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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 ≤ 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 $\{2_{001}|0, 0, \tfrac{1}{2}\}$, 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 $\{2_{001}|0, 0, \tfrac{1}{2}\}$ 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 $\{m_{100}|\tfrac{1}{2}, 0, \tfrac{1}{2}\}$ and $\{m_{010}|\tfrac{1}{2}, 0, 0\}$, 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 $\{m_{100}|\tfrac{1}{2}, 0, \tfrac{1}{2}\}$ and $\{m_{010}|\tfrac{1}{2}, 0, 0\}$ 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_α 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_α 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

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

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_α 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_α 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 $(O; \mathbf{a}, \mathbf{b}, \mathbf{c})$ be the coordinate system in which the group $\mathcal{F}(\mathcal{D})$ is defined. O is the origin of the coordinate system, and $\mathbf{a}$, $\mathbf{b}$ and $\mathbf{c}$ are the basis vectors of the coordinate system. $\mathbf{a}$, $\mathbf{b}$ and $\mathbf{c}$ 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 $(O + \mathbf{p}; \mathbf{a}', \mathbf{b}', \mathbf{c}')$, 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 $\mathcal{D}$. $O + \mathbf{p}$ 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 $O + \mathbf{p}$. On translating the origin from O to $O + \mathbf{p}$, 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 $\mathbf{a}$, $\mathbf{b}$ and $\mathbf{c}$ to $\mathbf{a}'$, $\mathbf{b}'$ and $\mathbf{c}'$, respectively. The basis vectors $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$ define the conventional unit cell of the non-primed subgroup $\mathcal{D}$ of $\mathcal{F}(\mathcal{D})$ in the coordinate system $(O; \mathbf{a}, \mathbf{b}, \mathbf{c})$ in which $\mathcal{F}(\mathcal{D})$ is defined. $(O + \mathbf{p}; \mathbf{a}', \mathbf{b}', \mathbf{c}')$ 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	$P2/m'$	$P2$ $(0, 0, 0; \mathbf{a}, \mathbf{b}, \mathbf{c})$	$\{1|0\}$ $\{2_{010}|0\}$ $\{1|0\}'$ $\{m_{010}|0\}'$

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.

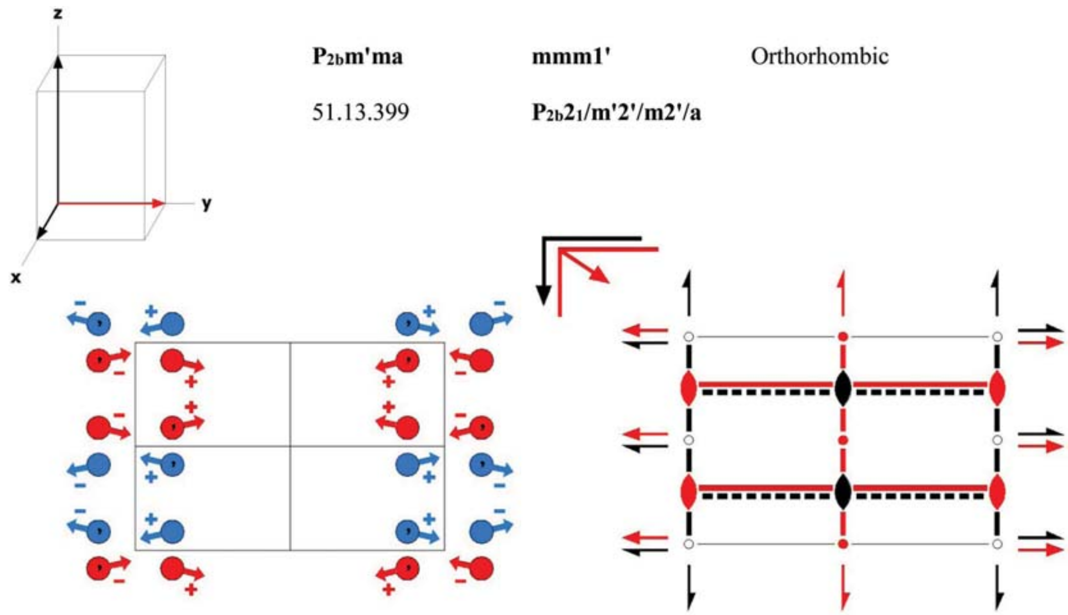
3.6.3.2. Heading

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



Origin at center (2'/m) at $2_1$2/ma

Asymmetric unit 0 ≤ x ≤ ¼; 0 ≤ y ≤ ½; 0 ≤ z ≤ 1

Symmetry Operations

For (0,0,0) + set

(1) 1	(2) 2' ¼,0,z	(3) 2' 0,y,0	(4) 2 (½,0,0) x,0,0
{1 | 0}	{2_{001} | ½,0,0}'	{2_{010} | 0}'	{2_{100} | ½,0,0}
(5) $\bar{1}$'	(6) a (½,0,0) x,y,0	(7) m x,0,z	(8) m' ¼,y,z
{$\bar{1}$ | 0}'	{m_{001} | ½,0,0}	{m_{010} | 0}	{m_{100} | ½,0,0}'

For (0,1,0)' + set

(2) t' (0,1,0)'	(2) 2 ¼,½,z	(3) 2 (0,1,0) 0,y,0	(4) 2' (½,0,0) x,½,0
{1 | 0,1,0}'	{2_{001} | ½,1,0}	{2_{010} | 0,1,0}	{2_{100} | ½,1,0}'
(5) $\bar{1}$ (0, ½,0)	(6) n' (½,1,0) x,y,0	(7) m' x,½,z	(8) b (0,1,0) ¼,y,z
{$\bar{1}$ | 0,1,0}	{m_{001} | ½,1,0}'	{m_{010} | 0,1,0}'	{m_{100} | ½,1,0}

Figure 3.6.3.1
Table of properties of the three-dimensional magnetic space group 51.13.399 $P_{2b}m'ma$.

