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Tables of crystallographic properties of magnetic space groups

D. 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

Tables of crystallographic properties of the reduced magnetic superfamilies of space groups, *i.e.* the 7 one-dimensional, 80 two-dimensional and 1651 three-dimensional group types, commonly referred to as *magnetic space groups*, are presented. The content and format are similar to that of non-magnetic space groups and subperiodic groups given in *International Tables for Crystallography*. Additional content for each representative group of each magnetic space-group type includes a diagram of general positions with corresponding general magnetic moments, Seitz notation used as a second notation for symmetry operations, and general and special positions listed with the components of the corresponding magnetic moments allowed by symmetry.

1. Introduction

Magnetic groups are symmetry groups of arrangements of non-zero magnetic moments (spins). These groups were introduced by Landau & Lifschitz (1951*a*,*b*, 1957, 1960) by reinterpreting the operation of 'change in color' in two-color (black and white) crystallographic groups as 'time inversion'. Crystallographic two-color groups of rotations had been given by Heesch (1930) and Shubnikov (1951; Holser, 1964*b*). The 1651 types of two-color three-dimensional space groups were derived by Belov *et al.* (1955, 1957; see also Holser, 1964*a*) and by Zamorzaev (1953, 1957*a*,*b*) and called *Shubnikov groups*. Koptsik (1966, 1971) applied these groups to determine crystallographic and physical properties of magnetic structures.

The three-dimensional magnetic space groups were rederived and a new list of symbols for 1191 types of three-dimensional magnetic space groups was given by Opechowski & Guccione (1965) (see also Opechowski, 1986; Litvin, 2001). This number plus 230 three-dimensional space-group types, which are also invariance groups of arrangements of non-zero magnetic moments, gives 1421 types of three-dimensional magnetic groups. The 230 types of groups which are the direct product of a space group and the time-inversion group are not magnetic groups as the time-inversion element in each such group precludes non-zero magnetic moments. To include these groups, Opechowski (1986) used the concept of a *magnetic superfamily*, giving a total of 1651 types of groups in the magnetic superfamilies of three-dimensional space groups. Let **F** denote a crystallographic group. The *magnetic superfamily* (Opechowski, 1986) of this crystallographic group **F** consists of[1]

1. The group **F**.
2. The group **F1**′, where **1**′ denotes time-inversion group consisting of the identity 1 and time inversion 1′.
3. The set of all groups **F**(**D**) = **D** + (**F** − **D**)1′, where **D** is a subgroup of index two of **F**.

The *reduced* magnetic superfamily of **F** is defined as above with the third component replaced with

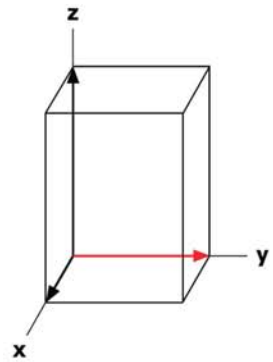
3*. The set of all *non-equivalent* groups **F**(**D**) = **D** + (**F** − **D**)1′, where **D** is a subgroup of index two of **F**.

The Opechowski & Guccione (1965) list consists of a listing of a symbol for one representative magnetic space group from each type. To uniquely specify the meaning of the Opechowski & Guccione symbols requires a specification of the meaning of the symbols for the 230 types of space groups. This specification was made in conjunction with Volume I of *International Tables for X-ray Crystallography* (1952) (abbreviated here as *ITC*52). In particular, this specification of one space group from each type was based on the specific form of the coordinate triplets of the set of general positions explicitly printed in *ITC*52.

