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Guidelines for communicating commensurate magnetic structures. A report of the International Union of Crystallography Commission on Magnetic Structures

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A report from the International Union of Crystallography Commission on Magnetic Structures outlining the recommendations for communicating commensurate magnetic structures.

1. Introduction

Since 1949, thousands of magnetic structures have been determined and reported. However, the lack of a standardization of their description has hampered a comprehensive and unambiguous exchange of information about them. Under these circumstances, the development of a database of magnetic structures was for many years an impossible objective. The International Union of Crystallography (IUCr) established the Commission on Magnetic Structures (CMS) in 2011 with the purpose, among other things, of improving this situation by establishing a set of standards for the description and dissemination of magnetic structures. Under its auspices and the direction of CMS Chair, Branton J. Campbell, and with the supervision of the IUCr Committee for the maintenance of the CIF standard (COMCIFS), the so-called magnetic CIF dictionary[1] (magCIF), which extends the CIF (Crystallographic Information Framework) standard (Hall & McMahon, 2005) to magnetic structures, began its development in 2014 and was approved by the IUCr in 2016. As it is done for ordinary structures, the magCIF format presents the constraints of the magnetic symmetry group in a standardized

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

[1] https://www.iucr.org/__data/iucr/cifdic_html/3/MAGNETIC_CIF/index.html

form to provide a simple and unambiguous description, which restricts the listing of the magnetic moments and atomic positions to an asymmetric unit.

In recent years, the magCIF standard has been implemented in most mainstream computer tools available for the analysis, visualization and determination of magnetic structures (*ISOTROPY*: Stokes *et al.*, 1995; Bilbao Crystallographic Server: Perez-Mato *et al.*, 2015; *VESTA*: Momma & Izumi, 2011; *JMOL*: Hanson, 2010; *JANA2020*: Petříček *et al.*, 2023; *FullProf*: Rodríguez-Carvajal, 1993; *GSAS-II*: Toby & Von Dreele, 2013). This standard format allows magnetic-structure information to be interchanged between all these programs. It has also enabled the development of MAGNDATA (Gallego *et al.*, 2016*a*,*b*), a free database of magnetic structures with more than 2000 entries. Each entry, which can be downloaded as a magCIF file, contains an unambiguous description and a correctly applied magnetic symmetry group.

The magCIF standard and the new software tools that employ it provide an opportunity for the magnetic-structure research community to work together to standardize the communication of magnetic structure information across many intersecting scientific disciplines. This report makes an effort in that direction by presenting guidelines and illustrative examples on how to unambiguously report a commensurate magnetic structure, making use of its magnetic space-group symmetry.

Except for some general considerations, where incommensurate structures are explicitly mentioned, these guidelines are intended for commensurate structures. Though they are not addressed by the current report, the magCIF standard also supports incommensurate magnetic structures and their magnetic superspace-group symmetries. They require however a different methodology and therefore they will be the subject of a separate report. As an additional comment, it is important to state that this report addresses magnetic structures that can be described in the 'atomic approximation', where the magnetic moment density is expressed in terms of real-valued magnetic moments localized at atomic sites, which sometimes in the following will be referred to as *spins*. This document does not contain recommendations or guidelines on the reporting of experimental data or experimental details.

By recommending the crystallographic description of magnetic structures, which employs magnetic symmetry groups, the present guidelines break from the traditional approach of describing a magnetic structure in terms of spin basis vectors (or *symmetry modes*) of the irreducible representations (*irreps*) of the parent non-magnetic space group. In contrast with the representation analysis, the crystallographic description of a magnetic structure is a straightforward standalone description that does not refer to any other structure. Historically, many researchers considered the use of magnetic symmetry groups and irreps as mutually exclusive alternatives. Nevertheless, in fact, the two approaches are complementary and work together perfectly when applied with sufficient generality. Thus, the theoretical and practical (computational) progress of the past decade now permits a harmonious combination of both magnetic space groups and magnetic irreps in the characterization of commensurate magnetic structures. These guidelines are a consequence of this progress and in no way diminish the importance of group-representation analysis, which can be routinely used for the construction of the relevant magnetic space groups in each case.

This report is comprehensive, including lengthy arguments on which the recommendations are based. Therefore, in order to facilitate a quick and simple reference, a brief appendix is included, with two examples of magnetic CIF files, where the minimal set of items that are necessary for communicating commensurate magnetic structures are highlighted.

2. General considerations

The guidelines, which will be enumerated in the next section, are based on the following general principles and considerations.

(i) Standardization necessarily implies complicating the description of simple structures for the benefit of simplifying the description of complex ones under a common framework.

If one looks at how the structure of NaCl is described in a standard CIF file, it may be surprising to see the complete listing of the 192 symmetry operations (defining its space group). This description based on the CIF format may appear inefficient and excessive given the simplicity of the structure. However, the advantage of this common standard description is that it can be used for much more complicated structures, without a significant increase in format complexity. This is also the case when standardization is applied to the description of a magnetic structure.

(ii) The characterization of a commensurate magnetic structure must include the identification of its magnetic space group (MSG).

Whatever the method employed to determine a three-dimensional magnetic structure, the model being reported, or the format used to describe it, if the model is commensurate, its symmetry group is necessarily one of the 1421 possible types of magnetic space groups (MSGs), also known as Shubnikov groups (Koptsik, 1966), having excluded the 230 gray MSGs associated with structures without magnetic order. This MSG must be identified and reported, as it dictates the symmetry constraints on the atomic magnetic moments themselves and on any possible effect that the magnetic ordering may induce. Among other things, the MSG allows the identification of the point group symmetry of the system, which is required for any systematic analysis of its crystal tensor and twinning properties.

(iii) The identification of the MSG of a magnetic structure should not be limited to the assignment of an MSG symbol and/or index, but must also adequately specify the symmetry operations of the relevant MSG relative to the basis (unit cell and origin) employed for the description of the structure.

The various listings of the symmetry operations of the MSG types, which are available on the internet, are all coincident, and some of them are computer readable. They can therefore be considered as the *standard* or reference setting of the MSGs [see point (vi) below]. However, the unit cell and origin

(henceforth *basis*) used for the description of a magnetic structure often does not correspond to the standard setting of its MSG. Therefore, in such cases the identification of the MSG should not be limited to the assignment of the symbol and/or numerical index of the corresponding MSG type. In addition, enough information should be given to communicate unambiguously the symmetry operations of the MSG in the current basis (the basis being used in the description). The simplest way to do this is to supplement the MSG symbol with the transformation from the current basis to that of the *standard* setting of the MSG, which can then be used (inversely) to transform the listed operations of the MSG type in the standard setting to the current setting.

When the structural description employs a non-standard setting of the MSG, in order to prevent any misunderstanding, it is also recommended that the MSG symmetry operations for the current basis be also listed explicitly. As these two forms of defining the MSG of the structure are redundant, they allow a possible crosscheck of their mutual consistency.

(iv) In the case that alternative magnetic orderings with different MSGs are equally compatible with the available data, the structure should be reported making an arbitrary choice among the possible MSGs, preferably an MSG of maximal symmetry, though the other possible MSGs should also be indicated.

In some cases, due to limitations of the experimental data, alternative spin arrangements with different MSGs may fit the data equally well. One should be aware that these different possible MSGs generally imply physically non-equivalent phases. Typical examples are systems with a uniaxial paramagnetic phase, where the absolute orientation of the atomic magnetic moments on the basal plane remains undetermined, single-**k** or multi-**k** models equally fitting the data, or magnetic modulations with a propagation vector inside the Brillouin zone, such that the actual spin arrangement depends on the global phase of the modulation, to which the magnetic diffraction is insensitive. If no additional argument exists to make preferable one of the possible solutions, one is then obliged to make an arbitrary choice among the possible MSGs. We recommend, in such a case, choosing an arrangement corresponding to an MSG of higher symmetry. However, the arbitrariness of this choice and details of any other possible MSGs should be communicated clearly. These alternative MSGs may imply, for instance, rather different macroscopic properties, which could be investigated by other means to resolve the ambiguity in future work.

(v) A magnetic structure can be described using its MSG, as a direct generalization of the well established methodology of ordinary crystallography, *i.e.* a crystallographic description. This approach is simple, compact, unambiguous and robust. These guidelines are based on this method, which is also the basis for the magCIF format.

In the same way as it is done for ordinary structures, a commensurate magnetic structure can be described using its symmetry group (*i.e.* its MSG) to reduce the listing of atomic positions and magnetic moments to a set of symmetry-independent atoms, the so-called asymmetric unit. The atomic positions and magnetic moments of the remaining atoms can be generated by applying the symmetry operations of the MSG.

In the case of atoms in the asymmetric unit that lie at some special position, the MSG also determines their symmetry constraints, both for their positions and their magnetic moments. In this way, all new degrees of freedom, both magnetic and structural ones, present in the magnetic phase as a consequence of the symmetry loss caused by the magnetic ordering, become explicit.

