and then go to case 1, to follow the procedure explained there.

These are the steps that can be followed for case 2:

1) Upload your magCIF file with no symmetry, except the trivial one, in the online program ISOCIF on the ISOTROPY Software Suite (https://stokes.byu.edu/iso/isotropy.php).

ISOCIF will show then a first output page where the MSG corresponding to the model described in the uploaded file is identified, and a series of options for further editing and manipulating the file data are presented. Here below it is shown a very partial screenshot of this first output/menu page for a particular example. One can see that the program identifies the MSG in the file as P1 (N. 1.1) in the BNS notation. i.e. the trivial simplest symmetry group with no symmetry except the identity and the lattice translations defined by the given unit cell.

ISOCIF: modify and save CIF file

Help for this page

Magnetic Space Group: 1.1 P1 (1.1.1 P1), Lattice parameters: a=3.63000, b=3.63000, c=11.96000, alpha=90.00000, beta=90.00000, gar
Fe1_1 1a (x,y,z;mx,my,mz), x=0.00000, y=0.00000, z=0.00000, mx=0.00000, my=0.95000, mz=0.00000, Fe1_2 1a (x,y,z;mx,my,mz), x=0.0
my=-0.95000, mz=0.00000, Fe1_3 1a (x,y,z;mx,my,mz), x=0.50000, y=0.50000, z=0.00000, mx=0.00000, my=0.95000, mz=0.00000, Fe1_
y=0.50000, z=0.50000, mx=0.00000, my=-0.95000, mz=0.00000, Fe2_1 1a (x,y,z;mx,my,mz), x=0.00000, y=0.50000, z=0.16500, mx=0.0(
(x,y,z;mx,my,mz), x=0.00000, y=0.50000, z=-0.33500, mx=0.00000, my=-1.52000, mz=0.00000, Fe2_3 1a (x,y,z;mx,my,mz), x=0.50000, y
my=1.52000, mz=0.00000, Fe2_4 1a (x,y,z;mx,my,mz), x=0.50000, y=0.00000, z=0.33500, mx=0.00000, my=-1.52000, mz=0.00000, As1_
z=0.36750, As1_2 1a (x,y,z), x=0.00000, y=0.50000, z=-0.13250, As1_3 1a (x,y,z), x=0.50000, y=0.00000, z=-0.36750, As1_4 1a (x,y,z), x=
Nearest neighbor distances: This information is not displayed when there are more than ten Wyckoff sites.

[ISOVIZ file]

Atomic radius (Angstroms): 0.4   Maximum bond length (Angstroms): 2.5   Length of magnetic moment vectors (Angstrom

(pixels): 1024

Viewing range: xmin 0   xmax 1   ymin 0   ymax 1   zmin 0   zmax 1

[Change lattice and origin] You may change the lattice vectors and/or origin if desired. The transformation matrix must have a deter
space-group setting (i.e., the operators must retain the same form).

2) Among the options listed in the output/menu page click on the button termed "detect higher symmetry":

The program then detects the actual magnetic space group (MSG) of the structure being described by the uploaded file and produces a new output/menu webpage. Below we show a very partial screenshot of this page for the present example:

The program has identified the MSG type of the structure. In the case of our example this is P$_a$nma (N. 64.450) in the BNS notation, and lists a set of atomic positions and moments of an asymmetric unit under this MSG. **It is important to remark that for this description the program automatically introduces a transformation of the basis in order to have the MSG in its standard setting**. This transformation is indicated on the last row of the text, which precedes the multiple options. For our example this transformation is: (**c**, **b**, **-a**; 3/4, 1/4, 1/2). Therefore not only the unit cell vectors have been interchanged, but also its origin has been shifted to the position (3/4,1/4,1/2) of the original unit cell (*note that the transformed unit cell lattice vectors in ISOCIF are indicated as row vectors, in*

contrast with the description in the programs of the Bilbao server, where they are the columns of a 3x3 matrix).

3) Among the options listed in the new output/menu page go to the option termed "Save CIF file", at the end of the page. **Choose there the option with the text: "Use alternate (possibly nonstandard) setting in CIF file".** Introduce then in the spaces available the desired unit cell and origin to be used for the description. Subsequently click on the button: "Save CIF file". The program then creates and provides the desired magCIF file. Download and save this file in your computer using the extension ".mcif".

