International Tables for Crystallography (2016). Vol. A, Section 3.6.2.1, pp. 852–853.

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; **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**)	$\{1\|0\}$	$\{2_{100}\|0\}$	$\{2_{010}\|0, 0, 1\}$	$\{2_{001}\|0, 0, 1\}$
			$\{\bar{1}\|\frac{1}{2}, \frac{1}{2}, 1\}$	$\{m_{100}\|\frac{1}{2}, \frac{1}{2}, 1\}$	$\{m_{010}\|\frac{1}{2}, \frac{1}{2}, 0\}$	$\{m_{001}\|\frac{1}{2}, \frac{1}{2}, 0\}$

references