(vi) There are two alternative settings and notations for the MSG types that can be considered standard: the Belov–Neronova–Smirnova (BNS) and the Opechowski–Guccione (OG) notations.

The listings of the operations in these two alternative notations of each MSG type are readily accessible in Litvin (2013) for the OG setting, and both in the BNS and OG settings in resources like *ISOSPACEGROUP* in the *ISOTROPY* Software Suite (Stokes *et al.*, 1995) and *MGENPOS* in the Bilbao Crystallographic Server (Perez-Mato *et al.*, 2015). These Tables are also available in *ISO_MAG* (Stokes *et al.* (1995) and we take them as the standard setting for the MSGs. The magCIF dictionary supports both settings, so that magnetic CIF files can, in principle, be produced using either of the two settings and notations, which only differ in the description of MSGs of type 4.

For MSGs of type 4 (*i.e.* those groups having translations combined with time reversal – the so-called anti-translations), the OG description employs a unit cell, which does not generate the periodic lattice possessed by the structure when the magnetic degrees of freedom are considered. This breaks with a key convention of ordinary crystallography, thereby making more difficult the development of appropriate software via simple extensions of crystallographic software tools available for non-magnetic structures. This problem does not arise with BNS settings, which is probably the reason why all major software tools that employ magnetic space groups in the analysis and/or description of magnetic structures support only the BNS description. For this reason, and to keep this report as simple as possible, the present guidelines will only consider the BNS settings for the MSGs.

In the future, new software may be developed and/or currently available software may be upgraded to support OG settings and notation, in which case, these guidelines can be easily adapted and extended to include them.

(vii) Unified (UNI) symbols for MSG types have been proposed recently as a new step towards standardizing MSG use.

These new symbols, together with the numerical indices of the BNS notation, are intended as unified labels for the MSG types, independent of the use of the BNS or OG setting (Campbell *et al.*, 2022). The UNI symbols resolve some weaknesses of the two traditional notations, being transparent in all cases about the underlying magnetic point groups (MPGs) and about their differences from ordinary space groups. It is therefore expected that in the future these UNI

symbols will be generally adopted. In the present guidelines, for the sake of clarity, they are included in the examples alongside the traditional BNS symbol.

(viii) An explicit statement about the magnetic point group (MPG) of the reported structure is recommended, although this information can be derived from the MSG.

The magnetic point group (MPG) associated with an MSG can be trivially derived from the knowledge of the MSG symmetry operations. The MPG alone determines the symmetry constraints of all crystal tensor properties, and some of these properties, primarily the basic ones, can be directly inferred from the MPG label and the orientations of the MPG operations with respect to the basis being used. The MPG, compared with the point group of the paramagnetic phase is also the basis for deriving the possible orientational domain states of the crystal and the switching properties of any tensor property. It is therefore convenient that the report of a magnetic structure includes the explicit statement of its MPG.

(ix) The report of a magnetic structure is incomplete without information about the positions of the non-magnetic atoms.

The MSG of a magnetic structure, and therefore its properties, depends in general on the positions of the non-magnetic atoms. The report of a commensurate magnetic structure should therefore specify not only the positions and moments of the magnetic atoms, but also the positions (at least approximate) of the non-magnetic ones. Hence, the crystalline arrangement of all the atoms should be indicated. This crystalline structure is often termed *nuclear structure*, or *chemical structure*. Here we will simply denote it as *crystal structure*, in the sense that it defines the atomic positional crystalline arrangement present in the magnetic structure. In the crystallographic description recommended in this report both the crystal structure and the spin arrangement are described within a unique framework, applying the MSG of the system.

This means that in the frequent case where the positions of the non-magnetic atoms have not been necessary for determining the spin arrangement, the crystal structure should however be part of the report, even if it is only approximate and corresponds to a different temperature, run, sample or literature work. At the very least, a specific literature reference to the assumed crystal structure should be provided.

(x) The MSG of a magnetic structure not only describes the symmetry of the arrangement of the magnetic moments, but it is also the symmetry group that constrains the non-magnetic degrees of freedom, as for instance lattice strain and atomic positions.

This means that in many cases, the symmetry loss caused by the magnetic ordering reduces the symmetry constraints on the non-magnetic degrees of freedom as well. This is, for instance, the ultimate origin of the magnetically induced ferroelectricity observed in type II multiferroics, and it is also the cause of some 'concomitant' structural transitions, which are in fact induced magneto-structural effects.

If the crystal structure is described under the MSG of the system, as recommended in these guidelines, all possible new structural degrees of freedom that are released by the magnetic ordering become explicit, showing in particular the resulting Wyckoff site splitting of both magnetic and non-magnetic atoms and the symmetry-allowed lattice strain. This should be the starting point of any quantitative investigation of possible magneto-structural effects.

(xi) Magnetic-induced structural effects are often too weak to be observed, which has previously encouraged separate descriptions of the magnetic and non-magnetic parts of the magnetic structure. Because such a separation hampers portability, both non-magnetic and magnetic structural details should be communicated within a common crystallographic framework, as recommended in these guidelines.

Structural effects induced by magnetic ordering are often weak enough to be neglected, such that the crystal structure can be approximated by that of the paramagnetic phase or its space group can be assumed within experimental resolution to be still valid in the magnetic phase, independently of the symmetry loss produced by the magnetic ordering. This allows, when fitting the diffraction data, a handy separation of the magnetic and non-magnetic parts, as if they were 'two phases'. This *two-phase* separation has also been traditionally maintained in the final description of the magnetic structure. This separation however hampers the portability of the model and its use in other studies, such as DFT calculations. For any practical use, the *two-phase* information must be somehow merged in a common framework and treated as a *single* phase, which it really is. It is therefore recommended, independently of the method employed for the determination of the structure, to avoid the two-phase description and instead report the crystal structure within the same framework as the spin arrangement, *i.e.* under its MSG in the crystallographic form described by these guidelines. As explained in point (x) this allows one to explicitly indicate which non-magnetic structural constraints are relaxed due to the magnetic ordering, even if these changes are negligible within the resolution of the structure-determination experiment.

If for any reason, the crystal structure is described separately from the spin arrangement, then the report must include the setting transformation that relates the basis (unit cell and origin) used for the crystal structure and its space group to the basis used for the spin arrangement and its MSG.

(xii) Group-representation analysis should be considered as a complement rather than an alternative to the crystallographic description of a magnetic structure under its MSG.

The group-representation method, which employs spin basis modes (or vectors) adapted to the irreducible representations (irreps) of the parent space group (usually the space group of the paramagnetic structure), is a powerful and systematic way to explore and enumerate possible spin arrangements. The early existence of efficient computer programs applying this method has facilitated its extensive use in the determination and description of magnetic structures. In contrast, the lack of data and software infrastructure for magnetic symmetry groups greatly limited the adoption of the crystallographic description of magnetic structures. Fortunately, there are now a variety of powerful and freely accessible computer tools that support the investigation of any

commensurate magnetic structure using a complementary and self-consistent combination of both magnetic symmetry groups and group-representation analysis.

(xiii) The crystallographic description of a magnetic structure under its MSG does not require a comparison with any other structure, while the description in terms of irrep basis modes is based on a comparison with a specified non-magnetic parent structure.

The determination of a magnetic structure usually starts from the knowledge of the corresponding paramagnetic structure, which provides a natural reference or *parent structure*, from which to characterize the magnetic ordering. However, once the magnetic structure has been determined, it can be described in a crystallographic form, as recommended in these guidelines, without reference to any other structure.

The crystallographic description under an MSG is a straightforward standalone description, while a group-representational description in terms of irrep spin basis vectors is inherently a comparison against a parent paramagnetic structure. In fact, once the magnetic structure is defined under its MSG, its group-representational description can be derived if a parent structure is specified.

For most magnetic structures, the MSG is only compatible with a single irrep of its parent paramagnetic space group [see the next point (xiv)]. In the most general case, however, the MSG of the structure may permit contributions from multiple irreps. Commonly, some of the MSG-compatible irreps do not contribute to the observed spin arrangement, and as a consequence, the magnetic structure has additional spin correlations which cannot be explained by its MSG. These are precisely the situations where the crystallographic description is best complemented by the additional presentation of irrep basis vectors. In such cases, the joint use of an MSG and irrep basis vectors provides a more complete description of a magnetic structure.

Any irrep that must necessarily contribute to the spin arrangement in order to reduce the symmetry of the crystal from the parent paramagnetic space group down to the observed MSG are called *primary*. The remaining MSG-compatible irreps, which may also be present in the spin arrangement under the constraints of the MSG, but are not necessary to arrive at the MSG, are termed *secondary*, since if present, they can usually be considered as secondary effects.

It is important to remark that although the choice of the paramagnetic parent structure is in most cases obvious, it is formally not unique, and in the case of materials with several paramagnetic phases or with a paramagnetic phase having some pseudo-symmetry, it can be a matter of choice.