The program when detecting the actual MSG of the structure in step 2), transforms the structure into the standard setting of the MSG. Therefore, in order to create a magCIF file, which uses the detected MSG, **but keeps the original unit cell and origin of your input file, you have to indicate here the transformation from the basis used by the program to your original unit cell and origin**. This means that you have to introduce **the inverse transformation of the one that was done automatically by the program**, which is indicated at the top of the webpage. In our example this inverse transformation is then: (**-c**, **b**, **a**; -1/2, -1/4, 3/4).

Of course, at this point, you can also choose and introduce any other basis that you may consider appropriate, as long as it is consistent with the MSG, or you may keep the standard setting basis, which was chosen by the program.

4) Go to Case 1 with the magCIF file that you have obtained.

Note that the ISOCIF in general will have made a rather arbitrary choice (among the existing possibilities) of the atoms listed in the file as symmetry independent, and it will also have assigned to these atoms some new atomic labels, which may be not the ones that you desire. You will be able to change these choices made by ISOCIF in the procedure explained above for case 1 (see step 18 therein).

==

Case 3: You do NOT have yet a magCIF file of any kind, but you have a model of the magnetic structure using some parameterization.

You are supposed to have an unambiguous model of the magnetic structure, with any kind of parameterization, like for instance the traditional representation method, but you do NOT have available yet a magCIF file, which could be used either in the procedure described in case 1 or in case 2.

In this case, the most obvious and direct approach seems to prepare a primary magCIF file of the type required for the case 2 above, with no symmetry included and listing all atoms and moments within a unit cell of the structure. This process will be explained in detail below as a second possible approach, but it may however become rather long and tedious, and in any case it will require afterwards to follow consecutively both the procedures explained above for case 2 and case 1.

For simple structures, especially those where a single irrep is involved in the magnetic arrangement, an initial magCIF file, which is fully consistent with the MSG of the structure and can be used for case 1, can be directly obtained using free computer tools available in internet. This method using internet computer tools can be very efficient and rapid, as it permits afterwards to go directly to the procedure of case 1.

We therefore propose for case 3 the two following alternate procedures:

1st Procedure: How to create a magCIF file of a magnetic structure fully consistent with its magnetic symmetry to be used directly in the procedure explained above as Case 1. (Use of MAXMAGN, k-SUBGROUPSMAG plus MAGMODELIZE or use of ISODISTORT):

1) If you do not have it yet, create or retrieve an ordinary CIF file describing the structure of your system in its paramagnetic phase, or even better: if you have available the positional structure in the magnetic phase, described under the space group of the paramagnetic phase, create or retrieve the corresponding ordinary CIF file of this structure. This file will have to be used as input in the next steps.

2) **Use of MAXMAGN:** If your magnetic structure is a 1k structure, i.e. with a single propagation vector, and it is rather simple, in particular if the structure is described with a single one dimensional irreducible representation (irrep), then MAXMAGN in the Bilbao Crystallographic Server is a very simple and efficient tool to create the desired magCIF file. This program can also very be efficient in the case of a single multi-dimensional irrep, if the parent structure is not trigonal, rhombohedral or cubic. In more complex cases, it is recommended to go directly to point 3) below, for the alternative of using k-SUBGROUPSMAG.

The steps of the process when using MAXMAGN are the following (several tutorials with more detailed information are available on the webpage of the program):

2.1) Introduce in the first input page of the program the relevant propagation vector and check the box: "Structure data of the paramagnetic phase will be included" and submit.

2.2) On the next page, upload the CIF file of the paramagnetic phase or the one corresponding to the positional structure in the magnetic phase (described in the space group of the paramagnetic phase), if available. In the next menu, indicate the atoms that should be considered magnetic. The program will then enumerate all possible alternative magnetic models corresponding to maximal symmetries consistent with the propagation vector that has been introduced.

2.3) In the list of possible alternative symmetries, for each of them click on the last column entitled "Magnetic Structure" to produce a model of the magnetic structure consistent with this symmetry. In many cases, the model described in the resulting webpage can be discarded immediately as the shown symmetry constraints on the moments are incompatible with your structure. In some other cases, the inspection of the variation of the moments among the atoms within the Wyckoff orbits of the magnetic atoms, which are listed in this page, can also be sufficient to discard some models. In any other case, fill with approximate values, consistent with those in your structure, the menu boxes available for the moment components of the symmetry independent magnetic atoms, and produce a graphical representation of the structure with the tool of the program. Compare the 3D graphical representation with your structure: In most cases this comparison will be sufficient to identify the model that agrees with your structure (There can only be one model that is coincident with your structure!).

