



A recapitulation of magnetic space groups and their UNI symbols

B. J. Campbell,^{a*} H. T. Stokes,^a J. M. Perez-Mato^b and J. Rodriguez-Carvajal^c

^aDepartment of Physics and Astronomy, Brigham Young University, Provo, UT 84602, USA, ^bFacultad de Ciencia y Tecnología, Universidad del País Vasco, UPV/EHU, Apartado 644, 48080 Bilbao, Spain, and ^cInstitut Laue-Langevin (ILL), 71 avenue des Martyrs, 38042 Grenoble, France. *Correspondence e-mail: branton_campbell@byu.edu

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The mathematical structure, description and classification of magnetic space groups is briefly reviewed, with special emphasis on the recently proposed notation, the so-called UNI symbols [Campbell *et al.* (2022). *Acta Cryst. A* **78**, 99–106]. As illustrative examples, very simple magnetic space groups from each of the four possible types are described in detail.

1. Introduction

The mathematical structure of magnetic space groups (MSGs), also called Shubnikov groups, is well documented (Zamorzaev, 1957; Belov *et al.*, 1957; Opechowski & Guccione, 1965; Litvin, 2013). The four basic MSG construct types (Litvin, 2001) are referred to herein as types 1, 2, 3 and 4. Historically, two systems of MSG settings and symbols have seen wide use, which are the BNS system of Belov *et al.* (1957) and the OG system of Opechowski & Guccione (1965). The BNS and OG symbols for type-4 MSGs are quite different, and each have strengths and weaknesses. Both systems have been actively maintained, compared, and debated for years (Opechowski & Litvin, 1977; Litvin, 1998, 2008, 2013, 2016; Grimmer, 2009, 2010; Stokes & Campbell, 2010).

To address the weaknesses and the common misconceptions resulting from the two traditional notations, the unified (UNI) system of MSG symbols was proposed by Campbell *et al.* (2022). The UNI notation has since been endorsed by the Commission on Magnetic Structures of the International Union of Crystallography and adopted by many mainstream software tools for the determination, analysis, exploration, and visualization of magnetic structures, including the Bilbao Crystallographic Server (Perez-Mato *et al.*, 2015), *FullProf* (Rodríguez-Carvajal, 1993), *JANA2020* (Petříček *et al.*, 2023), and the *ISOTROPY Software Suite* (<https://iso.byu.edu>).

Magnetic symmetry operations differ from those of nonmagnetic symmetry operations by either including or explicitly omitting time-reversal. From a macroscopic atomic point of view, the action of time reversal in a magnetic structure is limited to a reversal of the directions of all atomic average magnetic moments present in the structure; it has no effect on the nonmagnetic degrees of freedom. The identity operation and the time-reversal operation comprise a two-element group called the *time-reversal group*, for which the time-reversal operation is the group generator. In general, a magnetic symmetry operation is constructed by combining an ordinary symmetry operation with one of the two elements of the time-reversal group.

MSG: Cc, 1'	
$\{1 000\}$	$x, y, z, +1$
$\{m_{010} 00\frac{1}{2}\}$	$x, -y, z + \frac{1}{2}, +1$
$\{1 \frac{1}{2}\frac{1}{2}0\}$	$x + \frac{1}{2}, y + \frac{1}{2}, z, +1$
$\{m_{010} \frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	$x + \frac{1}{2}, -y + \frac{1}{2}, z + \frac{1}{2}, +1$
$\{1' 000\}$	$x, y, z, -1$
$\{m'_{010} 00\frac{1}{2}\}$	$x, -y, z + \frac{1}{2}, -1$
$\{1' \frac{1}{2}\frac{1}{2}0\}$	$x + \frac{1}{2}, y + \frac{1}{2}, z, -1$
$\{m'_{010} \frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	$x + \frac{1}{2}, -y + \frac{1}{2}, z + \frac{1}{2}, -1$

MSG: P2 ₁ /c, 1'	
$\{1 000\}$	$x, y, z, +1$
$\{2_{010} 0\frac{1}{2}\frac{1}{2}\}$	$-x, y + \frac{1}{2}, -z + \frac{1}{2}, +1$
$\{-1 000\}$	$-x, -y, -z, +1$
$\{m_{010} 0\frac{1}{2}\frac{1}{2}\}$	$x, -y + \frac{1}{2}, z + \frac{1}{2}, +1$
$\{1' 000\}$	$x, y, z, -1$
$\{2'_{010} 0\frac{1}{2}\frac{1}{2}\}$	$-x, y + \frac{1}{2}, -z + \frac{1}{2}, -1$
$\{-1' 000\}$	$-x, -y, -z, -1$
$\{m'_{010} 0\frac{1}{2}\frac{1}{2}\}$	$x, -y + \frac{1}{2}, z + \frac{1}{2}, -1$

The UNI symbols are easier to interpret correctly than the BNS or OG symbols while also preserving the most important features of both the traditional BNS and OG symbols. The UNI MSG symbol is a modified BNS symbol, though for a type-4 MSG, the symbol of the nonmagnetic ordinary space group that applies to the nonmagnetic degrees of freedom (evident in the corresponding OG symbol) is also included in square brackets. The centring symbol at the front of the UNI MSG symbol indicates actual centring translations rather than anti-centring operations. In order to facilitate recognition of the magnetic point group (MPG), a generator from the time-reversal group is explicitly included at the end of each type-1, type-2 or type-4 UNI MSG symbol in order to make the MPG immediately recognizable. This emphasizes that type-1 MSGs do not include time-reversal symmetry but do allow non-zero magnetic moments, clearly differentiates type-1 and type-2 MSGs, and helps avoid the incorrect notion that a type-4 MSG can support a ferromagnetic moment (Gallego *et al.*, 2019). The translational component of an anti-translation operation is indicated as a subscript on the time-reversal generator in the UNI MSG symbol in a manner analogous to the notation used for glide planes and screw axes in ordinary space-group symbols. For each type-3 MSG, primes are used in the UNI symbol to indicate point-group operations that include time reversal.

