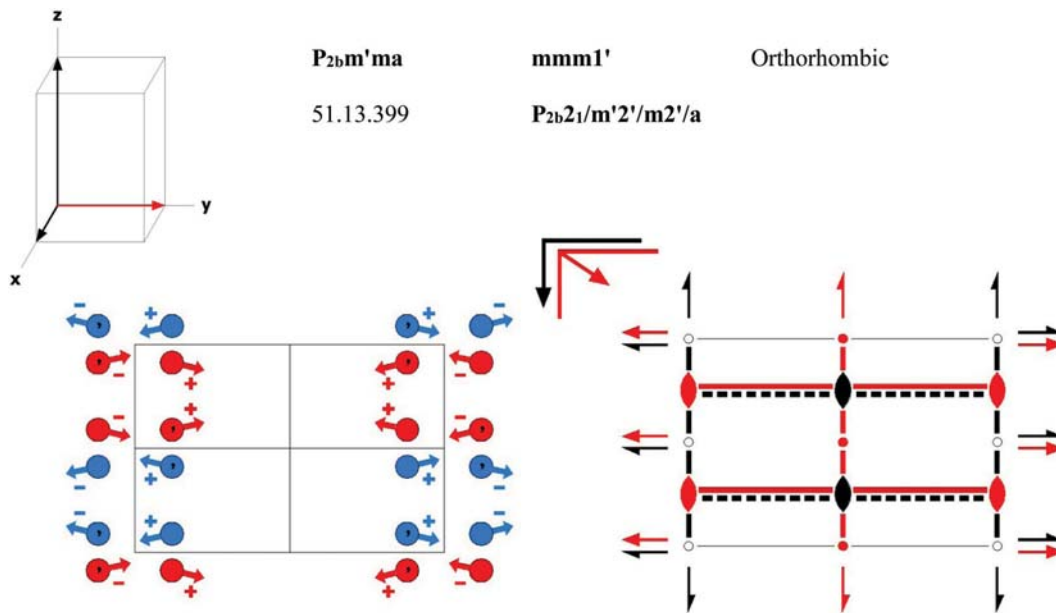


3. ADVANCED TOPICS ON SPACE-GROUP SYMMETRY



Origin at center ($2'/m$) at $2_12/ma$
Asymmetric unit $0 \leq x \leq 1/4$; $0 \leq y \leq 1/2$; $0 \leq z \leq 1$
Symmetry Operations

				For (0,0,0) + set
(1) 1	(2) $2' \frac{1}{4}, 0, z$	(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
(2) $t' (0, 1, 0)'$	(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) $b (0, 1, 0) 1/4, y, z$	
$\{\bar{1} 0, 1, 0\}$	$\{m_{001} 1/2, 1, 0\}'$	$\{m_{010} 0, 1, 0\}'$	$\{m_{100} 1/2, 1, 0\}$	

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

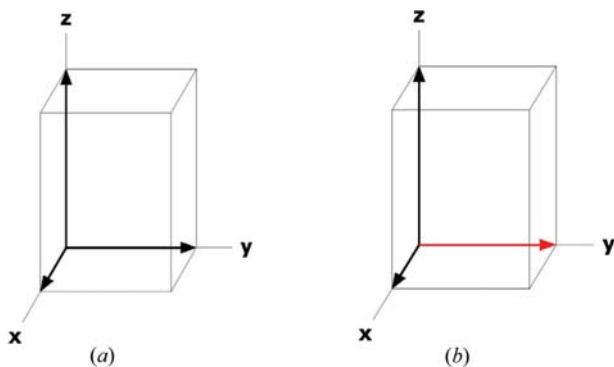


Figure 3.6.3.2
 Lattice diagrams of (a) the three-dimensional magnetic space group 26.1.168 $\mathcal{F} = Pmc2_1$ and (b) the three-dimensional magnetic space group 26.10.177 $\mathcal{M}_R = P_{2b}m'c'2_1 = \mathcal{F}(\mathcal{D}) = Pmc2_1(Pca2_1)$.

type. Given a coordinate system, this group is defined by the list of symmetry operations (see Section 3.6.3.6) given on the page with this Hermann–Mauguin symbol in the heading, or by the given list of general positions and magnetic moments (see Section 3.6.3.9).

- (2) The *short international* (Hermann–Mauguin) *point group symbol* for the geometric crystal class to which the magnetic space group belongs.
- (3) The crystal system or crystal system/Bravais system classification to which the magnetic space group belongs.

The second line has two additional entries:

- (4) The three-part numerical serial index of the magnetic group (see Section 3.6.2.2.1).
- (5) The *full international* (Hermann–Mauguin) *symbol* of the magnetic space group.

3.6. MAGNETIC SUBPERIODIC GROUPS AND MAGNETIC SPACE GROUPS

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, z [u, \bar{v}, w]	(4) $x + \frac{1}{2}, \bar{y}, z$ [u, \bar{v}, \bar{w}]	(5) \bar{x}, \bar{y}, z [$\bar{u}, \bar{v}, \bar{w}$]
		(6) $x + \frac{1}{2}, y, z$ [\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}]	$\frac{3}{4}, y, z$ [0, \bar{v}, w]	$\frac{3}{4}, \bar{y}, z$ [0, \bar{v}, \bar{w}]	
8 j .m'	$x, \frac{1}{2}, z$ [u,0,w]	$\bar{x} + \frac{1}{2}, \frac{1}{2}, z$ [$\bar{u}, 0, w$]	$\bar{x}, \frac{1}{2}, z$ [u,0,w]	$x + \frac{1}{2}, \frac{1}{2}, z$ [$\bar{u}, 0, w$]	
8 i .m	$x, 0, z$ [0,v,0]	$\bar{x} + \frac{1}{2}, \frac{1}{2}, z$ [0,v,0]	$\bar{x}, 0, z$ [0, $\bar{v}, 0$]	$x + \frac{1}{2}, 0, z$ [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]	$\frac{3}{4}, \frac{1}{2}, z$ [0,0,w]			
4 e m'm'2'	$\frac{1}{4}, 0, z$ [0,v,0]	$\frac{3}{4}, 0, z$ [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 $a^* = -a/2$ $b^* = b$ Origin at 0,0,z		Along [1,0,0] p_{2a}^*2mm $a^* = b$ $b^* = c$ Origin at x,0,0		Along [0,1,0] $p_{2mg}1'$ $a^* = -a$ $b^* = c$ 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 projec-

tions. 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