It is important that one must take care of the fact that the program only lists by default one of the possible equivalent domain-related MSGs and this may be not the one that corresponds to your model if your structure is quite complex. In this case, one has to use the option in the program of enumerating all possible domain-related descriptions (conjugate MSGs) to be able to identify the one that corresponds to your structure.

If despite checking all domain-related descriptions for the listed alternative symmetries, none of them can be identified with your structure, then your structure must have a lower symmetry than those listed by MAXMAGN. Therefore the symmetry associated with your structure **is not maximal** for the observed propagation vector, and in this case it is recommended to go to point 3) below, where the use of the most general tool k-SUBGROUPSMAG is explained

Note however that if the magnetic ordering in your structure corresponds to a single 1-dimensional irrep, then the MSG of your structure **must necessarily be maximal** for the observed propagation vector (k-maximal), and therefore must correspond to one of the models listed by MAXMAGN. In general, about 70% of all published magnetic structures have k-maximal magnetic symmetries and any structure of this type will necessarily be among those listed by MAXMAGN.

2.4) If in the previous step you have identified the MSG corresponding to your structure, download and save the magCIF file created by MAXMAGN for the model and MSG, which describes your structure.

In general, the symmetry breaking represented by the MSG of the magnetic structure may imply for the positional structure new degrees of freedom both in the unit cell and the atomic position, including the splitting of some atomic sites, both magnetic and non-magnetic ones. In the **very improbable** case that the magneto-structural coupling in your structure is so strong that you have been able to detect some structural distortion related with these new structural degrees of freedom, these deviations from the constraints of the original parent space group symmetry can be introduced manually at this point in the atomic positions and unit cell listed in the saved magCIF file.

2.5) If necessary, if previously only approximate moment values were used, fill in the obtained magCIF file the exact values of the moment components for the magnetic atoms listed in the file,

2.6) Go to Case 1 with the magCIF file that you have obtained.

==

3) **Use of k-SUBGROUPSMAG and MAGMODELIZE:** In the case that your magnetic structure could not be identified with one of the models enumerated by MAXMAGN, or in the case that your structure is quite complex, like for instance it is a multi-k structure with several propagation vectors, or it has a multi-dimensional irrep with a parent space group that has one o more three-fold axes, or it has several irreps involved, then the program k-SUBGROUPSMAG combined with MAGMODELIZE (both in the Bilbao Crystallographic Server) can be used in a similar way as MAXMAGN to enumerate possible models consistent with the relevant propagation vectors, **but not restricted to be of maximal symmetry**. These models can then be compared with your magnetic structure in an analogous way as done in MAXMAGN, and again a visual and/or a graphical inspection is in most cases sufficient to identify the appropriate model (for more information on how to use these programs see the tutorials available on the programs webpages).

3.1) The list of possible models provided by k-SUBGROUPSMAG can be restricted to those that can be realised by a phase transition of "Landau-type", i.e. with only a single irrep involved in the magnetic ordering. If your structure satisfies this condition, then one (and only one) of the models in this restricted list provided by k-SUBGROUPSMAG must be adequate to describe your structure.

As stressed in the case of using MAXMAGN, here also one must take care of the fact that the program only lists by default one of the possible equivalent domain-related MSGs and this may be not the one that corresponds to your model. In this case, one has to use the option in the program of enumerating all possible domain-related descriptions (conjugacy class) to be able to identify the one that corresponds to your structure.

3.2) You can also restrict further in k-SUBGROUPSMAG the possible symmetries to those that can be realised for a specific irrep, and then proceed similarly as above, comparing the corresponding models with your structure.

3.3) In the most complex cases, if the model of your structure does not appear in the lists with the filters indicated above, one can still use K-SUBGROUPSMAG with less restrictive conditions, and proceed with the list of alternative symmetries in a similar way as in the previous cases. The program provides the group-subgroup hierarchy of all listed symmetries, and obviously the most reasonable way to proceed with the comparison with your structure is to follow this hierarchy, starting first with the MSGs of maximal symmetry and continue with their subgroups in a hierarchical way until the actual symmetry and model that can be identified with your structure is found.