(xiv) The MSGs of most commensurate magnetic structures are only compatible with a single irrep of the parent paramagnetic space group, and for these structures, the crystallographic description is especially advantageous.

Most magnetic structures have spin arrangements associated with a single irrep of the parent space group, and in a majority of these cases, the resulting MSG is only compatible with this specific irrep. This means that all other irreps are forbidden by the symmetry constraints defined by the MSG. In other words, these structures have MSGs, which automatically force their spin arrangements to comply with one and only one irrep of the parent space group. About 80% of the roughly 1900 commensurate magnetic structures in the MAGNDATA database are in this category.

In the case that the irrep compatible with the MSG is one-dimensional, so the irrep is necessarily real, there is a one-to-one correspondence between the free parameters of the crystallographic and group-representational descriptions. The crystallographic description is, however, more self-contained and straightforward to communicate to a broad audience.

In the case of a magnetic structure for which the only MSG-allowed irrep is multi-dimensional (*i.e.* the dimension is greater than 1), a variety of possible alternative MSGs might be possible depending on the 'direction' of the corresponding multi-dimensional magnetic order parameter (*i.e.* the specific linear combination of basis vectors of that irrep). In other words, the MSG of the structure depends on how the irrep's multiple basis vectors are combined. For such structures, the crystallographic description of the spin arrangement under its MSG generally requires fewer parameters than a group-representational description under the relevant multi-dimensional irrep.

Thus, in the very common case of an MSG that is compatible with only one magnetic irrep (either one-dimensional or multi-dimensional), the crystallographic description is especially preferred, even if the magnetic structure was originally determined using the group-representation method. Of course, the crystallographic description can always be supplemented with group-representational information.

(xv) When the MSG of the magnetic structure is compatible with more than one irrep, the combined use of the MSG and the spin basis vectors of these irreps is a more efficient and complete way to describe the structure.

If more than one irrep of the parent space group is compatible with the MSG of the magnetic structure, the magnetic degrees of freedom allowed by the MSG can be decomposed into contributions from these compatible irreps. In such cases, each irrep spin basis vector imposes constraints on the magnetic moments of the atoms within the asymmetric unit and/or some correlation amongst them, which are not enforced by the MSG itself. These are sufficient to define the irrep spin basis vector, because any additional relations with the magnetic moments of other atoms out of the asymmetric unit, which complete the spin arrangement of the spin basis vector, are taken into account by the symmetry relations enforced by the MSG.

Consequently, as mentioned in point (xiii), if only one of the several MSG-compatible irreps is active (something that happens quite often), the restriction of the magnetic arrangement to the spin basis vectors of this irrep implies additional constraints beyond those of the MSG. These additional restrictions, which decrease the number of parameters necessary to describe the spin arrangement, become explicit when the irrep basis vector(s) are invoked as a complement to the crystallographic description under the MSG.

(xvi) Commensurate magnetic structures with a propagation vector that allows magnetic odd harmonics necessarily have an MSG compatible with more than one irrep. The additional degrees of freedom corresponding to any higher harmonics are automatically included in the crystallographic description under its MSG.

The MSG description of a magnetic structure automatically includes all the degrees of freedom, which are released by the magnetic ordering as possible induced effects. This includes the possible presence of higher harmonics in the magnetic ordering. This happens for instance when the propagation vector **k** of the magnetic arrangement is such that 3**k** is not equivalent to **k**. In such cases, the MSG generally splits the magnetic-atom sites with respect to the parent space group so that some atomic magnetic moments become symmetry independent, which would otherwise be correlated if the magnetic arrangement were restricted to a single harmonic wave of the observed propagation vector.

These structures are examples where the MSG is compatible with more than one irrep, as the higher harmonics are necessarily associated with irreps that are different from that of the primary modulation. The MSG necessarily allows them, as they are possible secondary induced effects. The additional correlations coming from the restriction to the primary harmonic become explicit if the crystallographic description is complemented with the definition of the irrep basis vectors for all MSG-compatible irreps and the values of their amplitudes are given.

(xvii) There are two alternative labeling systems for the irrep notation, which are robust and unambiguous. It is recommended to use one of them. We advise against labeling the irreps arbitrarily or according to labels arbitrarily assigned by some programs.

There are two irrep notation systems, which are widely used and well supported in terms of software and documentation. The Cracknell, Davies, Miller and Love (CDML) irrep notation, originating in the tables of Cracknell *et al.* (1979), is presently used by many programs, including the *ISOTROPY* Software Suite (Stokes *et al.*, 1995), the Bilbao Crystallographic Server (Perez-Mato *et al.*, 2015), *JANA2020* (Petříček *et al.*, 2023), some options of *FullProf* (Rodríguez-Carvajal, 1993), *etc*. If one is working with a specific irrep with an arbitrary label, the equivalent CDML label can be easily identified by comparing the characters of a set of generators of the parent space group to those in the character tables under the CDML notation, which are readily accessible via resources like REPRESENTATIONS SG in the Bilbao Crystallographic Server (Perez-Mato *et al.*, 2015) or ISO-IR (Stokes *et al.*, 2013) in the *ISOTROPY* Software Suite (Stokes *et al.*, 1995).

The other robust and unambiguous irrep labeling system comes from the book by Kovalev (1965, 1993), which was transformed into digital form and is available in the program *SARAh* (Wills, 2000). Recently the *ISOTROPY* Software Suite has made available the mapping between the Kovalev and the CDML notations, both as listings and as computer readable files, such that the two notations can be easily interchanged.

If unfamiliar or arbitrary irrep labels are ultimately employed, the information is incomplete unless one also lists the irrep(s) characters for a set of generators of the parent space group. Otherwise, the arbitrary irrep labels are essentially useless to the reader.

(xviii) To avoid confusion with the irreps associated with non-magnetic distortions, and for the sake of a more comprehensive notation, the labeling of the irreps associated with magnetic orderings should explicitly indicate its odd character for time reversal, *i.e.* as irreps of the gray magnetic space group associated with the parent paramagnetic phase.

The traditional use of irreps of the non-magnetic parent space group to describe the transformation properties of magnetic orderings ignores an important additional transformation property of these distortions, namely its odd character with respect to time reversal. This contrasts, for instance, with the transformation properties of phonon modes, which are even under time reversal. If the transformation properties of a phonon mode and a spin mode were indeed described by the same irrep, they could couple bilinearly in the paramagnetic phase, which is physical nonsense.

Therefore, it is recommended to declare the irreps associated with a spin arrangement as belonging to the gray magnetic space group of the paramagnetic phase (not to the corresponding non-magnetic space group), and therefore explicitly possessing an odd character under time reversal. This is accomplished simply by adding an 'm' to the front of the usual irrep label. For instance, the irrep label X_1 becomes mX_1. This change of notation in the irrep labeling of magnetic distortions was initially introduced within the *ISOTROPY* Software Suite (Stokes *et al.*, 1995) and it is now used by many other computer tools. This simple change of notation makes it possible to consider together unambiguously both magnetic and non-magnetic distortions and to classify them consistently within a common framework.

(xix) The specific irrep or set of irreps associated with a magnetic arrangement may depend on the way the parent structure is described, in particular on the choice of origin.

The irrep or irreps associated with the spin arrangement in a magnetic structure may depend on the origin of the unit cell chosen for the description of the paramagnetic parent structure. This typically happens in the case of non-zero propagation vectors because a change of origin, compatible with the standard setting of the parent space group, generally interchanges some group operations though the corresponding irrep matrices describing the associated transformation properties of the spin arrangement cannot change. This mathematically implies in general a different mapping between the operations of the group and the matrices, and therefore a different irrep. Hence, even using a standard setting for the parent space group, the active irrep or irreps describing the observed spin arrangement may change depending on the way the parent structure is described. For example, in the case of space group $Pm\bar{3}m$, the choice to place the magnetic atom at the origin or at $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ will in general imply the association of a different irrep or irreps to the same spin arrangement, if it has a non-zero propagation vector.

(xx) Any magnetic ordering is described by real (not complex) atomic magnetic moments, and therefore necessarily transforms according to a real representation of the parent symmetry group. Complex irreps cannot describe the transformation properties of a commensurate magnetic arrangement.

This means that in the case of a complex irrep $m\tau$, the representation to be considered for the description of the transformation properties of a spin arrangement must be the direct sum of the pair of complex conjugate irreps: $m\tau+m\tau^*$, *i.e.* the so-called *physically irreducible* representation $m\tau\tau^*$. It should therefore be stressed that it is mathematically and physically incorrect to assign one (or more) complex irreps to a magnetic arrangement, without also including the corresponding complex conjugate irreps.

The CDML notation, extended to time-odd irreps, employs labels with one or more repeated letters, like mU_1U_3, mGM_2GM_3 or mA_1A_1, to indicate that two mathematical complex conjugated irreps are being added to produce a physically irreducible representation. In the case of a pseudo-real irrep label, such as mA_1A_1, the complex irrep and its complex conjugate are equivalent so that both the letter and its subscript are repeated.