*ITC*52 has been replaced by Volume A of *International Tables for Crystallography* (1983) (abbreviated here as *ITC-A*). One finds that, for some space groups, the set of coordinate triplets of the general positions explicitly printed in *ITC-A* differs from that explicitly printed in *ITC*52. As a consequence, if one attempts to interpret the Opechowski–Guccione symbols using *ITC-A*, one will, in many cases misinterpret the meaning of the symbol (Litvin, 1997, 1998).[2]

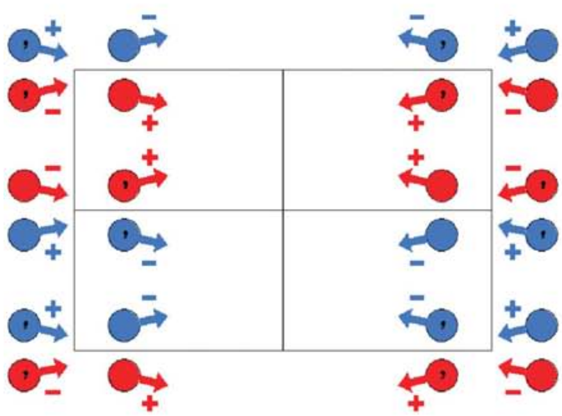
[1] A magnetic superfamily as defined by Zamorzaev (1957*a*,*b*) does not include groups of *F*.

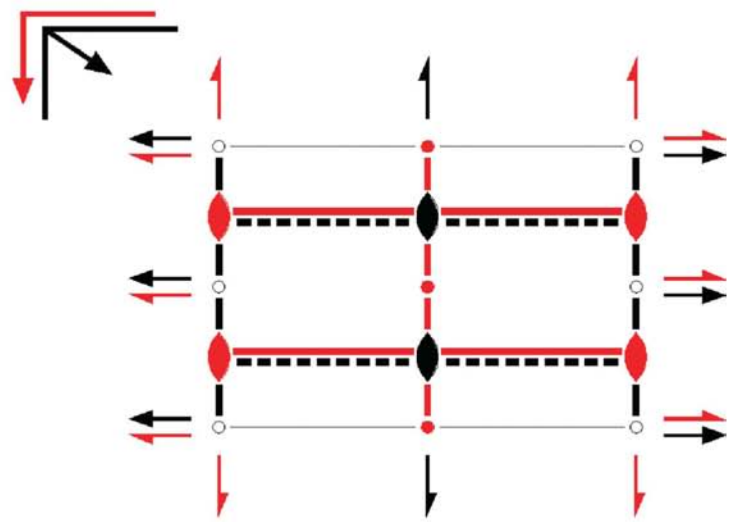
[2] It was suggested in these two papers that the original Opechowski–Guccione set of symbols should be modified so that one could correctly interpret them using *ITC-A* instead of *ITC*52. Adopting this ill advised suggestion would have required in the future a new modification of the Opechowski–Guccione set of symbols whenever changes were made to the explicit coordinate triplets of the general positions in *ITC-A*. Consequently, the meaning of the original Opechowski–Guccione list of symbols was specified by Litvin (2001).



P_{2b} m'ma' | mmm1' | Orthorhombic

51.15.401 | $P_{2b}\,2_1$ '/m'2/m2'/a'





Origin at center (2/m) at 2_1 '2/ma'

Asymmetric unit $0 \le x \le 1/4$; $0 \le y \le ½$; $0 \le z \le 1$

Symmetry Operations

For (0,0,0) + set

(1) 1 $(1 \mid 0,0,0)$	(2) 2' 1/4,0,z $(2_z \mid 1/2,0,0)'$	(3) 2 0,y,0 $(2_y \mid 0,0,0)$	(4) 2' (1/2,0,0) x,0,0 $(2_x \mid 1/2,0,0)'$
(5) $\bar{1}$ $(\bar{1} \mid 0,0,0)$	(6) a' (1/2,0,0) x,y,0 $(m_z \mid 1/2,0,0)'$	(7) m x,0,z $(m_y \mid 0,0,0)$	(8) m' 1/4,y,z $(m_x \mid 1/2,0,0)'$

For (0,1,0)' + set

(1) t' (0,1,0) $(1 \mid 0,1,0)'$	(2) 2 1/4,1/2,z $(2_z \mid 1/2,1,0)$	(3) 2' (0,1,0) 0,y,0 $(2_y \mid 0,1,0)'$	(4) 2 (1/2,0,0) x,1/2,0 $(2_x \mid 1/2,1,0)$
(5) $\bar{1}$' 0,1/2,0 $(\bar{1} \mid 0,1,0)'$	(6) n (1/2,1,0) x,y,0 $(m_z \mid 1/2,1,0)$	(7) m' x,1/2,z $(m_y \mid 0,1,0)'$	(8) b (0,1,0) 1/4,y,z $(m_x \mid 1/2,1,0)$

Figure 1
Example table of crystallographic properties of magnetic space groups, the three-dimensional magnetic space group $P_{2b}m'ma'$.