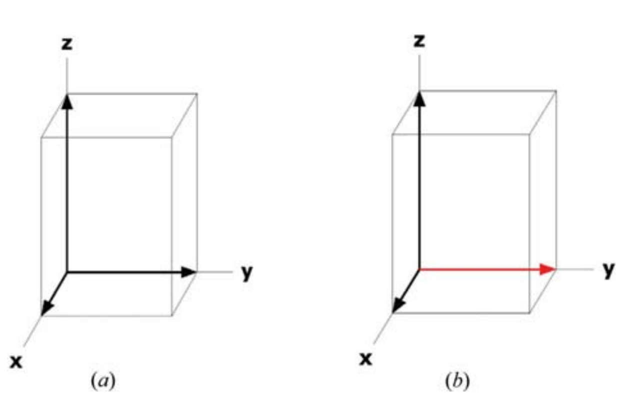


Figure 3.6.3.2
Lattice diagrams of (*a*) the three-dimensional magnetic space group 26.1.168 $\mathcal{F} = Pmc2_1$ and (*b*) the three-dimensional magnetic space group 26.10.177 $\mathcal{M}_R = P_{2b}m'c'2_1 = \mathcal{F}(\mathcal{D}) = Pmc2_1(Pca2_1)$.

type. Given a coordinate system, this group is defined by the list of symmetry operations (see Section 3.6.3.6) given on the page with this Hermann–Mauguin symbol in the heading, or by the given list of general positions and magnetic moments (see Section 3.6.3.9).

(2) The *short international* (Hermann–Mauguin) *point group symbol* for the geometric crystal class to which the magnetic space group belongs.

(3) The crystal system or crystal system/Bravais system classification to which the magnetic space group belongs.

The second line has two additional entries:

(4) The three-part numerical serial index of the magnetic group (see Section 3.6.2.2.1).

(5) The *full international (Hermann–Mauguin) symbol* of the magnetic space group.

Continued 51.13.399 **P_{2b}m'ma**

Generators selected (1); t (1,0,0); t (0,1,0)'; t (0,0,1); (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site Symmetry

Coordinates

(0,0,0) + (0,1,0)' +

Multiplicity, Wyckoff letter, Site Symmetry				
16 l 1	(1) x,y,z [u,v,w]	(2) $\bar{x}$+½,$\bar{y}$,z [u,v,$\bar{w}$]	(3) $\bar{x}$,y,$\bar{z}$ [u,$\bar{v}$,w]	(4) x+½,$\bar{y}$,$\bar{z}$ [u,$\bar{v}$,$\bar{w}$]
	(5) $\bar{x}$,$\bar{y}$,$\bar{z}$ [$\bar{u}$,$\bar{v}$,$\bar{w}$]	(6) x+½,y,$\bar{z}$ [$\bar{u}$,$\bar{v}$,w]	(7) x,$\bar{y}$,z [$\bar{u}$,v,$\bar{w}$]	(8) $\bar{x}$+½,y,z [$\bar{u}$,v,w]
8 k m'..	¼,y,z [0,v,w]	¼,$\bar{y}$,z [0,v,$\bar{w}$]	¾,y,$\bar{z}$ [0,$\bar{v}$,w]	¾,$\bar{y}$,$\bar{z}$ [0,$\bar{v}$,$\bar{w}$]
8 j .m'.	x,½,z [u,0,w]	$\bar{x}$+½,½,z [$\bar{u}$,0,w]	$\bar{x}$,½,$\bar{z}$ [u,0,w]	x+½,½,$\bar{z}$ [$\bar{u}$,0,w]
8 i .m.	x,0,z [0,v,0]	$\bar{x}$+½,½,z [0,v,0]	$\bar{x}$,0,$\bar{z}$ [0,$\bar{v}$,0]	x+½,0,$\bar{z}$ [0,$\bar{v}$,0]
8 h .2'.	0,y,½ [u,0,w]	½,$\bar{y}$,½ [u,0,$\bar{w}$]	0,$\bar{y}$,½ [$\bar{u}$,0,$\bar{w}$]	½,y,½ [$\bar{u}$,0,w]
8 g .2'.	0,y,0 [u,0,w]	½,$\bar{y}$,0 [u,0,$\bar{w}$]	0,$\bar{y}$,0 [$\bar{u}$,0,$\bar{w}$]	½,y,0 [$\bar{u}$,0,w]
4 f m'm'2	¼,½,z [0,0,w]	¾,½,$\bar{z}$ [0,0,w]		
4 e m'm2'	¼,0,z [0,v,0]	¾,0,$\bar{z}$ [0,$\bar{v}$,0]		
4 d .2'/m'.	0,½,½ [u,0,w]	½,½,½ [$\bar{u}$,0,w]		
4 c .2'/m.	0,0,½ [0,0,0]	½,0,½ [0,0,0]		
4 b .2'/m'.	0,½,0 [u,0,w]	½,½,0 [$\bar{u}$,0,w]		
4 a .2'/m.	0,0,0 [0,0,0]	½,0,0 [0,0,0]		

Symmetry of Special Projections

Along [0,0,1] **p_{c*}2mm**
a* = -**a**/2 **b*** = **b**
Origin at 0,0,z

Along [1,0,0] **p_{2a*}2mm**
a* = **b** **b*** = **c**
Origin at x,0,0

Along [0,1,0] **p2mg1'**
a* = -**a** **b*** = **c**
Origin at 0,y,0

Figure 3.6.3.1
Table of properties of the three-dimensional magnetic space group 51.13.399 $P_{2b}m'ma$ continued.

