

3.6. MAGNETIC SUBPERIODIC GROUPS AND MAGNETIC SPACE GROUPS

**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	$\mathcal{F}$	$\mathcal{F}'$	$\mathcal{F}(\mathcal{D})$	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  $\mathcal{F}'$  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  $\mathcal{F}$ ,  $\mathcal{F}'$  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  $\mathcal{F}'$  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  $\mathcal{F}$ ,  $\mathcal{F}'$  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  $\mathcal{F}'$  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.*  $Pm_{xy}' m_{xy}' 2_z$ , 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 <sub>010</sub>  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 <sub>010</sub>  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 <sub>010</sub>  0, 1, 0}	{ $\bar{1}$  0, 1, 0}	{ $m_{010}$  0}
50.10.386	$P_{2c}b'a'n'$	$Pnnn(\frac{1}{3}, \frac{1}{4}, \frac{1}{2}; \mathbf{a}, 2\mathbf{c}, \mathbf{b})$	{1 0}	{2 <sub>100</sub>  0}	{2 <sub>010</sub>  0, 0, 1}	{2 <sub>001</sub>  0, 0, 1}
			{ $\bar{1}$   $\frac{1}{2}, \frac{1}{2}, 1$ }	{ $m_{100}$   $\frac{1}{2}, \frac{1}{2}, 1$ }	{ $m_{010}$   $\frac{1}{2}, \frac{1}{2}, 0$ }	{ $m_{001}$   $\frac{1}{2}, \frac{1}{2}, 0$ }