3.6. MAGNETIC SUBPERIODIC GROUPS AND MAGNETIC SPACE GROUPS

symmetry element also appears coupled with time inversion is represented by a red $1'$ printed between and above the general-position and symmetry diagrams. Because groups of this type contain the time-inversion symmetry, the magnetic moments are all identically zero, and no arrows appear in the general-position diagram. An example, the diagrams of the magnetic space group $P4_1221'$ are shown in Fig. 3.6.3.5. For triclinic, monoclinic/oblique, monoclinic/rectangular and orthorhombic rod groups, the colour coding of the general positions is extended according to the positive or negative values of the x and z components of the coordinates of the general position, see Fig. 3.6.3.6.

VRML (Virtual Reality Modeling Language) general-position diagrams are available for the two- and three-dimensional magnetic subperiodic groups (Cordisco & Litvin, 2004), and for the one-, two- and non-cubic three-dimensional magnetic space groups (Burke *et al.*, 2006). These diagrams can be rotated and zoomed in on to aid in the visualization of the general-position diagrams, and include both the general positions of the atoms and the general orientations of the associated magnetic moments.

3.6.3.4. Origin

If the magnetic space group is centrosymmetric, then the inversion centre 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 site symmetry is higher than 1, the origin is placed on a screw axis, a glide plane or at the intersection of several such symmetries.

In 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, for the magnetic space group $I4/mcm$, one finds '**Origin** at center $(4/m)$ at $4/mc2_1/c$'. The site symmetry is $4/m$ and, in addition, two glide planes perpendicular to the y and z axes, and a screw axis parallel to the z axis, pass through the origin.

3.6.3.5. Asymmetric unit

An asymmetric unit is a simply connected smallest part of space which, by application of all symmetry operations of the magnetic group, exactly fills the whole space. For subperiodic groups, because the translational symmetry is of a lower dimension than that of the space, the asymmetric unit is infinite in size. The asymmetric unit for subperiodic groups is defined by setting the limits on the coordinates of points contained in the asymmetric unit. For example, the asymmetric unit for the magnetic layer group 32.3.199 $pm'2_1n'$ is

Asymmetric unit $0 < x < \frac{1}{2}$; $0 < y < 1$; $0 < z$

Since the translational symmetry of a magnetic space group is of the same dimension as that of the space, the subymmetric unit is a finite part of space. The asymmetric unit is defined, as above, by setting the limits on the coordinates of points contained in the asymmetric unit. For example, for the magnetic space group 140.3.1198 $I4/m'cm$ one has

Table 3.6.3.1
Symmetry operations of magnetic space group 51.14.400 $P_{2b}mma'$

Symmetry operations			
	For $(0, 0, 0)+$ set		
(1) 1	(2) 2 1/4, 0, z	(3) $2'$ 0, y, 0	(4) $2'$ (1/2, 0, 0) x, 0, 0
$\{1\|0\}$	$\{2_{001}\|1/2, 0, 0\}$	$\{2_{010}\|0\}'$	$\{2_{100}\|1/2, 0, 0\}'$
(5) $\bar{1}'$	(6) a' (1/2, 0, 0) x, y, 0	(7) m x, 0, z	(8) m 1/4, y, z
$\{\bar{1}\|0\}'$	$\{m_{001}\|1/2, 0, 0\}'$	$\{m_{010}\|0\}$	$\{m_{100}\|1/2, 0, 0\}$
	For $(0, 1, 0)'+$ set		
(1) t' (0, 1, 0)	(2) $2'$ 1/4, 1/2, z	(3) 2 (0, 1, 0) 0, y, 0	(4) 2 (1/2, 0, 0) x, 1/2, 0
$\{1\|0, 1, 0\}'$	$\{2_{001}\|1/2, 1, 0\}'$	$\{2_{010}\|0, 1, 0\}$	$\{2_{100}\|1/2, 1, 0\}$
(5) $\bar{1}$ 0, 1/2, 0	(6) n (1/2, 1, 0) x, y, 0	(7) m' x, 1/2, z	(8) b (0, 1, 0) 1/4, y, z
$\{\bar{1}\|0, 1, 0\}$	$\{m_{001}\|1/2, 1, 0\}$	$\{m_{010}\|0, 1, 0\}'$	$\{m_{100}\|1/2, 1, 0\}'$

Asymmetric unit $0 < x < \frac{1}{2}$; $0 < y < \frac{1}{2}$; $0 < z < \frac{1}{4}$; $y < \frac{1}{2} - x$

Drawings showing the boundary planes occurring in the tetragonal, trigonal and hexagonal systems, together with their algebraic equations, are given in Fig. 2.1.3.11. Drawings of asymmetric units for cubic groups have been published by Koch & Fischer (1974). The asymmetric units have complicated shapes in the trigonal, hexagonal and cubic crystal systems, and consequently are also specified by giving the vertices of the asymmetric unit. For example, for the magnetic space group 176.1.1374 $P6_3/m$ one finds

Asymmetric unit	$0 < x < 2/3$;	$0 < y < 2/3$;	$0 < z < 1/4$;		
	$x < (1 + y)/2$;	$y < \min(1 - x, (1 + x)/2)$			
Vertices	0, 0, 0	1/2, 0, 0	2/3, 1/3, 0	1/3, 2/3, 0	0, 1/2, 0
	0, 0, 1/4	1/2, 0, 1/4	2/3, 1/3, 1/4	1/3, 2/3, 1/4	0, 1/2, 1/4

Because the asymmetric unit is invariant under time inversion, all magnetic space groups $\mathcal{F}$, $\mathcal{F}1'$ and $\mathcal{F}(\mathcal{D})$ of the magnetic superfamily of type $\mathcal{F}$ have identical asymmetric units, the asymmetric unit of the group $\mathcal{F}$ (as in the present volume).

3.6.3.6. Symmetry operations

Listed under the heading of *Symmetry operations* is the geometric description of the symmetry operations of the magnetic group. A symbol denoting the geometric description of each symmetry operation is given. Details of this symbolism, except for the use of prime to denote time inversion, are given in Sections 1.4.2 and 2.1.3.9. For glide planes and screw axes, the glide and screw part are always explicitly given in parentheses by fractional coordinates, *i.e.* by fractions of the basis vectors of the coordinate system of $\mathcal{F}$ of the superfamily of the magnetic group. A coordinate triplet indicating the location and orientation of the symmetry element is given, and for rotation-inversions the location of the inversion point is also given. These symbols, with the addition of a prime to denote time inversion, follow those used in the present volume, *IT* E and Litvin (2005, 2008b). In addition, each symmetry operation is also given in Seitz (1934, 1935a,b, 1936) notation (see Section 3.6.2.2.3), *e.g.* see Table 3.6.3.1 for the symmetry operations of the magnetic space group 51.14.400 $P_{2b}mma'$.

The corresponding coordinate triplets of the *General positions,* see Section 3.6.3.9, may be interpreted as a second description of the symmetry operations, a description in matrix form. The numbering (1), (2), ..., (p), ... of the entries in the blocks *Symmetry operations* is the same as the numbering of the corresponding coordinate triplets of the *General position*, the first block below *Positions*. For all magnetic groups with primitive

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) $\bar{x}+1/2, y, z \; [u, \bar{v}, \bar{w}]$

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.

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.

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