



Introducing a unified magnetic space-group symbol

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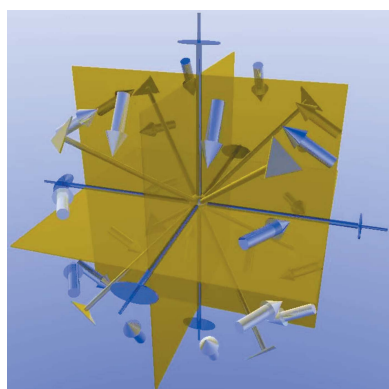
The two commonly used systems of magnetic space-group (MSG) symbols, with accompanying numbers and settings, are those of Belov–Neronova–Smirnova (BNS) and Opechowski–Guccione (OG). The symbols from both systems have been used for several decades now. Both have advantages and disadvantages. Both present challenges of interpretation to novice and expert users alike, which can inhibit understanding and lead to errors in published magnetic structures. To address each of these challenges going forward, a new unified (UNI) MSG symbol is introduced, which combines a modified BNS symbol with essential information from the OG symbol.

1. Introduction

The inequivalent types of symmetry groups of three-dimensional commensurate magnetic crystals, which are often referred to as Shubnikov groups or magnetic space groups (MSGs), were first enumerated by Zamorzaev (1957). Litvin (2016) mentions several different systems for assigning descriptive symbols to MSGs. The most common and widely used among them are those of Belov *et al.* (1957) and Opechowski & Guccione (1965). The Opechowski–Guccione (OG) symbols were refined by Litvin (1998), and the Belov–Neronova–Smirnova (BNS) symbols, which were notably employed by Bradley & Cracknell (1972), were later corrected by Opechowski & Litvin (1977). Both the BNS and OG systems, if understood correctly, can be robustly interpreted and unambiguously identified with the corresponding MSGs. Litvin (2016) provides a concise comparison of these two systems.

The extensive tables of Litvin (2013) provide both graphical and symbolic data on each of the 1651 MSGs, including representative operations and Wyckoff positions presented in the OG setting, with a format similar to the *International Tables of Crystallography* Vol. A (Aroyo, 2016). The ISO-MAG tables (Stokes & Campbell, 2010) further provide computer-readable data for each MSG, including the number, symbol, representative operations and Wyckoff positions in both the BNS and OG settings. The *MGENPOS* and *MWYCPOS* programs (Perez-Mato *et al.*, 2015) of the Bilbao Crystallographic Server then present MSG data derived from the ISO-MAG tables in a user-friendly on-demand format.

Noting that the BNS system has distinct advantages over the OG system, Grimmer (2009) presented a way to interpret BNS-setting information from the tables and diagrams of Litvin (2016). Grimmer (2010) then suggested a modified OG system of symbols that is easier to interpret. However, as explained below, both the BNS and OG symbols for MSGs



have properties that tend to confuse and mislead both novice and expert practitioners alike. To address these challenges, we introduce a new unified (UNI) system of MSG symbols, which are more informative and much easier to read and use than either BNS or OG symbols.

2. Definitions

2.1. The magnetic point group of a magnetic space group

For an MSG M_s with translation subgroup T , the magnetic point group (MPG) M_p of M_s is isomorphic to the factor group M_s/T of cosets of T in M_s . Each coset of T in M_s corresponds to a specific point group operation of M_p .

2.2. The magnetic component of a magnetic symmetry operation

Each operation of an MPG can be represented as $\{\mathbf{P}, \theta\}$, where $\mathbf{P}$ is a Euclidean point operation and θ indicates whether the operation includes time reversal ($\theta = -1$) or not ($\theta = +1$). Similarly, each operation of an MSG can be represented as $\{\mathbf{P}, \theta \mid \mathbf{t} + \mathbf{L}\}$, where $\mathbf{L}$ is a lattice translation, $\mathbf{t}$ is either zero or a fractional (*i.e.* non-lattice) translation within the unit cell, and $\{\mathbf{P}, \theta \mid \mathbf{t}\}$ is a coset representative of the MSG with respect to the translation subgroup T .

Because it is common to attach a prime character (') to a time-reversed generator in the symbol of an MPG or MSG, we will use the terms 'primed' and 'time-reversed' interchangeably, and will use the terms 'unprimed' and 'non-time-reversed' interchangeably.

Because a magnetic moment $\mathbf{m}$ is an axial vector, the action of an MPG or MSG operation on $\mathbf{m}$ is expressed as $\mathbf{m}' = [\theta \det(\mathbf{P})\mathbf{P}] \cdot \mathbf{m}$, where $\det(\mathbf{P})$ is the determinant of $\mathbf{P}$, which is +1 for proper operations (*e.g.* rotations) or -1 for improper operations (*e.g.* mirror planes or the inversion). In contrast, its action on a polar vector (*e.g.* atomic displacement) $\mathbf{p}$ is expressed as $\mathbf{p}' = \mathbf{P}\mathbf{p}$.

2.3. Mapping an MPG or MSG to a non-magnetic group

For a magnetic point group M_p , the 'family point group' (FPG) F_p of M_p is the non-magnetic point group obtained by removing the time reversal from each time-reversed operation of M_p without eliminating the operation, and is also the point group possessed by the non-magnetic variables of a magnetic structure. M_p is a member of the 'family' (also known as 'superfamily') of MPGs derived from F_p .

