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# 3.6. Magnetic subperiodic groups and magnetic space groups

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## 3.6.1. Introduction

The *magnetic subperiodic groups* in the title refer to generalizations of the crystallographic subperiodic groups, *i.e.* frieze groups (two-dimensional groups with one-dimensional translations), crystallographic rod groups (three-dimensional groups with one-dimensional translations) and layer groups (three-dimensional groups with two-dimensional translations). There are seven frieze-group types, 75 rod-group types and 80 layer-group types, see *International Tables for Crystallography*, Volume E, *Subperiodic Groups* (2010; abbreviated as *IT* E). The magnetic *space groups* refer to generalizations of the one-, two- and three-dimensional crystallographic space groups, *n*-dimensional groups with *n*-dimensional translations. There are two one-dimensional space-group types, 17 two-dimensional space-group types and 230 three-dimensional space-group types, see Part 2 of the present volume (*IT* A).

Generalizations of the crystallographic groups began with the introduction of an operation of 'change in colour' and the 'two-colour' (black and white, antisymmetry) crystallographic point groups (Heesch, 1930; Shubnikov, 1945; Shubnikov *et al.*, 1964). Subperiodic groups and space groups were also extended into two-colour groups. Two-colour subperiodic groups consist of 31 two-colour frieze-group types (Belov, 1956*a*,*b*), 394 two-colour rod-group types (Shubnikov, 1959*a*,*b*; Neronova & Belov, 1961*a*,*b*; Galyarski & Zamorzaev, 1965*a*,*b*) and 528 two-colour layer-group types (Neronova & Belov, 1961*a*,*b*; Palistrant & Zamorzaev, 1964*a*,*b*). Of the two-colour space groups, there are seven two-colour one-dimensional space-group types (Neronova & Belov, 1961*a*,*b*), 80 two-colour two-dimensional space-group types (Heesch, 1929; Cochran, 1952) and 1651 two-colour three-dimensional space-group types (Zamorzaev, 1953, 1957*a*,*b*; Belov *et al.*, 1957). See also Zamorzaev (1976), Shubnikov & Koptsik (1974), Koptsik (1966, 1967), and Zamorzaev & Palistrant (1980). [Extensive listings of references on colour symmetry, magnetic symmetry and related topics can be found in the books by Shubnikov *et al.* (1964), Shubnikov & Koptsik (1974), and Opechowski (1986).]

The so-called *magnetic groups*, groups to describe the symmetry of spin arrangements, were introduced by Landau & Lifschitz (1951, 1957) by re-interpreting the operation of 'change in colour' in two-colour crystallographic groups as 'time inversion'. This chapter introduces the structure, properties and symbols of *magnetic* subperiodic groups and *magnetic* space groups as given in the extensive tables by Litvin (2013), which are an extension of the classic tables of properties of the two- and three-dimensional subperiodic groups found in *IT* E and the one-, two- and three-dimensional space groups found in the present volume. A survey of magnetic group types is also presented in Litvin (2013), listing the elements of one representative group in each *reduced superfamily* of the two- and three-dimensional magnetic subperiodic groups and one-, two- and three-dimensional magnetic space groups. Two notations for magnetic groups, the Opechowski–Guccione notation (OG notation) (Guccione, 1963*a*,*b*; Opechowski & Guccione, 1965; Opechowski, 1986) and the Belov–Neronova–Smirnova notation (BNS notation) (Belov *et al.*, 1957) are compared. The maximal subgroups of index $\leq 4$ of the magnetic subperiodic groups and magnetic space groups are also given.

## 3.6.2. Survey of magnetic subperiodic groups and magnetic space groups

We review the concept of a reduced magnetic superfamily (Opechowski, 1986) to provide a classification scheme for magnetic groups. This is used to obtain the survey of the two- and three-dimensional magnetic subperiodic group types and the one-, two- and three-dimensional magnetic space groups given in Litvin (2013). In that survey a specification of a single representative group from each group type is provided.

### 3.6.2.1. Reduced magnetic superfamilies of magnetic groups

Let $\mathcal{F}$ denote a crystallographic group. The magnetic superfamily of $\mathcal{F}$ consists of the following set of groups:

(1) The group $\mathcal{F}$.
(2) The group $\mathcal{F}1' \equiv \mathcal{F} \times 1'$, the direct product of the group $\mathcal{F}$ and the time-inversion group $1'$, the latter consisting of the identity 1 and time inversion $1'$.
(3) All groups $\mathcal{F}(\mathcal{D}) \equiv \mathcal{D} \cup (\mathcal{F} - \mathcal{D})1' \equiv \mathcal{F} \underline{\times} 1'$, subdirect products of the groups $\mathcal{F}$ and $1'$. $\mathcal{D}$ is a subgroup of index 2 of $\mathcal{F}$. Groups of this kind will also be denoted by $\mathcal{M}$.

The third subset is divided into two subdivisions:

(3*a*) Groups $\mathcal{M}_T$, where $\mathcal{D}$ is an equi-translational (*translationengleiche*) subgroup of $\mathcal{F}$.
(3*b*) Groups $\mathcal{M}_R$, where $\mathcal{D}$ is an equi-class (*klassengleiche*) subgroup of $\mathcal{F}$.[1]

Two magnetic groups $\mathcal{F}_1(\mathcal{D}_1)$ and $\mathcal{F}_2(\mathcal{D}_2)$ are called *equivalent* if there exists an affine transformation that maps $\mathcal{F}_1$ onto $\mathcal{F}_2$ and $\mathcal{D}_1$ onto $\mathcal{D}_2$ (Opechowski, 1986). If only non-equivalent groups $\mathcal{F}(\mathcal{D})$ are included, then the above set of groups is referred to as the reduced magnetic superfamily of $\mathcal{F}$.

*Example*

We consider the crystallographic point group $\mathcal{F} = 2_x2_y2_z$. The magnetic superfamily of the group $2_x2_y2_z$ consists of five groups: $\mathcal{F} = 2_x2_y2_z$, the group $\mathcal{F}1' = 2_x2_y2_z1'$, and the three groups $\mathcal{F}(\mathcal{D}) = 2_x2_y2_z(2_x)$, $2_x2_y2_z(2_y)$ and $2_x2_y2_z(2_z)$. Since the latter three groups are all equivalent, the reduced magnetic superfamily of the group $\mathcal{F} = 2_x2_y2_z$ consists of only three groups: $2_x2_y2_z$, $2_x2_y2_z1'$, and one of the three groups $2_x2_y2_z(2_x)$, $2_x2_y2_z(2_y)$ and $2_x2_y2_z(2_z)$.