Continued 51.15.401 P_{2b} m'ma'

Generators selected (1); t(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry. — Coordinates

(0,0,0) + (0,1,0)' +

16	l	1	(1) x,y,z [u,v,w]	(2) $\bar{x}$+1/2,$\bar{y}$,z [u,v,$\bar{w}$]	(3) $\bar{x}$,y,$\bar{z}$ [$\bar{u}$,v,$\bar{w}$]	(4) x+1/2,$\bar{y}$,$\bar{z}$ [$\bar{u}$,v,w]
			(5) $\bar{x}$,$\bar{y}$,$\bar{z}$ [u,v,w]	(6) x+1/2,y,$\bar{z}$ [u,v,$\bar{w}$]	(7) x,$\bar{y}$,z [$\bar{u}$,v,$\bar{w}$]	(8) $\bar{x}$+1/2,y,z [$\bar{u}$,v,w]
8	k	m'..	1/4,y,z [0,v,w]	1/4,$\bar{y}$,z [0,v,$\bar{w}$]	3/4,y,$\bar{z}$ [0,v,$\bar{w}$]	3/4,$\bar{y}$,$\bar{z}$ [0,v,w]
8	j	.m'.	x,1/2,z [u,0,w]	$\bar{x}$+1/2,1/2,z [$\bar{u}$,0,w]	$\bar{x}$,1/2,$\bar{z}$ [$\bar{u}$,0,$\bar{w}$]	x+1/2,1/2,$\bar{z}$ [u,0,$\bar{w}$]
8	i	.m.	x,0,z [0,v,0]	$\bar{x}$+1/2,0,z [0,v,0]	$\bar{x}$,0,$\bar{z}$ [0,v,0]	x+1/2,0,$\bar{z}$ [0,v,0]
8	h	.2.	0,y,1/2 [0,v,0]	1/2,$\bar{y}$,1/2 [0,v,0]	0,$\bar{y}$,1/2 [0,v,0]	1/2,y,1/2 [0,v,0]
8	g	.2.	0,y,0 [0,v,0]	1/2,$\bar{y}$,0 [0,v,0]	0,$\bar{y}$,0 [0,v,0]	1/2,y,0 [0,v,0]
4	f	m'm'2	1/4,1/2,z [0,0,w]	3/4,1/2,$\bar{z}$ [0,0,$\bar{w}$]		
4	e	m'm2'	1/4,0,z [0,v,0]	3/4,0,$\bar{z}$ [0,v,0]		
4	d	.2/m'.	0,1/2,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
4	c	.2/m.	0,0,1/2 [0,v,0]	1/2,0,1/2 [0,v,0]		
4	b	.2/m'.	0,1/2,0 [0,0,0]	1/2,1/2,0 [0,0,0]		
4	a	.2/m.	0,0,0 [0,v,0]	1/2,0,0 [0,v,0]		

Symmetry of Special Projections

Along [0,0,1] p_{2a^*} 2'mm'
a* = -**b** **b*** = **a**/2
Origin at 0,0,z

Along [1,0,0] p_{2a^*} 2'mm'
a* = **b** **b*** = **c**
Origin at x,0,0

Along [0,1,0] p2mg1'
a* = -**a** **b*** = **c**
Origin at 0,y,0

Figure 1 (continued)

The meaning of the set of Opechowski–Guccione symbols (1965) was then specified, independently of *International Tables for Crystallography*, by Litvin (2001). For each symbol, this was done by explicitly specifying a set of coset representatives, called the *standard set of coset representatives*, of the decomposition of the group represented by the symbol with respect to its translational subgroup.

