International Tables for Crystallography (2016). Vol. A, Section 3.6.3.10, pp. 862–863.

Table 3.6.3.2
General positions of magnetic space group 51.14.400 $P_{2b}mma'$

Positions	Coordinates			
	(0, 0, 0)+ (0, 1, 0)′+			
16 *l* 1	(1) x, y, z $[u, v, w]$	(2) $\bar{x}+1/2, \bar{y}, z$ $[\bar{u}, \bar{v}, w]$	(3) $\bar{x}, y, \bar{z}$ $[u, \bar{v}, w]$	(4) $x+1/2, \bar{y}, \bar{z}$ $[\bar{u}, v, w]$
	(5) $\bar{x}, \bar{y}, \bar{z}$ $[\bar{u}, \bar{v}, \bar{w}]$	(6) $x+1/2, y, \bar{z}$ $[u, v, \bar{w}]$	(7) $x, \bar{y}, z$ $[\bar{u}, v, \bar{w}]$	(8) $\bar{x}+1/2, y, z$ $[u, \bar{v}, \bar{w}]$

lattices, the two lists, *Symmetry operations* and *General position*, have the same number of entries.

For magnetic groups with centred cells, only one block of several (two, three or four) blocks of the general positions is explicitly given, see Table 3.6.3.2. A set of two, three or four centring translations is given below the subheading *Coordinates*. Each of these translations is added to the given block of general positions to obtain the complete set of blocks of general positions. While one of the several blocks of general positions is explicitly given, the corresponding symmetry operations are all explicitly given. Each corresponding block of symmetry operations is listed under a subheading of 'centring translation + set' for each centring translation listed below the subheading *Coordinates*.

3.6.3.7. Abbreviated headline

On the second and subsequent pages of the tables for a specific magnetic group there is an abbreviated headline. This abbreviated headline contains three items: (1) the word 'Continued', (2) the three-part number of the magnetic group type, and (3) the short international (Hermann–Mauguin) symbol for the magnetic group type.

3.6.3.8. Generators selected

The line *Generators selected* lists the symmetry operations selected to generate the symmetry-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 the *Symmetry operations*.

3.6.3.9. General and special positions with spins (magnetic moments)

The entries under *Positions*, referred to as *Wyckoff positions*, consist of the *General position*, the upper block, followed by blocks of *Special positions*. The upper block of positions, the general position, is a set of symmetry-equivalent points where each point is left invariant only by the identity operation or, for magnetic groups $\mathcal{F}1'$, by the identity operation and time inversion, but by no other symmetry operations of the magnetic group. The lower blocks, the special positions, are sets of symmetry-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 $\mathcal{F}1'$, in addition to the identity operation and time inversion.

For each block of positions the following information is provided:

Multiplicity: The multiplicity is the number of equivalent positions in the conventional unit cell of the non-primed group $\mathcal{F}$ associated with the magnetic 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. This group is isomorphic to a subgroup of the point group of the magnetic group. An 'oriented' symbol is used to show how the symmetry elements at a site are related to the conventional crystallographic basis, and the sequence of characters in the symbol correspond to the sequence of symmetry directions in the magnetic group symbol. Sets of equivalent symmetry directions that do not contribute any element to the site symmetry are represented by dots. Sets of symmetry directions having more than one equivalent direction may require more than one character if the site-symmetry group belongs to a lower crystal system. For example, for the $2c$ position of the magnetic space group $P4'm'm$ (99.3.825) the site-symmetry group is '$2m'm'.$'. The two characters $m'm'$ represent the secondary set of tetragonal symmetry directions, whereas the dot represents the tertiary tetragonal symmetry directions.

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. 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.

3.6.3.10. Symmetry of special projections

The symmetry of special projections is given for the two- and three-dimensional magnetic groups. For each three-dimensional magnetic group, the symmetry is given for three projections, projections onto planes normal to the projection directions. If there are three symmetry directions, the three projection directions correspond to primary, secondary and tertiary symmetry directions. If there are fewer than three symmetry directions, the additional projection direction or directions are taken along coordinate axes. For two-dimensional magnetic groups, there are two orthogonal projections. The projections are onto lines normal to the projection directions.