(xxi) If a magnetic ordering has a single propagation vector k, and if k and −k are inequivalent, then −k is necessarily also involved in the spin arrangement, and both vectors must be considered when irrep basis functions are constructed.

When the propagation vector **k** of the magnetic ordering is not translationally equivalent to −**k** under the symmetry operations of the parent paramagnetic space group, it has traditionally been assumed that atomic sites related by a parent symmetry operation that switches **k** with −**k** have independent irrep spin basis vectors. This is not correct. The irrep spin basis vectors of these assumed 'split' atomic sites are necessarily correlated to satisfy the transformation properties defined by a single irrep. These correlations, when refined using irrep spin basis vectors, have usually been introduced *a posteriori*, either *ad hoc* or as the result of the refinement process; but in fact, they are inherent to the relevant irrep, and are automatically introduced in a crystallographic description via the corresponding MSG.

When **k** and −**k** are not related by a symmetry operation of the parent space group, the irreps associated with **k** and −**k** are distinct and are complex conjugates of one another, so that a physically irreducible irrep is constructed as their direct sum [as described in point (**xx**) above].

In the case where the symmetry operations of the parent space group transform a propagation vector **k** into non-equivalent vectors distinct from −**k**, the full irrep includes all these symmetry-related propagation vectors, and as a consequence, multi-**k** spin arrangements are possible for a single irrep. These possible multi-**k** models associated with a single irrep and their MSGs can be readily obtained from the mentioned internet resources, which combine the use of magnetic space groups and representation analysis, and generally allow higher symmetries than the possible single-**k** models.

3. How to report a commensurate magnetic structure under its magnetic space group

Here we list the items required for a complete and unambiguous report of a commensurate magnetic structure in a crystallographic form under its MSG, and the representation-analysis information that may complement this description. For the sake of simplicity these guidelines only use the BNS setting for an MSG, which is the one generally supported by available software resources. The extension to a description using the OG setting is rather straightforward.

The necessary items in the description of a magnetic structure under its MSG are analogous to those necessary for the crystallographic description of a non-magnetic structure. The assignment of an MSG permits one to reduce the listing of atomic positions and magnetic moments to those of an 'asymmetric unit', all other atomic positions and magnetic moments being trivially generated by application of the MSG symmetry operations.

As illustrative examples, Tables 1 and 2 describe the magnetic structures of $Dy_2Co_3Al_9$ and Mn_3Sn in the crystallographic recommended form, with Tables 3 and 4 complementing this description with additional representation analysis information. These structures were reported by Gorbunov *et al.* (2018) and Brown *et al.* (1990), respectively, and their magCIF files can be retrieved from MAGNDATA (Gallego *et al.*, 2016*b*) (entries 1.267 and 0.199). The MSG of $Dy_2Co_3Al_9$ is compatible with only one irrep of the parent paramagnetic space group, while Mn_3Sn is an example of the less frequent case, where the MSG is compatible with more than one irrep. They are representatives of the two different basic situations, which are possible when MSG symmetry and representation analysis are applied together.

The items listed below are divided in two sets:

(*a*) Crystallographic information sufficient to describe the magnetic structure itself, complemented by basic information on the relationship between the magnetic structure and its parent paramagnetic structure. These items (§3.1.1–§3.1.13) are all supported by the magCIF format (examples given in Tables 1 and 2).

(*b*) Detailed representation-analysis information relating the magnetic structure to its parent paramagnetic structure. These items (§3.2.1–§3.2.6) are not yet supported by the magCIF format (examples given in Tables 3 and 4).

3.1. Crystallographic information (examples in Tables 1 and 2)

3.1.1. Parent space group

Symbol of the space group of the parent paramagnetic structure. If the parent space group is being considered in a non-standard setting, the details of this setting should be clearly indicated. In the case of space groups with alternative standard settings that vary the origin, the choice made should be explicitly mentioned. Origin choice 2 (inversion center at the origin) is strongly recommended, as it is taken as the default by most programs.

Table 1
Magnetic structure of $Dy_2Co_3Al_9$ (Gorbunov *et al.*, 2018) described under its MSG (crystallographic description), with basic information about its relation with its parent paramagnetic structure.

All entries in the table are supported by the magnetic CIF (magCIF) format.

Compound	$Dy_2Co_3Al_9$ (MAGNDATA #1.267)	
Parent space group	*Cmcm* (No. 63)	
Propagation vector(s)	$(0, 0, \frac{1}{2})$	
Transformation from parent basis to the one used	(**a**, **b**, 2**c**; 0, 0, 0)	
MSG symbol	A_amm2 (UNI: $Amm2.1'_a$)	
MSG number	38.192	
Transformation from basis used to standard setting of MSG	(**c**, **a**, **b**; 0, 0, $-\frac{1}{8}$)	
Magnetic point group	$mm2.1'$ (**c**, **a**, **b**) or $m2m.1'$	
Unit-cell parameters (Å, °)	a = 12.72390, α = 90	
	b = 7.45860, β = 90	
	c = 18.59880, γ = 90	
MSG symmetry operations	$x, y, z, +1$	$\{1 \mid 0, 0, 0\}$
	$-x, y, -z+\frac{3}{4}, +1$	$\{2_{010} \mid 0, 0, \frac{3}{4}\}$
	$-x, y, z, +1$	$\{m_{100} \mid 0, 0, 0\}$
	$x, y, -z+\frac{3}{4}, +1$	$\{m_{001} \mid 0, 0, \frac{3}{4}\}$
MSG symmetry centering operations	$x, y, z, +1$	$\{1 \mid 0, 0, 0\}$
	$x+\frac{1}{2}, y+\frac{1}{2}, z, +1$	$\{1 \mid \frac{1}{2}, \frac{1}{2}, 0\}$
	$x, y, z+\frac{1}{2}, -1$	$\{1' \mid 0, 0, \frac{1}{2}\}$
	$x+\frac{1}{2}, y+\frac{1}{2}, z+\frac{1}{2}, -1$	$\{1' \mid \frac{1}{2}, \frac{1}{2}, \frac{1}{2}\}$
Positions of magnetic atoms	Dy1_1 Dy 0.33940 0.33290 0.12500	
	Dy1_2 Dy 0.66060 0.66710 0.37500	
Positions of non-magnetic atoms	Co1 Co 0.32880 0.00000 0.00000	
	Co2 Co 0.00000 0.00000 0.00000	
	Al1_1 Al 0.00000 0.1249 0.125	
	Al1_2 Al 0.00000 0.8751 0.375	
	Al2_1 Al 0.1079 0.4459 0.125	
	Al2_2 Al 0.8921 0.5541 0.375	
	Al3_1 Al 0.0000 0.3322 0.2714	
	Al3_2 Al 0.00000 0.6678 0.5214	
	Al4_1 Al 0.1686 0.3330 0.03585	
	Al4_2 Al 0.8314 0.6670 0.28585	
Magnetic moment components (μ_B) of magnetic atoms, symmetry constraints and moment magnitudes	Dy1_1 1.34 (2) 8.35 (2) 0.0 (m_x, m_y, 0) 8.46 (2)	
	Dy1_2 0.0 0.0 1.38 (1) (0, 0, m_z) 1.38 (1)	

Table 2
Magnetic structure of Mn_3Sn (Brown *et al.*, 1990) described under its MSG (crystallographic description), with basic information about its relation with its parent paramagnetic structure.

All entries in the table are supported by the magnetic CIF (magCIF) format.

	Mn_3Sn (MAGNDATA #0.199)	
Parent space group	$P6_3/mmc$ (No. 194)	
Propagation vector(s)	(0, 0, 0)	
Transformation from parent basis to the one used	(**a**, **b**, **c**; 0, 0, 0)	
MSG symbol	$Cmc'm'$	
MSG number	63.463	
Transformation from basis used to standard setting of MSG	(−**b**, 2**a**+**b**, **c**; 0, 0, 0)	
Magnetic point group	$m'm'm$ (2**a**+**b**, **c**, −**b**)	
Unit-cell parameters (Å, °)	a = 5.665, α = 90	
	b = 5.665, β = 90	
	c = 4.531, γ = 120	
MSG symmetry operations	$x, y, z, +1$	$\{1 \mid 0, 0, 0\}$
	$-x, -x+y, -z, +1$	$\{2_{010} \mid 0, 0, 0\}$
	$-x, -y, -z, +1$	$\{-1 \mid 0, 0, 0\}$
	$x, x-y, z, +1$	$\{m_{010} \mid 0, 0, 0\}$
	$x, x-y, -z+\frac{1}{2}, -1$	$\{2'_{210} \mid 0, 0, \frac{1}{2}\}$
	$-x, -y, z+\frac{1}{2}, -1$	$\{2'_{001} \mid 0, 0, \frac{1}{2}\}$
	$-x, -x+y, z+\frac{1}{2}, -1$	$\{m'_{210} \mid 0, 0, \frac{1}{2}\}$
	$x, y, -z+\frac{1}{2}, -1$	$\{m'_{001} \mid 0, 0, \frac{1}{2}\}$
Positions of magnetic atoms	Mn1_1 Mn 0.8388 0.6776 0.25	
	Mn1_2 Mn 0.3224 0.1612 0.25	
Positions of non-magnetic atoms	Sn1 Sn 0.33333 0.66667 0.25	
Magnetic moment components (μ_B) of magnetic atoms, symmetry constraints and moment magnitudes	Mn1_1 3.00 (1) 3.00 0.0 (m_x, m_y, 0) 3.00 (1)	
	Mn1_2 0.0 −3.00 0.0 (0, m_y, 0) 3.00 (1)	

3.1.2. Propagation vector(s)

Wavevector(s) associated with the spin arrangement. The spin arrangement of any magnetic structure can be considered as a modulated disposition of the atomic magnetic moments with respect to the parent structure according to one or more reciprocal-space wavevectors, which can be zero in the simplest case. These so-called *propagation vectors* of the magnetic structure should be expressed as unitless relative components with respect to the conventional reciprocal unit cell of the parent space group.