We have compiled an electronic book entitled *Magnetic Space Groups*.[3] This book presents tables of crystallographic properties of the reduced magnetic superfamilies of one-, two- and three-dimensional space-group types, which we shall refer to simply as one-, two- and three-dimensional magnetic space groups. Unlike the work of Koptsik (1966, 1971), this work is based on that of Opechowski & Guccione (1965), their symbols, and the format and content of *International Tables for Crystallography* and that of Litvin (2005). In §2, we detail the form and content of these tables, which are similar to the form and content of tables of properties of non-magnetic space-group types and subperiodic group types given in *International Tables for Crystallography* (1983, 2002) and in tables of properties of magnetic subperiodic groups (Litvin, 2005). In §3, we discuss additional material, as comparisons of magnetic and black and white group notation and tables of magnetic space-group symbols and elements, contained in this electronic book.

2. Tables of properties of magnetic space groups

The content of the magnetic group tables consists of the following.

Lattice diagram
Headline
Diagrams of symmetry elements and of the general positions
Origin
Asymmetric unit
Symmetry operations
Generators selected
Positions, with multiplicities, site symmetries, coordinates and magnetic moments
Symmetry of special projections

An example of these tables, for the three-dimensional magnetic space group $P_{2b}m'ma'$, is given in Fig. 1.

2.1. Lattice diagram

In the upper left hand corner of the first page of tables for each magnetic space group is the lattice diagram of the magnetic space group. This lattice diagram depicts (i) the coordinate system used, (ii) the conventional unit cell of the space group **F**, the magnetic space group's magnetic superfamily type, and (iii) the generators of the translational subgroup of the magnetic space group. The generating lattice vectors are color coded. Those colored black are not coupled with time inversion while those colored red are coupled with time inversion. In Fig. 1, the lattice diagram shows the orthorhombic P_{2b} lattice with the generating lattice vector in the y direction coupled with time inversion.

[3] This electronic book is available from the IUCr electronic archives (Reference: PZ5052). Services for accessing these archives are described at the back of the journal. This electronic book may also be downloaded from http://www.bk.psu.edu/faculty/Litvin/download.html and is also available on CD on request from the author at u3c@psu.edu.

2.2. Headline

To the right of the lattice diagram is a two-line heading, *e.g.* from Fig. 1:

$P_{2b}m'ma'$ $mmm1'$ Orthorhombic
51.15.401 $P_{2b}\ 2_1'/m'2/m2'/a'$

On the upper line, starting on the left, are three entries.

(i) The *short international* (Hermann–Mauguin) *symbol* of the magnetic space group. Each symbol has two meanings: the first is that of the Hermann-Mauguin symbol of a magnetic space-group type; the second is that of a specific magnetic space group which belongs to this magnetic space-group type. Given a coordinate system, this group is defined both by the list of symmetry operations given on the page with this Hermann–Mauguin symbol in the heading, or by the given list of general positions and magnetic moments.

(ii) The *short international* (Hermann–Mauguin) *point-group symbol* for the geometric class to which the magnetic space group belongs.

(iii) The crystal system to which the magnetic space group belongs.

The second line has two additional entries:

(i) the three-part numerical serial index of the magnetic space group;

(ii) the *long international (Hermann–Mauguin) symbol* of the magnetic space group.

2.3. Diagrams of symmetry elements and of the general positions

There are two types of diagrams, symmetry diagrams and general position diagrams. The symmetry diagrams show (i) the relative locations and orientations of the symmetry elements and (ii) the locations and orientations of the symmetry elements relative to a given coordinate system. The general position diagrams show, in that coordinate system, the arrangement of a set of symmetrically equivalent points and relative orientations of magnetic moments on this set of equivalent points relative to the symmetry elements.

In the general position diagrams, the general positions and corresponding magnetic moments are color-coded. Positions with a z component of $+z$ are circles color-coded red and with a z component of $-z$ are circles color-coded blue. The magnetic moments are color-coded to the general position with which they are associated, their direction in the plane of the diagram is given by an arrow in the direction of the magnetic moment. A + or − sign near the tip of the arrow indicates the magnetic moment is inclined, respectively, above or below the plane of diagram.