For a magnetic space group M_s , the 'family space group' (FSG) F_s of M_s is the non-magnetic space group (SG) obtained by removing the time reversal from each time-reversed operation of M_s without eliminating the operation, and is also the SG possessed by the non-magnetic variables of a magnetic structure. M_s is a member of the 'family' (also known as 'superfamily') of MSGs derived from F_s (Litvin, 1998, 2016; Grimmer, 2009).

The 'maximal point subgroup' (XPG) D_p of M_p is the point group obtained by removing all time-reversed operations from

M_p . It is the maximal point group contained in M_p with only unprimed operations.

The 'maximal space subgroup' (XSG) D_s of M_s is the SG obtained by removing time-reversed operations from M_s . It is the maximal SG contained in M_s with only unprimed operations.

2.4. Magnetic point-group construct types

Here, and throughout the remainder of the paper, the explicit use of the symbols 1 and 1' in group equations or MPG/MSG symbols will refer to elements of the two-element time-reversal group, $\{1, 1'\}$, consisting of the identity and the time-reversal operation. The MPGs of a given family can be constructed by combining the elements of the FPG with those of $\{1, 1'\}$ as follows:

(Type 1) $M_p = F_p 1$: construct M_p with only the operations of F_p , but with their actions extended to the magnetic degrees of freedom as non-time-reversed operations. Though it is not strictly necessary to explicitly combine the identity operation with each element of F_p , we do so to emphasize the relationship to the time-reversal group, $\{1, 1'\}$. This construct type is sometimes referred to as 'colorless'.

(Type 2) $M_p = F_p 1 + F_p 1'$: construct M_p by creating two operations from each operation of F_p , one unprimed (combined with 1) and one primed (combined with 1'). This construct type is often referred to as 'gray' or 'paramagnetic'.

(Type 3) $M_p = D_p 1 + (F_p - D_p) 1'$: given an index-2 subgroup D_p of F_p , construct M_p by priming each operation in $F_p - D_p$ (the complement of D_p in F_p) while leaving each operation in D_p unprimed. This construct type is sometimes referred to as 'bi-colored' or 'black and white'.

2.5. Commonly used MPG symbols

The 122 MPGs belonging to three-dimensional crystals are listed by Litvin (2013). Their commonly used MPG symbols are constructed from the point-group symbols of F_p as follows:

(Type 1) The symbol for M_p is identical to that of F_p .

(Type 2) The symbol for M_p is obtained by appending the symbol for the time-reversal generator (1') to the end of the symbol for F_p . Conversely, the symbol for F_p is obtained from that of M_p by removing the 1' at the end.

(Type 3) The symbol for M_p is obtained from that of F_p by adding a prime (') to the symbol of each point-group generator of F_p that is time-reversed in M_p . Conversely, the symbol for F_p is obtained from that of M_p by removing the prime from each time-reversed generator of M_p .

2.6. Magnetic space-group construct types

The MSGs of a given family can be constructed by combining the elements of the FSG with those of $\{1, 1'\}$ (Litvin, 2001) as follows:

(Type 1) $M_s = F_s 1$: construct M_s with only the operations of F_s , but with their action extended to the magnetic degrees of freedom as non-time-reversed operations. This construct type is sometimes referred to as 'colorless'.

(Type 2) $M_s = F_s 1 + F_s 1'$: construct M_s by creating two operations from each operation of F_s , one unprimed and one primed. This construct type is often referred to as ‘gray’ or ‘paramagnetic’.

(Type 3) $M_s = D_s 1 + (F_s - D_s) 1'$: given an index-2 *translationengleiche* subgroup D_s of F_s , construct M_s by priming each operation in $F_s - D_s$ while leaving each operation in D_s unprimed. This construct has been alternatively referred to as ‘3a’ or M_T by Litvin (2013, 2016), and as ‘BW1’ by Grimmer (2009, 2010).

(Type 4) $M_s = D_s 1 + (F_s - D_s) 1'$: given an index-2 *klas-sengleiche* subgroup D_s of F_s , construct M_s by priming each operation in $F_s - D_s$ while leaving each operation in D_s unprimed. For the coset representatives with respect to the translation subgroup T , such an MSG can also be described as $D_s 1 + D_s \{1'|\mathbf{t}\}$, where the operation $\{1'|\mathbf{t}\}$ is an anti-centering translation (also known as ‘anti-translation’), which combines the time-reversal generator of the MPG with a fractional (*i.e.* non-lattice) translation $\mathbf{t}$. This construct has been alternatively referred to as ‘3b’ or M_R by Litvin (2013, 2016), and as ‘BW2’ by Grimmer (2009, 2010).

For both MPGs and MSGs, the *International Tables of Crystallography* Vol. D (Borovik-Romanov *et al.*, 2013) switch the type-1 and type-2 labels relative to the usual convention described above, thus assigning gray groups to type 1 and colorless groups to type 2.