*Example*

In the reduced magnetic space group superfamily of $\mathcal{F} = Pnn2$ there are five groups: $\mathcal{F} = Pnn2$, $\mathcal{F}1' = Pnn21'$, and three groups $\mathcal{F}(\mathcal{D}) = Pnn2(Pc)$, $Pnn2(P2)$ and $Pnn2(Fdd2)$. The

[1] Replacing time inversion $1'$ by an operation of 'changing two colours', the two-colour groups corresponding to the types 1, 2, 3*a* and 3*b* magnetic groups are known as type I, II, III and IV Shubnikov groups, respectively (Bradley & Cracknell, 1972).

**Table 3.6.2.1**
Numbers of types of groups in the reduced magnetic superfamilies of one-, two- and three-dimensional crystallographic point groups, subperiodic groups and space groups

| Type of group | $\mathcal{F}$ | $\mathcal{F}1'$ | $\mathcal{F}(\mathcal{D})$ | Total |
|---|---|---|---|---|
| One-dimensional magnetic point groups | 2 | 2 | 1 | 5 |
| Two-dimensional magnetic point groups | 10 | 10 | 11 | 31 |
| Three-dimensional magnetic point groups | 32 | 32 | 58 | 122 |
| Magnetic frieze groups | 7 | 7 | 17 | 31 |
| Magnetic rod groups | 75 | 75 | 244 | 394 |
| Magnetic layer groups | 80 | 80 | 368 | 528 |
| One-dimensional magnetic space groups | 2 | 2 | 3 | 7 |
| Two-dimensional magnetic space groups | 17 | 17 | 46 | 80 |
| Three-dimensional magnetic space groups | 230 | 230 | 1191 | 1651 |

groups $Pnn2(Pc)$ and $Pnn2(P2)$ are equi-translational magnetic space groups $\mathcal{M}_T$ and $Pnn2(Fdd2)$ is an equi-class magnetic space group $\mathcal{M}_R$.

A magnetic group has been defined as a symmetry group of a spin arrangement $\mathbf{S}(r)$ (Opechowski, 1986). With this definition, since $1'\mathbf{S}(r) = -\mathbf{S}(r)$, a group $\mathcal{F}1'$ is then not a magnetic group. However, there is not universal agreement on the definition or usage of the term *magnetic group*. Two definitions (Opechowski, 1986) have magnetic groups as symmetry groups of spin arrangements, with one having only groups $\mathcal{F}(\mathcal{D})$, of the three types of groups $\mathcal{F}$, $\mathcal{F}1'$ and $\mathcal{F}(\mathcal{D})$, defined as magnetic groups, while a second having both group $\mathcal{F}$ and $\mathcal{F}(\mathcal{D})$ defined as magnetic groups. Here we shall refer to all groups in a magnetic superfamily of a group $\mathcal{F}$ as magnetic groups, while cognizant of the fact that groups $\mathcal{F}1'$ cannot be a symmetry group of a spin arrangement.

### 3.6.2.2. Survey of magnetic point groups, magnetic subperiodic groups and magnetic space groups

The survey consists of listing the reduced magnetic superfamily of one group from each type of one-, two- and three-dimensional crystallographic point groups, two- and three-dimensional crystallographic subperiodic groups, and one-, two- and three-dimensional space groups (Litvin, 1999, 2001, 2013). The numbers of types of groups $\mathcal{F}$, $\mathcal{F}1'$ and $\mathcal{F}(\mathcal{D})$ in the reduced superfamilies of these groups is given in Table 3.6.2.1. The one group from each type, called the *representative group* of that type, is specified by giving a symbol for its translational subgroup and listing a set of coset representatives, called the standard set of coset representatives, of the decomposition of the group with respect to its translational subgroup. The survey provides the following information for each magnetic group type and its associated representative group:

(1) The serial number of the magnetic group type.
(2) A Hermann–Mauguin-like symbol of the magnetic group type which serves also as the symbol of the group type's representative group.
(3) For group types $\mathcal{F}(\mathcal{D})$: The symbol of the group type of the non-primed subgroup $\mathcal{D}$ of index 2 of the representative group $\mathcal{F}(\mathcal{D})$, and the position and orientation of the coordinate system of the representative group $\mathcal{D}$ of the group type $\mathcal{D}$ in the coordinate system of the representative group $\mathcal{F}(\mathcal{D})$.
(4) The standard set of coset representatives of the decomposition of the representative group with respect to its translational subgroup.

Examples of entries in the survey of magnetic groups are given in Table 3.6.2.2. The survey of the three-dimensional magnetic space groups (Litvin, 2001, 2013) was incorporated into the survey of three-dimensional magnetic space groups given by Stokes & Campbell (2009) and the coset representatives can also be found on the Bilbao Crystallographic Server (http://www.cryst.ehu.es; Aroyo *et al.*, 2006).

#### 3.6.2.2.1. Magnetic group type serial number

For each set of magnetic group types, one-, two- and three-dimensional crystallographic magnetic point groups, magnetic subperiodic groups and magnetic space groups, a separate numbering system is used. A three-part composite number $N_1.N_2.N_3$ is given in the first column, see Table 3.6.2.2. $N_1$ is a sequential number for the group type to which $\mathcal{F}$ belongs. $N_2$ is a sequential numbering of the magnetic group types of the reduced magnetic superfamily of $\mathcal{F}$. Group types $\mathcal{F}$ always have the assigned number $N_1.1.N_3$, and group types $\mathcal{F}1'$ the assigned number $N_1.2.N_3$. $N_3$ is a global sequential numbering for each set of magnetic group types. The sequential numbering $N_1$ for subperiodic groups and space groups follows the numbering in *IT* E and *IT* A, respectively.

#### 3.6.2.2.2. Magnetic group type symbol

A Hermann–Mauguin-like type symbol is given for each magnetic group type in the second column. This symbol denotes both the group type and the representative group of that type. For example, the symbol for the three-dimensional magnetic space-group type 25.4.158 is $Pm'm'2$. This symbol denotes both the group type, which consists of an infinite set of groups, and the representative group $Pm'_xm'_y2_z$. While this representative group may be referred to as 'the group $Pm'm'2$', other groups of this group type, *e.g.* $Pm_{xy}'m_{\bar{x}y}'2_z$, will always be written with subindices. The representative group of the magnetic group type is defined by its translational subgroup, implied by the first letter in the magnetic group type symbol and defined in Table 1.1 of Litvin (2013), and a given set of coset representatives, called the *standard set of coset representatives*, of the representative group with respect to its translational subgroup.