Whereas Campbell *et al.* (2022) defined the UNI notation in rigorous detail and introduced the UNI symbol for the standard setting of each MSG, in the present work, we focus on the interpretation and utilization of the UNI MSG symbols. For each type of magnetic space group, we provide a summary of its description and its properties before working through several examples. In order to emphasize the practical aspects of the symbols, we have minimized mathematical and theoretical considerations.

2. Definitions and notation

Magnetic space groups (MSGs) can be constructed as an extension of ordinary crystallographic space groups by allowing certain space group elements to be augmented by the time reversal operation, which we denote as $1'$. Consequently, a generic operation of an MSG can be expressed as $\{R, \theta | \mathbf{t}\}$, where R is a proper or improper rotation, t is a translation, and θ is -1 if time reversal is included or $+1$ otherwise. If the operation $\{R, \theta | \mathbf{t}\}$ belongs to the MSG of a crystalline structure with atomic density $\rho(\mathbf{r})$ and magnetic moment density $\mathbf{M}(\mathbf{r})$, the system must remain invariant after the action of the operation, which means that the following equations must be satisfied:

$$\rho(\mathbf{r}) = \rho(\{R | \mathbf{t}\}^{-1} \mathbf{r}), \quad (1)$$

$$\mathbf{M}(\mathbf{r}) = \theta \det(R) R \cdot \mathbf{M}(\{R | \mathbf{t}\}^{-1} \mathbf{r}), \quad (2)$$

where $\det(R)$ accounts for the fact that the magnetic moment is an axial vector. Alternatively, if we consider an atomic description for any atom i in the structure, with position $\mathbf{r}_i$ and

magnetic moment $\mathbf{M}_i$, there must be another atom j of the same species, with position $\mathbf{r}_j$ and magnetic moment $\mathbf{M}_j$ that satisfies:

$$\mathbf{r}_j = \{R | \mathbf{t}\} \mathbf{r}_i, \quad (3)$$

$$\mathbf{M}_j = \theta \det(R) R \cdot \mathbf{M}_i. \quad (4)$$

An alternative approach is to use the Seitz notation (Glazer *et al.*, 2014) to describe an MSG operation. This allows the inclusion of time reversal to be indicated by adding a prime ($'$) to the spatial operation (R'). We then have that $\{R' | \mathbf{t}\}$ is equivalent to $\{R, -1 | \mathbf{t}\}$ for a time-reversed operation, whereas $\{R | \mathbf{t}\}$, in the context of an MSG, is equivalent to $\{R, +1 | \mathbf{t}\}$ and explicitly excludes time reversal. In the present paper, we will sometimes refer to an operation as 'primed' if it involves time reversal and as 'non-primed' if it does not involve time reversal.

The product of two MSG operations is computed as $\{R_2, \theta_2 | \mathbf{t}_2\} \cdot \{R_1, \theta_1 | \mathbf{t}_1\} = \{R_2 R_1, \theta_2 \theta_1 | R_2 \mathbf{t}_1 + \mathbf{t}_2\}$, where individual time-reversal components are simply multiplied. The multiplication rule above shows that the product of the time-reversal with itself is the identity operation: $\{1' | 000\} \cdot \{1' | 000\} = \{1 | 000\}$. We can also see that pure time reversal commutes with every other MSG operation: $\{1' | 000\} \cdot \{R, \theta | \mathbf{t}\} = \{R, \theta | \mathbf{t}\} \cdot \{1' | 000\} = \{R, -\theta | \mathbf{t}\}$. Finally, we can observe that the product of two MSG operations has a prime ($'$) only if exactly one of the two operations is primed, and lacks a prime if the two operations are either both primed or both non-primed.

Another commonly used notation is an extension of that used in the *International Tables for Crystallography* (1983) for ordinary space groups. In this notation, the operations $\{R | \mathbf{t}\}$ are described by their action on a generic position vector described by its components (x, y, z) with respect to a given basis. Simply, a ' -1 ' is appended to the symbol of a primed operation, while a ' $+1$ ' is appended to the symbol of a non-primed operation. The following examples illustrate the aforementioned notation.

$$\begin{aligned} \{m_{001} | \tfrac{1}{2} 0 0\} &= x + \tfrac{1}{2}, y, -z, +1 \\ \{1' | 0 \tfrac{1}{2} \tfrac{1}{2}\} &= x, y + \tfrac{1}{2}, z + \tfrac{1}{2}, -1 \\ \{-1 | 0 0 \tfrac{1}{2}\} &= -x, -y, -z + \tfrac{1}{2}, +1 \\ \{4'_{001} | 000\} &= -y, x, z, -1 \end{aligned}$$

The detailed form of the 3×3 Euclidean point-operation matrix and the three-dimensional translation vector within each MSG operation depends on the basis (unit cell and origin) selected to describe the magnetic structure. Consequently, two MSGs defined by their respective sets of operations (in one of the forms shown above) are considered equivalent if a change of basis can transform one set into the other. Under this equivalence condition, the number of possible distinct non-equivalent MSGs is 1651.

As with ordinary space groups, each non-equivalent MSG possesses a *standard* description, which is referred to as the standard setting. This is given by a specific form for the group operations. In the case of MSGs, there is not yet a volume of the *International Tables for Crystallography* to provide a list of standard settings. However, there are various resources

available, which fully describe the 1651 MSGs (Litvin, 2013; Stokes & Campbell, 2010; Perez-Mato *et al.*, 2015; González-Platas *et al.*, 2021; Campbell *et al.*, 2022). The listed operations for the MSGs described by these resources are mutually consistent and can therefore be taken together to define the standard setting of each MSG. The MSG examples presented below are all described in their standard settings, although it should be noted that it is common to describe an MSG in a nonstandard setting. Consequently, the explicit form of the group operations of the MSG to be considered in this case will then differ from their standard form.