2.7. BNS and OG symbols for MSGs

The BNS and OG symbols of an MSG have similarities and differences. For MSGs of types 1–3, the BNS and OG settings and symbols are identical and based on the symbols of the corresponding FSG. For a type-4 MSG, the OG setting and symbol are based on those of the corresponding FSG (*i.e.* F_s in Section 2.3), while the BNS setting and symbol are based on those of the corresponding XSG (*i.e.* D_s in Section 2.3).

(Type 1) The BNS and OG symbols for M_s are identical to that of F_s .

(Type 2) The BNS and OG symbols for M_s are obtained by appending a 1' to the end of the symbol for F_s . Conversely, the symbol for F_s is obtained from that of M_s by removing the 1' at the end.

(Type 3) The BNS and OG symbols for M_s are obtained from that of F_s by adding a prime to the symbol of each SG generator of F_s that is time-reversed in M_s . Conversely, the symbol for F_s is obtained from that of M_s by removing the prime from each primed generator of M_s .

(Type 4) The BNS symbol for M_s is obtained from that of D_s by adding a subscript to the lattice-centering character indicating the location of the anti-centering translation within the unit cell, which necessarily exists for a type-4 MSG (see the previous section). In contrast, the OG symbol for M_s is obtained from that of F_s by adding a subscript to the lattice-centering character indicating the basis vectors of the magnetic lattice of M_s relative to those of D_s , and by adding a prime to the symbol of each SG generator of F_s whose representative operation in the 1952 edition of the *Inter-*

tional Tables of X-ray Crystallography Vol. I (Henry & Lonsdale, 1952) is time-reversed in M_s . Conversely, the SG symbol for D_s is obtained by removing the subscript from the BNS lattice-centering symbol, whereas the space-group symbol for F_s is obtained by removing the subscript from the OG lattice-centering symbol and by removing the primes from any primed generators.

2.8. Primitive unit-cell volumes (PUCV)

The BNS and OG symbols of an MSG must be interpreted in a particular crystallographic setting. We refer here to the ‘lattice’ of an SG or MSG as its translation subgroup, which does not include anti-translations. Given a primitive basis $\{\mathbf{a}_p, \mathbf{b}_p, \mathbf{c}_p\}$ for the lattice of an SG or MSG, the primitive unit-cell volume (PUCV) is computed as the triple product $(\mathbf{a}_p \times \mathbf{b}_p) \cdot \mathbf{c}_p$.

Recall that for a type-3 MSG, the BNS and OG symbols of M_s are identical and based on that of F_s . F_s , D_s and M_s all have the same primitive lattice bases, and hence the same PUCVs. This equivalence of the PUCVs of F_s and M_s makes equating their primitive settings very convenient in the sense that every distinct integer combination of primitive basis vectors of F_s represents a distinct lattice vector of M_s .

For a type-4 MSG, the PUCVs of D_s and M_s are equal to one another and both twice that of F_s . Thus, in a primitive BNS setting (based on D_s), each distinct integer combination of primitive basis vectors of D_s is a distinct lattice vector of M_s . However in a primitive OG setting (based on F_s), only half of the possible integer combinations of primitive basis vectors of F_s are lattice vectors of M_s , so that it becomes inconvenient to keep track of which integer triplets are lattice vectors of a type-4 MSG and which are not. This departure from the usual crystallographic convention makes it more difficult to extend existing crystallographic software to treat magnetism, and explains why BNS settings and symbols are far more widely supported than OG settings and symbols in magnetic crystallography software.

2.9. An example of each MSG construct type

We provide an example of each construct type, all four examples being from the same MSG family.

The type-1 MSG described as *Fmm2* (BNS No. 42.219 or OG No. 42.1.309). Its FSG and XSG are both *Fmm2* (No. 42) in the same conventional setting as the MSG. Its type-1 MPG is *mm2.1* (symbol enhanced as in Section 3.5), and its FPG and XPG are both *mm2*.

The type-2 MSG described as *Fmm21'* (BNS No. 42.220 or OG No. 42.2.310). Its FSG and XSG are both *Fmm2* (No. 42) in the same conventional setting as the MSG. Its type-2 MPG is *mm2.1'* (symbol enhanced as in Section 3.5), and its FPG and XPG are both *mm2*.

The type-3 MSG described as *Fm'm'2* (BNS No. 42.222 or OG No. 42.4.312). Its FSG is *Fmm2* (No. 42) and its XSG is *F2* (No. 5, an alternative setting of *C2*) in the same conventional setting as the MSG. Its type-3 MPG is *m'm'2*, its FPG is *mm2* and its XPG is 2.

Table 1

BNS, OG and UNI symbols for a few example MSGs, with the corresponding MPG symbols (with newly implemented separation of magnetic and non-magnetic generators), and the basis transformations from the conventional setting of the FSG to the conventional setting of the MSG.