3.6.3.3. Diagrams of symmetry elements and of the general positions

There are two types of diagrams: symmetry diagrams and general-position diagrams. The symmetry diagrams show (1) the relative locations and orientations of the symmetry elements and (2) the absolute locations and orientations of these symmetry elements in a given coordinate system. The general-position diagrams show, in that coordinate system, the arrangement of a set of symmetry-equivalent general points and the relative orientations of magnetic moments on this set of points. Figs. 3.6.3.3 and 3.6.3.4 show the symmetry diagram and general-position diagram, respectively, of the three-dimensional magnetic space group $P4_12'2'$.

All diagrams of three-dimensional magnetic space groups and three-dimensional subperiodic groups are orthogonal projections. The projection direction is along a basis vector of the conventional crystallographic coordinate system, see Table 1.1 of Litvin (2013). If the other two basis vectors are not parallel to the plane of the diagram, they are indicated by a subscript p, *e.g.* $\mathbf{a}_p$, $\mathbf{b}_p$ and $\mathbf{c}_p$. Schematic representations of the diagrams, showing their conventional coordinate systems, *i.e.* the origin O and basis vectors, are given in Table 2.1 of Litvin (2013). For two-dimensional magnetic space groups and magnetic frieze groups, the diagrams are in the plane defined by the group's conventional coordinate system.

The graphical symbols used in the symmetry diagrams are listed in Table 2.2 of Litvin (2013) and are an extension of those used in the present volume, *IT* E and Litvin (2008*b*). For symmetry planes and symmetry axes parallel to the plane of diagram, for rotation-inversions and for centres of symmetry, the 'heights' h along the projection direction above the plane of the

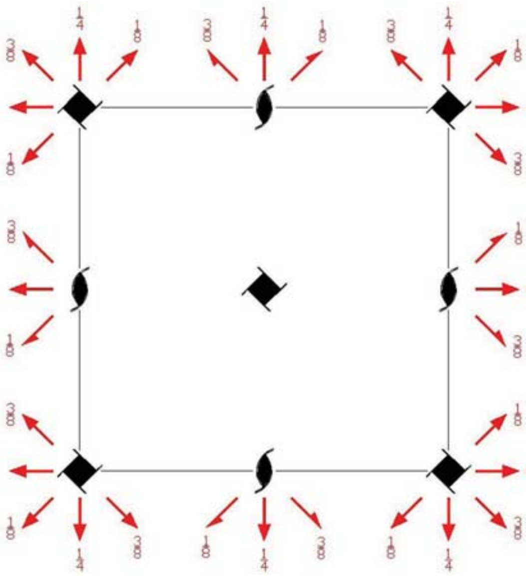


Figure 3.6.3.3
Symmetry diagram of $P4_12'2'$

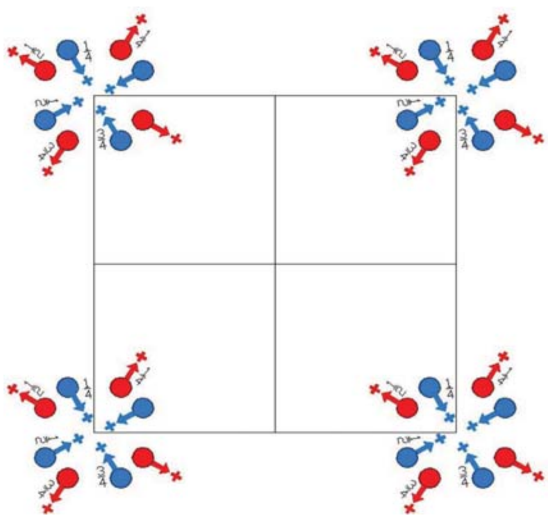


Figure 3.6.3.4
General-position diagram of $P4_12'2'$.

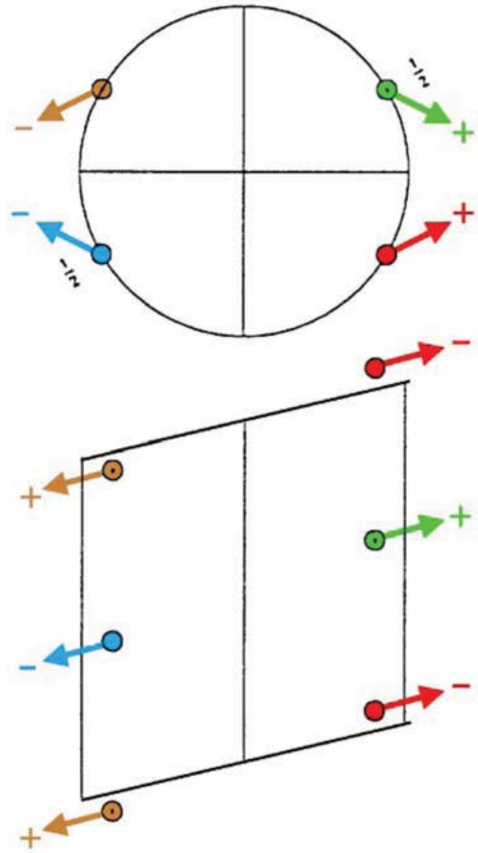


Figure 3.6.3.6
General-position diagram of rod group 2.3.29 $P2/c'11$. The positional colour coding is red for $x > 0$ and $z > 0$; blue for $x > 0$ and $z < 0$; green for $x < 0$ and $z > 0$; and brown for $x < 0$ and $z < 0$.