3. Magnetic space groups of type-2

From the preceding discussion, it might be surmised that MSGs alter the symmetries of the underlying nonmagnetic structure (the paramagnetic parent) or introduce new symmetries that are only applicable to the magnetic order. In fact, the opposite is true. Magnetic ordering breaks the symmetries that are already present in the paramagnetic parent structure. Those parent symmetries that remain in the magnetically ordered phase form the MSG, which is always a subgroup of the symmetry group of the paramagnetic parent. In this sense, any magnetic structure can be considered as *distorted* with respect to its paramagnetic parent. This implies that all the symmetry operations present in the MSG of the magnetic phase must also be present in the symmetry group associated with the corresponding paramagnetic structure. In order to describe the symmetry of a magnetic structure, it is not necessary to add symmetry operations with respect to the paramagnetic structure; rather, it is sufficient to remove some of them.

According to equations (2) and (4), the pure time reversal operation (*i.e.* with zero translation) $\{1' | 000\}$, which reverses the direction of all non-zero magnetic moments, is a trivial symmetry operation of any paramagnetic structure. If flipping all the magnetic moments does not change the structure, then those moments must be zero to begin with. According to the definition of paramagnetism, the average local magnetic moment over the whole structure is zero, and all average atomic magnetic moments are zero. Consequently, the actual symmetry group of any paramagnetic structure is described by an MSG containing the operation. This is a very special kind of MSG, where every non-primed operation $\{R | \mathbf{t}\}$ is accompanied by a corresponding primed operation $\{R' | \mathbf{t}\} = \{1' | 000\} \cdot \{R | \mathbf{t}\}$. Therefore, the number of operations in such an MSG is twice that of the corresponding nonmagnetic space group. This kind of MSG is said to be of *type-2*.

The symbol $\mathcal{G}$ is used to denote the set of operations of the ordinary space group of a paramagnetic structure. The symbol M_2 is introduced to denote the corresponding type-2 MSG describing the complete symmetry group of this paramagnetic structure. Thus $\mathcal{G}$ is a subgroup of M_2 for which any operation explicitly does *not* involve time reversal. However, even without time reversal, the operations of $\mathcal{G}$ have a well defined action on the magnetic moments. M_2 can be constructed from $\mathcal{G}$ as follows:

$$M_2 = \mathcal{G} + \{1' | 000\} \mathcal{G}. \quad (5)$$

In the context of group theory, this is referred to as a coset decomposition, where each term in the sum is a coset. The first coset in (5) is $\mathcal{G}$, which is a subgroup of M_2 . However, the second coset, which contains a time-reversed copy of each element of $\mathcal{G}$, is not a subgroup of M_2 .

A type-2 MSG is also commonly referred to as a *gray* MSG or a *paramagnetic* MSG. This is because a type-2 MSG necessarily contains the time reversal operation $\{1' | 000\}$, which precludes it from being the symmetry group of a magnetically ordered structure. Obviously there must be exactly 230 different MSGs of type-2, one for each ordinary space group.

The BNS and OG symbols used for MSGs of type-2 are simple extensions of the ordinary space group symbols, with the addition of $1'$ at the end. The UNI notation differs slightly by adding $.1'$ instead, which serves to separate the time-reversal group generator symbol from the rest of the space-group symbol with a dot. This new convention is particularly useful when the symbols are presented in ASCII text format, as it allows for the clear distinction between the time reversal group generator symbol and visually similar symbols such as those of the time-reversed spatial inversion $-1'$ and the time-reversed screw axis $2_{-1}'$.

If $\mathcal{G}$ in (5) is the Hermann–Mauguin symbol of the ordinary space group, then the UNI symbol for M_2 is $\mathcal{G}.1'$. Consequently, $Cc.1'$, $P2_1/c.1'$, $Pnma.1'$ and $Fd\bar{3}m.1'$ are symbols of gray MSGs. The UNI symbol for the corresponding MPG, which is formed by the point-operational parts of the elements of the MSG, follows the same rule. For instance, the MPGs of these four examples are $m.1'$, $2/m.1'$, $mmm.1'$ and $m\bar{3}m.1'$, respectively.

For illustrative purposes, Table 1 provides a detailed account of the operations of the MSGs $Cc.1'$ and $P2_1/c.1'$. The listings demonstrate how each ordinary space-group operation appears both with and without time reversal included.

It is paradoxical that the time-reversal symmetry, which is implicit in any paramagnetic phase, is most appreciated when it is absent, *e.g.* after it has been broken by the emergence of magnetic order. Indeed, the MSG of any magnetic structure with non-zero magnetic moments is formed as a subgroup (not containing the operation $\{1' | 000\}$) of the type-2 MSG of its paramagnetic phase. These other possible MSGs are classified into three additional types.

4. Magnetic space groups of type-1

The simplest subgroups of a gray MSG that lack pure time-reversal symmetry are those with no primed operations at all. These subgroups constitute the MSGs of type-1. By comparison with (5), a type-1 MSG M_1 can be expressed as

$$M_1 = \mathcal{G}, \quad (6)$$

where $\mathcal{G}$ in (6) is mathematically an ordinary space group, but is considered as an MSG whose operations explicitly do not include time reversal as part of their definition. For this

Table 1

List of all operations (not equivalent by unit-cell lattice translations) of type-2 MSGs $Cc.1'$ and $P2_1/c.1'$.

In this and subsequent tables, operations are shown both in Seitz notation and in (x, y, z) form, and operations involving time reversal are highlighted in red.