For the three-dimensional magnetic space groups, each projection gives rise to a two-dimensional magnetic space group. For two-dimensional magnetic space groups, each projection gives rise to a one-dimensional magnetic space group. For magnetic rod groups and magnetic layer groups, a projection along the [001] direction gives rise, respectively, to a two-dimensional magnetic point group and a two-dimensional magnetic space group. All other projections give rise to magnetic frieze groups. For magnetic frieze groups, projections give rise to either a one-dimensional magnetic space group or a one-dimensional magnetic point group. The international (Hermann–Mauguin) symbol of the symmetry group of each projection is given. Below this symbol, the basis vector(s) of the projected symmetry group and the origin of the projected symmetry group are given in terms of the basis vector(s) of the projected magnetic group. The location of the origin of the symmetry group of the

Table 3.6.4.1
Comparisons of three-dimensional OG and BNS magnetic group type symbols

Serial No.	OG	BNS	$\mathcal{F}(\mathcal{D})$
44.1.324	$Imm2$		
44.2.325	$Imm21'$		
44.3.326	$Im'm2'$		
44.4.327	$Im'm'2$		
44.5.328	I_Pmm2	P_Imm2	$Imm2(Pmm2)$
44.6.329	$I_Pmm'2'$	P_Imm2_1	$Imm2(Pmm2_1)$
44.7.330	$I_Pm'm'2$	P_Inn2	$Imm2(Pnn2)$

projection is given with respect to the unit cell of the magnetic group from which it has been projected.

3.6.4. Comparison of OG and BNS magnetic group type symbols

There are other notations for magnetic group type symbols than the notations of Opechowski & Guccione (1965) and Belov, Neronova & Smirnova (1957): for example for the three-dimensional magnetic group 55.10.450 $P_{2c}b'a'm$ the Shubnikov notation is Ш^{403}_{58} (Koptsik, 1966; Shubnikov & Koptsik, 1974) or Sh^{403}_{58} (Ozerov, 1969*a*,*b*) (see also Zamorzaev, 1976). There are also the variations of the Opechowski & Guccione notation put forward by Grimmer (2009, 2010). We shall limit ourselves here to a detailed comparison of the Opechowski & Guccione and Belov, Neronova & Smirnova notations.

For all group types in the reduced magnetic superfamily of $\mathcal{F}$, the Opechowski & Guccione (1965) magnetic group type symbols (OG symbols) are based on the symbol of the group $\mathcal{F}$. Belov, Neronova & Smirnova (1957) also base their symbols (BNS symbols) on the symbol of the group $\mathcal{F}$, but only for magnetic groups of the type $\mathcal{F}$, $\mathcal{F}1'$ and $\mathcal{M}_T$. For magnetic groups $\mathcal{M}_R = \mathcal{F}(\mathcal{D}) = \mathcal{D} \cup (\mathcal{F} - \mathcal{D})1'$, where $\mathcal{D}$ is an equi-class subgroup of $\mathcal{F}$, the BNS symbol is based on the symbol of the group $\mathcal{D}$, the non-primed subgroup of index 2. A magnetic group $\mathcal{M}_R$ can be written as $\mathcal{M}_R = \mathcal{F}(\mathcal{D}) = \mathcal{D} \cup t_\alpha{}'\mathcal{D}$, where t_α is a translation of $\mathcal{F}$ not in $\mathcal{D}$. The BNS symbol for a magnetic group of the type $\mathcal{M}_R$ is the symbol for the group type $\mathcal{D}$ with a subindex inserted on the symbol for the translational subgroup of $\mathcal{D}$ to denote the translation $t_\alpha{}'$.

Example

The representative three-dimensional space group $\mathcal{F} = Pmm2$ has a translational subgroup generated by the three translations $\{1|1, 0, 0\}$, $\{1|0, 1, 0\}$ and $\{1|0, 0, 1\}$ and the standard set of coset representatives

$$\{1|0\} \quad \{m_{100}|0\} \quad \{m_{010}|0\} \quad \{2_{001}|0\}.$$

The three-dimensional magnetic space group 25.10.165 $\mathcal{F}(\mathcal{D}) = Pmm2(Pcc2)$ has a subgroup $\mathcal{D}$ with a translational subgroup generated by the three translations $\{1|1, 0, 0\}$, $\{1|0, 1, 0\}$ and $\{1|0, 0, 2\}$, $t_\alpha{}' = \{1|0, 0, 1\}'$, and a set of coset representatives

$$\{1|0\} \quad \{m_{100}|0, 0, 1\} \quad \{m_{010}|0, 0, 1\} \quad \{2_{001}|0\}.$$

The OG magnetic group type symbol is, see Section 3.6.2.2.4, $P_{2c}m'm'2$, *i.e.* based on the symbol for the group type $\mathcal{F} = Pmm2$. The BNS symbol is P_ccc2, *i.e.* based on the symbol for the subgroup $\mathcal{D} = Pcc2$ of $\mathcal{F}$, with a subindex 'c' attached to 'P' to denote the translation $t_\alpha{}' = \{1|0, 0, 1\}'$ in $\mathcal{M}_R = \mathcal{F}(\mathcal{D}) = \mathcal{D} \cup t_\alpha{}'\mathcal{D}$.

