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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).

references