MSG: $Cc.1'$	
$\{1 0 0 0\}$	$x, y, z, +1$
$\{m_{010} 0 0 \frac{1}{2}\}$	$x, -y, z + \frac{1}{2}, +1$
$\{1 \frac{1}{2} \frac{1}{2} 0\}$	$x + \frac{1}{2}, y + \frac{1}{2}, z, +1$
$\{m_{010} \frac{1}{2} \frac{1}{2} \frac{1}{2}\}$	$x + \frac{1}{2}, -y + \frac{1}{2}, z + \frac{1}{2}, +1$
$\{1' 0 0 0\}$	$x, y, z, -1$
$\{m'_{010} 0 0 \frac{1}{2}\}$	$x, -y, z + \frac{1}{2}, -1$
$\{1' \frac{1}{2} \frac{1}{2} 0\}$	$x + \frac{1}{2}, y + \frac{1}{2}, z, -1$
$\{m'_{010} \frac{1}{2} \frac{1}{2} \frac{1}{2}\}$	$x + \frac{1}{2}, -y + \frac{1}{2}, z + \frac{1}{2}, -1$

MSG: $P2_1/c.1'$	
$\{1 0 0 0\}$	$x, y, z, +1$
$\{2_{010} 0 \frac{1}{2} \frac{1}{2}\}$	$-x, y + \frac{1}{2}, -z + \frac{1}{2}, +1$
$\{-1 0 0 0\}$	$-x, -y, -z, +1$
$\{m_{010} 0 \frac{1}{2} \frac{1}{2}\}$	$x, -y + \frac{1}{2}, z + \frac{1}{2}, +1$
$\{1' 0 0 0\}$	$x, y, z, -1$
$\{2'_{010} 0 \frac{1}{2} \frac{1}{2}\}$	$-x, y + \frac{1}{2}, -z + \frac{1}{2}, -1$
$\{-1' 0 0 0\}$	$-x, -y, -z, -1$
$\{m'_{010} 0 \frac{1}{2} \frac{1}{2}\}$	$x, -y + \frac{1}{2}, z + \frac{1}{2}, -1$

Table 2

List of all operations (not equivalent by unit-cell lattice translations) of type-1 MSGs $Cc.1$ and $P2_1/c.1$.

All operations in these groups are non-primed.

MSG: $Cc.1$	
$\{1 0 0 0\}$	$x, y, z, +1$
$\{m_{010} 0 0 \frac{1}{2}\}$	$x, -y, z + \frac{1}{2}, +1$
$\{1 \frac{1}{2} \frac{1}{2} 0\}$	$x + \frac{1}{2}, y + \frac{1}{2}, z, +1$
$\{m_{010} \frac{1}{2} \frac{1}{2} \frac{1}{2}\}$	$x + \frac{1}{2}, -y + \frac{1}{2}, z + \frac{1}{2}, +1$

MSG: $P2_1/c.1$	
$\{1 0 0 0\}$	$x, y, z, +1$
$\{2_{010} 0 \frac{1}{2} \frac{1}{2}\}$	$-x, y + \frac{1}{2}, -z + \frac{1}{2}, +1$
$\{-1 0 0 0\}$	$-x, -y, -z, +1$
$\{m_{010} 0 \frac{1}{2} \frac{1}{2}\}$	$x, -y + \frac{1}{2}, z + \frac{1}{2}, +1$

reason, a UNI notation for a type-1 MSG adds '.1' after the corresponding ordinary space group symbol. It should be noted that for both type-1 and type-2 MSGs, the symbol following the dot indicates an element of the time-reversal group. For a type-1 MSG, this is the identity operation 1, whereas for a type-2 MSG, this is the time-reversal operation $1'$. There are 230 different MSGs of type-1, one for each ordinary space group.

According to (6), if $\mathcal{G}$ is represented by its Hermann–Mauguin symbol, then the UNI MSG symbol for M_1 is $\mathcal{G}.1$. For example, $Cc.1$, $P2_1/c.1$, $Pnma.1$ and $Fd\bar{3}m.1$ are UNI symbols of type-1 MSGs. The MPG corresponding to a type-1 MSG containing no primed point operations is also distinguished from the corresponding ordinary point group in a similar manner. The UNI symbols of the MPGs of the above MSGs are $m.1$, $2/m.1$, $mmm.1$ and $m\bar{3}m.1$, respectively. Table 2 provides illustrative examples of two type-1 MSGs, $Cc.1$ and $P2_1/c.1$, and their operations.

Table 3

List of all operations (not equivalent by unit-cell lattice translations) of the type-3 MSGs Cc' and $P2_1'/c$.

MSG: Cc'	
$\{1 0 0 0\}$	$x, y, z, +1$
$\{1 \frac{1}{2} \frac{1}{2} 0\}$	$x + \frac{1}{2}, y + \frac{1}{2}, z, +1$
$\{m'_{010} 0 0 \frac{1}{2}\}$	$x, -y, z + \frac{1}{2}, -1$
$\{m'_{010} \frac{1}{2} \frac{1}{2} \frac{1}{2}\}$	$x + \frac{1}{2}, -y + \frac{1}{2}, z + \frac{1}{2}, -1$

MSG: $P2_1'/c$	
$\{1 0 0 0\}$	$x, y, z, +1$
$\{m_{010} 0 \frac{1}{2} \frac{1}{2}\}$	$x, -y + \frac{1}{2}, z + \frac{1}{2}, +1$
$\{-1' 0 0 0\}$	$-x, -y, -z, -1$
$\{2'_{010} 0 \frac{1}{2} \frac{1}{2}\}$	$-x, y + \frac{1}{2}, -z + \frac{1}{2}, -1$

5. Magnetic space groups of type-3

A type-3 MSG is defined as one in which half of the operations are primed, and none of the primed operations are translations. In other words, each primed operation has a non-trivial point operation ($R \neq 1$). The coset decomposition of a type-3 MSG M_3 can be expressed as

$$M_3 = \mathcal{G} + \{R' | \mathbf{t}\} \mathcal{G} \quad (7)$$

where $\mathcal{G}$ is an ordinary space group (no primed operations) and $\{R' | \mathbf{t}\}$ is some primed operation with a non-trivial R not contained in the MPG of $\mathcal{G}$ (note that in this case M_3 is not a subgroup of $\mathcal{G}.1'$). This partitions M_3 into two cosets of equal size, one consisting of $\mathcal{G}$ itself (all elements of which are non-primed), and the other consisting of all primed operations. Each element of the second coset is obtained as the product of the same operation $\{R' | \mathbf{t}\}$ with each operation of $\mathcal{G}$.

If in equation (7) we remove the prime from each primed operation in the second coset, the result is an ordinary space group, denoted as F , with the coset decomposition $F = \mathcal{G} + \{R | \mathbf{t}\} \mathcal{G}$. This ordinary space group F is called the family space group (FSG) of the MSG. Furthermore, the MSG M_3 in equation (7) is a subgroup $F.1'$ of the corresponding gray MSG. The FSG is the effective ordinary space group applicable to the nonmagnetic degrees of freedom in a magnetic phase with M_3 as its MSG, since time reversal is irrelevant for nonmagnetic degrees of freedom.