Only the relative lengths and mutual orientations of the translation vectors of the translational subgroup are given, see Table 1.2 of Litvin (2013). The symmetry directions of symmetry operations represented by characters in the Hermann–Mauguin symbols are implied by the character's position in the symbol and are given in Table 1.3 of Litvin (2013). The standard set of coset representatives are given with respect to an implied coordinate

**Table 3.6.2.2**
Examples of the format of the survey of magnetic groups of three-dimensional magnetic space-group types

| Serial No. | Symbol | Non-primed subgroup of index 2 | Standard set of coset representatives | | | |
|---|---|---|---|---|---|---|
| 10.1.49 | $P2/m$ | | $\{1\|0\}$ | $\{2_{010}\|0\}$ | $\{\bar{1}\|0\}$ | $\{m_{010}\|0\}$ |
| 10.3.51 | $P2'/m$ | $Pm$ $(0, 0, 0; \mathbf{a}, \mathbf{b}, \mathbf{c})$ | $\{1\|0\}$ | $\{2_{010}\|0\}$ | $\{\bar{1}\|0\}'$ | $\{m_{010}\|0\}'$ |
| 10.9.57 | $P_{2b}2'/m$ | $P2_1/m$ $(0, \frac{1}{2}, 0; \mathbf{a}, 2\mathbf{b}, \mathbf{c})$ | $\{1\|0\}$ | $\{2_{010}\|0, 1, 0\}$ | $\{\bar{1}\|0, 1, 0\}$ | $\{m_{010}\|0\}$ |
| 50.10.386 | $P_{2c}b'a'n'$ | $Pnnn$ $(\frac{1}{4}, \frac{1}{4}, \frac{1}{2}; \mathbf{a}, 2\mathbf{c}, \mathbf{b})$ | $\{1\|0\}$ | $\{2_{100}\|0\}$ | $\{2_{010}\|0, 0, 1\}$ | $\{2_{001}\|0, 0, 1\}$ |
| | | | $\{\bar{1}\|\frac{1}{2}, \frac{1}{2}, 1\}$ | $\{m_{100}\|\frac{1}{2}, \frac{1}{2}, 1\}$ | $\{m_{010}\|\frac{1}{2}, \frac{1}{2}, 0\}$ | $\{m_{001}\|\frac{1}{2}, \frac{1}{2}, 0\}$ |

system. The absolute lengths of translation vectors, the position in space of the origin of the coordinate system and the orientation in that space of the basis vectors of that coordinate system are not explicitly given.

*3.6.2.2.3. Standard set of coset representatives*

The standard set of coset representatives of each representative group is listed on the right-hand side of the survey of magnetic group types, see *e.g.* Table 3.6.2.2. Each coset in the standard set of coset representatives is given in Seitz notation (Seitz, 1934, 1935*a*,*b*, 1936), *i.e.* $\{\boldsymbol{R}|\boldsymbol{\tau}\}$ or $\{\boldsymbol{R}|\boldsymbol{\tau}\}'$. $\boldsymbol{R}$ denotes a proper or improper rotation (rotation-inversion), $\boldsymbol{\tau}$ a non-primitive translation with respect to the non-primed translational subgroup of the magnetic group, and the prime denotes that $\{\boldsymbol{R}|\boldsymbol{\tau}\}$ is coupled with time inversion. The subindex notation on $\boldsymbol{R}$, denoting the orientation of the proper or improper rotation, is given in Table 1.4 of Litvin (2013). [Note that the Seitz notation used in Litvin (2013) predates and is different from the IUCr standard convention for Seitz symbolism, see Section 1.4.2.2 and Glazer *et al.* (2014).]

*3.6.2.2.4. Opechowski–Guccione magnetic group type symbols and the standard set of coset representatives*

The specification of the magnetic group type symbol and the standard set of coset representatives of the magnetic group type's representative group is based on the conventions introduced by Opechowski and Guccione (Opechowski & Guccione, 1965; Opechowski, 1986) for three-dimensional magnetic space groups. The specification was made in conjunction with Volume I of *International Tables for X-ray Crystallography* (1969) (abbreviated here as *ITXC* I). One finds in *ITXC* I, for each group type $\mathcal{F}$, a specification of the coordinate system used, and, in terms of that coordinate system, a specification of the subgroup of translations $\mathcal{T}$ of the representative space group of that group type, and also indirectly a specification of a set of coset representatives of $\mathcal{T}$ of that representative group of group type $\mathcal{F}$. These coset representatives are uniquely determined from the coordinate triplets of the explicitly printed general position of the space group. The symbol $\mathcal{F}$ for the space group is taken to be the space-group symbol at the top of the page listing these coordinate triplets. The symbol for a group type $\mathcal{F}1'$ is that of the group type $\mathcal{F}$ followed by $1'$, and the coset representatives of the representative group of the group type $\mathcal{F}1'$ consist of the set of coset representatives of $\mathcal{F}$ and this set multiplied by $1'$.

*Example*

In *ITXC* I, on the page for $\mathcal{F} = P2/m$ one finds the following coordinate triplets of the general position:

$$x, y, z; \quad x, y, \bar{z}; \quad \bar{x}, \bar{y}, z; \quad \bar{x}, \bar{y}, \bar{z}$$

determining the coset representative of the representative group $P2/m$:

$$\{1|0\}; \quad \{m_{001}|0\}; \quad \{2_{001}|0\}; \quad \{\bar{1}|0\}.$$

The coset representatives of the representative group $P2/m1'$ are then:

$$\begin{array}{llll} \{1|0\}; & \{m_{001}|0\}; & \{2_{001}|0\}; & \{\bar{1}|0\} \\ \{1|0\}'; & \{m_{001}|0\}'; & \{2_{001}|0\}'; & \{\bar{1}|0\}'. \end{array}$$

*ITXC* I has been replaced by *IT* A. Ones finds that, for some space groups, the set of coordinate triplets of the general positions explicitly printed in *IT* A differs from that explicitly printed in *ITXC* I. As a consequence, if one attempts to interpret the Opechowski–Guccione symbols (OG symbols) for magnetic groups using *IT* A, one will, in many cases misinterpret the meaning of the symbol (Litvin, 1997, 1998). [It was suggested in these two papers that the original set of OG symbols should be modified so one could correctly interpret them using *IT* A instead of *ITXC* I. Adopting this ill-advised suggestion would have required in the future a new modification of the OG symbols whenever changes were made to the choices of coordinate triplets of the general position in *IT* A. Consequently, the meaning of the original OG symbols was specified by Litvin (2001) by explicitly giving the coset representatives of the representative groups of each three-dimensional magnetic space group.]