For magnetic space groups of the type **F**(**D**), where **D** is an equi-class subgroup, the general position and symmetry diagram do not encompass, in all cases, the conventional unit cell of the non-magnetic subgroup of the magnetic space group. The diagrams of the group $P_{2b}m'ma'$ in Fig. 1 are examples of this. For the symmetry diagram, there is no necessity for explicitly enlarging the diagram, as the symmetry diagram is periodic with respect to all translations of the space group **F** of the magnetic space group (Kopsky, 1993*a*,*b*). The general position diagram, in such cases, can be easily enlarged as one knows the translations of the magnetic space group, *i.e.* the general position diagram is periodic in the direction of non-primed translations and in the direction of primed translations the magnetic moments are inverted.

2.4. Origin

If the magnetic space group is centrosymmetric then the inversion center or a position of high site symmetry, as on the fourfold axis of tetragonal groups, is chosen as the origin. For noncentrosymmetric groups, the origin is at a point of highest site symmetry. If no symmetry is higher than 1, the origin is placed on a screw axis, a glide plane or at the intersection of several such symmetries.

On the *Origin* line below the diagrams, the site symmetry of the origin is given. An additional symbol indicates all symmetry elements that pass through the origin. For example, from Fig. 1, for the three-dimensional magnetic space group $P_{2b}m'ma'$, one finds "**Origin** at center ($2/m$) at $2_1'2/ma'$". The site symmetry is $2/m$, at the upper left corner of the symmetry diagram, and in addition passing through the origin is a twofold primed screw axis along the x direction and a primed glide plane perpendicular to the z axis.

2.5. Asymmetric unit

An asymmetric unit of a magnetic space group is a simply connected smallest part of space which, by application of all symmetry operations of the magnetic space group, exactly fills the whole space. Since the magnetic space groups contain a translational subgroup, the asymmetric unit is a finite part of space. We define the asymmetric unit by setting the limits on the coordinates of points contained in the asymmetric unit. For example, for the three-dimensional magnetic space group $P_{2b}m'ma'$ we have an asymmetric unit defined by

$$0 < x < \tfrac{1}{4};\ 0 < y < \tfrac{1}{2};\ 0 < z < 1.$$

Because the asymmetric unit is invariant under time inversion, all magnetic space groups **F**, **F1**$'$ and **F**(**D**) of the magnetic superfamily of type **F** have identical asymmetric units.

2.6. Symmetry operations

Listed under the heading of *Symmetry operations* is the geometric description of the symmetry operations of the magnetic space group. In addition, each symmetry operation is also given in Seitz notation (Burns & Glazer, 1990). For example, the mirror plane $m'1/4,y,z$ is in Seitz notation $(m_x|1/2,0,0)'$, where the prime denotes that the mirror plane is coupled with time inversion.

2.7. Generators selected

The line *Generators selected* lists the symmetry operations selected to generate the symmetrically equivalent points of the *General position* from a point with coordinates x, y, z. The first generator is always the identity operation given by (1) followed by generating translations. Additional generators are given as numbers (p) which refer to the coordinate triplets of the *General position* and to corresponding symmetry operations in the first block, if more than one, of *Symmetry operations*.

2.8. Positions, with multiplicities, site symmetries, coordinates and magnetic moments

The entries under *Positions*, referred to as *Wyckoff positions*, consists of the *General positions*, the upper block, followed by blocks of *Special positions*. The upper block of positions, the general positions, is a set of symmetrically equivalent points where each point is left invariant only by the identity operation or, for magnetic groups **F1**$'$, by the identity operation and time inversion, but by no other symmetry operations of the magnetic space group. The lower blocks, the special positions, are a set of symmetrically equivalent points where each point is left invariant by at least one additional operation in addition to the identity operation or, for magnetic space groups **F1**$'$, in addition to the identity operation and time inversion.

For each block of positions information is provided.

Multiplicity: The multiplicity is the number of equivalent positions in the conventional unit cell of the non-magnetic group **F** associated with the magnetic space group.