Case	BNS No.	BNS	OG No.	OG	UNI MSG	UNI MPG	FSG → MSG
[1]	2.7	$P_5\bar{1}$	2.4.7	$P_{25}\bar{1}$	$P\bar{1}.1'_c[P\bar{1}]$	$\bar{1}.1'$	a, b, 2c
[2]	42.223	F_5mm2	25.9.163	P_1mm2	$Fmm2.1'_l[Pmm2]$	$mm2.1'$	2a, 2b, 2c
[3]	161.72	R_73c	160.5.1299	R_R3m'	$R3c.1'_c[R3m]$	$3m.1'$	−a, −b, 2c
[4]	218.84	$P_1\bar{4}3n$	217.5.1584	$I_P\bar{4}'3m'$	$P\bar{4}3n.1'_l[I\bar{4}3m]$	$\bar{4}3m.1'$	a, b, c
[5]	140.550	I_c4/mcm	123.19.1017	P_14/mmm'	$I4/mcm.1'_c[rP4/mmm]$	$4/mmm.1'$	a − b, a + b, 2c
[6]	28.96	P_Bma2	39.7.284	A_Pbm2	$Pma2.1'_B[Bma2]$	$mm2.1'$	b, −a, c
[7]	1.2	$P11'$	1.2.2	$P11'$	$P1.1'$	$1.1'$	a, b, c
[8]	1.1	$P1$	1.1.1	$P1$	$P1.1$	1.1	a, b, c
[9]	62.441	$Pnma$	62.1.502	$Pnma$	$Pnma.1$	$mmm.1$	a, b, c
[10]	62.448	$Pn'ma'$	62.8.509	$Pn'ma'$	$Pn'ma'$	$m'mm'$	a, b, c

The type-4 MSG described as C_Amc2_1 (BNS No. 36.179) or $F_Cmm'2'$ (OG No. 42.7.315). Its FSG is $Fmm2$ (No. 42) and its XSG is $Cmc2_1$ (No. 36). Its type-2 MPG is $mm2.1'$ (symbol enhanced as in Section 3.5), and both its FPG and XPG are $mm2$. The conventional C -centered unit cell of the MSG and XSG is identical to the conventional F -centered cell of the FSG, except for an origin shift of $(0, \frac{1}{4}, 0)$, which makes the PUCV of the MSG and XSG two times larger than that of the FSG, as expected. In the setting of the MSG, the anti-translation is $(0, \frac{1}{2}, \frac{1}{2})'$, which justifies the anti-translation subscript 'A' on the BNS symbol.

3. Unified (UNI) magnetic space-group symbols

The traditional BNS and OG symbols have several practical weaknesses, which are straightforward to address with the new UNI MSG symbols. Each weakness, together with the UNI-symbol feature that addresses it, is presented below and illustrated by one or more examples in Table 1. Some of the UNI-symbol features also imply modifications to the commonly used MPG symbols, so that each UNI MSG symbol is associated with a UNI MPG symbol.

3.1. Unambiguous anti-translation subscript

To achieve a Hermann–Mauguin-like symbol, the subscript on any generator should specify an unambiguous fractional translation. This should also be the case for an anti-translation operation, which combines the time-reversal generator of the MPG with a fractional translation.

The lattice-symbol subscripts of OG symbols specify basis transformations rather than individual translations, and so are not suitable for a Hermann–Mauguin-like symbol. However, the BNS-symbol subscripts are suitable for this purpose.

In all cases, the BNS-system subscripts 'a', 'b', 'c', 'A', 'B', 'C' and 'T' unambiguously specify an intrinsic translation. However, the BNS subscript 'S' does not unambiguously specify an intrinsic translation, and therefore needs to be changed. For triclinic groups possessing an anti-translation, the subscript 'S' should be replaced with 'a', 'b', 'c', 'A', 'B', 'C'

or 'T' depending on the setting used (Case 1 in Table 1). For orthorhombic and cubic MSGs for which D_s has a face-centered conventional cell, the subscript 'S' could be replaced with any one of 'a', 'b', 'c' or 'T' in principle, but should be consistently replaced with 'T' so as to specify an actual translation in the least arbitrary way (Case 2 in Table 1).

Just as for space-group symbols, the anti-translation subscript must depend on the setting used; this is in order to accurately convey the actual generator employed in the current setting. For rhombohedral MSGs with an anti-translation, the subscript 'c' should be used for a hexagonal axis setting because the anti-translation is $(0, 0, \frac{1}{2})$ (Case 3 in Table 1).

These changes are employed in the UNI symbols, which have the following unambiguous anti-translation subscripts: 'a' = $(\frac{1}{2}, 0, 0)$, 'b' = $(0, \frac{1}{2}, 0)$, 'c' = $(0, 0, \frac{1}{2})$, 'A' = $(0, \frac{1}{2}, \frac{1}{2})$, 'B' = $(\frac{1}{2}, 0, \frac{1}{2})$, 'C' = $(\frac{1}{2}, \frac{1}{2}, 0)$ and 'T' = $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$.

The anti-translation subscript of the OG symbol for a type-4 MSG advantageously implies the basis vectors of the conventional unit cell of M_s (and hence D_s) relative to those of F_s . Though this information is not explicitly included in the UNI symbol, it can be easily inferred from the UNI symbol for a given combination of the lattice symbol at the front of the UNI symbol and the anti-translation subscript on the time-reversal generator at the end of the UNI symbol. The possibilities are as follows:

- 'P', 'A', 'T' with subscript 'a' → (2a, b, c).
- 'P', 'B', 'T' with subscript 'b' → (a, 2b, c).
- 'P', 'C', 'T', 'R' with subscript 'c' → (a, b, 2c).
- 'A' with subscripts 'b' or 'c' → (a, 2b, 2c).
- 'B' with subscripts 'a' or 'c' → (2a, b, 2c).
- 'C' with subscripts 'a' or 'b' → (2a, 2b, c).
- 'P', 'A', 'B', 'C' with subscripts 'A', 'B' or 'C' → (a, b, c).
- 'P' with subscript 'T' → (a, b, c).
- 'R' with subscript 'T' → (b + c, a + c, a + b).
- 'F' with subscript 'T' → (2a, 2b, 2c).