*Magnetic groups $\mathcal{M}_T$*

The symbol for a magnetic group type $\mathcal{M}_T = \mathcal{F}(\mathcal{D}) = \mathcal{D} \cup (\mathcal{F} - \mathcal{D})1'$ and its representative group is based on the symbol for the group type $\mathcal{F}$. $\mathcal{D}$ is an equi-translational subgroup of $\mathcal{F}$, *i.e.* the translational subgroup $\mathcal{T}^{\mathcal{M}_T}$ of the magnetic group $\mathcal{M}_T$ is $\mathcal{T}$, the translational subgroup of $\mathcal{F}$. The translational part of the group type symbol of an $\mathcal{M}_T$ group is then the same as that of the group type $\mathcal{F}$. A number or letter in the remaining part of the symbol of $\mathcal{F}$ appears unchanged in the symbol for $\mathcal{M}_T$ if it is associated with a coset representative of the representative group $\mathcal{F}$ that is also an element contained in the subgroup $\mathcal{D}$ of $\mathcal{F}$. If not in $\mathcal{D}$, *i.e.* if in $\mathcal{F} - \mathcal{D}$, the number or letter appears in the symbol for $\mathcal{M}_T$ with a prime to denote that the element in $\mathcal{M}_T$ is coupled with $1'$.

*Example*

The orthorhombic space-group type $\mathcal{F} = Pca2_1$ has the magnetic space-group type number 29.1.198. The representative group is defined by a orthorhombic translational subgroup $\mathcal{T}$ denoted by the letter $P$ in $Pca2_1$ and the standard set of coset representatives

$$\{1|0\} \quad \{m_{100}|\tfrac{1}{2}, 0, \tfrac{1}{2}\} \quad \{m_{010}|\tfrac{1}{2}, 0, 0\} \quad \{2_{001}|0, 0, \tfrac{1}{2}\}.$$

The magnetic space-group type 29.5.202 is a group $\mathcal{M}_T$ whose symbol is $Pc'a'2_1$. In this case we have $Pc'a'2_1 = P2_1 \cup (Pca2_1 - P2_1)1'$, *i.e.* $\mathcal{F} = Pca2_1$ and $\mathcal{D} = P2_1$. The symbol '$2_1$' in the symbol for $\mathcal{F} = Pca2_1$ refers to the coset representative $\{2_{001}|0, 0, \frac{1}{2}\}$, an element in $\mathcal{D} = P2_1$. Consequently, the symbol '$2_1$' appears unprimed in the symbol for $\mathcal{M}_T$ ($Pc'a'2_1$) and the coset representative $\{2_{001}|0, 0, \frac{1}{2}\}$ appears as an unprimed coset representative in the standard set of coset representatives of $\mathcal{M}_T$. The symbols '$c$' and '$a$' in $\mathcal{F} = Pca2_1$ refer to the coset representatives $\{m_{100}|\frac{1}{2}, 0, \frac{1}{2}\}$ and $\{m_{010}|\frac{1}{2}, 0, 0\}$, respectively, neither of which are contained in $\mathcal{D}$. Consequently, both symbols appear primed in the symbol $Pc'a'2_1$ for $\mathcal{M}_T$ and the coset representatives $\{m_{100}|\frac{1}{2}, 0, \frac{1}{2}\}$ and $\{m_{010}|\frac{1}{2}, 0, 0\}$ appear as primed coset representatives in the standard set of coset representatives of $\mathcal{M}_T$. The representative magnetic space group $Pc'a'2_1$ then has the orthorhombic translational subgroup $\mathcal{T}$ denoted by the letter $P$ and the standard set of coset representatives

$$\{1|0\} \quad \{m_{100}|\tfrac{1}{2}, 0, \tfrac{1}{2}\}' \quad \{m_{010}|\tfrac{1}{2}, 0, 0\}' \quad \{2_{001}|0, 0, \tfrac{1}{2}\}.$$

*Magnetic groups $\mathcal{M}_R$*

The symbol for a group type $\mathcal{M}_R = \mathcal{F}(\mathcal{D}) = \mathcal{D} \cup (\mathcal{F} - \mathcal{D})1'$ and its representative group is also based on the symbol for the group $\mathcal{F}$. [This is in contradistinction to the BNS symbols of $\mathcal{M}_R$ groups (Belov *et al.*, 1957), where the symbol for an $\mathcal{M}_R$ group type is based on the symbol for the group $\mathcal{D}$, see Section 3.6.4.] As this is an equi-class magnetic group, half the translations of $\mathcal{F}$ are now coupled with $1'$ in $\mathcal{M}_R$ and half the translations remain unprimed in $\mathcal{M}_R$. The unprimed translations constitute the translational subgroup $\mathcal{T}^{\mathcal{D}}$ of $\mathcal{D}$. We can then write the coset decomposition of the translational subgroup $\mathcal{T}$ of $\mathcal{F}$ with respect to the translational subgroup $\mathcal{T}^{\mathcal{D}}$ of $\mathcal{D}$ as

$$\mathcal{T} = \mathcal{T}^{\mathcal{D}} \cup t_\alpha \mathcal{T}^{\mathcal{D}},$$

where $t_\alpha$ denotes a chosen coset representative, a translation of $\mathcal{F}$ which appears primed (coupled with $1'$) in $\mathcal{M}_R$. The translational subgroup $\mathcal{T}^{\mathcal{M}_R}$ of $\mathcal{M}_R$ can then be written as

$$\mathcal{T}^{\mathcal{M}_R} = \mathcal{T}^{\mathcal{D}} \cup t_\alpha{}' \mathcal{T}^{\mathcal{D}}.$$

Symbols for the translational groups $\mathcal{T}$, the translational subgroups $\mathcal{T}^{\mathcal{D}}$ of $\mathcal{T}$, the translational groups $\mathcal{T}^{\mathcal{M}_R}$ of $\mathcal{M}_R$ and the choice of the translations $t_\alpha$ are given in Fig. 1 of Litvin (2013).

The symbol for a magnetic group type $\mathcal{M}_R = \mathcal{F}(\mathcal{D})$ and its representative group is based on the symbol of the group type $\mathcal{F}$, and is also a symbol for the subgroup $\mathcal{D}$ of unprimed elements: the translational part of the symbol of $\mathcal{F}$ is replaced by the symbol for the translational subgroup $\mathcal{T}^{\mathcal{D}}$ of $\mathcal{D}$. If a coset representative $\{\boldsymbol{R}|\boldsymbol{\tau}(\boldsymbol{R})\}$ of $\mathcal{T}$ in $\mathcal{F}$ appears as the coset representative $\{\boldsymbol{R}|\boldsymbol{\tau}(\boldsymbol{R}) + \boldsymbol{t}_\alpha\}$ of $\mathcal{T}^{\mathcal{D}}$ in $\mathcal{D}$, then the number or letter corresponding to $\{\boldsymbol{R}|\boldsymbol{\tau}(\boldsymbol{R})\}$ in the symbol for $\mathcal{F}$ is primed. If $\{\boldsymbol{R}|\boldsymbol{\tau}(\boldsymbol{R})\}$ appears unchanged as a coset representative of $\mathcal{T}^{\mathcal{D}}$ in $\mathcal{D}$, then the number or letter corresponding to $\{\boldsymbol{R}|\boldsymbol{\tau}(\boldsymbol{R})\}$ in the symbol for $\mathcal{F}$ is unchanged (Opechowski & Litvin, 1977). The resulting symbol is a symbol for $\mathcal{D}$ based on the symbol for $\mathcal{F}$ and is also a symbol for the magnetic group $\mathcal{M}_R = \mathcal{F}(\mathcal{D})$: the symbol specifies not only $\mathcal{D}$ but also $\mathcal{F}$; by deleting the subindex on the translational part of the symbol and the primes on the rotational part, one obtains the symbol specifying $\mathcal{F}$. Having specified $\mathcal{D}$ and $\mathcal{F}$, one has specified the group $\mathcal{M}_R = \mathcal{F}(\mathcal{D})$.