The traditional and UNI symbols for type-3 MSGs and their MPGs are identical. Starting with the Hermann–Mauguin symbol of the FSG F , one simply adds a prime to each FSG generator in the symbol that includes the time reversal in the MSG. Consequently, the symbols Cc' , $P2_1'/c$, $Pn'ma$ and $Fd'\bar{3}'m$ represent type-3 MSGs, while the corresponding MPGs are m' , $2'/m$, $m'mm$ and $m'\bar{3}'m$, respectively. The total number of type-3 MSGs is 674.

Table 3 provides a detailed account of the operations of the MSGs Cc' and $P2_1'/c$ in their standard settings, which are identical to those of their FSGs (ordinary space groups Cc and $P2_1/c$) listed in *Volume A* of the *International Tables for Crystallography* (1983), with the exception of the primes on the operations listed in red. The operations without time

Table 4

List of all operations (not equivalent by unit-cell lattice translations) of the type-3 MSG $P2_1'/c$.

MSG: $P2_1'/c$	
$\{1 0 0 0\}$	$x, y, z, +1$
$\{m_{010} 0 0 \frac{1}{2}\}$	$x, -y, z + \frac{1}{2}, +1$
$\{-1 0 0 0\}$	$-x, -y, -z, -1$
$\{2_{010} 0 0 \frac{1}{2}\}$	$-x, y, -z + \frac{1}{2}, -1$

reversal (in black) define the subgroup denoted as $\mathcal{G}$ in (7), while the first primed operation in the list can be taken as the representative $\{R' | t\}$ of the second coset in (7). In the case of Cc' , the non-primed subgroup $\mathcal{G}$ from (7) is the centered triclinic group $C1$, and the representative $\{R' | t\}$ of the second coset is $\{m'_{010} | 0 0 \frac{1}{2}\}$, which can be expressed as

$$Cc' = C1 + \{m'_{010} | 0 0 \frac{1}{2}\}C1. \quad (8)$$

In the case of $P2_1'/c$, the non-primed subgroup $\mathcal{G}$ from (7) is Pc (but in a nonstandard setting), and the representative $\{R' | t\}$ of the second coset is the primed spatial inversion $\{-1' | 0 0 0\}$. A complete description of the subgroup $\mathcal{G}$ must include the details of its setting. The c glide operation perpendicular to the b axis is represented as $\{m_{010} | 0 \frac{1}{2} \frac{1}{2}\}$ instead of the standard $\{m_{010} | 0 0 \frac{1}{2}\}$. It is then sufficient to shift the origin by $(0 \frac{1}{4} 0)$ to have the operation in the latter form. Thus, the transformation of the basis and origin one would need in order to bring the non-primed subgroup Pc in Table 3 into the standard setting can be described as $(\mathbf{a}, \mathbf{b}, \mathbf{c}; 0 \frac{1}{4} 0)$. This can then be written as:

$$P2_1'/c = Pc(\mathbf{a}, \mathbf{b}, \mathbf{c}; 0 \frac{1}{4} 0) + \{-1' | 0 0 0\}Pc(\mathbf{a}, \mathbf{b}, \mathbf{c}; 0 \frac{1}{4} 0). \quad (9)$$

A different but related type-3 MSG, namely $P2'/c$, when presented in its standard setting as shown in Table 4, has coset decomposition

$$P2'/c = Pc + \{-1' | 0 0 0\}Pc, \quad (10)$$

where the transformation of the subgroup Pc to the standard setting is not specified because it is already in the standard setting. Although equations (9) and (10) appear similar, these coset decompositions define two distinct MSGs because the non-primed subgroups Pc and $Pc(\mathbf{a}, \mathbf{b}, \mathbf{c}; 0 \frac{1}{4} 0)$ are different. Despite being equivalent by a transformation, the resulting total groups are not equivalent when the second coset is added.

6. Magnetic space groups of type-4

A Type-4 MSG is defined as an MSG that possesses anti-translations, that is, translations combined with time reversal. The coset decomposition of a type-4 MSG M_4 can be expressed as

$$M_4 = \mathcal{G} + \{1' | \mathbf{t}_o\}\mathcal{G}, \quad (11)$$

where $\mathcal{G}$ is an ordinary space group with time-reversal explicitly excluded, *i.e.* without primed operations, and $\mathbf{t}_o$ is necessarily non-zero. As for all MSGs except type-1, half of the operations of M_4 are non-primed (first coset) and form a

subgroup of the MSG, while the other half (second coset) are primed and do not form a subgroup. Each operation of the second coset differs from the corresponding operation of the first coset only by the inclusion of a prime and the addition of the translation $\mathbf{t}_o$. This implies that for each primitive lattice translation $\{1 | \mathbf{T}\}$ of the group $\mathcal{G}$, the MSG also possesses the anti-translation $\{1' | \mathbf{T} + \mathbf{t}_o\}$.

Unlike type-3 MSGs, the FSG of a type-4 MSG has a different lattice to that of the MSG itself, so the number of lattice translations in the FSG is twice that of the MSG. This implies that a primitive unit cell of the FSG is half the size of the primitive unit cell of the MSG. The FSG of M_4 can be decomposed according to $F = \mathcal{G} + \{1 | \mathbf{t}_o\}\mathcal{G}$, so that the lattice translations of M_4 are exactly those of $\mathcal{G}$. The translation $\mathbf{t}_o$ in (11) must necessarily have the properties that $2\mathbf{t}_o$ belongs to the primitive lattice of M_4 , and $\mathbf{t}_o$ belongs to the primitive lattice of F but not to the primitive lattice of M_4 . Therefore, in a description of the MSG using a unit cell (centered if necessary) that generates the lattice of the MSG, the translation $\mathbf{t}_o$ in (11) must be a fractional translation within that unit cell. This is the so-called BNS description of a type-4 MSG.