Note that there are some tetragonal MSGs for which the lattice-centering 'P' together with anti-translation subscript 'C' is associated with the relative basis (a − b, a + b, c), or for which the lattice-centering 'T' together with anti-translation

subscript 'c' is associated with the relative basis ($\mathbf{a} - \mathbf{b}$, $\mathbf{a} + \mathbf{b}$, $2\mathbf{c}$).

Naturally, the conventional setting transformation from F_s to M_s (and hence D_s) includes not only a basis transformation, but also an origin shift, which is not displayed in the last column of Table 1.

On a related note, recent versions of the *International Tables for Crystallography*, Vol. A (IT-A), designate five SGs (Nos. 39, 41, 64, 67, 68) as having double glide planes, meaning that there are two superposed glide operations with orthogonal intrinsic translations in the same geometric plane. In the spirit of a Hermann–Mauguin system of unambiguous generator translations, the UNI symbol does not use 'e' for such a generator, but instead reverts to the traditional 'a', 'b' or 'c'.

3.2. Explicit inclusion of the time-reversal generator for type-4 MSGs

It is highly desirable that the MPG of an MSG should be explicitly evident in the MSG symbol simply by removing any translational detail from each generator given in the symbol. This is always possible for space-group symbols in IT-A, and also for the BNS and OG symbols for type-1, type-2 and type-3 MSGs. For type-4 MSGs, however, the time-reversal generator is not explicitly presented in either the BNS or OG symbols. The fact that the MPG of a type-4 MSG is always of type 2, and therefore includes the pure time-reversal operation, is not explicitly evident from the symbol itself. To mitigate this weakness, the UNI symbol for a type-4 MSG explicitly includes the time-reversal generator symbol ($1'$) at the end, following the other point-operation generator symbols (Cases 1–6 in Table 1). Furthermore, the OG symbol of a type-4 MSG assigns primes to generators in a technically precise way based on a historical convention, but tends to lead users to incorrectly conclude that the corresponding generators have only a time-reversed instance in the MPG and MSG, when in fact all spatial point operations of F_p have both primed and unprimed instances in the MPG and MSG. The UNI symbol of a type-4 MSG only includes a prime on the magnetic time-reversal generator (Cases 1–6 in Table 1), making it abundantly clear to users that a type-4 MSG has a type-2 (gray) rather than a type-3 MPG. This clarity helps to prevent the misinterpretation of magnetic tensor properties (Gallego *et al.*, 2019), which has affected even experienced practitioners.

3.3. Explicit inclusion of the $\{1,1'\}$ identity generator for type-1 MSGs

The fact that the BNS and OG symbols for a type-1 MSG are identical to that of its FSG lead some practitioners to consider the group as an ordinary space group, to refer to such a group as 'non-magnetic', and even to assume that any magnetic structure having such a symmetry group cannot support magnetic moments. To clarify that a type-1 MSG is in fact a 'magnetic' space group, its UNI symbol appends ' 1 ' to the end of the symbol, as illustrated in Cases 8–9 in Table 1, where the identity operation following the period is that of the

two-element time-reversal group $\{1, 1'\}$. Here, the explicit addition of an identity generator is reminiscent of the long Hermann–Mauguin symbol of a monoclinic group (*e.g.* $P121$).

3.4. Separation of the $\{1,1'\}$ generator from the rest of the symbol

The OG and BNS symbols for type-2 groups append the magnetic time-reversal generator symbol ($1'$) to the end of the MSG symbol, which is helpful, though it can still be difficult to visually determine whether the $1'$ indicates a time-reversal generator, a primed inversion symmetry or a primed rotation generator with a subscripted 1. The same issue now arises for both type-1 and type-4 UNI MSG symbols, to which either 1 or $1'$ should be, respectively, appended.

To improve readability and understanding, the UNI MSG symbol uses a period (':') to separate the symbol of the generator of group $\{1, 1'\}$ from the rest of the symbol for each type-1 MSG (Cases 8–9), type-2 MSG (Case 7) or type-4 MSG (Cases 1–6) symbol, as illustrated in Table 1. This feature does not apply to a type-3 MSG (Case 10), which has no need of the extra generator symbol.

3.5. MPG symbol

Observe that these new features of the UNI MSG symbol also lend themselves to analogous use in the MPG symbol. For a type-3 MPG, the UNI and commonly used MPG symbols are identical. But there are differences for type-1 and type-2 MPGs, as illustrated in each case of Table 1. Firstly, for a type-1 MPG, the symbol 1 for the identity generator of the two-element time-reversal group, $\{1, 1'\}$, is explicitly included at the end of the UNI MPG symbol. Secondly, for both type-1 and type-2 MPGs, the UNI MPG symbol employs a period to separate the symbol of the generator of group $\{1, 1'\}$ from the rest of the symbol. The UNI symbols of the 122 three-dimensional crystallographic MPGs (*i.e.* those obtainable as translation factor groups of three-dimensional MSGs) are listed in Table S1 of the supporting information, and numbered according to Litvin (2013).