*Example*

Consider again the group 29.1.198, $\mathcal{F} = Pca2_1$, where

$$\mathcal{F} = \{1|0\}\mathcal{T} \cup \{m_{100}|\tfrac{1}{2},0,\tfrac{1}{2}\}\mathcal{T} \cup \{m_{010}|\tfrac{1}{2},0,0\}\mathcal{T} \cup \{2_{001}|0,0,\tfrac{1}{2}\}\mathcal{T}.$$

The symbol for the $\mathcal{M}_R = \mathcal{F}(\mathcal{D})$ group type 29.7.204 is $P_{2b}c'a'2_1$ and is based on the symbol for $\mathcal{F} = Pca2_1$. The translational subgroup $\mathcal{T}^{\mathcal{D}}$ of $\mathcal{D}$ is given by the symbol $P_{2b}$ where $t_\alpha = \{1|0, 1, 0\}$, *i.e.* $\mathcal{T}^{\mathcal{D}}$ is generated by the three translations $\{1|1, 0, 0\}$, $\{1|0, 2, 0\}$ and $\{1|0, 0, 1\}$ of $\mathcal{T}$, and the translational subgroup $\mathcal{T}^{\mathcal{M}_R}$ of $P_{2b}c'a'2_1$ is given by $\mathcal{T}^{\mathcal{M}_R} = \mathcal{T}^{\mathcal{D}} \cup t_\alpha{}'\mathcal{T}^{\mathcal{D}}$. The two primed symbols $c'$ and $a'$ in $P_{2b}c'a'2_1$ refer to the fact that the two coset representatives $\{m_{100}|\tfrac{1}{2},0,\tfrac{1}{2}\}$ and $\{m_{010}|\tfrac{1}{2},0,0\}$ that appear in the set of standard coset representatives of $\mathcal{T}$ in $\mathcal{F}$ appear as the coset representatives $\{m_{100}|\tfrac{1}{2},1,\tfrac{1}{2}\}$ and $\{m_{010}|\tfrac{1}{2},1,0\}$ in the set of standard coset representatives of $\mathcal{T}^{\mathcal{D}}$ in $\mathcal{D}$. As the symbol $2_1$ in $P_{2b}c'a'2_1$ is not primed, the coset representative $\{2_{001}|0, 0, \tfrac{1}{2}\}$ of $\mathcal{T}$ in $\mathcal{F}$ remains unchanged as a coset representative of $\mathcal{T}^{\mathcal{D}}$ in $\mathcal{D}$. We have then the subgroup

$$\mathcal{D} = \{1|0\}\mathcal{T}^{\mathcal{D}} \cup \{m_{100}|\tfrac{1}{2},1,\tfrac{1}{2}\}\mathcal{T}^{\mathcal{D}} \cup \{m_{010}|\tfrac{1}{2},1,0\}\mathcal{T}^{\mathcal{D}} \cup \{2_{001}|0,0,\tfrac{1}{2}\}\mathcal{T}^{\mathcal{D}}.$$

We note that these same coset representatives of $\mathcal{T}^{\mathcal{D}}$ in $\mathcal{D}$ are also the coset representatives of the standard set of coset representatives of $\mathcal{T}^{\mathcal{M}_R}$ in $\mathcal{M}_R$.

$$\mathcal{M}_R = \{1|0\}\mathcal{T}^{\mathcal{M}_R} \cup \{m_{100}|\tfrac{1}{2},1,\tfrac{1}{2}\}\mathcal{T}^{\mathcal{M}_R} \cup \{m_{010}|\tfrac{1}{2},1,0\}\mathcal{T}^{\mathcal{M}_R} \cup \{2_{001}|0,0,\tfrac{1}{2}\}\mathcal{T}^{\mathcal{M}_R}$$

and the standard set of coset representatives of $P_{2b}c'a'2_1$ listed in the tables is the same set of coset representatives:

$$\{1|0\} \quad \{m_{100}|\tfrac{1}{2},1,\tfrac{1}{2}\} \quad \{m_{010}|\tfrac{1}{2},1,0\} \quad \{2_{001}|0,0,\tfrac{1}{2}\}.$$

Since $\mathcal{T}^{\mathcal{M}_R} = \mathcal{T}^{\mathcal{D}} \cup t_\alpha{}'\mathcal{T}^{\mathcal{D}}$, it follows that $\mathcal{M}_R = \mathcal{D} \cup (\mathcal{F} - \mathcal{D})1'$ and

$$\begin{aligned}\mathcal{M}_R = {} & \{1|0\}\mathcal{T}^{\mathcal{D}} \cup \{m_{100}|\tfrac{1}{2},1,\tfrac{1}{2}\}\mathcal{T}^{\mathcal{D}} \cup \{m_{010}|\tfrac{1}{2},1,0\}\mathcal{T}^{\mathcal{D}} \\ & \cup \{2_{001}|0,0,\tfrac{1}{2}\}\mathcal{T}^{\mathcal{D}} \cup \{1|0,1,0\}'\mathcal{T}^{\mathcal{D}} \cup \{m_{100}|\tfrac{1}{2},0,\tfrac{1}{2}\}'\mathcal{T}^{\mathcal{D}} \\ & \cup \{m_{010}|\tfrac{1}{2},0,0\}'\mathcal{T}^{\mathcal{D}} \cup \{2_{001}|0,1,\tfrac{1}{2}\}'\mathcal{T}^{\mathcal{D}}.\end{aligned}$$

