Acta Crystallographica Section A
Foundations of Crystallography
ISSN 0108-7673

Magnetic group maximal subgroups of index ≤ 4

Daniel B. Litvin

Department of Physics, The Eberly College of Science, The Pennsylvania State University, Penn State Berks, PO Box 7009, Reading, PA 19610-6009, USA. Correspondence e-mail: u3c@psu.edu

Received 6 August 2007
Accepted 14 November 2007

The one-, two- and three-dimensional magnetic space groups and the two- and three-dimensional magnetic subperiodic groups are considered. The maximal subgroups of index ≤ 4 of a *representative group* of each type in the *reduced superfamilies* of these magnetic groups are tabulated.

1. Introduction

Group–subgroup relations find applications in the Landau theory of phase transitions (Iziumov & Syromiatnikov, 1990), domain structure analysis (Janovec & Přívratská, 2003), symmetry mode analysis (Aroyo & Perez-Mato, 1998) and relations between crystal structures (Bärnighausen, 1980). In phase transitions, Ascher (1966, 1967) pointed out the important role played by maximal subgroups. Maximal subgroups play a central role in determining all subgroups of a group because any subgroup can be obtained by a chain of maximal subgroups. A historical review of group–subgroup relations and the derivation of maximal subgroups of non-magnetic groups can be found in Volume A1 of *International Tables for Crystallography* (2004).

A complete listing of the maximal subgroups of the two- and three-dimensional non-magnetic space groups has also been published in Volume A1 of *International Tables for Crystallography* (2004). The maximal subgroups of index <4 of the three-dimensional non-magnetic space groups and three-dimensional non-magnetic subperiodic groups can also be found on the Bilbao Crystallographic Server, http://www.cryst.ehu.es/ (Aroyo *et al.*, 2006).

With the advent of spintronics and multiferroic systems and their industrial applications, magnetic structures have received renewed attention (Schmid, 2004). The investigation of complex magnetic materials and of their potential applications requires an in-depth knowledge of their symmetries, such as their group–subgroup relations and maximal subgroups. However, little has been published presenting tabulations of, or on methods of determining, the maximal subgroups of magnetic groups. The maximal subgroups of the magnetic frieze groups have been tabulated (Litvin, 1996) as have *all* equi-translational subgroups of the magnetic subperiodic groups (Litvin, 2005), which includes all maximal equi-translational subgroups. An Abstract was published by Belguith & Billiet (1977) of a method for deriving the subgroups of two-colored space groups, and in the paper by Sayari & Billiet (1977) the following reference is given to this method: 'Belguith, J. & Billiet, Y. (1978). In preparation.' As two-colored space groups and magnetic space groups are mathematically isomorphic, this method would also be a method for the derivation of subgroups of magnetic space groups. This paper has not, to our knowledge, been published. An algorithmic procedure to determine the maximal subgroups of magnetic space groups and magnetic subperiodic groups from the maximal subgroups of non-magnetic space groups and subperiodic groups was put forward by Litvin (1996). Here we use this methodology and the existing tables of maximal subgroups of non-magnetic groups to tabulate maximal subgroups of magnetic space groups and magnetic subperiodic groups.

In §2 we define the terminology which we use and in §3 the format and content of the maximal subgroup tables.[1]

2. Magnetic groups

Let $\mathbf{F}$ denote a non-magnetic crystallographic group. A crystallographic magnetic group is a subgroup of $\mathbf{F1}'$, where $\mathbf{1}'$ denotes the time inversion group consisting of the identity 1 and time inversion $1'$, *and* which is an invariance group of some spin arrangement $\mathbf{S}(\mathbf{r})$. Since $1'\mathbf{S}(\mathbf{r}) = -\mathbf{S}(\mathbf{r})$, a magnetic group cannot contain the subgroup $\mathbf{1}'$ and consequently groups $\mathbf{F1}'$ are not magnetic groups. We associate a group $\mathbf{F1}'$ with the magnetic groups which are subgroups of $\mathbf{F1}'$ by using the concept (Opechowski, 1986) of the *magnetic superfamily of crystallographic groups of type* $\boldsymbol{F}$: The magnetic superfamily of crystallographic groups of type $\mathbf{F}$ consists of

1. groups of type $\mathbf{F}$,
2. groups of type $\mathbf{F1}'$,
3. groups of type $\mathbf{F}(\mathbf{D}) = \mathbf{D} + (\mathbf{F} - \mathbf{D})\mathbf{1}'$, where $\mathbf{D}$ is a subgroup of index 2 of $\mathbf{F}$.

We note that only the first and third kinds are magnetic groups.

