International Tables for Crystallography (2016). Vol. A, Section 3.6.3.3, pp. 859–861.

Continued 51.13.399 **$P_{2b}m'ma$**

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

Symmetry of Special Projections

Along [0,0,1] **$p_{c^*}2mm$**	Along [1,0,0] **$p_{2a^*}2mm$**	Along [0,1,0] **p2mg1'**
a* = -a/2 b* = b	**a* = b b* = c**	**a* = -a b* = c**
Origin at 0,0,z	Origin at x,0,0	Origin at 0,y,0

Figure 3.6.3.1
Table of properties of the three-dimensional magnetic space group 51.13.399 $P_{2b}m'ma$ continued.

3.6.3.3. 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 (1) the relative locations and orientations of the symmetry elements and (2) the absolute locations and orientations of these symmetry elements in a given coordinate system. The general-position diagrams show, in that coordinate system, the arrangement of a set of symmetry-equivalent general points and the relative orientations of magnetic moments on this set of points. Figs. 3.6.3.3 and 3.6.3.4 show the symmetry diagram and general-position diagram, respectively, of the three-dimensional magnetic space group $P4_12'2'$.

All diagrams of three-dimensional magnetic space groups and three-dimensional subperiodic groups are orthogonal projections. The projection direction is along a basis vector of the conventional crystallographic coordinate system, see Table 1.1 of Litvin (2013). If the other two basis vectors are not parallel to the plane of the diagram, they are indicated by a subscript p, *e.g.* $\mathbf{a}_p$, $\mathbf{b}_p$ and $\mathbf{c}_p$. Schematic representations of the diagrams, showing their conventional coordinate systems, *i.e.* the origin O and basis vectors, are given in Table 2.1 of Litvin (2013). For two-dimensional magnetic space groups and magnetic frieze groups, the diagrams are in the plane defined by the group's conventional coordinate system.

The graphical symbols used in the symmetry diagrams are listed in Table 2.2 of Litvin (2013) and are an extension of those used in the present volume, *IT* E and Litvin (2008*b*). For symmetry planes and symmetry axes parallel to the plane of diagram, for rotation-inversions and for centres of symmetry, the 'heights' h along the projection direction above the plane of the

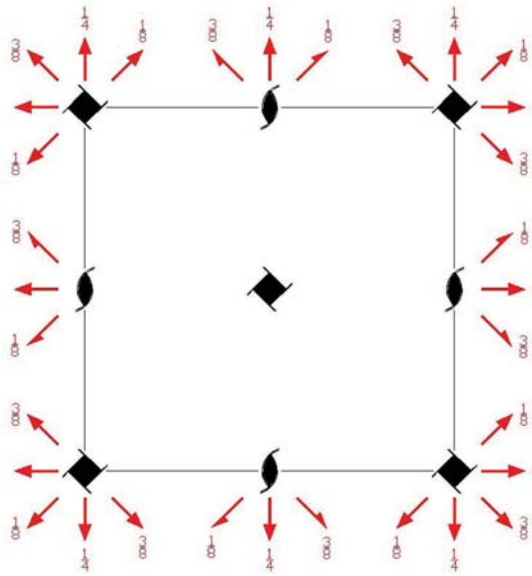

Figure 3.6.3.3
Symmetry diagram of $P4_12'2'$

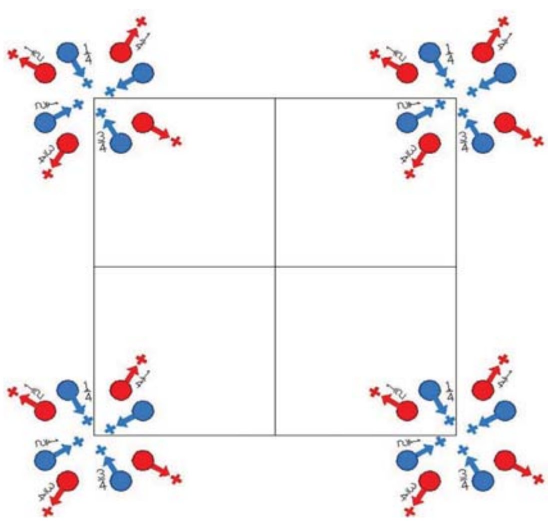

Figure 3.6.3.4
General-position diagram of $P4_12'2'$.