3.6. Location of the anti-translation subscript

In the BNS system, the MSG generators and lattice-centering symbol are already conveyed in the setting of the conventional unit cell of M_s (and hence D_s), rather than of F_s . However, the subscript on the lattice-centering character suggests that the presence of anti-translations (which are not lattice translations) somehow modifies the lattice of the MSG to be different from that indicated by the lattice-centering character, though this is not the case. In reality, the subscript is merely a code, which specifies an intrinsic fractional translation that combines with the time-reversal generator of the MPG, in the same way that mirror planes and rotation axes combine with intrinsic fractional translations to form glide planes and screw axes, respectively. Consistent with the presentation of translational components of non-magnetic space-group generators, the UNI symbols move the subscript

from the BNS lattice-centering character to the time-reversal generator symbol (Cases 1–6 in Table 1).

3.7. Reference, alternative and non-standard MSG settings

Like a BNS or OG symbol, the UNI MSG symbol must be interpreted in a particular crystallographic setting. The UNI reference setting of an MSG is the standard IT-A setting of the FSG (types 1, 2, 3) or XSG (type 4), assuming (i) a conventional rather than primitive unit cell, (ii) a unique monoclinic 'b' axis, (iii) the monoclinic cell choice 1, (iv) the default orthorhombic 'abc' axis permutation, (v) an *R*-centered hexagonal cell for each rhombohedral group and (vi) an inversion symmetry at the origin (origin choice 2) when relevant. We note that the UNI reference setting of an MSG is identical to that of the ISO-MAG tables of Stokes & Campbell (2010), and is also consistent with the corresponding BNS symbol when the setting can be unambiguously obtained from the BNS symbol.

The space-group symbols presented in the IT-A are based on a finite set of alternative settings for each group, which might involve different monoclinic unique axes and cell choices, axes permutations, origin choices, or primitive versus conventional cells. Due to its dependence on the space-group symbols of the XSG and FSG, the UNI symbols for a type-4 MSG can also employ these same alternative IT-A settings in a natural way. An alternative setting transformation that permutes the unit-cell axes and corresponding MSG generators also transforms the translational component of each generator (including that of the time-reversal generator) in a predictable way, and any primes follow their generators through the permutation. In this way, the UNI MSG symbol of any alternative setting supported by the IT-A is well defined. For example, the alternative setting of type-3 MSG, $Pm'a/2$ (No. 28.91), obtained from setting transformation (**b**, **c**, **a**; 0, 0, 0), yields the alternative MSG symbol, $Pc'2m'$. As another example, the alternative setting of type-4 MSG, $Pma2.1'_b$ (No. 28.93), obtained from setting transformation (**b**, **c**, **a**; 0, 0, 0), yields the alternative MSG symbol, $Pc2m.1'_a$.

When an alternative MSG setting is used, we strongly suggest that the basis and origin transformation to the above-mentioned reference setting of the MSG be presented together with the setting-adapted UNI MSG symbol, even if one could reasonably determine this transformation from the symbol.

Due to the desire to have the unit cell of the MSG align with that of some real or hypothetical non-magnetic parent SG, it is very common to employ a non-standard MSG setting, *i.e.* one for which the FSG (types 1, 2, 3) or XSG (type 4) setting is not supported in IT-A. When working in a non-standard setting, one should never attempt to adapt the UNI symbol to the non-standard setting. Rather, the UNI symbol of the reference setting of the MSG should be presented together with the basis and origin transformation that takes the non-standard setting to the reference setting.

For example, the MAGNDATA (Gallego *et al.*, 2016) entry for the magnetic structure of $NiCr_2O_4$, based on the work of

Tomiyasu & Kagomiya (2004), describes the MSG as $Fd'd'd$, which is the reference setting for No. 70.530, but also specifies ($-\mathbf{a} + \mathbf{b}$, **c**, $\mathbf{a} + \mathbf{b}$; $\frac{1}{2}$, 1, $\frac{1}{2}$) as the transformation to the reference ('ref') setting from the non-standard ('n.s.') setting used by the authors. In other words, $\mathbf{a}_{\text{ref}} = -\mathbf{a}_{\text{n.s.}} + \mathbf{b}_{\text{n.s.}}$, $\mathbf{b}_{\text{ref}} = \mathbf{c}_{\text{n.s.}}$, $\mathbf{c}_{\text{ref}} = \mathbf{a}_{\text{n.s.}} + \mathbf{b}_{\text{n.s.}}$, and the origin of the reference setting is located at the point ($\frac{1}{2}$, 1, $\frac{1}{2}$) in the non-standard setting. This transformation is in general not unique, but, in order to fully define the relevant MSG, it is sufficient to indicate one of the possible ones.