A *reduced magnetic superfamily of crystallographic groups of type* $\boldsymbol{F}$ (Opechowski, 1986) consists of a list of one group of type $\mathbf{F}$, one group of type $\mathbf{F1}'$ and one group from each type of groups $\mathbf{F}(\mathbf{D})$. A survey of magnetic groups consists of listings of a set of coset representatives, of the decomposition of the group with respect to its translational subgroup, of each group in each reduced magnetic superfamily. The set of coset representatives chosen is called the *standard set of coset representatives* and the one group of each type the *representative group* of that type. Surveys of magnetic space groups and magnetic subperiodic groups are given, with appropriate references, in Litvin (1999, 2001). Below we tabulate the maximal subgroups of index <4 of the representative groups of the reduced magnetic superfamilies of one-, two- and three-dimensional magnetic space groups and two- and three-dimensional magnetic subperiodic groups, the latter set consisting of the two-dimensional magnetic

[1] The complete set of tables is available from the IUCr electronic archives (Reference: PZ5045). Services for accessing these data are described at the back of the journal. These tables, which constitute an electronic monograph entitled *Maximal Subgroups of Index ≤ 4 of the 1, 2, and 3 Dimensional Magnetic Space Groups and 2 and 3 Dimensional Magnetic Subperiodic Groups*, may also be downloaded from http://www.bk.psu.edu/faculty/Litvin and are also available on CD on request from the author at u3c@psu.edu.

Table 1
The maximal subgroups of index ≤4 of the representative magnetic layer group of type $pb'aa'$.

43.5.302	$pb'aa'$	$(0, 0, 0; a, b, c)$	$(1\|000)$	$(2_x\|0\,\frac{1}{2}\,0)'$	$(2_y\|\frac{1}{2}\,\frac{1}{2}\,0)$	$(2_z\|\frac{1}{2}\,0\,0)'$
			$(\bar{1}\|000)$	$(m_x\|0\,\frac{1}{2}\,0)'$	$(m_y\|\frac{1}{2}\,\frac{1}{2}\,0)$	$(m_z\|\frac{1}{2}\,0\,0)'$
$p112'/a'$	2	$(0, 0, 0; a, b, c)$	$(1\|000)$	$(2_z\|\frac{1}{2}\,0\,0)'$	$(\bar{1}\|000)$	$(m_z\|\frac{1}{2}\,0\,0)'$
$p2'/b'11$	2	$(0, 0, 0; a, b, c)$	$(1\|000)$	$(2_x\|0\,\frac{1}{2}\,0)'$	$(\bar{1}\|000)$	$(m_x\|0\,\frac{1}{2}\,0)'$
$p2_1/b11$	2	$(0, 0, 0; b, \bar{a}, c)$	$(1\|000)$	$(2_y\|\frac{1}{2}\,\frac{1}{2}\,0)$	$(\bar{1}\|000)$	$(m_y\|\frac{1}{2}\,\frac{1}{2}\,0)$
$p2_12'2'$	2	$(\frac{1}{4}, 0, 0; b, \bar{a}, c)$	$(1\|000)$	$(2_x\|0\,\frac{1}{2}\,0)'$	$(2_y\|\frac{1}{2}\,\frac{1}{2}\,0)$	$(2_z\|\frac{1}{2}\,0\,0)'$
$pba'2'$	2	$(\frac{1}{4}, 0, 0; b, \bar{a}, c)$	$(1\|000)$	$(m_x\|0\,\frac{1}{2}\,0)'$	$(m_y\|\frac{1}{2}\,\frac{1}{2}\,0)$	$(2_z\|\frac{1}{2}\,0\,0)'$
$pb'2b'$	2	$(0, \frac{1}{4}, 0; b, \bar{a}, c)$	$(1\|000)$	$(2_x\|0\,\frac{1}{2}\,0)'$	$(m_y\|\frac{1}{2}\,\frac{1}{2}\,0)$	$(m_z\|\frac{1}{2}\,0\,0)'$
$pb'2_1a'$	2	$(\frac{1}{4}, 0, 0; a, b, c)$	$(1\|000)$	$(m_x\|0\,\frac{1}{2}\,0)'$	$(2_y\|\frac{1}{2}\,\frac{1}{2}\,0)$	$(m_z\|\frac{1}{2}\,0\,0)'$
$pb'aa'$	3	$(0, 0, 0; a, 3b, c)$	$(1\|000)$	$(2_x\|0\,\frac{3}{2}\,0)'$	$(2_y\|\frac{1}{2}\,\frac{3}{2}\,0)$	$(2_z\|\frac{1}{2}\,0\,0)'$
			$(\bar{1}\|000)$	$(m_x\|0\,\frac{3}{2}\,0)'$	$(m_y\|\frac{1}{2}\,\frac{3}{2}\,0)$	$(m_z\|\frac{1}{2}\,0\,0)'$
$pb'aa'$	3	$(0, 1, 0; a, 3b, c)$	$(1\|000)$	$(2_x\|0\,\frac{7}{2}\,0)'$	$(2_y\|\frac{1}{2}\,\frac{3}{2}\,0)$	$(2_z\|\frac{1}{2}\,2\,0)'$
			$(\bar{1}\|020)$	$(m_x\|0\,\frac{3}{2}\,0)'$	$(m_y\|\frac{1}{2}\,\frac{7}{2}\,0)$	$(m_z\|\frac{1}{2}\,0\,0)'$
$pb'aa'$	3	$(0, 2, 0; a, 3b, c)$	$(1\|000)$	$(2_x\|0\,\frac{11}{2}\,0)'$	$(2_y\|\frac{1}{2}\,\frac{3}{2}\,0)$	$(2_z\|\frac{1}{2}\,4\,0)'$
			$(\bar{1}\|040)$	$(m_x\|0\,\frac{3}{2}\,0)'$	$(m_y\|\frac{1}{2}\,\frac{11}{2}\,0)$	$(m_z\|\frac{1}{2}\,0\,0)'$
$pb'aa'$	3	$(0, 0, 0; 3a, b, c)$	$(1\|000)$	$(2_x\|0\,\frac{1}{2}\,0)'$	$(2_y\|\frac{3}{2}\,\frac{1}{2}\,0)$	$(2_z\|\frac{3}{2}\,0\,0)'$
			$(\bar{1}\|000)$	$(m_x\|0\,\frac{1}{2}\,0)'$	$(m_y\|\frac{3}{2}\,\frac{1}{2}\,0)$	$(m_z\|\frac{3}{2}\,0\,0)'$
$pb'aa'$	3	$(1, 0, 0; 3a, b, c)$	$(1\|000)$	$(2_x\|0\,\frac{1}{2}\,0)'$	$(2_y\|\frac{7}{2}\,\frac{1}{2}\,0)$	$(2_z\|\frac{7}{2}\,0\,0)'$
			$(\bar{1}\|200)$	$(m_x\|2\,\frac{1}{2}\,0)'$	$(m_y\|\frac{3}{2}\,\frac{1}{2}\,0)$	$(m_z\|\frac{3}{2}\,0\,0)'$
$pb'aa'$	3	$(2, 0, 0; 3a, b, c)$	$(1\|000)$	$(2_x\|0\,\frac{1}{2}\,0)'$	$(2_y\|\frac{11}{2}\,\frac{1}{2}\,0)$	$(2_z\|\frac{11}{2}\,0\,0)'$
			$(\bar{1}\|400)$	$(m_x\|4\,\frac{1}{2}\,0)'$	$(m_y\|\frac{3}{2}\,\frac{1}{2}\,0)$	$(m_z\|\frac{3}{2}\,0\,0)'$