The UNI MSG symbol of a type-4 MSG can be considered as a modified BNS symbol. In the UNI symbol (in its abbreviated form), the Hermann–Mauguin symbol of the ordinary space group $\mathcal{G}$ is followed by a dot and a subscripted time-reversal symbol that specifies the anti-translation $\{1' | \mathbf{t}_o\}$ in (11). For example, $1'_a, 1'_c, 1'_c, 1'_l$ are symbols of the operations $\{1' | \frac{1}{2} 0 0\}$, $\{1' | 0 0 \frac{1}{2}\}$, $\{1' | \frac{1}{2} \frac{1}{2} 0\}$ and $\{1' | \frac{1}{2} \frac{1}{2} \frac{1}{2}\}$, respectively. Thus $Pc.1'_c, P2_1/c.1'_a, P2_1/c.1'_c, Pnma.1'_A$ and $Fd\bar{3}m.1'_l$ are all UNI symbols of type-4 MSGs. Table 5 provides the operations of three of these MSGs and their corresponding FSGs. The total number of type-4 MSGs is 517.

The UNI symbol of a type-4 MSG does not place a prime on any generator of the ordinary space group $\mathcal{G}$. Since every non-primed operation g of $\mathcal{G}$ in M_4 has a corresponding primed operation of the form $\{1' | \mathbf{t}_o\} \cdot g$ in M_4 , there is no need to prime any of the generators of $\mathcal{G}$.

The above MSG symbols explicitly indicate that the associated MPGs are $m.1', 2/m.1', 2/m.1', mmm.1'$ and $m\bar{3}m.1'$, respectively, which are all gray groups. In fact, the MPG P_4 of type-4 MSG M_4 also has a coset decomposition like that of (11), namely $P_4 = P + \{1' | \mathbf{t}_o\}P$, where P is the ordinary point group of $\mathcal{G}$. This implies that the MPG of every type-4 MSG must be gray. A type-4 MSG can definitely support magnetic order, although its gray MPG implies that it only allows macroscopic tensor properties that would also be permitted in a paramagnetic phase with the same gray MPG. Consequently, macroscopic magnetization, linear magnetoelectricity, and other analogous phenomena are precluded in magnetic structures with a type-4 MSG.

In the so-called OG description of a magnetic structure, the operations of a type-4 MSG are described with respect to the lattice of its FSG. The OG symbol of a type-4 MSG is based on the symbol of its FSG (the group F) rather than on the symbol of the ordinary space group $\mathcal{G}$ from (11), which contains all the non-primed operations of the MSG. As previously stated, the UNI symbol of a type-4 MSG is based on the symbol of $\mathcal{G}$.

Table 5

List of all operations (not equivalent by unit-cell lattice translations) of the type-4 MSGs $Pc.1'_c$, $P2_1/c.1'_a$ and $P2_1/c.1'_c$, as well as the corresponding FSGs.

The complete form of the UNI symbol of a type-4 MSG includes the FSG symbol in square brackets.

MSG: $Pc.1'_c$ [Cc]		FSG: Cc	
$\{1 0 0 0\}$	$x, y, z, +1$	$\{1 0 0 0\}$	x, y, z
$\{m_{010} 0 0 \frac{1}{2}\}$	$x, -y, z + \frac{1}{2}, +1$	$\{m_{010} 0 0 \frac{1}{2}\}$	$x, -y, z + \frac{1}{2}$
$\{1' \frac{1}{2} \frac{1}{2} 0\}$	$x + \frac{1}{2}, y + \frac{1}{2}, z, -1$	$\{1 \frac{1}{2} \frac{1}{2} 0\}$	$x + \frac{1}{2}, y + \frac{1}{2}, z$
$\{m'_{010} \frac{1}{2} \frac{1}{2} \frac{1}{2}\}$	$x + \frac{1}{2}, -y + \frac{1}{2}, z + \frac{1}{2}, -1$	$\{m_{010} \frac{1}{2} \frac{1}{2} \frac{1}{2}\}$	$x + \frac{1}{2}, -y + \frac{1}{2}, z + \frac{1}{2}$

MSG: $P2_1/c.1'_a$ [$P2_1/c$]		FSG: $P2_1/c$	
$\{1 0 0 0\}$	$x, y, z, +1$	$\{1 0 0 0\}$	x, y, z
$\{2_{010} 0 \frac{1}{2} \frac{1}{2}\}$	$-x, y + \frac{1}{2}, -z + \frac{1}{2}, +1$	$\{2_{010} 0 \frac{1}{2} \frac{1}{2}\}$	$-x, y + \frac{1}{2}, -z + \frac{1}{2}$
$\{-1 0 0 0\}$	$-x, -y, -z, +1$	$\{-1 0 0 0\}$	$-x, -y, -z$
$\{m_{010} 0 \frac{1}{2} \frac{1}{2}\}$	$x, -y + \frac{1}{2}, z + \frac{1}{2}, +1$	$\{m_{010} 0 \frac{1}{2} \frac{1}{2}\}$	$x, -y + \frac{1}{2}, z + \frac{1}{2}$
$\{1' \frac{1}{2} 0 0\}$	$x + \frac{1}{2}, y, z, -1$	$\{1 \frac{1}{2} 0 0\}$	$x + \frac{1}{2}, y, z$
$\{2'_{010} \frac{1}{2} \frac{1}{2} \frac{1}{2}\}$	$-x + \frac{1}{2}, y + \frac{1}{2}, -z + \frac{1}{2}, -1$	$\{2_{010} \frac{1}{2} \frac{1}{2} \frac{1}{2}\}$	$-x + \frac{1}{2}, y + \frac{1}{2}, -z + \frac{1}{2}$
$\{-1' \frac{1}{2} 0 0\}$	$-x + \frac{1}{2}, -y, -z, -1$	$\{-1 \frac{1}{2} 0 0\}$	$-x + \frac{1}{2}, -y, -z$
$\{m'_{010} \frac{1}{2} \frac{1}{2} \frac{1}{2}\}$	$x + \frac{1}{2}, -y + \frac{1}{2}, z + \frac{1}{2}, -1$	$\{m_{010} \frac{1}{2} \frac{1}{2} \frac{1}{2}\}$	$x + \frac{1}{2}, -y + \frac{1}{2}, z + \frac{1}{2}$