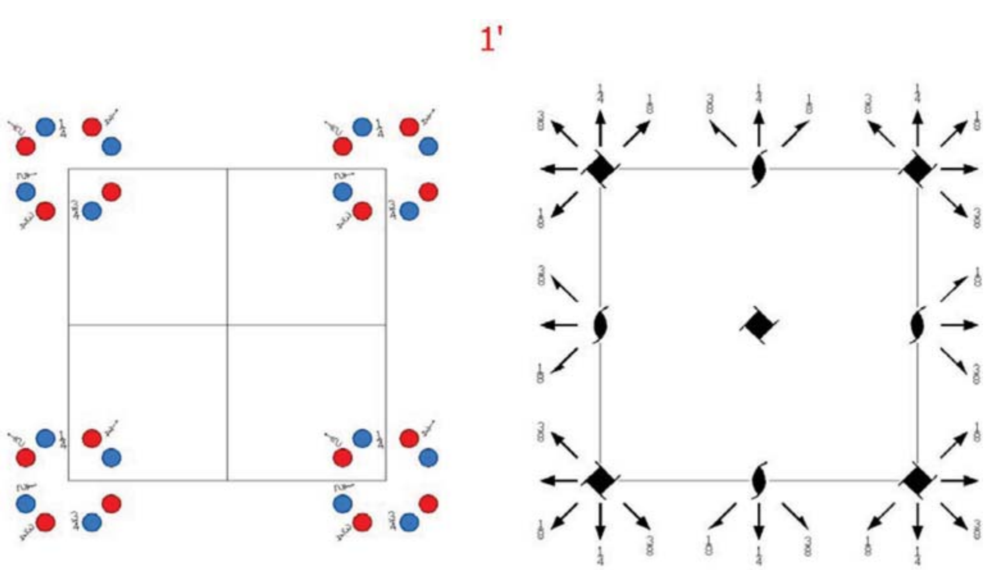


Figure 3.6.3.5
Diagrams of the magnetic space group $P4_1221'$.

diagram are given. The heights are given as fractions of the shortest translation along the projection direction and, if different from zero, are printed next to the graphical symbol, see Fig. 3.6.3.3.

In the general-position diagrams, the general positions and corresponding magnetic moments are colour coded. Positions with a z component of $+z$ are shown as red circles and those with a z component of $-z$ are shown as blue circles. If the z component is either $h + z$ or $h - z$ with $h \neq 0$, then the height h is printed next to the general position, see Fig. 3.6.3.4. If two general positions have the same x component and y component, but one has a z component $+z$ and the other $-z$, the positions are shown as a circle with one half coloured red, the other half blue. The magnetic moments are colour coded to the general position to which they are associated, their direction in the plane of projection is given by an arrow in the direction of the projected magnetic moment. A + or − sign near the tip of the arrow indicates that the magnetic moment is inclined, respectively, above or below the plane of projection.

For magnetic space groups of the type $\mathcal{F}1'$, the symmetry diagram is that of the group $\mathcal{F}$. That each symmetry element also appears coupled with time inversion is represented by a red $1'$ printed between and above the general-position and symmetry diagrams. Because groups of this type contain the time-inversion symmetry, the magnetic moments are all identically zero, and no arrows appear in the general-position diagram. An example, the diagrams of the magnetic space group $P4_1221'$ are shown in Fig. 3.6.3.5. For triclinic, monoclinic/oblique, monoclinic/rectangular and orthorhombic rod groups, the colour coding of the general positions is extended according to the positive or negative values of the x and z components of the coordinates of the general position, see Fig. 3.6.3.6.

VRML (Virtual Reality Modeling Language) general-position diagrams are available for the two- and three-dimensional magnetic subperiodic groups (Cordisco & Litvin, 2004), and for the one-, two- and non-cubic three-dimensional magnetic space groups (Burke *et al.*, 2006). These diagrams can be rotated and zoomed in on to aid in the visualization of the general-position diagrams, and include both the general positions of the atoms and the general orientations of the associated magnetic moments.

Table 3.6.3.1
Symmetry operations of magnetic space group 51.14.400 $P_{2b}mma'$

Symmetry operations			
	For (0, 0, 0)+ set		
(1) 1 {1|0}	(2) 2 1/4, 0, z $\{2_{001}\|1/2, 0, 0\}$	(3) $2'$ 0, y, 0 $\{2_{010}\|0\}'$	(4) $2'$ (1/2, 0, 0) x, 0, 0 $\{2_{100}\|1/2, 0, 0\}'$
(5) $\bar{1}'$ $\{\bar{1}\|0\}'$	(6) a' (1/2, 0, 0) x, y, 0 $\{m_{001}\|1/2, 0, 0\}'$	(7) m x, 0, z $\{m_{010}\|0\}$	(8) m 1/4, y, z $\{m_{100}\|1/2, 0, 0\}$
	For (0, 1, 0)′+ set		
(1) t' (0, 1, 0) $\{1\|0, 1, 0\}'$	(2) $2'$ 1/4, 1/2, z $\{2_{001}\|1/2, 1, 0\}'$	(3) 2 (0, 1, 0) 0, y, 0 $\{2_{010}\|0, 1, 0\}$	(4) 2 (1/2, 0, 0) x, 1/2, 0 $\{2_{100}\|1/2, 1, 0\}$
(5) $\bar{1}$ 0, 1/2, 0 $\{\bar{1}\|0, 1, 0\}$	(6) n (1/2, 1, 0) x, y, 0 $\{m_{001}\|1/2, 1, 0\}$	(7) m' x, 1/2, z $\{m_{010}\|0, 1, 0\}'$	(8) b (0, 1, 0) 1/4, y, z $\{m_{100}\|1/2, 1, 0\}'$

3.6.3.4. Origin

If the magnetic space group is centrosymmetric, then the inversion centre or a position of high site symmetry, as on the fourfold axis of tetragonal groups, is chosen as the origin. For noncentrosymmetric groups, the origin is at a point of highest site symmetry. If no site symmetry is higher than 1, the origin is placed on a screw axis, a glide plane or at the intersection of several such symmetries.