Consequently, a primed number or letter in the symbol for $\mathcal{M}_R$ (which is also a symbol for $\mathcal{D}$) denotes that the corresponding coset representative appears in $\mathcal{D}$ coupled with $t_\alpha$ and primed in $(\mathcal{F} - \mathcal{D})1'$, *e.g.* $a'$ in $P_{2b}c'a'2_1$ denotes that the coset $\{m_{100}|\tfrac{1}{2},0,\tfrac{1}{2}\}$ appears as $\{m_{100}|\tfrac{1}{2},1,\tfrac{1}{2}\}$ in $\mathcal{D}$ and as $\{m_{100}|\tfrac{1}{2},0,\tfrac{1}{2}\}'$ in $(\mathcal{F} - \mathcal{D})1'$. An unprimed number or letter in the symbol for $\mathcal{M}_R$ (which is also a symbol for $\mathcal{D}$) denotes that the corresponding element appears unchanged in $\mathcal{D}$ and coupled with $t_\alpha$ and primed in $(\mathcal{F} - \mathcal{D})1'$, *e.g.* the symbol $2_1$ in $P_{2b}c'a'2_1$ denotes that $\{2_{001}|0,0,\tfrac{1}{2}\}$ is in $\mathcal{D}$ and $\{2_{001}|1,0,\tfrac{1}{2}\}'$ is in $(\mathcal{F} - \mathcal{D})1'$.

For two-dimensional magnetic space groups with square and hexagonal lattices, three-dimensional magnetic space groups with tetragonal, hexagonal, rhombohedral and cubic lattices, and magnetic layer and rod groups with tetragonal, trigonal or hexagonal lattices, each letter or number in the group type symbol may represent not a single symmetry direction but a set of symmetry directions, see Table 1.3 in Litvin (2013), Table 2.1.3.1 in the present volume and Table 1.2.4.1 in *IT* E. Stokes & Campbell (2009) have pointed out that this can lead to not being able to determine the standard set of coset representatives in $\mathcal{M}_R$ groups from the Opechowski–Guccione magnetic group symbol. Consequently, we introduce the convention that in determining the standard set of coset representatives, each letter or number in the group type symbol in these groups refers to the first symmetry direction of each set of symmetry directions listed in the aforementioned tables.

*Example*

The standard set of coset representatives of 94.1.786 $P4_22_12$ is

$$\begin{array}{llll}\{1|0\}; & \{4_{001}|\tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2}\}; & \{2_{001}|0\}; & \{4_{001}|\tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2}\} \\ \{2_{100}|\tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2}\}; & \{2_{010}|\tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2}\}; & \{2_{110}|0\}; & \{2_{1\bar{1}0}|0\}.\end{array}$$

For the three-dimensional magnetic group 94.7.792 $P_{2c}4_2'2_1'2$, the standard set of coset representatives is

$$\begin{array}{llll}\{1|0\}; & \{4_{001}|\tfrac{1}{2},\tfrac{1}{2},\tfrac{3}{2}\}; & \{2_{001}|0,0,1\}; & \{4_{001}|\tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2}\} \\ \{2_{100}|\tfrac{1}{2},\tfrac{1}{2},\tfrac{3}{2}\}; & \{2_{010}|\tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2}\}; & \{2_{110}|0,0,1\}; & \{2_{1\bar{1}0}|0\}.\end{array}$$

The secondary position in the Hermann–Mauguin symbol $P_{2c}4_2'2_1'2$ denotes the set of symmetry directions {[100], [010]}. With this convention, the primed symbol $2_1'$ denotes that the corresponding coset representative $\{2_{100}|\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}\}$ of $P4_22_12$ appears in the coset representatives of $P_{2c}4_2'2_1'2$ coupled with the translation $t_\alpha = \{1|0, 0, 1\}$. The third position in the Hermann–Mauguin symbol $P_{2c}4_2'2_1'2$ denotes the set of symmetry directions $\{[1\bar{1}0], [110]\}$. The unprimed symbol 2 denotes that the coset representative $\{2_{1\bar{1}0}|0\}$ of $P4_22_12$ appears unchanged in the coset representatives of $P_{2c}4_2'2_1'2$.

The impact of this convention is that nine Opechowski–Guccione symbols of three-dimensional magnetic space groups need to be changed:

| | Old symbol | New symbol |
|---|---|---|
| 93.6.781 | $P_{2c}4_222$ | $P_{2c}4_222'$ |
| 93.8.783 | $P_I4_222$ | $P_I4_222'$ |
| 93.9.784 | $P_{2c}4_2'22'$ | $P_{2c}4_2'22$ |
| 153.4.1270 | $P_{2c}3_112$ | $P_{2c}3_112'$ |
| 154.4.1274 | $P_{2c}3_121$ | $P_{2c}3_12'1$ |
| 180.6.1401 | $P_{2c}6_222$ | $P_{2c}6_222'$ |
| 180.7.1402 | $P_{2c}6_2'22'$ | $P_{2c}6_2'22$ |
| 181.6.1408 | $P_{2c}6_422$ | $P_{2c}6_422'$ |
| 181.7.1409 | $P_{2c}6_4'2'2$ | $P_{2c}6_4'2'2'$ |

To have all $\mathcal{M}_R$ group symbols represent subgroups $\mathcal{D}$, six symbols for three-dimensional magnetic space groups were based (Opechowski & Guccione, 1965) on the symbol of the subgroup $\mathcal{D}$ instead of the symbol for $\mathcal{F}$. These are the groups 144.3.1236 $P_{2c}3_2$, 145.3.1239 $P_{2c}3_1$, 151.4.1262 $P_{2c}3_212$, 152.4.1266 $P_{2c}3_221$, 153.4.1270 $P_{2c}3_112$ and 154.4.1274 $P_{2c}3_121$. Additional groups are the rod groups 43.3.231 $\not{p}_{2c}3_2$, 44.3.234 $\not{p}_{2c}3_1$, 47.4.246 $\not{p}_{2c}3_212$ and 48.4.250 $\not{p}_{2c}3_112$.

#### 3.6.2.2.5. *Symbol of the subgroup $\mathcal{D}$ of index 2 of $\mathcal{F}(\mathcal{D})$*

For magnetic group types $\mathcal{F}(\mathcal{D})$, the magnetic group type symbol of the subgroup $\mathcal{D}$ is given in the third column of the survey of magnetic groups, see *e.g.* Table 3.6.2.2. If $\mathcal{F}(\mathcal{D})$ is a group $\mathcal{M}_T$, then the subgroup $\mathcal{D}$ is defined by the translational group of $\mathcal{F}(\mathcal{D})$ and the unprimed coset representatives of $\mathcal{F}(\mathcal{D})$.