MSG: $P2_1/c.1'_c$ [$P2_1/m$]		FSG: $P2_1/m$	
$\{1 0 0 0\}$	$x, y, z, +1$	$\{1 0 0 0\}$	x, y, z
$\{2_{010} 0 \frac{1}{2} \frac{1}{2}\}$	$-x, y + \frac{1}{2}, -z + \frac{1}{2}, +1$	$\{2_{010} 0 \frac{1}{2} \frac{1}{2}\}$	$-x, y + \frac{1}{2}, -z + \frac{1}{2}$
$\{-1 0 0 0\}$	$-x, -y, -z, +1$	$\{-1 0 0 0\}$	$-x, -y, -z$
$\{m_{010} 0 \frac{1}{2} \frac{1}{2}\}$	$x, -y + \frac{1}{2}, z + \frac{1}{2}, +1$	$\{m_{010} 0 \frac{1}{2} \frac{1}{2}\}$	$x, -y + \frac{1}{2}, z + \frac{1}{2}$
$\{1' 0 0 \frac{1}{2}\}$	$x, y, z + \frac{1}{2}, -1$	$\{1 0 0 \frac{1}{2}\}$	$x, y, z + \frac{1}{2}$
$\{2'_{010} 0 \frac{1}{2} 0\}$	$-x, y + \frac{1}{2}, -z, -1$	$\{2_{010} 0 \frac{1}{2} 0\}$	$-x, y + \frac{1}{2}, -z$
$\{-1' 0 0 \frac{1}{2}\}$	$-x, -y, -z + \frac{1}{2}, -1$	$\{-1 0 0 \frac{1}{2}\}$	$-x, -y, -z + \frac{1}{2}$
$\{m'_{010} 0 \frac{1}{2} 0\}$	$x, -y + \frac{1}{2}, z, -1$	$\{m_{010} 0 \frac{1}{2} 0\}$	$x, -y + \frac{1}{2}, z$

It should be noted that in the examples presented in Table 5, if we were to ignore the primes in all primed operations of the MSG, the operations of the MSG and the FSG would be identical. However, since the anti-translations of a type-4 MSG become actual translations of the FSG, the unit cells of the FSG and the MSG have different sizes and can sometimes even have different orientations (e.g. different by a 45° rotation). For this reason, the UNI symbol of this type of MSG has an extended or complete form, which may be optionally employed for the provision of more comprehensive information, specifically the space group of the FSG is also indicated in square brackets.

In the first example, $Pc.1'_c$ contains the anti-translation $\{1' | \frac{1}{2} \frac{1}{2} 0\}$, which becomes a C -centring translation in the FSG. Therefore, the extended symbol for this MSG is $Pc.1'_c [Cc]$, which communicates both the MSG and the FSG.

In the second example, $P2_1/c.1'_a$ contains the anti-translation, which becomes the lattice translation $\{1 | \frac{1}{2} 0 0\}$ in the FSG (when described in the setting of the MSG). Since this translation halves the unit-cell size along the a direction, it can be described as $\{1 | 1 0 0\}$ in the FSG setting. Note that the last four operations of the FSG differ from the first four only by this lattice translation. Based on the first four operations, it can be seen that the FSG is a space group of type $P2_1/c$ (in the half-sized unit cell). Therefore, the extended UNI symbol for this MSG is $P2_1/c.1'_a [P2_1/c]$.

Table 6

List of all operations (not equivalent by unit-cell lattice translations) of the MSG $P2_1/c.1'_c (-c, b, a; \frac{1}{4} 0 0)$.

This represents MSG type $P2_1/c.1'_c$ in a nonstandard setting. In order to take each group operation to its form in the standard setting of the MSG, as listed in Table 5, it is sufficient to apply the indicated transformation, $(-c, b, a; \frac{1}{4} 0 0)$, which is also part of the MSG label.

MSG: $P2_1/c.1'_c (-c, b, a; \frac{1}{4} 0 0)$	
$\{1 0 0 0\}$	$x, y, z, +1$
$\{2_{010} 0 \frac{1}{2} 0\}$	$-x, y + \frac{1}{2}, -z, +1$
$\{-1 \frac{1}{2} 0 0\}$	$-x + \frac{1}{2}, -y, -z, +1$
$\{m_{010} \frac{1}{2} \frac{1}{2} 0\}$	$x + \frac{1}{2}, -y + \frac{1}{2}, z, +1$
$\{1' \frac{1}{2} 0 0\}$	$x + \frac{1}{2}, y, z, -1$
$\{2'_{010} \frac{1}{2} \frac{1}{2} 0\}$	$-x + \frac{1}{2}, y + \frac{1}{2}, -z, -1$
$\{-1' 0 0 0\}$	$-x, -y, -z, -1$
$\{m'_{010} 0 \frac{1}{2} 0\}$	$x, -y + \frac{1}{2}, z, -1$

A different situation occurs in the third example, $P2_1/c.1'_c$, which contains the anti-translation $\{1' | 0 0 \frac{1}{2}\}$. This becomes the lattice translation $\{1 | 0 0 \frac{1}{2}\}$ in the FSG (described in the setting of the MSG). Since this translation halves the unit cell of the FSG along c , it can be described as $\{1 | 0 0 1\}$ in the setting of the FSG. In this case, the MSG has a c -glide plane perpendicular to b at $y = \frac{1}{4}$, described by the operation $\{m_{010} | 0 \frac{1}{2} \frac{1}{2}\}$. Additionally, it has a primed ordinary mirror plane at the same location, described by the operation $\{m'_{010} | 0 \frac{1}{2} 0\}$. These MSG operations become the ordinary mirror planes $\{m_{010} | 0 \frac{1}{2} 1\}$ and $\{m_{010} | 0 \frac{1}{2} 0\}$ in the FSG (and in the setting of the FSG), which are translationally equivalent geometric mirror planes. Similarly, the primed and non-primed twofold screw axes of the MSG condense into the same ordinary twofold screw axis in the FSG. The FSG is therefore a space group of type $P2_1/m$, and the extended UNI symbol for the MSG is $P2_1/c.1'_c [P2_1/m]$. This UNI symbol implies that the MSG is a subgroup of the gray MSG $P2_1/m.1'$ and not of $P2_1/c.1'$.