Wyckoff letter: This letter is a coding scheme for the blocks of positions, starting with *a* at the bottom block and continuing upwards in alphabetical order.

Site symmetry: The site-symmetry group is the largest subgroup of the magnetic space group that leaves invariant the first position in each block of positions. An 'oriented' symbol is used to show how the symmetry elements at a site are related to the conventional crystallographic basis. Sets of equivalent symmetry directions that do not contribute any element to the site symmetry are represented by dots.

Coordinates of positions and components of magnetic moments: In each block of positions, the coordinates of each position are given. Immediately following each set of position coordinates are the components of the symmetry-allowed magnetic moment at that position. The components of the magnetic moment of the first position are determined from the given site-symmetry group. For magnetic space group $P_{2b}m'ma'$ at special positions with Wyckoff letter c we have

$$c \quad .2/m. \quad 0,0,1/2[0,v,0] \quad 1/2,0,1/2[0,v,0].$$

The site symmetry at $0,0,\frac{1}{2}$ is $.2/m.$ and consequently the magnetic moment is $[0,v,0]$. The components of the magnetic moments at the remaining positions are determined by applying the symmetry operations to the components of that magnetic moment at the first position. Applying the element

$2'$ 1/4,0,z [in Seitz notation $(2_z|1/2,0,0)'$] to the magnetic moment $[0,v,0]$ at $0,0,\frac{1}{2}$, we obtain the magnetic moment $[0,v,0]$ at the second position $\frac{1}{2},0,\frac{1}{2}$.

2.9. Symmetry of special projections

Under the heading *Symmetry of special projections*, the following information is given for the projections of each two- and three-dimensional magnetic space group.

Projection direction: All projections are orthogonal, *i.e.* the projection, for three-dimensional magnetic space groups, is onto a plane normal to the projection direction. For two-dimensional magnetic space groups, the projection is onto a line normal to the projection direction.

Basis vectors: For three-dimensional magnetic space groups, the relationship between the basis vectors $\mathbf{a}^*$, $\mathbf{b}^*$ of the two-dimensional magnetic space-group symmetry of the projection is given in terms of the basis vectors **a**, **b**, **c** of the three-dimensional magnetic space group. For triclinic and monoclinic three-dimensional magnetic space groups where basis vectors **a**, **b** or **c** are inclined to the plane of projection, these basis vectors are replaced by $\mathbf{a}_p$, $\mathbf{b}_p$ or $\mathbf{c}_p$, respectively.

For two-dimensional magnetic space groups, the relationship between the basis vector $\mathbf{a}^*$ of the one-dimensional magnetic space-group symmetry of the projection is given in terms of the basis vectors **a** and **b** of the two-dimensional magnetic space group. For oblique two-dimensional magnetic space groups where basis vectors **a** or **b** are inclined to the plane of projection, these basis vectors are replaced by $\mathbf{a}_p$ or $\mathbf{b}_p$, respectively.

Location of origin: For three-dimensional magnetic space groups, the location of the origin of the two-dimensional magnetic space-group symmetry of the projection is given with respect to the unit cell of the three-dimensional magnetic space group. For two-dimensional magnetic space groups, the location of the origin of the one-dimensional magnetic space-group symmetry of the projection is given with respect to the unit cell of the two-dimensional magnetic space group.

3. Additional material

In addition to the tables of crystallographic properties of the magnetic space groups discussed in the previous section, the electronic book[4] contains a list of the changes in the symbols listed in Opechowski & Guccione (1965) and Opechowski (1986), and those used in these tables. A comparison of the symbols introduced by Opechowski & Guccione (1965) and the black and white space-group symbols of Belov *et al.* (1955, 1957), and used in the work of Koptsik (1966, 1971), is discussed and a side-by-side comparison is given.

The symbols used for the reduced magnetic superfamilies of one- and two-dimensional space groups, *i.e.* one- and two-dimensional magnetic space groups, are given along with a specification of a representative group of each type. A side-by-side comparison of the symbols used for these groups with those used for black and white groups by Niggli (1964) and Belov & Tarkhova (1956*a*,*b*) is also given.

[4] See deposition footnote.

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