*Example*

Consider the three-dimensional magnetic space-group type 16.3.101 $P2'2'2$. The representative group $P2'2'2$ is defined by the translational subgroup $\mathcal{T}$ denoted by the letter $P$ generated by the translations

$$\{1|1,0,0)\}\quad\{1|0,1,0\}\quad\{1|0,0,1\}$$

and the standard set of coset representatives

$$\{1|0\}\quad\{2_{100}|0\}'\quad\{2_{010}|0\}'\quad\{2_{001}|0\}.$$

The subgroup $\mathcal{D}$ of index 2 of the representative group $\mathcal{F}(\mathcal{D}) = P2'2'2$ is defined by the translational group $\mathcal{T}$ denoted by the letter $P$ and the cosets $\{1|0\}$ and $\{2_{001}|0\}$, and is a group of type $P2$.

If $\mathcal{F}(\mathcal{D})$ is a group $\mathcal{M}_R$, then the subgroup $\mathcal{D}$ is defined by the non-primed translational group of $\mathcal{F}(\mathcal{D})$ and all the cosets of the standard set of coset representatives of the group $\mathcal{F}(\mathcal{D})$.

*Example*

Consider the three-dimensional magnetic space-group type 16.4.102 $P_{2a}222$. The representative group $P_{2a}222$ is defined by the translational group $\mathcal{T}$ denoted by the symbol $P_{2a}$ generated by the translations

$$\{1|1,0,0\}'\quad\{1|0,1,0\}\quad\{1|0,0,1\}$$

and the standard set of coset representatives

$$\{1|0\}\quad\{2_{100}|0\}\quad\{2_{010}|0\}\quad\{2_{001}|0\}.$$

The subgroup $\mathcal{D}$ of index 2 of the representative group $\mathcal{F}(\mathcal{D}) = P_{2a}222$ is defined by the translational subgroup $\mathcal{T}$ denoted by the symbol $P_{2a}$, *i.e.* the translations generated by

$$\{1|2,0,0\}\quad\{1|0,1,0\}\quad\{1|0,0,1\}$$

and the standard set of cosets of $P_{2a}222$. The group $\mathcal{D}$ is a group of type $P222$.

While the group type symbol of $\mathcal{D}$ is given, the coset representatives of the subgroup $\mathcal{D}$ of $\mathcal{F}(\mathcal{D})$ derived from the standard set of coset representatives of $\mathcal{F}(\mathcal{D})$ may not be identical with the standard set of coset representatives of the representative group of type $\mathcal{D}$ found in the survey of magnetic group types. Consequently, to show the relationship between this subgroup $\mathcal{D}$ and the listed representative group of groups of type $\mathcal{D}$ additional information is provided: a new coordinate system is defined in which the coset representatives of this subgroup $\mathcal{D}$ are identical with the standard set of coset representatives listed for the representative group of groups of type $\mathcal{D}$: Let ($O$; **a**, **b**, **c**) be the coordinate system in which the group $\mathcal{F}(\mathcal{D})$ is defined. $O$ is the origin of the coordinate system, and **a**, **b** and **c** are the basis vectors of the coordinate system. **a**, **b** and **c** represent a set of basis vectors of a primitive cell for primitive lattices and of a conventional cell for centred lattices. A second coordinate system, defined by ($O$ + **p**; **a**′, **b**′, **c**′), is given in which the coset representatives of this subgroup $\mathcal{D}$ are identical with the standard set of coset representatives listed for the representative group of groups of type $\mathcal{D}$. $O$ + **p** is referred to as the *location* of the subgroup $\mathcal{D}$ in the coordinate system of the group $\mathcal{F}(\mathcal{D})$ (Kopský, 2011). The origin is first translated from $O$ to $O$ + **p**. On translating the origin from $O$ to $O$ + **p**, a coset representative $\{\boldsymbol{R}|\boldsymbol{\tau}\}$ becomes $\{\boldsymbol{R}|\boldsymbol{\tau} + \boldsymbol{Rp} - \boldsymbol{p}\}$ (Litvin, 2005, 2008*b*; see also Section 1.5.2.3). This is followed by changing the basis vectors **a**, **b** and **c** to **a**′, **b**′ and **c**′, respectively. The basis vectors **a**′, **b**′, **c**′ define the conventional unit cell of the non-primed subgroup $\mathcal{D}$ of $\mathcal{F}(\mathcal{D})$ in the coordinate system ($O$; **a**, **b**, **c**) in which $\mathcal{F}(\mathcal{D})$ is defined. ($O$ + **p**; **a**′, **b**′, **c**′) is given immediately following the group type symbol for the subgroup $\mathcal{D}$ of $\mathcal{F}(\mathcal{D})$. [In Litvin (2013), for typographical simplicity, the symbols '$O$ +' are omitted.]

*Example*

For the three-dimensional magnetic space-group type 10.4.52, $\mathcal{F}(\mathcal{D}) = P2/m'$, one finds in Litvin (2013)[2]

| Serial No. | Symbol | Non-primed subgroup of index 2 | Standard set of coset representatives |
|---|---|---|---|
| 10.4.52 | $P2/m'$ | $P2$ (0, 0, 0; **a**, **b**, **c**) | $\{1|0\}$ $\{2_{010}|0\}$<br>$\{1|0\}'$ $\{m_{010}|0\}'$ |

The translational subgroup of the subgroup $\mathcal{D} = P2$ of $\mathcal{F}(\mathcal{D}) = P2/m'$ is generated by the translations $\{1|1,0,0\}$, $\{1|0,1,0\}$ and $\{1|0,0,1\}$ and the coset representatives of this group are $\{1|0\}$ and $\{2_{010}|0\}$, the unprimed coset representatives on the right. This subgroup $\mathcal{D}$ is of type $P2$. In Litvin (2013), listed for the group type 3.1.8, $P2$, one finds the identical two coset representatives. Consequently, there is no change in the coordinate system, *i.e.* $\mathbf{p} = (0,0,0)$ and $\mathbf{a}' = \mathbf{a}$, $\mathbf{b}' = \mathbf{b}$ and $\mathbf{c}' = \mathbf{c}$. In the coordinate system of the magnetic group $P2/m'$, the coset representatives of its subgroup $\mathcal{D} = P2$ are identical with the standard set of coset representatives of the group type $P2$.

[2] In Litvin (2013) the terminology 'non-magnetic' is used in place of 'non-primed' in the column headings in these tables.