3.4) Once the symmetry and model describing your structure is identified, one can proceed similarly as in 2) above, to produce an appropriate magCIF file to be used in the procedure of case 1.

4) **Use of ISODISTORT:** As an alternative to MAXMAGN or K-SUBGROUPSMAG, you can use in a similar form ISODISTORT in the ISOTROPY Software Suite at (https://stokes.byu.edu/iso/isotropy.php) applying its so-called "Method 2", specially in the case of complex cases. The program enumerates possible active irreps and resulting magnetic symmetries, and provides for each of them a magCIF files, a graphical representation, etc. However, when enumerating possible symmetries for the structure, this program chooses arbitrarily one of the possible equivalent domain-related MSGs (if there is more than one,), and it does not have the option, as the other programs, to generate possible alternative descriptions corresponding to the other conjugate MSGs. Therefore in these cases the identification of the model corresponding to your structure may fail, UNLESS you do the comparison after transforming your structure to the basis chosen by ISODISTORT in order to have the MSG in its standard setting.

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2ⁿᵈ Procedure: How to construct a simple magCIF file of any magnetic structure with only the unit cell defining the lattice and listing all the atomic positions and moments within the unit cell, to be used in the procedure explained in Case 2 above.

In principle, if you have an unambiguous model of your structure in any form of description, there must be no problem to produce either manually or via a computer tool a list of all atomic positions and of all atomic moments (described in terms of their components along the crystallographic axes and in Bohr magnetons) within a unit cell that defines the periodicity of the magnetic arrangement. For simplicity this unit cell can be a supercell. This is the only information needed. Once having these lists, it only remains the task of transferring these values to a template of a magCIF file with no symmetry except the identity operation (MSG: P1). Such template is included in the zip file, which contained these instructions. It

is also reproduced below, but filled with an example (template in blue, filled data in red), where an acceptable format for the data to be filled can be seen.

```
#\#CIF_2.0

data_1
_cell_length_a          3.63000
_cell_length_b          3.63000
_cell_length_c          11.96000
_cell_angle_alpha        90.00000
_cell_angle_beta        90.00000
_cell_angle_gamma         90.00000

loop_
_space_group_symop_magn_operation.id
_space_group_symop_magn_operation.xyz
1 x,y,z,+1

loop_
_space_group_symop_magn_centering.id
_space_group_symop_magn_centering.xyz
1 x,y,z,+1

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Fe1_1 Fe 0.00000 0.00000 0.00000 1.0000
Fe1_2 Fe 0.00000 0.00000 0.50000 1.0000
Fe1_3 Fe 0.50000 0.50000 0.00000 1.0000
Fe1_4 Fe 0.50000 0.50000 0.50000 1.0000
Fe2_1 Fe 0.00000 0.50000 0.16500 1.0000
Fe2_2 Fe 0.00000 0.50000 0.66500 1.0000
Fe2_3 Fe 0.50000 0.00000 0.83500 1.0000
Fe2_4 Fe 0.50000 0.00000 0.33500 1.0000
As1_1 As 0.00000 0.50000 0.36750 1.0000
As1_2 As 0.00000 0.50000 0.86750 1.0000
As1_3 As 0.50000 0.00000 0.63250 1.0000
As1_4 As 0.50000 0.00000 0.13250 1.0000

loop_
_atom_site_moment.label
_atom_site_moment.crystalaxis_x
_atom_site_moment.crystalaxis_y
_atom_site_moment.crystalaxis_z
Fe1_1  0.0 0.95 0.0
Fe1_2  0.0 -0.95 0.0
Fe1_3  0.0 0.95 0.0
Fe1_4  0.0 -0.95 0.0
Fe2_1  0.0 1.52 0.0
Fe2_2  0.0 -1.52 0.0
```

Fe2_3 0.0 1.52 0.0
Fe2_4 0.0 -1.52 0.0

The data to be included in the template is quite self-explanatory, and an acceptable format can be seen in the example above (in red). Note that the magnetic moment must be specified in terms of its components (in Bohr magnetons) along the three main crystallographic axes defined by the unit cell parameters.

Once this simple magCIF file is constructed, one can then follow consecutively the processes for Case 2 and Case 1, explained above.