

## 2. GUIDE TO THE USE OF THE SPACE-GROUP TABLES

Table 2.2.5.1. Patterson symmetries for two and three dimensions

Laue class	Lattice type	Patterson symmetry (with space-group number)			
<i>Two dimensions</i>					
2	<i>p</i>	<i>p</i> 2 (2)			
2 <i>mm</i>	<i>p c</i>	<i>p</i> 2 <i>mm</i> (6)	<i>c</i> 2 <i>mm</i> (9)		
4	<i>p</i>	<i>p</i> 4 (10)			
4 <i>mm</i>	<i>p</i>	<i>p</i> 4 <i>mm</i> (11)			
6	<i>p</i>	<i>p</i> 6 (16)			
6 <i>mm</i>	<i>p</i>	<i>p</i> 6 <i>mm</i> (17)			
<i>Three dimensions</i>					
$\bar{1}$	<i>P</i>	$P\bar{1}$ (2)			
2/ <i>m</i>	<i>P C</i>	<i>P</i> 2/ <i>m</i> (10)	<i>C</i> 2/ <i>m</i> (12)		
<i>mmm</i>	<i>P C I F</i>	<i>P</i> <i>mmm</i> (47)	<i>C</i> <i>mmm</i> (65)	<i>I</i> <i>mmm</i> (71)	<i>F</i> <i>mmm</i> (69)
4/ <i>m</i>	<i>P I</i>	<i>P</i> 4/ <i>m</i> (83)		<i>I</i> 4/ <i>m</i> (87)	
4/ <i>mmm</i>	<i>P I</i>	<i>P</i> 4/ <i>mmm</i> (123)		<i>I</i> 4/ <i>mmm</i> (139)	
$\bar{3}$	<i>P R</i>	$P\bar{3}$ (147)			$R\bar{3}$ (148)
{ $\bar{3}m1$ $\bar{3}1m$	<i>P R</i>	$P\bar{3}m1$ (164)			$R\bar{3}m$ (166)
	<i>P R</i>	$P\bar{3}1m$ (162)			
6/ <i>m</i>	<i>P</i>	<i>P</i> 6/ <i>m</i> (175)			
6/ <i>mmm</i>	<i>P</i>	<i>P</i> 6/ <i>mmm</i> (191)			
$m\bar{3}$	<i>P I F</i>	$Pm\bar{3}$ (200)		$Im\bar{3}$ (204)	$Fm\bar{3}$ (202)
$m\bar{3}m$	<i>P I F</i>	$Pm\bar{3}m$ (221)		$Im\bar{3}m$ (229)	$Fm\bar{3}m$ (225)

## 2.2.6. Space-group diagrams

The space-group diagrams serve two purposes: (i) to show the relative locations and orientations of the symmetry elements and (ii) to illustrate the arrangement of a set of symmetrically equivalent points of the general position.

All diagrams are orthogonal projections, *i.e.* the projection direction is perpendicular to the plane of the figure. Apart from the descriptions of the rhombohedral space groups with 'rhombohedral axes' (*cf.* Section 2.2.6.6), the projection direction is always a cell axis. If other axes are not parallel to the plane of the figure, they are indicated by the subscript *p*, as *a<sub>p</sub>*, *b<sub>p</sub>* or *c<sub>p</sub>*. This applies to one or two axes for triclinic and monoclinic space groups (*cf.* Figs. 2.2.6.1 to 2.2.6.3), as well as to the three rhombohedral axes in Fig. 2.2.6.9.

The graphical symbols for symmetry elements, as used in the drawings, are displayed in Chapter 1.4.

In the diagrams, 'heights' *h* above the projection plane are indicated for symmetry planes and symmetry axes *parallel* to the projection plane, as well as for centres of symmetry. The heights are given as fractions of the shortest lattice translation normal to the projection plane and, if different from 0, are printed next to the graphical symbols. Each symmetry element at height *h* is accompanied by another symmetry element of the same type at height  $h + \frac{1}{2}$  (this does not apply to the horizontal fourfold axes in the cubic diagrams). In the space-group diagrams, only the symmetry element at height *h* is indicated (*cf.* Chapter 1.4).

Schematic representations of the diagrams, displaying the origin, the labels of the axes, and the projection direction [*uvw*], are given in Figs. 2.2.6.1 to 2.2.6.10 (except Fig. 2.2.6.6). The general-position diagrams are indicated by the letter G.

## 2.2.6.1. Plane groups

Each description of a plane group contains two diagrams, one for the symmetry elements (left) and one for the general position (right). The two axes are labelled *a* and *b*, with *a* pointing downwards and *b* running from left to right.

## 2.2.6.2. Triclinic space groups

For each of the two triclinic space groups, three elevations (along *a*, *b* and *c*) are given, in addition to the general-position diagram G (projected along *c*) at the lower right of the set, as illustrated in Fig. 2.2.6.1.

The diagrams represent a reduced cell of type II for which the three interaxial angles are non-acute, *i.e.*  $\alpha, \beta, \gamma \geq 90^\circ$ . For a cell of type I, all angles are acute, *i.e.*  $\alpha, \beta, \gamma < 90^\circ$ . For a discussion of the two types of reduced cells, reference is made to Section 9.2.2.

 2.2.6.3. Monoclinic space groups (*cf.* Sections 2.2.2 and 2.2.16)

The 'complete treatment' of each of the two settings contains four diagrams (Figs. 2.2.6.2 and 2.2.6.3). Three of them are projections of the symmetry elements, taken along the unique axis (upper left) and along the other two axes (lower left and upper right). For the general position, only the projection along the unique axis is given (lower right).

The 'synoptic descriptions' of the three cell choices (for each setting) are headed by a pair of diagrams, as illustrated in Fig. 2.2.6.4. The drawings on the left display the symmetry elements and the ones on the right the general position (labelled G). Each diagram is a projection of four neighbouring unit cells along the unique axis. It contains the outlines of the three cell choices drawn as heavy lines. For the labelling of the axes, see Fig. 2.2.6.4. The headline of the description of each cell choice contains a small-scale drawing, indicating the basis vectors and the cell that apply to that description.

## 2.2.6.4. Orthorhombic space groups and orthorhombic settings

The space-group tables contain a set of four diagrams for each orthorhombic space group. The set consists of three projections of the symmetry elements [along the *c* axis (upper left), the *a* axis (lower left) and the *b* axis (upper right)] in addition to the general-position diagram, which is given only in the projection along *c*