Because the primitive OG cell volume of a type-4 MSG is half that of the PUCV of the XSG, the OG setting of the XSG is not a supported alternative IT-A setting of the XSG. Thus, when working in the OG setting of a type-4 MSG, one should present both the UNI reference symbol and reference transformation.

The primitive rhombohedral setting of a rhombohedral SG is a supported IT-A alternative to the *R*-centered hexagonal setting. For apparently historical reasons, the IT-A employs the symbols $R3c$ and $R\bar{3}c$ for the primitive rhombohedral settings of space groups Nos. 161 and 167, respectively, despite the fact that the glide plane is a '*c*' = (0, 0, $\frac{1}{2}$) glide only in the hexagonal setting. Fig. 1.5.1.6(a) of IT-A (Aroyo, 2016) shows that this intrinsic glide translation is actually ($\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$) in the primitive rhombohedral setting, so that this generator would be more appropriately listed as '*n*' rather than '*c*'. Furthermore, in a primitive setting, the lattice symbol should be '*P*' rather than '*R*'. Rather than implying FSG/XSG symbols that are much different from the historical space-group symbols in IT-A, the UNI system simply declares all primitive settings of MSGs with centered lattices to be non-standard. Thus, a primitive rhombohedral setting is treated as non-standard within the UNI system, even though it is a supported alternative setting in IT-A. So, when working in a primitive rhombohedral MSG setting, the UNI-reference MSG symbol and the UNI-reference transformation, (**a** − **b**, **b** − **c**, **a** + **b** + **c**; 0, 0, 0), should be presented together.

For each of the 1651 three-dimensional MSGs, Table S2 of the supporting information compares the UNI MSG symbol with the BNS and OG symbols, and also gives the UNI symbol of the corresponding MPG, while Table S3 of the supporting information unambiguously specifies the UNI-reference setting via two redundant approaches: (i) the explicit *xyz* forms of the generators in the UNI MSG symbol, and (ii) the magnetic Hall symbol of the MSG (González-Platas *et al.*, 2021).

3.8. The oriented FSG symbol

The OG symbol of a type-4 MSG is derived from the corresponding FSG symbol, which provides important information about the ordinary space-group symmetry of the non-magnetic degrees of freedom of the structure. This information is entirely lacking in the BNS symbol. To communicate this otherwise missing information, the UNI symbol for a type-4 MSG includes the symbol of the FSG explicitly as additional information in square brackets ('[]'), as illustrated in Cases 1–6

in Table 1. Though the result tends to be bulky, this extra information is quite valuable.

The utility of augmenting the symbol of a type-4 MSG with the corresponding FSG symbol is maximized by presenting the FSG symbol in an alternative setting such that the FSG cell axes are nicely aligned with the corresponding cell axes of the current setting of the XSG. The resulting FSG symbol will be called the 'oriented FSG symbol'. This is illustrated in Case 6 in Table 1, where the OG symbol is A_pbm2 and the FSG symbol is $Abm2$ in the standard IT-A space-group setting of the FSG, and where the BNS symbol is P_bma2 and the XSG symbol is $Pma2$ in the standard IT-A setting of the XSG. The basis transformation from the FSG/OG to the BNS/XSG setting is $(-b, a, c)$, which takes the standard IT-A setting of the FSG ($Abm2$) into that of the oriented FSG ($Bma2$). The resulting UNI symbol, $Pma2.1'_B[Bma2]$, includes the modified BNS symbol at the front, followed by the oriented FSG symbol in square brackets.

For those tetragonal MSGs in which the IT-A settings of the XSG and FSG unavoidably differ in orientation by a 45° rotation in the plane perpendicular to the tetragonal axis, the character 'r' (meaning 'rotated') is prepended to the front of the oriented FSG symbol, as illustrated in Case 5 in Table 1.

Like the Hermann–Mauguin symbol for a space group, the UNI symbol of an MSG can be presented in its short, full or extended form. Furthermore, any one of the short, full and extended forms of the UNI symbol of a type-4 MSG can either be presented in truncated or complete form, depending on whether the oriented FSG symbol is omitted or included. For instance, the short truncated and short complete forms of the UNI symbol in Case 6 in Table 1 are $Pma2.1'_B$ and $Pma2.1'_B[Bma2]$, respectively. The complete form of the UNI symbol of a type-4 MSG is recommended for most applications, though one can also use the truncated form when convenient.

4. MSG numbers

The BNS and OG numbers emphasize different ways to classify MSGs. The first part of both numbers indicates a standard IT-A space-group number. For a type-4 MSG, the first part of the OG number indicates the FSG while the first part of the BNS number indicates the XSG. For a type-1, -2, -3 MSG, the first part of both the BNS and OG numbers indicates the FSG. The second part of the BNS number indexes all MSGs in a given crystal system, whereas the second part of the OG number indexes all MSGs with a given FSG. The OG number also has a third part, which indexes all MSGs in a linear fashion. Because the main part of the UNI MSG symbol is a modified BNS symbol, we recommend that it be presented together with the corresponding BNS number for a given MSG.

5. Conclusion

A unified (UNI) magnetic space-group symbol is introduced, which combines a modified BNS symbol in a BNS setting with

essential information from the OG symbol. The UNI symbol is easier to interpret correctly than previous MSG symbols, at the expense of some compactness.