In the example given in Table 1, the propagation vector is $(0, 0, \frac{1}{2})$, which implies a doubling of the unit cell for the lattice periodicity of the MSG (see §3.1.3), while it is (0, 0, 0) in the case of Table 2, where the lattice periodicity of the parent phase is maintained.

3.1.3. Transformation from parent basis to the basis of the magnetic structure

Transformation of the basis (unit cell and origin) of the parent space group to the *current* basis used for the description of the magnetic structure (see §3.1.8). This transformation can include not only a change of the unit cell vectors, but also an origin shift, which should be expressed in unitless relative components with respect to the conventional unit cell of the parent space group. Because this transformation can be combined with any operation of the MSG, it is in general not unique.

In the example given in Table 1, this transformation is (**a**, **b**, 2**c**; 0, 0, 0), *i.e.* the origin and orientation of the unit-cell parameters in the *Cmcm* parent space group are maintained, except for the **c** parameter, which is necessarily doubled, due to the propagation vector $(0, 0, \frac{1}{2})$ of the magnetic ordering.

In the example given in Table 2, this transformation is the identity, because the magnetic propagation vector is null. Although the MSG in its standard setting is C-centered orthorhombic, the parent primitive unit cell and origin are also used for the description of the magnetic structure in order to facilitate the comparison with the paramagnetic hexagonal structure.

Table 3
Representation analysis of the magnetic structure of $Dy_2Co_3Al_9$, which complements the crystallographic description in Table 1.

This is a typical case, where only one irrep of the parent space group is compatible with the MSG of the structure. In such cases, the irrep constraints are fully taken into account by the MSG. irrep spin basis vectors or modes are not necessary.

	$Dy_2Co_3Al_9$
Primary irrep(*s*) label(s) with dimension	mZ1 (two-dimensional) (special direction)
Description of the primary irrep	mZ1: $\{2_{001} \mid 0, 0, \frac{1}{2}\}$: (0, −1; 1, 0) $\{2_{010} \mid 0, 0, \frac{1}{2}\}$: (1, 0; 0, −1) $\{-1 \mid 0, 0, 0\}$: (0, −1; −1, 0) $\{1 \mid 0, 0, 1\}$: (−1, 0; 0, −1) $\{1 \mid 0, 1, 0\}$: (1, 0; 0, 1) $\{1 \mid 1, 0, 0\}$: (1, 0; 0, 1) $\{1 \mid \frac{1}{2}, \frac{1}{2}, 0\}$: (1, 0; 0, 1)
Secondary irrep(*s*) label(s)	Not allowed

Table 4
Representation analysis of the magnetic structure Mn_3Sn (Brown *et al.*, 1990), which complements its crystallographic description in Table 2.

This is an example, where more than one irrep, namely two irreps of the parent space group, are compatible with the MSG of the structure. One of them is observed, being responsible for the symmetry break (primary irrep), while the other one corresponds to a possible induced effect (secondary irrep). The magnetic arrangement described in Table 2 is decomposed into components associated with the two irreps. The irrep basis modes are defined describing the corresponding additional constraints and/or correlations for the atoms in the asymmetric unit of the crystallographic description.

	Mn_3Sn
Primary irrep(*s*) label(s) with dimension	mGM6+ (two-dimensional) (special direction)
Description of primary irrep(*s*)	mGM6+: $\{6_{001} \mid 0, 0, \frac{1}{2}\}$: $(\frac{1}{2}, -\sqrt{\frac{3}{2}}, \sqrt{\frac{3}{2}}, \frac{1}{2})$ $\{-1 \mid 0, 0, 0\}$: (1, 0; 0, 1) $\{m_{010} \mid 0, 0, 0\}$: $(\frac{1}{2}, \sqrt{\frac{3}{2}}, \sqrt{\frac{3}{2}}, -\frac{1}{2})$
Secondary irrep(*s*) label(s) with dimension	mGM3+ (one-dimensional)
Description of secondary irrep(*s*)	mGM3+: $\{6_{001} \mid 0, 0, \frac{1}{2}\}$: −1 $\{-1 \mid 0, 0, 0\}$: 1 $\{m_{010} \mid 0, 0, 0\}$: 1
Primary basis mode(s) and amplitude(s) C_i (in μ_B)	mGM6+, mode 1: Mn1_1 (1, 1, 0) C_1 = 3.00 (1) Mn1_2 (0, −1, 0) mGM6+, mode 2: Mn1_1 (0, 1, 0) C_2 = 0.0 Mn1_2 (0, 1, 0)
Secondary basis mode(s) and amplitude(s) C_i (in μ_B)	mGM3+, mode 3: Mn1_1 (1, 0, 0) C_3 = 0.0 Mn1_2 (0, 1, 0)

3.1.4. MSG symbol

Symbol in the BNS notation of the MSG of the magnetic structure. MSG symbols and their numerical indices in the BNS notation, and listings of the corresponding symmetry operations in their standard setting, can be found in the *ISOTROPY* Software Suite (Stokes *et al.*, 1995) and in the Bilbao Crystallographic Server (Perez-Mato *et al.*, 2015). Alternatively, or as a complement, the UNI symbol (Campbell *et al.*, 2022), also available in these resources, can be used. Another complementary symbol that may be provided is the magnetic Hall symbol (González-Platas *et al.*, 2021).

The MSG of the example given in Table 1 is of type 4, where UNI symbols differ considerably from those in the BNS notation. In this case, the UNI symbol $Amm2.1'_a$ makes explicit that the time-reversal operation is part of the magnetic point group. In the example of Table 2, the MSG is of type 3, and in this case, the BNS, OG and UNI symbols coincide.

3.1.5. MSG numerical index

It is recommended to include as an additional very robust identification of the MSG, its numerical index in the BNS setting (Stokes *et al.*, 1995; Perez-Mato *et al.*, 2022), which is also used in the UNI notation.

3.1.6. Transformation to standard setting of the MSG

In the case that the MSG is not employed in its standard setting, the MSG symbol should be complemented with the transformation from the current basis of the MSG (unit-cell vectors and origin used in the magnetic-structure description) to a basis where the MSG acquires its BNS standard setting. This transformation must include not only the relation of the unit-cell vectors in the standard setting with those being used, but the required origin shift, which should be expressed in unitless relative components with respect to the current unit cell. Generally, there may be more than one transformation possible and it is sufficient to indicate one of them. If no transformation accompanies the MSG, the standard setting of the MSG is to be assumed.

In the example given in Table 1 the transformation (**c**, **a**, **b**; 0, 0, $-\frac{1}{8}$) means that the MSG would take its standard form if the unit-cell parameters $\mathbf{a}_s$, $\mathbf{b}_s$, $\mathbf{c}_s$ were chosen as $\mathbf{a}_s = \mathbf{c}$, $\mathbf{b}_s = \mathbf{a}$, $\mathbf{c}_s = \mathbf{b}$, and the origin were located at $-\frac{1}{8}\mathbf{c}$, where **a**, **b**, **c** are the vectors defining the current unit cell used.

In the example given in Table 2, the parent paramagnetic phase is hexagonal and the magnetic structure is orthorhombic. The MSG setting of $Cmc'm'$ employed here is related to the standard BNS setting of the MSG by transformation (−**b**, 2**a**+**b**, **c**; 0, 0, 0), as the parent hexagonal unit cell is used in the description of the magnetic structure. The transformation defines the standard C-centered orthorhombic unit cell of the MSG, embedded in the lattice generated by the oblique primitive unit cell being used. Notice that this primitive unit cell is symmetry-allowed to exhibit some strain, but in a restricted form to maintain the orthorhombic C-centered lattice (**a** and **b** must maintain equal lengths, but the β angle can deviate from 120°).