*Example*

For the three-dimensional magnetic space-group type 16.7.105, $\mathcal{F}(\mathcal{D}) = P_{2c}22'2'$ one has

| Serial No. | Symbol | Non-primed subgroup of index 2 | Standard set of coset representatives |
|---|---|---|---|
| 16.7.105 | $P_{2c}22'2'$ | $P222_1$ (0, 0, 0; **a**, **b**, 2**c**) | $\{1\|0\}$ $\{2_{100}\|0\}$ $\{2_{010}\|0, 0, 1\}$ $\{2_{001}\|0, 0, 1\}$ |

The translational subgroup of the subgroup $\mathcal{D} = P222_1$ of $\mathcal{F}(\mathcal{D}) = P_{2c}22'2'$ is generated by the translations $\{1|1, 0, 0\}$, $\{1|0, 1, 0\}$ and $\{1|0, 0, 2\}$, and the coset representatives of this group are all those coset representatives on the right. This subgroup $\mathcal{D}$ is of type $P222_1$. Listed for the group type 17.1.106 $P222_1$, one finds a different set of coset representatives:

$$\{1|0\} \quad \{2_{100}|0\} \quad \{2_{010}|0, 0, \tfrac{1}{2}\} \quad \{2_{001}|0, 0, \tfrac{1}{2}\}.$$

Consequently, to show the relationship between this subgroup $\mathcal{D}$ of $\mathcal{F}(\mathcal{D})$ and the listed representative group of the group type $P222_1$ we change the coordinate system in which $\mathcal{D}$ is defined to (0, 0, 0; **a**, **b**, 2**c**). In this new coordinate system the coset representatives of the subgroup $\mathcal{D}$ are identical with the coset representatives of the representative group of the group type $P222_1$.

*Example*

For the three-dimensional magnetic space-group type 18.4.116, $P2_12_1'2'$, one has

| Serial No. | Symbol | Non-primed subgroup of index 2 | Standard set of coset representatives |
|---|---|---|---|
| 18.4.116 | $P2_12_1'2'$ | $P2_1$ (0, $\frac{1}{4}$, 0; **c**, **a**, **b**) | $\{1\|0\}$ $\{2_{100}\|\frac{1}{2}, \frac{1}{2}, 0\}$ $\{2_{010}\|\frac{1}{2}, \frac{1}{2}, 0\}'$ $\{2_{001}\|0\}'$ |

The translational subgroup of $\mathcal{D}$ is generated by the translations $\{1|1, 0, 0\}$, $\{1|0, 1, 0\}$ and $\{1|0, 0, 1\}$ and the coset representatives of this group are $\{1|0\}$ and $\{2_{100}|\frac{1}{2}, \frac{1}{2}, 0\}$, the unprimed coset representatives on the right. The group $\mathcal{D}$ is of type $P2_1$. For the magnetic group type 4.1.15 $P2_1$ one finds a different set of coset representatives: $\{1|0\}$ and $\{2_{010}|0, \frac{1}{2}, 0\}$. Consequently, to show the relationship between the subgroup $\mathcal{D}$ of $\mathcal{F}(\mathcal{D})$ and the listed representative group of the group type $P2_1$, we change the coordinate system in which the subgroup $\mathcal{D}$ is defined to (0, $\frac{1}{4}$, 0; **c**, **a**, **b**). The origin is first translated from $O$ to $O + \mathbf{p}$, where $\mathbf{p} = (0, \frac{1}{4}, 0)$, and then a new set of basis vectors, $\mathbf{a}' = \mathbf{c}$, $\mathbf{b}' = \mathbf{a}$ and $\mathbf{c}' = \mathbf{b}$, is defined. In this new coordinate system the coset representatives of the subgroup $\mathcal{D}$ are identical with the standard set of coset representatives of the representative group of the group type $P2_1$.

## 3.6.3. Tables of properties of magnetic groups

In this section we present a guide to the tables of properties of the two- and three-dimensional magnetic subperiodic groups and the one-, two- and three-dimensional magnetic space groups given by Litvin (2013). The format and content of these magnetic group tables are similar to the format and content of the space-group tables in the present volume, the subperiodic group tables in *IT* E, and previous compilations of magnetic subperiodic groups (Litvin, 2005) and magnetic space groups (Litvin, 2008*b*). An example of one these tables is given in Fig. 3.6.3.1. The tables of properties of magnetic groups contain:

First page:
(1) Lattice diagram
(2) Headline
(3) Diagrams of symmetry elements and of the general positions
(4) Origin
(5) Asymmetric unit
(6) Symmetry operations

Subsequent pages:
(7) Abbreviated headline
(8) Generators selected
(9) General and special positions with spins (magnetic moments)
(10) Symmetry of special projections

Tabulations of properties of three-dimensional magnetic space groups can also be found in Koptsik (1968) (note that the general-position diagrams are of 'black and white' objects, not spins). Neutron-diffraction extinctions can be found in the work of Ozerov (1969*a*,*b*) and on the Bilbao Crystallographic Server, http://www.cryst.ehu.es (Aroyo *et al.*, 2006). General positions and Wyckoff positions of the three-dimensional magnetic space groups can also be found on the Bilbao Crystallographic Server.

### 3.6.3.1. Lattice diagram

For each three-dimensional magnetic space group, a three-dimensional lattice diagram is given in the upper left-hand corner of the first page of the tables of properties of that group. (For all other magnetic groups, the corresponding lattice diagram is given within the symmetry diagram, see Section 3.6.3.3 below.) This lattice diagram depicts the coordinate system used, the conventional unit cell of the space group $\mathcal{F}$, the magnetic space group's magnetic superfamily type and the generators of the translational subgroup of the magnetic space group. In Fig. 3.6.3.2 we show lattice diagrams for two orthorhombic magnetic space groups: (*a*) $Pmc2_1$ and (*b*) $P_{2b}m'c'2_1$. The generating lattice vectors are colour coded. Those coloured black are not coupled with time inversion, while those coloured red are coupled with time inversion. In the group $Pmc2_1$, a magnetic group of the type $\mathcal{F}$, the lattice is an orthorhombic $P$ lattice, see Fig. 3.6.3.2(*a*), and no generating translation is coupled with time inversion. In the second group, $P_{2b}m'c'2_1$, a magnetic group of type $\mathcal{M}_R$, the lattice is an orthorhombic $P_{2b}$ lattice, see Fig. 3.6.3.2(*b*), and the generating lattice vector in the $y$ direction is coupled with time inversion.

### 3.6.3.2. Heading

Each table begins with a headline consisting of two lines with five entries, for example

| | | |
|---|---|---|
| $P4/m'mm$ | $4/m'mm$ | Tetragonal |
| 123.3.1001 | $P4/m'2'/m2'/m$ | |

For three-dimensional magnetic space groups, this headline is to the right of the lattice diagram. On the upper line, starting on the left, are three entries:

(1) The *short international* (Hermann–Mauguin) *symbol* of the magnetic space group. Each symbol has two meanings: The first is that of the Hermann–Mauguin symbol of a magnetic space-group type. The second is that of a specific magnetic space group, the representative magnetic space group (see Section 3.6.2.2), which belongs to this magnetic space-group



references