In the *Origin* line below the diagrams, the site symmetry of the origin is given. An additional symbol indicates all symmetry elements that pass through the origin. For example, for the magnetic space group $I4/mcm$, one finds '**Origin** at center ($4/m$) at $4/mc2_1/c$'. The site symmetry is $4/m$ and, in addition, two glide planes perpendicular to the y and z axes, and a screw axis parallel to the z axis, pass through the origin.

3.6.3.5. Asymmetric unit

An asymmetric unit is a simply connected smallest part of space which, by application of all symmetry operations of the magnetic group, exactly fills the whole space. For subperiodic groups, because the translational symmetry is of a lower dimension than that of the space, the asymmetric unit is infinite in size. The asymmetric unit for subperiodic groups is defined by setting the limits on the coordinates of points contained in the asymmetric unit. For example, the asymmetric unit for the magnetic layer group 32.3.199 $pm'2_1n'$ is

Asymmetric unit $0 < x < \frac{1}{2}$; $0 < y < 1$; $0 < z$

Since the translational symmetry of a magnetic space group is of the same dimension as that of the space, the asymmetric unit is a finite part of space. The asymmetric unit is defined, as above, by setting the limits on the coordinates of points contained in the asymmetric unit. For example, for the magnetic space group 140.3.1198 $I4/m'cm$ one has

Asymmetric unit $0 < x < \frac{1}{2}$; $0 < y < \frac{1}{2}$; $0 < z < \frac{1}{4}$; $y < \frac{1}{2} - x$

Drawings showing the boundary planes occurring in the tetragonal, trigonal and hexagonal systems, together with their algebraic equations, are given in Fig. 2.1.3.11. Drawings of asymmetric units for cubic groups have been published by Koch & Fischer (1974). The asymmetric units have complicated shapes in the trigonal, hexagonal and cubic crystal systems, and consequently are also specified by giving the vertices of the asymmetric unit. For example, for the magnetic space group 176.1.1374 $P6_3/m$ one finds

Asymmetric unit		$0 < x < 2/3$;	$0 < y < 2/3$;	$0 < z < 1/4$;	
		$x < (1 + y)/2$;	$y < \min(1 - x, (1 + x)/2)$		
Vertices	0, 0, 0	1/2, 0, 0	2/3, 1/3, 0	1/3, 2/3, 0	0, 1/2, 0
	0, 0, 1/4	1/2, 0, 1/4	2/3, 1/3, 1/4	1/3, 2/3, 1/4	0, 1/2, 1/4

Because the asymmetric unit is invariant under time inversion, all magnetic space groups $\mathcal{F}$, $\mathcal{F}1'$ and $\mathcal{F}(\mathcal{D})$ of the magnetic superfamily of type $\mathcal{F}$ have identical asymmetric units, the asymmetric unit of the group $\mathcal{F}$ (as in the present volume).

3.6.3.6. Symmetry operations

Listed under the heading of *Symmetry operations* is the geometric description of the symmetry operations of the magnetic group. A symbol denoting the geometric description of each symmetry operation is given. Details of this symbolism, except for the use of prime to denote time inversion, are given in Sections 1.4.2 and 2.1.3.9. For glide planes and screw axes, the glide and screw part are always explicitly given in parentheses by fractional coordinates, *i.e.* by fractions of the basis vectors of the coordinate system of $\mathcal{F}$ of the superfamily of the magnetic group. A coordinate triplet indicating the location and orientation of the symmetry element is given, and for rotation-inversions the location of the inversion point is also given. These symbols, with the addition of a prime to denote time inversion, follow those used in the present volume, *IT* E and Litvin (2005, 2008*b*). In addition, each symmetry operation is also given in Seitz (1934, 1935*a*,*b*, 1936) notation (see Section 3.6.2.2.3), *e.g.* see Table 3.6.3.1 for the symmetry operations of the magnetic space group 51.14.400 $P_{2b}mma'$.

The corresponding coordinate triplets of the *General positions,* see Section 3.6.3.9, may be interpreted as a second description of the symmetry operations, a description in matrix form. The numbering (1), (2), ..., (p), ... of the entries in the blocks *Symmetry operations* is the same as the numbering of the corresponding coordinate triplets of the *General position*, the first block below *Positions*. For all magnetic groups with primitive

Table 3.6.3.2
General positions of magnetic space group 51.14.400 $P_{2b}mma'$

Positions	Coordinates			
	(0, 0, 0)+ (0, 1, 0)′+			
16 *l* 1	(1) x, y, z $[u, v, w]$	(2) $\bar{x}+1/2, \bar{y}, z$ $[\bar{u}, \bar{v}, w]$	(3) $\bar{x}, y, \bar{z}$ $[u, \bar{v}, w]$	(4) $x+1/2, \bar{y}, \bar{z}$ $[\bar{u}, v, w]$
	(5) $\bar{x}, \bar{y}, \bar{z}$ $[\bar{u}, \bar{v}, \bar{w}]$	(6) $x+1/2, y, \bar{z}$ $[u, v, \bar{w}]$	(7) $x, \bar{y}, z$ $[\bar{u}, v, \bar{w}]$	(8) $\bar{x}+1/2, y, z$ $[u, \bar{v}, \bar{w}]$

lattices, the two lists, *Symmetry operations* and *General position*, have the same number of entries.

For magnetic groups with centred cells, only one block of several (two, three or four) blocks of the general positions is explicitly given, see Table 3.6.3.2. A set of two, three or four centring translations is given below the subheading *Coordinates*. Each of these translations is added to the given block of general positions to obtain the complete set of blocks of general positions. While one of the several blocks of general positions is explicitly given, the corresponding symmetry operations are all explicitly given. Each corresponding block of symmetry operations is listed under a subheading of 'centring translation + set' for each centring translation listed below the subheading *Coordinates*.

3.6.3.7. Abbreviated headline

On the second and subsequent pages of the tables for a specific magnetic group there is an abbreviated headline. This abbreviated headline contains three items: (1) the word 'Continued', (2) the three-part number of the magnetic group type, and (3) the short international (Hermann–Mauguin) symbol for the magnetic group type.