The transformation to standard in Table 1 implies we could have used the MSG symbol $Cm2m.1_c$ instead of $Amm2.1_a$, obviating the transformation of the unit-cell vectors, but this alternative setting still requires an origin shift $-\frac{1}{8}\mathbf{c}$, which should then be also indicated. In general, one can always use the standard symbol of the MSG and indicate unambiguously the transformation to its standard setting, including the necessary origin shift.

3.1.7. Magnetic point group symbol

Symbol of the magnetic point group (MPG) associated with the MSG of the structure. One system of labeling and numbering of MPGs, which can be taken as standard, can be found in Litvin (2013). Another option is the UNI MPG symbols from which the new UNI MSG symbols (Campbell *et al.*, 2022) are derived. The UNI MPG symbols are now used by a number of software tools including the *ISOTROPY* Software Suite (Stokes *et al.*, 1995) and the Bilbao Crystallographic server (Perez-Mato *et al.*, 2015).

The form of the operations of the MPG in the current basis may not coincide with those of its standard setting. Therefore, in such cases it is necessary to include additional information that defines the transformation from the current basis to one where the operations of the MPG acquire their standard form. For point groups only the transformation of the unit cell is relevant.

In the example of Table 1, the MPG is denoted as $mm2.1'$ (**c**, **a**, **b**), because the twofold axis is along **c** in the standard description of the MPG, as shown in its label, while in the current unit cell it is along **b**. In this simple case, one could use a modified label of the form $m2m.1'$, though one should be aware that such a setting-adapted labeling of the MPG is not always possible because the orientation of the MPG standard setting can be oblique with respect to the current basis. In these cases, an indication of the transformation to standard of the MPG cannot be avoided (see, for instance, Table 2). In accordance with the UNI notation, the MPG symbol in Table 1 includes a dot separating the $1'$ symbol.

In the example of Table 2, the MPG is denoted as $m'm'm$ (2**a**+**b**, **c**, −**b**), so that the transformation to standard differs from that given for the MSG because the standard orientation of the MPG differs from that implied by the standard setting of the MSG. We can immediately discern from the MPG symbol and its transformation to standard that the *b* axis of the current unit cell is perpendicular to the non-primed mirror plane, and therefore admits a ferromagnetic moment.

3.1.8. Unit-cell parameters

Parameters defining the unit cell of the magnetic structure. This is the current unit cell employed to describe the operations of the MSG, the coordinates of the atomic positions and the components of the magnetic moments. It is often denoted as *magnetic unit cell*. Since we are considering a BNS setting this unit cell generates a lattice that describes the periodicity for both the atomic magnetic moments and atomic positions. When employing a conventional-centered or otherwise a non-standard setting of the MSG that uses a supercell, the definition of the lattice must be completed with additional centering translations, as described below in §3.1.10.

It is important that this unit cell does not necessarily coincide with that of the parent paramagnetic structure. In Table 1, it is a supercell with the *c* unit-cell parameter doubled relative to that of the parent paramagnetic unit cell since its magnetic ordering has propagation vector $(0, 0, \frac{1}{2})$. In the example given in Table 2, the propagation vector is (0, 0, 0) so that the MSG and paramagnetic parent space group share the same unit cell.

3.1.9. MSG symmetry operations

In the case that the magnetic structure is described with its MSG in a non-standard setting, it is strongly recommended to include the listing of the representative symmetry operations of the MSG relative to its current unit cell as given in §3.1.8. This can be a full set of translationally inequivalent operations, but this listing can be reduced to a minimal set of generators, especially in the case of an MSG with a large number of operations.

The listed MSG symmetry operations must be consistent with the reported MSG (see §3.1.4 and §3.1.5) and the given transformation to the MSG standard setting (see §3.1.6). When this list is not at hand, one can generate it by simply inverting the given transformation and applying it to each of the standard-setting MSG operations. Thus, in principle, the list of operations itself is redundant with the information given according to §3.1.4 (or §3.1.5) and §3.1.6. Nevertheless, if the MSG is not being applied in its standard setting, this explicit list of MSG operations eliminates any possible ambiguity. In fact, an explicit list of MSG operations in the current basis is obligatory in the magCIF format, whereas the MSG symbol, MSG numerical index and transformation to standard setting are merely strong recommendations.

The set of symmetry operations to be listed can be shortened if the set of centering and anti-centering translations are listed separately (see §3.1.10). But, if desired, they can be listed together including all their possible combinations, as is done in the standard CIF description of ordinary space groups.

The notation of the symmetry operations in the examples of Tables 1 and 2 follows the magCIF format in describing a transformation of a generic point (x, y, z), along with a ± 1 to indicate whether the operation is time reversed (-1) or not $(+1)$. Generalized Seitz symbols (Glazer *et al.*, 1990) are also presented in these tables as a possible easily interpreted alternative, to be used instead of the (x, y, z) notation. Other notations may also be used, so long as the operations are unambiguously defined.

Note that Table 1 includes MSG operations with translational parts equal to $(0, 0, \frac{3}{4})$, while these same operations in the standard setting of this MSG have translational parts equal to (0, 0, 0). The reason is that in order to facilitate its comparison with the parent paramagnetic structure, the magnetic structure and therefore the MSG, is being described keeping the unit-cell orientation and origin of the parent space group *Cmcm*. This introduces non-standard translations in the MSG operations, which would acquire its standard form if the basis is changed according to the transformation indicated in §3.1.6, which includes an appropriate origin shift.

3.1.10. MSG symmetry-centering and anti-centering operations

List of all the symmetry operations that are fractional translations and anti-translations within the current unit cell if

there are any. An anti-translation is the combination of the time-reversal operation with a translation and is analogous to a glide mirror plane operation or a screw rotation. As anti-translations are not lattice translations, they do not belong rigorously to a list of true centering operations. However, the magCIF format, because of its simplicity, allows and encourages the presentation of both centering and anti-centering operations in the same list when using the BNS description.

When the unit cell of the MSG is a supercell of the paramagnetic parent unit cell, one can often achieve a simpler comparison with the parent structure by choosing an equivalent or larger supercell whose basis vectors are parallel to those of the parent cell. In many cases, this results in a non-standard setting of the MSG requiring the inclusion of non-standard centering and anti-centering translations.

In Table 1, because the MSG is of type 4, it has anti-centering operations, the simplest of which has the form $\{1' \mid 0, 0, \frac{1}{2}\}$. This combines with the C-centering translation $\{1 \mid \frac{1}{2}, \frac{1}{2}, 0\}$ to generate the other non-zero anti-centering operation, $\{1' \mid \frac{1}{2}, \frac{1}{2}, \frac{1}{2}\}$. Notice that this MSG $Amm2.1'_a$ in its standard setting is A-centered and has an anti-centering translation along **a**. In Table 1, however, it was convenient to choose a basis for the MSG that preserves the shape and orientation of the C-centered parent unit cell, except for the necessary doubling of the cell along **c**. A transformation to the standard setting of the MSG would instead require a permutation of the unit cell axes of the parent (see §3.1.6).

In Table 2, the MSG is of type 3 so that no anti-centering can exist. Nor does the list include any non-trivial centering translations despite the MSG ($Cmc'm'$) being C-centered. Once again, an MSG basis is being used that preserves the unit cell of the parent hexagonal paramagnetic structure, which is oblique and primitive. The C-centering translation would only appear in the list if the structure is described in the standard setting of the MSG, which has an orthogonal unit cell (see §3.1.6).

3.1.11. Positions of magnetic atoms

Atomic positions, in relative coordinates with respect to the current MSG basis, of all symmetry-independent magnetic atoms forming an asymmetric unit for the MSG. Any split sites that were symmetry related in the space group of the paramagnetic phase but are not related by symmetry operations of the MSG should be listed separately within the asymmetric unit. If the magneto-structural coupling is weak enough, as it is often the case, the positions of split sites can still be related within experimental accuracy by the parent space-group symmetry, but their magnetic moments and hence their positions are truly independent in the magnetic structure.

In the example of Table 1, the atom Dy1 in the asymmetric unit of the parent space group *Cmcm* splits into two independent magnetic atoms in the asymmetric unit of the MSG, Dy1_1 and Dy1_2. Their positions are within experimental accuracy related by an inversion center in the parent space group, which is lost due to the magnetic ordering, such that their positions are (x, y, z) and $(1 - x, 1 - y, \frac{1}{2} - z)$, respectively. But this correlation between the two sites coming from the parent space group is no longer symmetry protected. Something similar happens in the case of Table 2, where the two MSG-independent atomic sites, Mn1_1 and Mn1_2, were symmetry related in the hexagonal parent space group.

3.1.12. Positions of non-magnetic atoms

Atomic positions, in relative coordinates with respect to the current MSG basis, of all symmetry-independent non-magnetic atoms forming an asymmetric unit for the MSG. Any split sites that were symmetry related in the space group of the paramagnetic phase but are not related by the symmetry operations of the MSG should be listed separately within the asymmetric unit of the MSG. If the magneto-structural coupling is weak enough, as it is often the case, the positions of the split sites may still be related within experimental accuracy by the parent space-group symmetry. But this correlation between the split positions is no longer symmetry protected, and the description considering only the MSG is convenient, in order to explicitly present all the new structural degrees of freedom that are released by the symmetry break caused by the magnetic order.