For a type-1, type-2 or type-3 MSG, the UNI symbol is very similar to the corresponding BNS and OG symbols. For a type-4 MSG, where the BNS and OG settings are necessarily different, the UNI symbol is a modified BNS symbol with appended information about the non-magnetic family space group (normally inferred from the OG symbol), and is true to the spirit of the system of Hermann–Mauguin symbols and settings employed for non-magnetic space groups in the IT-A.

The BNS symbol for a type-4 MSG indicates the conventional lattice centering of the MSG. The OG symbol reveals that of the underlying non-magnetic space group. The UNI symbol indicates both.

The BNS and OG symbols of a type-4 MSG fail to explicitly include the time-reversal generator ($1'$) together with the non-magnetic point-operation generators, which commonly leads even expert crystallographers to mistakenly conclude that the MPG is not gray and to thereby assume magnetic tensor properties and/or spin arrangements that are forbidden by a gray MPG. The UNI symbol of a type-4 MSG explicitly features the $1'$ generator, so that the MPG can be correctly deduced at a glance.

The primes on non-magnetic generators in the OG symbol of a type-4 MSG often lead users to erroneously assume that all of the corresponding group operations (combinations of the point operation with a translation) are primed, when in fact, only half of them are primed. The UNI symbol of a type-4 MSG only places a prime on the time-reversal generator.

The subscripted lattice symbols of type-4 BNS and OG symbols lend themselves to the common misconception of anti-translations as elements of the lattice of the MSG. The UNI symbol moves this subscript from the BNS lattice symbol to the $1'$ generator to clearly indicate the fractional translation of this magnetic point operation, which is analogous to the fractional translations of non-magnetic screw axes and glide planes.

The UNI symbols are designed to be interpreted like the Hermann–Mauguin symbols of the IT-A. The OG lattice-symbol subscript of a type-4 MSG indicates the relative basis of the magnetic lattice relative to that of the underlying non-magnetic lattice, and so is not suitable as a Hermann–Mauguin generator subscript for indicating the specific fractional translation of a representative point operation. The lattice-symbol subscript of the BNS symbol of a type-4 MSG would be suitable for such an interpretation except that it is sometimes ambiguous. The UNI symbol resolves this ambiguity.

The BNS and OG symbols for a type-2 MSG appropriately include the magnetic $1'$ generator, though it is often difficult (but not impossible) to visually discern whether it might indicate a primed inversion or a primed twofold screw axis instead. The UNI symbol always separates the magnetic generator from the rest of the symbol with a period (.) for type-1, type-2 and type-4 MSGs.

The complete UNI symbol preserves the most important features of both the BNS and OG symbols while resolving the

weaknesses of both systems. This symbol will make it much easier for both novice and expert practitioners to understand and use MSGs in the future. Though a new and improved MSG symbol may cause some initial confusion, we feel that its benefits will compound over time.

We note that the UNI symbol for an MSG will prove essential in constructing symbols for magnetic superspace groups, where the subscript on each generator of the MPG, including the time-reversal operation, combines with a phase shift indicator to convey a fractional superspace translation (Stokes & Campbell, 2022; Perez-Mato *et al.*, 2012).

6. Supporting information

For each of the 122 three-dimensional MPGs obtainable as a translation factor group of a three-dimensional MSG, Table S1 (included in a separate file) compares the new UNI MPG symbol to the commonly used MPG symbol. Differences arise only for type-1 (colorless) and type-2 (gray) MPGs, where the UNI symbol employs a period to isolate the relevant generator of the time-reversal group, $\{1, 1'\}$. The commonly used symbols were taken from and numbered according to Litvin (2013) with minor corrections ($2'm'$ should be $2'/m'$ and 17.4.64 should be 17.3.64).

Just as for non-magnetic point groups, the MPG symbol derived from an MSG symbol may differ from the equivalent entry in Table S1 due to the specific setting of the MSG or due to a different orientation of the point operations relative to the conventional lattice basis of the MSG. For example, orthorhombic $m'2m'$ (not listed) is obtained from $m'm'2$ (listed) by a permutation of the b and c axes. As another example, the orientation of tetragonal $\bar{4}m'2'$ (not listed) is related to that of $\bar{4}2'm'$ (listed) by a 45° rotation around the fourfold axis. Similarly, the orientation of trigonal MPG $3m'1$ is related to that of $31m'$ by a 30° c -axis rotation, and both are listed jointly as $3m'$ in Table S1 because it is customary to drop the identity generator when no crystal lattice is specified.

Table S2 (included as a separate file) lists (i) the BNS number, (ii) the BNS symbol, (iii) the OG number, (iv) the OG symbol, (v) the UNI MSG symbol corresponding to the UNI-reference setting, (vi) the UNI symbol of the MPG of the MSG, and (vii) the basis/origin transformation from the setting of the oriented FSG to the UNI-reference setting of the MSG.

Table S3 (included as a separate file) lists the following information for each of the 1651 three-dimensional MSGs: (i) the BNS number, (ii) the UNI symbol corresponding to the UNI-reference setting, (iii) the magnetic Hall symbol of the MSG, and (iv) the xyz forms of the generators in the UNI MSG symbol. See the article for terminology and citation details.

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