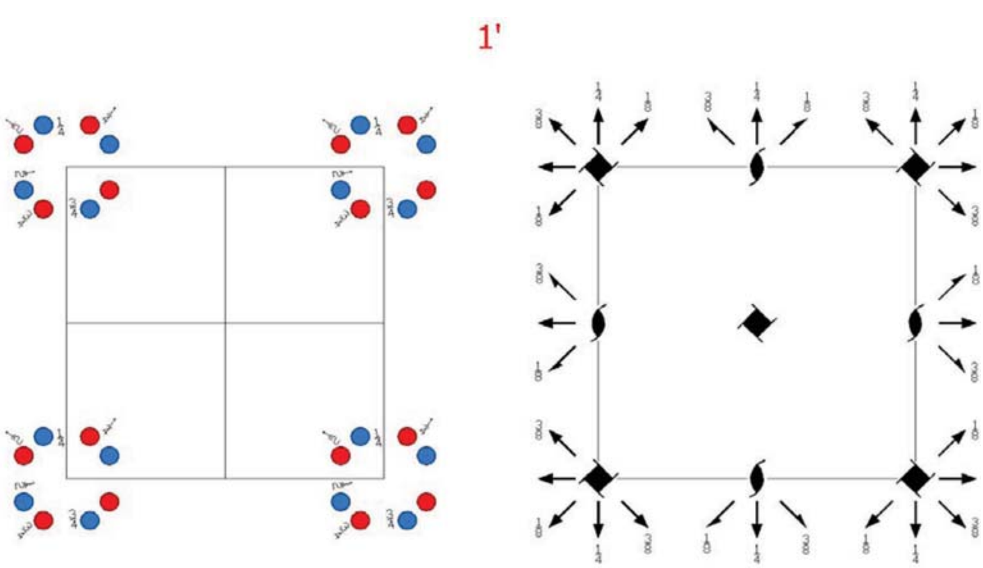

Figure 3.6.3.5
Diagrams of the magnetic space group $P4_1221'$.

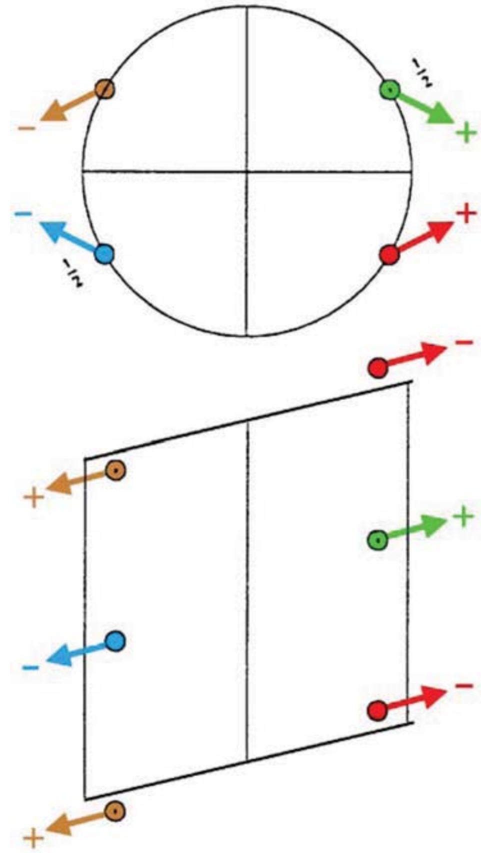

Figure 3.6.3.6
General-position diagram of rod group 2.3.29 $P2/c'11$. The positional colour coding is red for $x > 0$ and $z > 0$; blue for $x > 0$ and $z < 0$; green for $x < 0$ and $z > 0$; and brown for $x < 0$ and $z < 0$.

diagram are given. The heights are given as fractions of the shortest translation along the projection direction and, if different from zero, are printed next to the graphical symbol, see Fig. 3.6.3.3.

In the general-position diagrams, the general positions and corresponding magnetic moments are colour coded. Positions with a z component of $+z$ are shown as red circles and those with a z component of $-z$ are shown as blue circles. If the z component is either $h + z$ or $h - z$ with $h \neq 0$, then the height h is printed next to the general position, see Fig. 3.6.3.4. If two general positions have the same x component and y component, but one has a z component $+z$ and the other $-z$, the positions are shown as a circle with one half coloured red, the other half blue. The magnetic moments are colour coded to the general position to which they are associated, their direction in the plane of projection is given by an arrow in the direction of the projected magnetic moment. A + or − sign near the tip of the arrow indicates that the magnetic moment is inclined, respectively, above or below the plane of projection.

For magnetic space groups of the type $\mathcal{F}1'$, the symmetry diagram is that of the group $\mathcal{F}$. That each 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.

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
$\{\bar{1}\|0, 1, 0\}$	$\{m_{001}\|1/2, 1, 0\}$	$\{m_{010}\|0, 1, 0\}'$	$\{m_{100}\|1/2, 1, 0\}'$

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 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

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, 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

references