7. Notation of magnetic space groups in a nonstandard setting

In the nonmagnetic case, any distorted structure is usually described in a basis where its space group (a subgroup of the space group of its parent structure) is in its standard setting. This implies in many cases that the structure is described with a unit cell and origin different from those of the parent structure. In magnetic structures, the same approach can be taken, although in most cases the magneto-structural effects are relatively weak, meaning that the nonmagnetic structural degrees of freedom are rather insensitive to the symmetry breaking. Consequently, it is usual to keep the description of the magnetic ordering as close as possible to that of the parent structure. The spin arrangements are therefore typically envisioned in a structural framework associated with the parent structure. This implies that the magnetic structure is often described using a basis in which the magnetic space group is not in its standard setting.

The last MSG presented in Table 5 and the MSG presented in Table 6 are both of type $P2_1/c.1'_c$; however, the MSG of

Table 6 is presented in a nonstandard setting. This nonstandard setting can be realized, for instance, as the result of a magnetic ordering with propagation vector $(\frac{1}{2} 0 0)$ in a parent structure with ordinary space group *Pnma*, or rather with gray MSG *Pnma.1'*, if the resulting MSG is described by keeping the same origin and unit-cell orientation as the standard setting of space group *Pnma*. However, the *a* unit-cell parameter necessarily doubled due to the propagation vector; this is achieved by using the basis $(2\mathbf{a}, \mathbf{b}, \mathbf{c}; 0 0 0)$ relative to that of the standard setting of *Pnma*.

Except for the cell doubling, the symmetry operations of $P2_1/c.1'_c$ for the nonstandard setting in Table 6 are a subset of those of the standard setting of *Pnma.1'*, and necessarily differ from those of the standard setting of $P2_1/c.1'_c$ in Table 5. However, the basis transformation $(-\mathbf{c}, \mathbf{b}, \mathbf{a}; \frac{1}{4} 0 0)$ would be sufficient to make the operations of Table 6 acquire their standard form (in Table 5). Note that this basis transformation is defined relative to the basis being used in the description of the MSG, and therefore the unit-cell basis vector $\mathbf{a}$ in the transformation symbol is doubled with respect to the standard *Pnma* basis.

In order to facilitate such transformation calculations, it is beneficial to recall that the basis transformation to the standard setting can be expressed in the so-called augmented matrix form, of dimension 4×4 , which is expressed as:

$$P_a = \begin{pmatrix} P & \mathbf{p} \\ 0 & 1 \end{pmatrix}. \quad (12)$$

In this expression, the columns of the 3×3 submatrix P represent the basis vectors of the standard unit cell relative to the nonstandard one. The column vector $\mathbf{p}$ represents the origin of the standard cell in the coordinates of the nonstandard one. The value 0 at the lower-left position indicates that the row vector is $(0, 0, 0)$, and 1 in the lower-right corner is the number 1. For the current example involving MSG $P2_1/c.1'_c$, we have

$$P = (-\mathbf{c}, \mathbf{b}, \mathbf{a}) = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{pmatrix}, \quad \mathbf{p} = \begin{pmatrix} \frac{1}{4} \\ 0 \\ 0 \end{pmatrix}$$

The augmented matrix corresponding to the transformation $(-\mathbf{c}, \mathbf{b}, \mathbf{a}; \frac{1}{4} 0 0)$ is then given by

$$P_a = \begin{pmatrix} -\mathbf{c}, \mathbf{b}, \mathbf{a}; \frac{1}{4} 0 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 1 & \frac{1}{4} \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

If we define $\{R_s | \mathbf{t}_s\}$ and $\{R_{ns} | \mathbf{t}_{ns}\}$ as the forms of an MSG operation in the respective standard and nonstandard settings of the MSG, their corresponding augmented matrices

$$g_s = \begin{pmatrix} R_s & \mathbf{t}_s \\ 0 & 1 \end{pmatrix} \quad (13)$$

and

$$g_{ns} = \begin{pmatrix} R_{ns} & \mathbf{t}_{ns} \\ 0 & 1 \end{pmatrix} \quad (14)$$

are then related according to $g_{ns} = P_a g_s P_a^{-1}$. The character of the operation, whether primed or non-primed, is preserved by the transformation.

The transformation of the operations of MSG $P2_1/c.1'_c$ from the standard setting in Table 5 to the nonstandard setting in Table 6 can be verified by the reader, either by hand or by using software tools available in the internet, such as ISOSPACEGROUP (Stokes & Campbell, 2020), available within the *ISOTROPY Software Suite*, and Magnetic Symmetry Calculator, distributed within in the *FullProf Suite* (Rodríguez-Carvajal, 1993) and accessible from the toolbar through the Crystallographic Calculator. The former program requires the BNS number of the MSG (No. 14.82), while the latter requires either the selection of the group or just the name in text form as: $P2_1/c.1'_c[P2_1/m]$. Both programs require the input of the transformation from the standard setting to the nonstandard setting, which is $P_a^{-1} = (\mathbf{c}, \mathbf{b}, -\mathbf{a}; 0, 0, -\frac{1}{4})$. Also the tool MGENPOS in the Bilbao Crystallographic Server (Perez-Mato *et al.*, 2015) can be used to transform the list of the symmetry operations of any MSG to their form for any basis introduced by the user.

8. Conclusions

In this paper, we provide a comprehensive overview of the UNI notation for MSGs (Campbell *et al.*, 2022), which builds upon both the previous BNS and OG notations. We hope that the examples and explanations provided here will clarify the interpretation and use of the UNI MSG symbols and support their wide use by the scientific community concerned with the determination and communication of magnetic structures.

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