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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 $Pm'_x m'_y 2_z$. 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 sub-indices. 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; **a**, **b**, **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; **a**, 2**b**, **c**)	$\{1\|0\}$	$\{2_{010}\|0, 1, 0\}$	$\{\bar{1}\|0, 1, 0\}$	$\{m_{010}\|0\}$
50.10.386	$P_{2c}b'a'n'$	$Pnnn$ ($\frac{1}{4}$, $\frac{1}{4}$, $\frac{1}{2}$; **a**, 2**c**, **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 nonprimitive 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

references