3.6.3.8. Generators selected

The line *Generators selected* lists the symmetry operations selected to generate the symmetry-equivalent points of the *General position* from a point with coordinates x, y, z. The first generator is always the identity operation given by (1) followed by generating translations. Additional generators are given as numbers (p), which refer to the coordinate triplets of the *General position* and to corresponding symmetry operations in the first block, if more than one, of the *Symmetry operations*.

3.6.3.9. General and special positions with spins (magnetic moments)

The entries under *Positions*, referred to as *Wyckoff positions*, consist of the *General position*, the upper block, followed by blocks of *Special positions*. The upper block of positions, the general position, is a set of symmetry-equivalent points where each point is left invariant only by the identity operation or, for magnetic groups $\mathcal{F}1'$, by the identity operation and time inversion, but by no other symmetry operations of the magnetic group. The lower blocks, the special positions, are sets of symmetry-equivalent points where each point is left invariant by at least one additional operation in addition to the identity operation, or, for magnetic space groups $\mathcal{F}1'$, in addition to the identity operation and time inversion.

For each block of positions the following information is provided:

Multiplicity: The multiplicity is the number of equivalent positions in the conventional unit cell of the non-primed group $\mathcal{F}$ associated with the magnetic group.

Wyckoff letter: This letter is a coding scheme for the blocks of positions, starting with '*a*' at the bottom block and continuing upwards in alphabetical order.

Site symmetry: The site-symmetry group is the largest subgroup of the magnetic space group that leaves invariant the first position in each block of positions. This group is isomorphic to a subgroup of the point group of the magnetic group. An 'oriented' symbol is used to show how the symmetry elements at a site are related to the conventional crystallographic basis, and the sequence of characters in the symbol correspond to the sequence of symmetry directions in the magnetic group symbol. Sets of equivalent symmetry directions that do not contribute any element to the site symmetry are represented by dots. Sets of symmetry directions having more than one equivalent direction may require more than one character if the site-symmetry group belongs to a lower crystal system. For example, for the 2*c* position of the magnetic space group $P4'm'm$ (99.3.825) the site-symmetry group is '$2m'm'$.'. The two characters $m'm'$ represent the secondary set of tetragonal symmetry directions, whereas the dot represents the tertiary tetragonal symmetry directions.

Coordinates of positions and components of magnetic moments: In each block of positions, the coordinates of each position are given. Immediately following each set of position coordinates are the components of the symmetry-allowed magnetic moment at that position. The components of the magnetic moment of the first position are determined from the given site-symmetry group. The components of the magnetic moments at the remaining positions are determined by applying the symmetry operations to the components of that magnetic moment at the first position.

3.6.3.10. Symmetry of special projections

The symmetry of special projections is given for the two- and three-dimensional magnetic groups. For each three-dimensional magnetic group, the symmetry is given for three projections, projections onto planes normal to the projection directions. If there are three symmetry directions, the three projection directions correspond to primary, secondary and tertiary symmetry directions. If there are fewer than three symmetry directions, the additional projection direction or directions are taken along coordinate axes. For two-dimensional magnetic groups, there are two orthogonal projections. The projections are onto lines normal to the projection directions.

For the three-dimensional magnetic space groups, each projection gives rise to a two-dimensional magnetic space group. For two-dimensional magnetic space groups, each projection gives rise to a one-dimensional magnetic space group. For magnetic rod groups and magnetic layer groups, a projection along the [001] direction gives rise, respectively, to a two-dimensional magnetic point group and a two-dimensional magnetic space group. All other projections give rise to magnetic frieze groups. For magnetic frieze groups, projections give rise to either a one-dimensional magnetic space group or a one-dimensional magnetic point group. The international (Hermann–Mauguin) symbol of the symmetry group of each projection is given. Below this symbol, the basis vector(s) of the projected symmetry group and the origin of the projected symmetry group are given in terms of the basis vector(s) of the projected magnetic group. The location of the origin of the symmetry group of the

Table 3.6.4.1
Comparisons of three-dimensional OG and BNS magnetic group type symbols

Serial No.	OG	BNS	$\mathcal{F}(\mathcal{D})$
44.1.324	$Imm2$		
44.2.325	$Imm21'$		
44.3.326	$Im'm2'$		
44.4.327	$Im'm'2$		
44.5.328	I_Pmm2	P_Imm2	$Imm2(Pmm2)$
44.6.329	$I_Pmm'2'$	P_Imm2_1	$Imm2(Pmm2_1)$
44.7.330	$I_Pm'm'2$	P_Inn2	$Imm2(Pnn2)$

projection is given with respect to the unit cell of the magnetic group from which it has been projected.

3.6.4. Comparison of OG and BNS magnetic group type symbols

There are other notations for magnetic group type symbols than the notations of Opechowski & Guccione (1965) and Belov, Neronova & Smirnova (1957): for example for the three-dimensional magnetic group 55.10.450 $P_{2c}b'a'm$ the Shubnikov notation is $Ш^{403}_{58}$ (Koptsik, 1966; Shubnikov & Koptsik, 1974) or Sh^{403}_{58} (Ozerov, 1969*a*,*b*) (see also Zamorzaev, 1976). There are also the variations of the Opechowski & Guccione notation put forward by Grimmer (2009, 2010). We shall limit ourselves here to a detailed comparison of the Opechowski & Guccione and Belov, Neronova & Smirnova notations.

