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Magnetic space-group types[1]

D. B. Litvin

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

The interpretation of Opechowski–Guccione symbols for magnetic space-group types is based on coordinate triplets given in the now superceded *International Tables for X-ray Crystallography* [(1952), Vol. 1, edited by N. F. M. Henry & K. Lonsdale. Birmingham: Kynoch Press]. Changes to coordinate triplets in *International Tables for Crystallography* [(1983), Vol. A, edited by Th. Hahn. Dordrecht: Kluwer Academic Publishers] lead to misinterpretations of these symbols. A list is provided here of Opechowski–Guccione symbols for the 1651 magnetic space-group types with their original definitions given independent of *International Tables*.

1. Introduction

Opechowski & Guccione (1965) [see also Opechowski (1986) and Opechowski & Litvin (1977)] give a list of symbols, referred to here as OG symbols, for the 1191 types of magnetic space groups. [This number plus 230 space-group types and 230 types of groups which are the direct product of a space group and the time-inversion group gives a total of 1651 types of groups (Belov *et al.*, 1957).] The list consists of a listing of a symbol for one representative magnetic space group from each type. To uniquely specify the meaning of each symbol required the specification of a symbol for one representative space group from each of the 230 types of space groups. This specification was based on the specific form of the coordinate triplets of the set of general positions explicitly printed in *International Tables for X-ray Crystallography* (1952) (abbreviated here as *ITC*52).

*ITC*52 has now been replaced with Volume A of *International Tables for Crystallography* (1983) (abbreviated here as *ITC*83). One finds that for some space groups the set of coordinate triplets of the general positions explicitly printed in *ITC*83 differs from those explicitly printed in *ITC*52. As a consequence, if one attempts to interpret the OG symbols using *ITC*83, one will, in many cases, misinterpret the meaning of the symbol, or be led to erroneous conclusions as to the number of magnetic space-group types and to the validity of the list of OG symbols as a list of one magnetic space group from each type of magnetic space group (Litvin, 1997, 1998).

We here rectify this situation by providing, along with the original list of OG symbols of the magnetic space-group types, information defining the original meaning of each symbol. This is performed independent of any other tabulations which may or may not change in the future.

2. Magnetic space-group types

All space groups are classified into 230 classes, called the 230 space-group types (*ITC*52, *ITC*83). Let **F** denote a crystallographic space-group type. The *magnetic superfamily* (Opechowski, 1986) of crystallographic groups of type **F** consists of

(i) Groups of type **F**.

(ii) Groups of type **F1′**, the direct product of a group of the type **F** and the time inversion group **1′** consisting of the identity element 1 and time inversion 1′.

(iii) Groups of types $\mathbf{F(D)} = \mathbf{D} + (\mathbf{F} - \mathbf{D})1'$, where **D** is a subgroup of index 2 of **F**.

A survey of the crystallographic groups of the magnetic superfamily of crystallographic groups of type **F** is a classification of all these groups. It consists of the listing of the coset representatives

(*a*) of one group from the groups of type **F**,

(*b*) of one group from the groups of type **F1′**,

(*c*) of one group from the groups of each of the types **F(D)**.

The coset representatives, called the *standard set of coset representatives*, are of the decomposition of the group with respect to its translational subgroup. Such sets of coset representatives provide information analogous to the sets of general positions listed in *ITC*52 and *ITC*83. Each listed group is called the *representative group* of that type.[2] The symbol for each listed group is used to denote both the group and the group's type. Reference to the *group* **F**, **F1′** or **F(D)** will refer to the listed group and to the *group type* **F**, **F1′** or **F(D)** to that group's type.

The format of the tables of magnetic space-group types is:[3]

1. Serial number of the magnetic space-group type.

2. Symbol of the representative magnetic space group/magnetic space-group type.

3. Symbol of the subgroup **D** of index two of **F** for magnetic space groups **F(D)** and the position and orientation of the subgroup **D** in the coordinate system of the group **F(D)**, which is the same as the coordinate system of **F**.

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[2] Only the relative lengths and mutual orientations of the translation vectors and the standard set of coset representatives with respect to an implied coordinate system are given. 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 the coordinate system are not explicitly given.

[3] The complete tables entitled Magnetic Space Group Types with an extensive introduction is available from the IUCr electronic archives (Reference: DR0012). Services for accessing these data are described at the back of the journal.

Table 1
Magnetic space-group types of the magnetic superfamily of **Pca2$_1$**.

A three part numbering $N_1.N_2.N_3$ is used. N_1 is a sequential number for the group type to which **F** belongs, the same numbering as given in both *ITC*52 and *ITC*83. N_2 is a sequential number of the magnetic space-group types of the superfamily of **F** and N_3 is a global sequential number of the magnetic space-group types.

29.1.198	**Pca2$_1$**			(1 | 0, 0, 0)	(m_x | $\frac{1}{2}$, 0, $\frac{1}{2}$)	(m_y | $\frac{1}{2}$, 0, 0)	(2_z | 0, 0, $\frac{1}{2}$)
29.2.199	**Pca2$_1$1′**						
29.3.200	**Pc′a2$_1$′**	**Pc**	(0, 0, 0; c, $\bar{b}$, a)	(1 | 0, 0, 0)	(m_x | $\frac{1}{2}$, 0, $\frac{1}{2}$)′	(m_y | $\frac{1}{2}$, 0, 0)	(2_z | 0, 0, $\frac{1}{2}$)′
29.4.201	**Pca′2$_1$**′	**Pc**	($\frac{1}{4}$, 0, 0; b, $\bar{a}$, c)	(1 | 0, 0, 0)	(m_x | $\frac{1}{2}$, 0, $\frac{1}{2}$)	(m_y | $\frac{1}{2}$, 0, 0)′	(2_z | 0, 0, $\frac{1}{2}$)′
29.5.202	**Pc′a′2$_1$**	**P2$_1$**	(0, 0, 0; b, c, a)	(1 | 0, 0, 0)	(m_x | $\frac{1}{2}$, 0, $\frac{1}{2}$)′	(m_y | $\frac{1}{2}$, 0, 0)′	(2_z | 0, 0, $\frac{1}{2}$)
29.6.203	**P$_{2b}$ca2$_1$**	**Pca2$_1$**	(0, 0, 0; a, 2b, c)	(1 | 0, 0, 0)	(m_x | $\frac{1}{2}$, 0, $\frac{1}{2}$)	(m_y | $\frac{1}{2}$, 0, 0)	(2_z | 0, 0, $\frac{1}{2}$)
29.7.204	**P$_{2b}$c′a′2$_1$**	**Pna2$_1$**	(0, 0, 0; a, 2b, c)	(1 | 0, 0, 0)	(m_x | $\frac{1}{2}$, 1, $\frac{1}{2}$)	(m_y | $\frac{1}{2}$, 1, 0)	(2_z | 0, 0, $\frac{1}{2}$)

4. The standard set of coset representatives of the decomposition of the magnetic space group with respect to its translational subgroup.

An example from the tables is the survey of the magnetic space groups of the magnetic superfamily of **Pca2$_1$** is shown in Table 1.

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