

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

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

Since the translational symmetry of a magnetic space group is of the same dimension as that of the space, the asymmetric 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 {1 0}	(2) 2 1/4, 0, z {2 ₀₀₁ 1/2, 0, 0}	(3) 2' 0, y, 0 {2 ₀₁₀ 0}'	(4) 2' (1/2, 0, 0) x, 0, 0 {2 ₁₀₀ 1/2, 0, 0}'
(5) $\bar{1}$ { $\bar{1}$ 0}'	(6) a' (1/2, 0, 0) x, y, 0 {m ₀₀₁ 1/2, 0, 0}'	(7) m x, 0, z {m ₀₁₀ 0}	(8) m 1/4, y, z {m ₁₀₀ 1/2, 0, 0}
For (0, 1, 0)' + set			
(1) t' (0, 1, 0) {1 0, 1, 0}'	(2) 2' 1/4, 1/2, z {2 ₀₀₁ 1/2, 1, 0}'	(3) 2 (0, 1, 0) 0, y, 0 {2 ₀₁₀ 0, 1, 0}	(4) 2 (1/2, 0, 0) x, 1/2, 0 {2 ₁₀₀ 1/2, 1, 0}
(5) $\bar{1}$ 0, 1/2, 0 { $\bar{1}$ 0, 1, 0}	(6) n (1/2, 1, 0) x, y, 0 {m ₀₀₁ 1/2, 1, 0}	(7) m' x, 1/2, z {m ₀₁₀ 0, 1, 0}'	(8) b (0, 1, 0) 1/4, y, z {m ₁₀₀ 1/2, 1, 0}'

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

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

$$\begin{aligned} \text{Asymmetric unit } & 0 < x < 2/3; \quad 0 < y < 2/3; \quad 0 < z < 1/4; \\ & x < (1 + y)/2; \quad y < \min(1 - x, (1 + x)/2) \\ \text{Vertices } & 0, 0, 0 \quad 1/2, 0, 0 \quad 2/3, 1/3, 0 \quad 1/3, 2/3, 0 \quad 0, 1/2, 0 \\ & 0, 0, 1/4 \quad 1/2, 0, 1/4 \quad 2/3, 1/3, 1/4 \quad 1/3, 2/3, 1/4 \quad 0, 1/2, 1/4 \end{aligned}$$

Because the asymmetric unit is invariant under time inversion, all magnetic space groups \mathcal{F} , \mathcal{F}' and $\mathcal{F}(D)$ 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, 2008*b*). In addition, each symmetry operation is also given in Seitz (1934, 1935*a,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