A side-by-side comparison of OG magnetic group type symbols and BNS symbols is given in Litvin (2013). As the OG and BNS symbols are the same for magnetic groups $\mathcal{F}$, $\mathcal{F}1'$ and $\mathcal{M}_T$, BNS symbols are explicitly listed only for groups of type $\mathcal{M}_R$. Examples of this comparison are given in Table 3.6.4.1.

3.6.5. Maximal subgroups of index ≤ 4

We consider the maximal subgroups of index ≤ 4 of the one-, two- and three-dimensional magnetic space groups and the two- and three-dimensional magnetic subperiodic groups. A complete listing of the maximal subgroups of the two- and three-dimensional non-primed space groups can be found in *International Tables for Crystallography*, Volume A1, *Symmetry Relations Between Space Groups* (2010; *IT* A1). The maximal subgroups of index ≤ 4 of the three-dimensional non-primed space groups and non-primed layer and rod groups can also be found on the Bilbao Crystallographic Server (http://www.cryst.ehu.es; Aroyo *et al.*, 2006).

For magnetic groups, an abstract of a method for determining the maximal subgroups of magnetic groups was published by Sayari & Billiet (1977). The maximal subgroups of magnetic groups found in Litvin (2013) were derived from Litvin (2008*a*) using a method given by Litvin (1996).

Each maximal subgroup table is headed by the magnetic group type whose maximal subgroup types are to be listed.

Examples

For the three-dimensional magnetic space group type $Pb'a'm$, one finds (Litvin, 2013), in bold blue type, information which defines the representative group of this type in a coordinate system O; **a**, **b**, **c**:

$$55.5.445 \quad Pb'a'm \quad (0, 0, 0; \mathbf{a}, \mathbf{b}, \mathbf{c}) \quad \begin{array}{ll} \{1|0\} & \{2_{100}|\tfrac{1}{2}, \tfrac{1}{2}, 0\}' \\ \{2_{010}|\tfrac{1}{2}, \tfrac{1}{2}, 0\}' & \{2_{001}|0\} \\ \{\bar{1}|0\} & \{m_{100}|\tfrac{1}{2}, \tfrac{1}{2}, 0\}' \\ \{m_{010}|\tfrac{1}{2}, \tfrac{1}{2}, 0\}' & \{m_{001}|0\} \end{array}$$

The first column gives the global serial number of the group, followed in the second column by its magnetic group type symbol. In the third column, the symbol (O; **a**′, **b**′, **c**′) gives the origin O and basis vectors **a**′, **b**′, **c**′ of the conventional unit cell of the non-primed subgroup of the representative group of the type $Pb'a'm$. These basis vectors **a**′, **b**′, **c**′ imply both the magnetic and non-primed translational subgroups of the representative group. In this case, the P translational subgroup of the representative group is non-primed and generated by the basis vectors **a**, **b**, **c**. The standard set of coset representatives of this representative group is given on the right.

For the three-dimensional magnetic space-group type $P_{2b}ma2$ one finds (Litvin, 2013):

$$28.6.190 \quad P_{2b}ma2 \quad (0, 0, 0; \mathbf{a}, 2\mathbf{b}, \mathbf{c}) \quad \begin{array}{ll} \{1|0\} & \{m_{100}|\tfrac{1}{2}, 0, 0\} \\ \{m_{010}|\tfrac{1}{2}, 0, 0\} & \{2_{001}|0\} \end{array}$$

Note here that $\mathbf{a}' = \mathbf{a}$, $\mathbf{b}' = 2\mathbf{b}$, $\mathbf{c}' = \mathbf{c}$, being the basis vectors of the conventional unit cell of the non-primed subgroup of the representative group of $P_{2b}ma2$, implies that the translational subgroup of the representative group is P_{2b}, *i.e.* generated by the non-primed translations $\{1|1, 0, 0\}$, $\{1|0, 2, 0\}$, $\{1|0, 0, 1\}$ and the magnetic translation $\{1|0, 1, 0\}'$.

Following the subtable heading of each magnetic space-group type is a listing of the maximal subgroups of index ≤ 4 of the representative magnetic space group of this type.

references