frieze groups and the three-dimensional magnetic rod and magnetic layer groups.

3. Maximal subgroup tables

The maximal subgroup table of the representative magnetic layer group $pb'aa'$ is shown in Table 1. First is given information defining this representative group: a three-part serial number $N_1.N_2.N_3$ is assigned. N_1 is a sequential number for the superfamilies of groups of type **F**, and simultaneously for the groups of type **F**, emphasizing the relationship between the magnetic group and the non-magnetic space group **F**. N_2 is a sequential numbering of the groups of the reduced superfamily of type N_1. Group **F** is always assigned the number $N_1.1.N_3$ and group **F1′**, the number $N_1.2.N_3$. N_3 is a global sequential numbering of the groups being considered. In Table 1, 3.5.302 denotes that $pb'aa'$ belongs to the third superfamily of groups of type *pbaa*, the fifth group of the reduced superfamily of *pbaa*, and the 302nd group of the survey of magnetic layer groups. This is followed by a symbol denoting the origin and basis vectors of the non-magnetic translational subgroup of the representative group and then the standard set of coset representations.

Beneath the representative group are its maximal subgroups of index <4, there are no maximal subgroups of $pb'aa'$ of index 4. The equi-translational maximal subgroups are listed first followed by the equi-class maximal subgroups.

For each we give in successive columns:
1. the symbol for the subgroup type;
2. the subgroup index;
3. coordinate system: origin and basis vectors;
4. coset representatives.

