

## 1. SUBPERIODIC GROUP TABLES: FRIEZE-GROUP, ROD-GROUP AND LAYER-GROUP TYPES

Table 1.2.4.1. Sets of symmetry directions and their positions in the Hermann–Mauguin symbol

In the standard setting, periodic directions are [100] and [010] for the layer groups, [001] for the rod groups, and [10] for the frieze groups.

(a) Layer groups and rod groups.

	Symmetry direction (position in Hermann–Mauguin symbol)		
	Primary	Secondary	Tertiary
Triclinic	None		
Monoclinic	[100]	[010]	[001]
Orthorhombic			
Tetragonal	[001]	[100] [010]	[110] [110]
Trigonal	[001]	[100]	[110]
Hexagonal		[010] [110]	[120] [210]

(b) Frieze groups.

	Symmetry direction (position in Hermann–Mauguin symbol)		
	Primary	Secondary	Tertiary
Oblique	Rotation point in plane		
Rectangular		[10]	[01]

italic letter *c* for a centred cell. For rod and frieze groups there is only one centring type, the one-dimensional primitive cell, which is denoted by the lower-case script letter  $\rho$ .

(ii) The one or three entries after the centring letter refer to the one or three kinds of *symmetry directions* of the conventional crystallographic basis. Symmetry directions occur either as singular directions or as sets of symmetrically equivalent symmetry directions. Only one representative of each set is given. The sets of symmetry directions and their sequence in the Hermann–Mauguin symbol are summarized in Table 1.2.4.1.

Each position in the Hermann–Mauguin symbol contains one or two characters designating symmetry elements, axes and planes that occur for the corresponding crystallographic symmetry direction. Symmetry planes are represented by their normals; if a symmetry axis and a normal to a symmetry plane are parallel, the two characters are separated by a slash, e.g. the  $4/m$  in  $\rho 4/mcc$  (R40). Crystallographic symmetry directions that carry no symmetry elements are denoted by the symbol '1', e.g.  $p3m1$  (L69) and  $p112$  (L2). If no misinterpretation is possible, entries '1' at the end of the symbol are omitted, as in  $p4$  (L49) instead of  $p411$ . Subperiodic groups that have in addition to translations no symmetry directions or only centres of symmetry have only one entry after the centring letter. These are the layer-group types  $p1$  (L1) and  $p\bar{1}$  (L2), the rod-group types  $\rho 1$  (R1) and  $\rho\bar{1}$  (R2), and the frieze group  $\rho 1$  (F1).

### 1.2.5. Patterson symmetry

The entry *Patterson symmetry* in the headline gives the subperiodic group of the *Patterson function*, where Friedel's law is assumed, i.e. with neglect of anomalous dispersion. [For a discussion of the effect of dispersion, see Fischer & Knof (1987) and Wilson (2004).] The symbol for the Patterson subperiodic group can be deduced from the symbol of the subperiodic group in two steps:

(i) Glide planes and screw axes are replaced by the corresponding mirror planes and rotation axes.

Table 1.2.5.1. Patterson symmetries for subperiodic groups

(a) Layer groups.

Laue class	Lattice type	Patterson symmetry (with subperiodic group number)
$\bar{1}$	$p$	$p\bar{1}$ (L2)
$112/m$	$p$	$p112/m$ (L6)
$2/m11$	$p, c$	$p2/m11$ (L14), $c2/m11$ (L18)
$mmm$	$p, c$	$pmmm$ (L37), $cmmm$ (L47)
$4/m$	$p$	$p4/m$ (L51)
$4/mmm$	$p$	$p4/mmm$ (L61)
$\bar{3}$	$p$	$p\bar{3}$ (L66)
$\bar{3}1m$	$p$	$p\bar{3}1m$ (L71)
$\bar{3}m1$	$p$	$p\bar{3}m1$ (L72)
$6/m$	$p$	$p6/m$ (L75)
$6/mmm$	$p$	$p6/mmm$ (L80)

(b) Rod groups.

Laue class	Lattice type	Patterson symmetry (with subperiodic group number)
$\bar{1}$	$\rho$	$\rho\bar{1}$ (R2)
$2/m11$	$\rho$	$\rho 2/m11$ (R6)
$112/m$	$\rho$	$\rho 112/m$ (R11)
$mmm$	$\rho$	$\rho mmm$ (R20)
$4/m$	$\rho$	$\rho 4/m$ (R28)
$4/mmm$	$\rho$	$\rho 4/mmm$ (R39)
$\bar{3}$	$\rho$	$\rho\bar{3}$ (R48)
$\bar{3}m$	$\rho$	$\rho\bar{3}m$ (R51)
$6/m$	$\rho$	$\rho 6/m$ (R60)
$6/mmm$	$\rho$	$\rho 6/mmm$ (R73)

(c) Frieze groups.

Laue class	Lattice type	Patterson symmetry (with subperiodic group number)
2	$\rho$	$\rho 211$ (F2)
$2mm$	$\rho$	$\rho 2mm$ (F6)

(ii) If the resulting symmorphic subperiodic group is not centrosymmetric, inversion is added.

There are 13 different Patterson symmetries for the layer groups, ten for the rod groups and two for the frieze groups. These are listed in Table 1.2.5.1. The 'point-group part' of the symbol of the Patterson symmetry represents the *Laue class* to which the subperiodic group belongs (cf. Tables 1.2.1.1, 1.2.1.2 and 1.2.1.3).

### 1.2.6. Subperiodic group diagrams

There are two types of diagrams, referred to as *symmetry diagrams* and *general-position diagrams*. Symmetry diagrams show (i) the relative locations and orientations of the symmetry elements and (ii) the locations and orientations of the symmetry elements relative to a given coordinate system. General-position diagrams show the arrangement of a set of symmetrically equivalent points of general positions relative to the symmetry elements in that given coordinate system.

For the three-dimensional subperiodic groups, i.e. layer and rod groups, all diagrams are orthogonal projections. The projection direction is along a basis vector of the conventional crystallographic coordinate system (see Tables 1.2.1.1 and 1.2.1.2). If the other basis vectors are not parallel to the plane of the figure, they are indicated by subscript 'p', e.g.  $\mathbf{a}_p$ ,  $\mathbf{b}_p$  and  $\mathbf{c}_p$ .