For all group types in the reduced magnetic superfamily of $\mathcal{F}$, the Opechowski & Guccione (1965) magnetic group type symbols (OG symbols) are based on the symbol of the group $\mathcal{F}$. Belov, Neronova & Smirnova (1957) also base their symbols (BNS symbols) on the symbol of the group $\mathcal{F}$, but only for magnetic groups of the type $\mathcal{F}$, $\mathcal{F}1'$ and $\mathcal{M}_T$. For magnetic groups $\mathcal{M}_R = \mathcal{F}(\mathcal{D}) = \mathcal{D} \cup (\mathcal{F} - \mathcal{D})1'$, where $\mathcal{D}$ is an equi-class subgroup of $\mathcal{F}$, the BNS symbol is based on the symbol of the group $\mathcal{D}$, the non-primed subgroup of index 2. A magnetic group $\mathcal{M}_R$ can be written as $\mathcal{M}_R = \mathcal{F}(\mathcal{D}) = \mathcal{D} \cup t_\alpha'\mathcal{D}$, where t_α is a translation of $\mathcal{F}$ not in $\mathcal{D}$. The BNS symbol for a magnetic group of the type $\mathcal{M}_R$ is the symbol for the group type $\mathcal{D}$ with a subindex inserted on the symbol for the translational subgroup of $\mathcal{D}$ to denote the translation t_α'.

Example

The representative three-dimensional space group $\mathcal{F} = Pmm2$ has a translational subgroup generated by the three translations $\{1|1, 0, 0\}$, $\{1|0, 1, 0\}$ and $\{1|0, 0, 1\}$ and the standard set of coset representatives

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

The three-dimensional magnetic space group 25.10.165 $\mathcal{F}(\mathcal{D}) = Pmm2(Pcc2)$ has a subgroup $\mathcal{D}$ with a translational subgroup generated by the three translations $\{1|1, 0, 0\}$, $\{1|0, 1, 0\}$ and $\{1|0, 0, 2\}$, $t_\alpha' = \{1|0, 0, 1\}'$, and a set of coset representatives

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

The OG magnetic group type symbol is, see Section 3.6.2.2.4, $P_{2c}m'm'2$, *i.e.* based on the symbol for the group type $\mathcal{F} = Pmm2$. The BNS symbol is P_ccc2, *i.e.* based on the symbol for the subgroup $\mathcal{D} = Pcc2$ of $\mathcal{F}$, with a subindex 'c' attached to 'P' to denote the translation $t_\alpha' = \{1|0, 0, 1\}'$ in $\mathcal{M}_R = \mathcal{F}(\mathcal{D}) = \mathcal{D} \cup t_\alpha'\mathcal{D}$.

A side-by-side comparison of OG magnetic group type symbols and BNS symbols is given in Litvin (2013). As the OG and BNS symbols are the same for magnetic groups $\mathcal{F}$, $\mathcal{F}1'$ and $\mathcal{M}_T$, BNS symbols are explicitly listed only for groups of type $\mathcal{M}_R$. Examples of this comparison are given in Table 3.6.4.1.

3.6.5. Maximal subgroups of index ≤ 4

We consider the maximal subgroups of index ≤ 4 of the one-, two- and three-dimensional magnetic space groups and the two- and three-dimensional magnetic subperiodic groups. A complete listing of the maximal subgroups of the two- and three-dimensional non-primed space groups can be found in *International Tables for Crystallography*, Volume A1, *Symmetry Relations Between Space Groups* (2010; *IT* A1). The maximal subgroups of index ≤ 4 of the three-dimensional non-primed space groups and non-primed layer and rod groups can also be found on the Bilbao Crystallographic Server (http://www.cryst.ehu.es; Aroyo *et al.*, 2006).

For magnetic groups, an abstract of a method for determining the maximal subgroups of magnetic groups was published by Sayari & Billiet (1977). The maximal subgroups of magnetic groups found in Litvin (2013) were derived from Litvin (2008*a*) using a method given by Litvin (1996).

Each maximal subgroup table is headed by the magnetic group type whose maximal subgroup types are to be listed.

Examples

For the three-dimensional magnetic space group type $Pb'a'm$, one finds (Litvin, 2013), in bold blue type, information which defines the representative group of this type in a coordinate system O; **a**, **b**, **c**:

55.5.445	$Pb'a'm$	$(0, 0, 0; \mathbf{a}, \mathbf{b}, \mathbf{c})$	$\{1|0\}$	$\{2_{100}|\frac{1}{2}, \frac{1}{2}, 0\}'$
			$\{2_{010}|\frac{1}{2}, \frac{1}{2}, 0\}'$	$\{2_{001}|0\}$
			$\{\bar{1}|0\}$	$\{m_{100}|\frac{1}{2}, \frac{1}{2}, 0\}'$
			$\{m_{010}|\frac{1}{2}, \frac{1}{2}, 0\}'$	$\{m_{001}|0\}$

The first column gives the global serial number of the group, followed in the second column by its magnetic group type symbol. In the third column, the symbol $(O; \mathbf{a}', \mathbf{b}', \mathbf{c}')$ gives the origin O and basis vectors $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$ of the conventional unit cell of the non-primed subgroup of the representative group of the type $Pb'a'm$. These basis vectors $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$ imply both the magnetic and non-primed translational subgroups of the representative group. In this case, the P translational subgroup of the representative group is non-primed and generated by the basis vectors **a**, **b**, **c**. The standard set of coset representatives of this representative group is given on the right.

For the three-dimensional magnetic space-group type $P_{2b}ma2$ one finds (Litvin, 2013):

28.6.190	$P_{2b}ma2$	$(0, 0, 0; \mathbf{a}, 2\mathbf{b}, \mathbf{c})$	$\{1|0\}$	$\{m_{100}|\frac{1}{2}, 0, 0\}$
			$\{m_{010}|\frac{1}{2}, 0, 0\}$	$\{2_{001}|0\}$

Note here that $\mathbf{a}' = \mathbf{a}$, $\mathbf{b}' = 2\mathbf{b}$, $\mathbf{c}' = \mathbf{c}$, being the basis vectors of the conventional unit cell of the non-primed subgroup of the representative group of $P_{2b}ma2$, implies that the translational subgroup of the representative group is P_{2b}, *i.e.* generated by the non-primed translations $\{1|1, 0, 0\}$, $\{1|0, 2, 0\}$, $\{1|0, 0, 1\}$ and the magnetic translation $\{1|0, 1, 0\}'$.