In the example of Table 1, the Al sites in the asymmetric unit of parent space group *Cmcm* become split into two independent sites in the asymmetric unit of the MSG. The choice of the split sites in the asymmetric unit is not unique. For instance, the Al1_1 and Al1_2 atoms are related by the lost inversion operation, but the chosen Al4_1 and Al4_2 sites are related by the operation $\{2_{001} \mid 1, 1, \frac{1}{2}\}$ of the parent space group, which is also lost.

3.1.13. Magnetic moments of magnetic atoms and their MSG constraints

Magnetic moments of the magnetic atoms in the asymmetric unit of the MSG, as well as the MSG symmetry-constraints on these moments. It is recommended to parameterize the magnetic moments using vector components parallel to the crystallographic unit-cell axes (in Bohr magneton units). This description is presently supported by many software resources, including programs for structure refinement, analysis and visualization. The components of the moment should generally be complemented by the value of the moment modulus. The alternative parameterization based on the spherical coordinates of the moment vector, although supported by most refinement programs and by the magCIF standard, is not supported by most mainstream programs for analysis and visualization.

The magnetic moments on split sites that were symmetry related in the space group of the paramagnetic phase but are not related by symmetry operations of the MSG should be listed separately within the asymmetric unit of the MSG. The magnetic moments of atoms in the asymmetric unit of the MSG are symmetry independent, while the magnetic moments of all other atoms in the crystal are necessarily related to those

of the asymmetric unit by the symmetry operations of the MSG.

If a magnetic atom in the asymmetric unit lies on a special position, its magnetic moment may be subject to symmetry constraints due to the magnetic point group of the site. These symmetry constraints should be indicated so as to make explicit the degrees of freedom available to these moments under the MSG. Any additional constraints or correlations on the magnetic moments present in the model will then clearly have motivations unrelated to the MSG.

In Table 1, although the two independent magnetic sites are split from a single site in the paramagnetic phase, their symmetry constraints are completely different, one being restricted to the *ab* plane and the other being parallel to the *c* axis. Thus, there are three free parameters to define the spin arrangement and the reported model has determined the three of them as independent uncorrelated parameters. In the case of the second example, in Table 2, although the MSG also allows three free parameters in the description of the magnetic moments, the model includes a correlation between the three symmetry-independent parameters so that a single parameter has been determined to fully describe the model. As we will see below in Table 4, these additional correlations, which are not dictated by the MSG, are due to the compatibility of the MSG with two irreps of the parent space group and the absence of one of them in the spin arrangement, while the ferromagnetic order corresponding to the active irrep is also absent.

3.2. Representation-analysis information relating the magnetic structure to its parent paramagnetic structure (examples in Tables 3 and 4)

The crystallographic information listed above in §3.1 is sufficient to obtain an unambiguous description of a commensurate magnetic structure. The crystallographic description can then be complemented by a representation analysis of the deviations of the magnetic structure relative to the parent paramagnetic structure. In the common case of an MSG that is compatible with only a single irrep, the representation analysis is necessarily reduced to the identification of the relevant irrep, because the spin correlations and constraints dictated by the MSG fully coincide with those resulting from the irrep. When the MSG is compatible with more than one irrep, it is convenient to decompose the degrees of freedom allowed by the MSG into modes for each of the distinct compatible irreps, especially if some of the compatible irreps are inactive.

3.2.1. Primary irrep(s) label(s) and their dimension

The label (and dimension) of the primary irrep(s), either in the CDML or the Kovalev notation [see point (**xvii**) in Section 2]. For each primary irrep, it is also convenient to indicate if the order parameter must be restricted to a special direction within the irrep carrier space, or in other words, if its irrep basis vectors/modes must be in a specific linear combination to comply with the MSG. Because some software tools specify this so-called *order–parameter direction*, one should understand that its interpretation depends on the specific form of the irrep matrices used. Therefore, when presenting the order–parameter direction of an irrep, one should explicitly either include the relevant irrep matrices or reference a standard source of irrep-matrix data (see §3.2.3).

If the irrep has a single wavevector, the dimension of the small irrep associated with the small group of the wavevector (the one shown in some of the most popular software programs), is also the total dimension of the full irrep. But when the star of the irrep has more than one symmetry-related wavevector, the dimension of the full irrep is equal to the dimension of the small irrep multiplied by the number of symmetry-related wavevectors in the star. Thus, the dimensions of a multi-**k** irrep are partitioned equally amongst the wavevectors of the star of **k**.

A wavevector in the star of **k** is *active* if it is present in the spin arrangement. The effective dimension of the irrep within a given magnetic structure is the sum of the dimensions associated with the active wavevectors of that magnetic structure; the inactive **k** vectors of the irrep do not contribute. In the case of a single-**k** structure based on a multi-**k** primary irrep, the effective irrep dimension is the dimension of the small irrep, except for cases where $-\mathbf{k}$ is in the star of **k** but not equivalent to **k**, whereupon this dimension is doubled [see point (**xxi**) in Section 2].

For a structure with an MSG compatible with a single irrep, as in the example of Tables 1 and 3, this unique irrep is necessarily the primary one, and no other can contribute to the spin arrangement. The active irrep is mZ1 (CDML notation) with wavevector $(0, 0, \frac{1}{2})$, the irrep star containing only this single vector. Hence, the small irrep coincides with the full irrep and is two-dimensional. This means that the irrep is defined by 2×2 matrices, one for each operation of the parent space group.

For the example of Tables 2 and 4, the structure was determined restricting the arrangement to the single two-dimensional irrep mGM6+. However, the resulting MSG is also compatible with the one-dimensional irrep mGM3+, which can be considered secondary, since the presence of a magnetic component according to this irrep is not necessary in order to realize the observed MSG.

3.2.2. Description of the primary irrep(*s*)

The CDML label or the Kovalev label is sufficient to uniquely specify a space-group irrep because there are free online resources wherein these labels can be associated with unambiguous irrep matrices. A list of explicit irrep matrices is therefore not necessary when CDML or Kovalev irrep labels are used, though they may be optionally presented if desired for completeness. However, when arbitrary irrep labels are used, an explicit list of irrep(*s*) matrices is absolutely necessary. Either way, whenever explicit irrep matrices are provided, a minimal set of group generators is adequate.

In the example of Table 3, the list of 2×2 matrices defining the irrep mZ1 is limited to three adequately chosen opera-

tions, which together with those associated with lattice translations generate all the operations of the space group *Cmcm*. The matrices associated with the unit cell and centering translations can be trivially derived from the value of the propagation vector, but for completeness, they are included in the table.

It is important to note that the symmetry operations in these listings of irrep matrices, as shown in Tables 3 and 4, refer to the parent space group, while the symmetry operations listed to define the MSG, shown in Tables 1 and 2, refer to the MSG. Thus, these latter are generally defined with respect to a different basis (unit cell and origin) from that of the parent space group.

3.2.3. Secondary irrep(s) label(s) and their dimension

The label (and dimension) of the secondary irrep(*s*), either in the CDML or the Kovalev notation [see point (xvii) in §2], which are allowed by the MSG. About the constraints to a special irrep direction, the same considerations as in §3.2.1 apply.

In the example of Table 3, as the MSG is only compatible with a single irrep, no secondary irrep is to be considered, while in the example of Table 4, a one-dimensional secondary irrep mGM3+ (CDML notation) with wavevector (0, 0, 0) is indicated.

3.2.4. Description of the secondary irrep(s)

If the CDML or the Kovalev notation is used to label the secondary irrep(*s*), these labels are sufficient to define the irrep. But if desired for completeness, irrep matrices may be optionally included. However, when arbitrary irrep labels are used, an explicit list of irrep(s) matrices is absolutely necessary. Either way, whenever explicit irrep matrices are provided, a minimal set of group generators is adequate.

In the example given in Table 4, the secondary irrep mGM3+ is one-dimensional and the 1×1 matrices (values) for three adequately chosen group operations are sufficient to generate the irrep values for all the operations of parent space group $P6_3/mmc$. Thus, the list of values defining the irrep mGM3+ is limited to three operations. All lattice translations are trivially mapped to the identity matrix because of the null value of the irrep propagation vector.

3.2.5. Primary irrep mode(s) and their amplitude(s)

In the case of structures like the example given in Tables 1 and 3, where the MSG is only compatible with a single irrep, no additional information on the irreps involved in the magnetic ordering is necessary, as no additional irrep is possible, and the spin correlations associated with the irrep are already fully taken into account by the MSG operations.