The coset representatives of each subgroup are given in the coordinate system of the representative group whose maximal subgroups are listed, *i.e.* in this case of $pb'aa'$. If these coset representatives of the subgroup are identical with the coset representatives of the representative group of the subgroup, then the origin and basis vectors listed are unchanged. For example, in Table 1 we have the maximal subgroup

$$p112'/a' \quad 2 \quad (0,0,0;a,b,c) \quad (1|000) \quad (2_z|\tfrac{1}{2}00)' \quad (\bar{1}|000) \quad (m_z|\tfrac{1}{2}00)'$$

where the coset representatives listed here are the same as the coset representatives of the representative group $p112'/a'$ and consequently the coordinate system $(0,0,0; a,b,c)$ is not changed. For the maximal subgroup

$$p2_1/b11 \quad 2 \quad (0,0,0;b,\bar{a},c) \quad (1|000) \quad (2_y|\tfrac{1}{2}\tfrac{1}{2}0) \quad (\bar{1}|000) \quad (m_y|\tfrac{1}{2}\tfrac{1}{2}0),$$

the coset representatives listed are not the same as the coset representatives of the representative group $p2_1/b11$, which are:

$$(1|000) \quad (2_x|\tfrac{1}{2}\tfrac{1}{2}0) \quad (\bar{1}|000) \quad (m_x|\tfrac{1}{2}\tfrac{1}{2}0).$$

Consequently, a coordinate system transformation is required and is given by $(0, 0, 0; b, \bar{a}, c)$. For the maximal subgroup

$$pba'2' \quad 2 \quad (\tfrac{1}{4},0,0;b,\bar{a},c) \quad (1|000) \quad (m_x|0\tfrac{1}{2}0)' \quad (m_y|\tfrac{1}{2}\tfrac{1}{2}0) \quad (2_z|\tfrac{1}{2}00)',$$

the coset representatives are also not the same as the coset representatives of the representative group $pba'2'$, which are

$$(1|000) \quad (m_x|\tfrac{1}{2}\tfrac{1}{2}0) \quad (m_y|\tfrac{1}{2}\tfrac{1}{2}0)' \quad (2_z|000)'.$$

Consequently, a coordinate system transformation is required and is given by $(\frac{1}{4}, 0, 0; b, \bar{a}, c)$ which includes a change in origin.

In the tabulations of the maximal subgroups of groups of the type **F1′**, not all maximal subgroups are explicitly listed. If **G** is a maximal subgroup of **F**, then maximal subgroups **G1′** of **F1′** are not explicitly listed. All maximal subgroups **G** of **F** are listed under **F**. The maximal subgroups **G1′** of **F1′** are then found from the list of all maximal subgroups **G** of **F**, by multiplying each by **1′**. Also, in the listing of the coset representatives of a group **F1′**, only the coset representatives of the group **F** are explicitly listed. The second set of coset representatives of **F1′** are found by 'priming' each coset representative of **F**, *i.e.* multiplying each with 1′.

References

Aroyo, M. I. & Perez-Mato, J. M. (1998). *Acta Cryst.* A**54**, 19–30.
Aroyo, M. I., Perez-Mato, J. M., Capillas, C., Kroumova, E., Ivantchev, S., Madariaga, G., Kirov, A. & Wondratschek, H. (2006). *Z. Kristallogr.* **221**, 15–27.
Ascher, E. (1966). *Phys. Lett.* **20**, 352–354.
Ascher, E. (1967). *Chem. Phys. Lett.* **1**, 69–72.
Bärnighausen, H. (1980). *MATCH Commun. Math. Chem.* **9**, 139–175.
Belguith, J. & Billiet, Y. (1977). Fourth European Crystallographic Meeting, Oxford, Abstract PI.5, pp. 105–106.

International Tables for Crystallography (2004). Vol. A1, *Symmetry Relations between Space Groups*, edited by H. Wondratschek & U. Müller. Dordrecht: Kluwer Academic Publishers.

Iziumov, I. A. & Syromiatnikov, V. N. (1990). *Phase Transitions and Crystal Symmetry*. Dordrecht: Kluwer Academic Publishers.

Janovec, V. & Přívratská, J. (2003). *International Tables for Crystallography*, Vol. D. *Physical Properties of Crystals*, edited by A. Authier, ch. 3.4. Dordrecht: Kluwer Academic Publishers.

Litvin, D. B. (1996). *Acta Cryst.* A**52**, 681–685.

Litvin, D. B. (1999). *Acta Cryst.* A**55**, 963–964.

Litvin, D. B. (2001). *Acta Cryst.* A**57**, 729–730.

Litvin, D. B. (2005). *Acta Cryst.* A**61**, 382–385.

Opechowski, W. (1986). *Crystallographic and Metacrystallographic Groups*. Amsterdam: North Holland.

Sayari, A. & Billiet, Y. (1977). *Acta Cryst.* A**33**, 985–986.

Schmid, H. (2004). *Magnetoelectric Interaction Phenomena in Crystals*, edited by M. Fiebig, V. Eremenko & I. E. Chupis, pp. 1–34. Dordrecht: Kluwer Academic Publishers.