Following the subtable heading of each magnetic space-group type is a listing of the maximal subgroups of index ≤ 4 of the representative magnetic space group of this type.

Examples

From the list of maximal subgroups of the representative magnetic group of the type $Pb'a'm$ is the subgroup listed as

$Pb'a'2$	2	(0, 0, 0; **a**, **b**, **c**)	$\{1\|0\}$	$\{2_{001}\|0\}$
			$\{m_{010}\|\frac{1}{2},\frac{1}{2},0\}'$	$\{m_{100}\|\frac{1}{2},\frac{1}{2},0\}'$

The first column gives the magnetic group type symbol of the subgroup. The second column gives the subgroup index of this subgroup as a subgroup of the representative group of type $Pb'a'm$. In the third column, the symbol (O + **p**; **a**′, **b**′, **c**′) gives the origin 'O + **p**' and basis vectors **a**′, **b**′, **c**′ of the conventional unit cell of the non-primed subgroup, where **p**, a translation of the origin of the coordinate system of the representative group $Pb'a'm$, and the conventional unit cell are such that the coset representatives listed are transformed into the standard cosets of the representative group of the subgroup type $Pb'a'2$. In this case, since the listed coset representatives are the standard cosets of the representative group of type $Pb'a'2$, no translation of origin is required, and consequently O + **p** = 0, 0, 0. The conventional unit cell of the non-primed subgroup of the subgroup $Pb'a'2$ is the same as that of representative group of the type $Pb'a'2$ and consequently one finds **a**′ = **a**, **b**′ = **b**, **c**′ = **c**.

That the listed coset representatives of the subgroup are the same as those of the representative group of that subgroup type is not always the case:

Example

A subgroup of type $P2/m$ of the representative group $Pb'a'm$ is listed as

$P2/m$ 2 (0, 0, 0; **b**, **c**, **a**) $\{1|0\}$ $\{2_{001}|0\}$ $\{\bar{1}|0\}$ $\{m_{001}|0\}$

The standard set of coset representatives of the representative group $P2/m$ are

$$\{1|0\} \quad \{\bar{1}|0\} \quad \{2_{010}|0\} \quad \{m_{010}|0\}.$$

A change in setting to have the coset representatives of the subgroup be identical with the coset representatives of the representative group $P2/m$ is represented in the symbol (0, 0, 0; **b**, **c**, **a**), *i.e.* changing the setting from **a**, **b**, **c** to **b**, **c**, **a**.

Other cases may require a simultaneous change to both the origin and the setting of the conventional unit cell of the non-primed subgroup:

Example

A third subgroup of the representative group $Pb'a'm$ is the equi-class subgroup of the same type $Pb'a'm$:

$Pb'a'm$	2	(0, 0, $\frac{1}{2}$; **a**, **b**, 2**c**)	$\{1\|0\}$	$\{2_{100}\|\frac{1}{2},\frac{1}{2},1\}'$
			$\{2_{010}\|\frac{1}{2},\frac{1}{2},1\}'$	$\{2_{001}\|0\}$
			$\{\bar{1}\|0,0,1\}$	$\{m_{100}\|\frac{1}{2},\frac{1}{2},0\}'$
			$\{m_{010}\|\frac{1}{2},\frac{1}{2},0\}'$	$\{m_{001}\|0,0,1\}$

The listed coset representatives of this subgroup are not the same as the coset representatives of the representative group $Pb'a'm$, *i.e.* where the z component of the non-primitive translation associated with all coset representatives is zero. To have these listed coset representatives become identical with the coset representatives of the standard representative group of $Pb'a'm$, one must change the origin of the coordinate system. This information is provided in the symbol (0, 0, $\frac{1}{2}$; **a**, **b**, 2**c**) where O + **p** = 0, 0, $\frac{1}{2}$ denotes the translation under which all the non-zero z components of the coset representatives are transformed to zero. Note also that the P in the subgroup symbol denotes a non-primed translational subgroup which is determined by **a**′ = **a**, **b**′ = **b**, **c**′ = 2**c**, *i.e.* P denotes the translational group generated by the translations {1|1, 0, 0}, {1|0, 1, 0} and {1|0, 0, 2}.

In the tabulations of the maximal subgroups of groups of the type $\mathcal{F}1'$ not all maximal subgroups are explicitly listed. The maximal subgroup $\mathcal{F}$ of $\mathcal{F}1'$ is not listed. If $\mathcal{G}$ is a maximal subgroup of $\mathcal{F}$, then $\mathcal{G}1'$ is a maximal subgroup of $\mathcal{F}1'$ and is also not explicitly listed. All maximal subgroups $\mathcal{G}$ of $\mathcal{F}$ are listed under $\mathcal{F}$, and consequently, all maximal subgroups $\mathcal{G}1'$ of $\mathcal{F}1'$ are then found from the list of all maximal subgroups $\mathcal{G}$ of $\mathcal{F}$ by multiplying each by $1'$. For each listed maximal subgroup, its non-primed subgroup type is explicitly given. For example, a listed subgroup of $Pma21'$ is

$Pma'2'$	Pm	2	(0, 0, 0; **a**, **b**, **c**)	$\{1\|0\}$	$\{2_{001}\|0\}'$
				$\{m_{010}\|\frac{1}{2},0,0\}'$	$\{m_{100}\|\frac{1}{2},0,0\}$

where the non-primed subgroup type Pm of $Pma'2'$ is given in the second column.

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