In contrast, in structures like the example of Tables 2 and 4, where more than one irrep is compatible with the MSG, the magnetic arrangement of the structure can be decomposed into contributions from different irreps. These irrep components can be described in terms of collective *spin symmetry modes*, which define correlations not described by the MSG relations. These spin symmetry modes are traditionally called spin basis functions or spin basis vectors. Here they will be denoted as *irrep basis modes* or just *modes*.

The definition of the basis modes for each irrep can be limited to the set of magnetic atoms in the asymmetric unit of the MSG, which were symmetry related in the parent space group. If a magnetic atom in the asymmetric unit of the parent space group is split into several symmetry independent sites, the irrep basis vectors will generally introduce correlations between the magnetic moments of these split sites. If a magnetic atom is not split, the irrep basis modes can only introduce additional constraints on the moment direction that are not dictated by the MSG.

In the example of Table 4, the magnetic ordering according to the two-dimensional irrep mGM6+ is spanned by two basis modes. They are described by specific correlated arrangements of the magnetic moments of the two split Mn sites. Because the irrep mGM6+ is contained twice in the magnetic representation of the Mn site, a general mGM6+ spin arrangement would require four basis modes. The mGM6+ arrangement is however restricted to a specific order–parameter direction of the irrep carrier space to yield the relevant MSG. This means that the basis vectors are to be mixed by pairs in a specific linear combination, which reduces the number of possible basis modes complying with the MSG to two. One of them (mode 2 in Table 4) is a ferromagnetic *b*-axis arrangement of the split Mn-site moments: {Mn1_1: (0, 1, 0), Mn1_2: (0, 1, 0)}, which although absent in the reported structure would be possible as weak ferromagnetism within the MSG. The other mGM6+ mode (mode 1), described simply as {Mn1_1: (1, 1, 0), Mn1_2: (0, −1, 0)}, corresponds to the actual reported antiferromagnetic arrangement and is, therefore, the only mode with a non-zero amplitude. Notice that any non-zero value of the MSG-allowed ferromagnetic component associated with mGM6+ mode 2 is sufficient to break the exact equality of the magnitudes of the two MSG-independent Mn-site moments.

3.2.6. Secondary irrep mode(s) and their amplitude(s)

The description of the basis modes for the secondary irrep(*s*) can also be limited to the set of magnetic atoms present in the asymmetric unit, which were symmetry related in the parent space group.

In the example of Table 4, the secondary one-dimensional irrep mGM3+ spans a one-dimensional subspace in the magnetic representation of the Mn site and, therefore, it requires a single basis mode, which correlates the magnetic moments of the two split Mn sites in a different form than the two mGM6+ basis modes. This secondary irrep mode, absent in the reported model, when added to primary mode 1, would result in different moment magnitudes for the two split Mn atoms. Thus, although the structure described under its MSG has three free parameters, two for primary irrep mGM6+ and one for secondary irrep mGM3+, the refined and reported structure has only one free parameter, being fully described by mode 1.

To our knowledge, among the software publicly available, an irrep decomposition of the type described in §3.2.5 and §3.2.6, *i.e.* embedded within the crystallographic description of the magnetic structure, can only be obtained in an automatic form using the program *ISODISTORT* (Stokes *et al.*, 1995), and this program requires considerable proficiency and familiarity with its multiple options. Furthermore, an extension of the magCIF dictionary that accommodates representation analysis has not been yet developed. Therefore, we do not pretend that this mode decomposition should accompany all reports of magnetic structures with an MSG compatible with more than one irrep. It is presented for completeness to show the more comprehensive approach of combining representation analysis with a crystallographic description under an MSG.

4. Final remarks

This report presents a set of recommendations aimed at ensuring that newly determined commensurate magnetic structures are published in a standardized form, which facilitates their comprehension and portability and allows their digital storage. We basically recommend a crystallographic description of the structure that makes proper use of its magnetic space group, as supported by the magnetic extension of the CIF standard (magCIF). This description can be presented either in the main text of an article or as supplemental material, in a tabular form similar to the examples shown here. If a magCIF file of the structure is available, the necessary items to be reported can be easily retrieved therefrom. As an illustration, the appendices below reproduce in the magCIF format the essential contents of the two examples of Tables 1 and 2, where the use of red font indicates those items that are necessary for an unambiguous report of the magnetic structure.

It is then clear that reporting a magnetic structure in accordance with the present recommendations will require, especially in complex cases, the previous generation of an appropriate magCIF file. Presently there are numerous software resources that can be used for this purpose. Some of them allow an efficient combination of magnetic symmetry groups and representational analysis in the enumeration of and search of possible models of a magnetic structure, such that the structure can be directly refined under its crystallographic description, and the appropriate magCIF file can be directly generated after the refinement. But even if the magnetic structure is determined using the representation method alone or by any other method, the corresponding magCIF file can be easily obtained using freely available computer tools. First, a very simple magCIF file of the refined structure can be produced (either manually or by the refinement program) with the MSG limited to the trivial identity operation, and with a full list of all atomic positions and magnetic moments in a magnetic unit cell. Then internet software resources like ISOCIF or FINDSYM (Stokes *et al.*, 1995) can be used to read this file, to identify the actual MSG of the structure and to generate an appropriate magCIF file employing the correct MSG.

In any case, it is strongly recommended that a magCIF file be included as supplemental material when a magnetic structure is reported. Only by this means will there be the possibility of having a continually updated database of magnetic structures.

APPENDIX *A1*

Magnetic structure of $Dy_2Co_3Al_9$ (Table 1) as implemented in the magnetic CIF format (BNS setting)

Those items that are the minimal necessary for an unambiguous description of the magnetic structure are highlighted in red. It is supposed that the symmetry operators are provided in the unit-cell basis described in the 'cell_' tags.

```
 _parent_space_group.name_H-M_alt    'C m c m'
 _parent_space_group.IT_number    63
 _parent_space_group.transform_Pp_abc    'a,b,c;0,0,0'
 _parent_space_group.child_transform_Pp_abc
'a,b,2c;0,0,0'

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

 _space_group_magn.name_BNS    'A_a m m 2'
 _space_group_magn.number_BNS    38.192
 _space_group_magn.transform_BNS_Pp_abc
'c,a,b;0,0,-1/8'
 _space_group_magn.point_group_name "m m 2. 1' (c,a,b)"

 _cell_length_a    12.72390
 _cell_length_b    7.45860
 _cell_length_c    18.59880
 _cell_angle_alpha    90.00
 _cell_angle_beta    90.00
 _cell_angle_gamma    90.00

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

loop_
 _atom_site_label
 _atom_site_type_symbol
```

```
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
Dy1_1  Dy  0.33940  0.33290  0.12500
Dy1_2  Dy  0.66060  0.66710  0.37500
Co1  Co  0.32880  0.00000  0.00000
Co2  Co  0.00000  0.00000  0.00000
Al1_1  Al  0.00000  0.12490  0.12500
Al1_2  Al  0.00000  0.87510  0.37500
Al2_1  Al  0.10790  0.44590  0.12500
Al2_2  Al  0.89210  0.55410  0.37500
Al3_1  Al  0.00000  0.33220  0.27140
Al3_2  Al  0.00000  0.66780  0.52140
Al4_1  Al  0.16860  0.33300  0.03585
Al4_2  Al  0.83140  0.66700  0.28585

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
Dy1_1  1.34(2)  8.35(2)  0.00000  mx,my,0  8.46(2)
Dy1_2  0.00000  0.00000  1.38(1)  0,0,mz  1.38(1)
```

APPENDIX *A2*

Magnetic structure of Mn_3Sn (Table 2) as implemented in the magnetic CIF format (BNS setting)

Those items that are the minimal necessary for an unambiguous definition of the magnetic structure are highlighted in red.

```
 _parent_space_group.name_H-M_alt   'P 6_3/m m c'
 _parent_space_group.IT_number   194
 _parent_space_group.transform_Pp_abc   'a,b,c;0,0,0'
 _parent_space_group.child_transform_Pp_abc
'a,b,c;0,0,0'

loop_
 _parent_propagation_vector.id
 _parent_propagation_vector.kxkykz
k1  [0 0 0]
 _space_group_magn.name_BNS   "C m c' m'"
 _space_group_magn.number_BNS   63.463
 _space_group_magn.transform_BNS_Pp_abc
'-b,2a+b,c;0,0,0'
 _space_group_magn.point_group_name "m'm'm (2a+b,c,-b)"

 _cell_length_a   5.66500
 _cell_length_b   5.66500
 _cell_length_c   4.53100
 _cell_angle_alpha   90.00
 _cell_angle_beta   90.00
 _cell_angle_gamma   120.00

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

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

loop_
 _atom_site_label
 _atom_site_type_symbol
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
Mn1_1  Mn  0.83880  0.67760  0.25000
Mn1_2  Mn  0.32240  0.16120  0.25000
Sn1  Sn  0.33333  0.66667  0.25000

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
 Mn1_1  3.00(1)  3.00  0.00000  mx,my,0  3.00(1)
 Mn1_2  0.00000  -3.00  0.00000  0,my,0  3.00
```

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