International Tables for Crystallography (2006). Vol. E, Section 1.2.4, pp. 7–8.

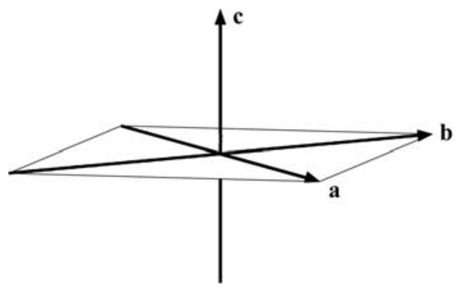

Fig. 1.2.1.2. Monoclinic/orthogonal basis vectors. For the monoclinic/orthogonal subdivision, $\alpha = \beta = 90^\circ$ and the plane containing the **a** and **b** non-lattice basis vectors is *orthogonal* to the lattice basis vector **c**.

The *conventional unit cell* of a subperiodic group is defined by the crystallographic origin and by those basis vectors which are also lattice vectors. For layer groups in the standard setting, the cell parameters, the magnitude of the lattice basis vectors **a** and **b**, and the angle between them, which specify the conventional cell, are given in the seventh column of Table 1.2.1.1. The conventional unit cell obtained in this manner turns out to be either *primitive* or *centred* and is denoted by *p* or *c*, respectively, in the eighth column of Table 1.2.1.1. For rod and frieze groups with their one-dimensional lattices, the single cell parameter to be specified is the magnitude of the lattice basis vector.

1.2.2. Contents and arrangement of the tables

The presentation of the subperiodic group tables in Parts 2, 3 and 4 follows the form and content of *IT* A (1983). The entries for a subperiodic group are printed on two facing pages or continuously on a single page, where space permits, in the following order (deviations from this standard format are indicated on the relevant pages):

Left-hand page:

(1) *Headline*;

(2) *Diagrams* for the symmetry elements and the general position;

(3) *Origin*;

(4) *Asymmetric unit*;

(5) *Symmetry operations*.

Right-hand page:

(6) *Headline* in abbreviated form;

(7) *Generators selected*: this information is the basis for the order of the entries under *Symmetry operations* and *Positions*;

(8) General and special *Positions*, with the following columns: *Multiplicity*; *Wyckoff letter*; *Site symmetry*, given by the oriented site-symmetry symbol; *Coordinates*; *Reflection conditions*;

(9) *Symmetry of special projections*;

(10) *Maximal non-isotypic non-enantiomorphic subgroups*;

(11) *Maximal isotypic subgroups and enantiomorphic subgroups of lowest index*;

(12) *Minimal non-isotypic non-enantiomorphic supergroups*.

1.2.2.1. *Subperiodic groups with more than one description*

For two monoclinic/oblique layer-group types with a glide plane, more than one description is available: *p*11*a* (L5) and *p*112/*a* (L7). The synoptic descriptions consist of abbreviated treatments for three 'cell choices', called 'cell choices 1, 2 and 3' [see Section 1.2.6, (i) *Layer groups*]. A complete description is given for cell choice 1 and it is repeated among the synoptic descriptions of cell choices 2 and 3. For three layer groups, *p*4/*n* (L52), *p*4/*nbm* (L62) and *p*4/*nmm* (L64), two descriptions are given (see Section 1.2.7). These two descriptions correspond to the choice of origin, at an inversion centre and on a fourfold axis. For 15 rod-group types, two descriptions are given, corresponding to two settings [see Section 1.2.6, (ii) *Rod groups*].

1.2.3. Headline

The description of a subperiodic group starts with a headline on a left-hand page, consisting of two or three lines which contain the following information when read from left to right.

First line:

(1) The *short international* (Hermann–Mauguin) *symbol* of the subperiodic group type. Each symbol has two meanings. The first is that of the Hermann–Mauguin symbol of the subperiodic group type. The second meaning is that of a specific subperiodic group which belongs to this subperiodic group type. Given a coordinate system, this group is defined by the list of symmetry operations (see Section 1.2.9) given on the page headed by that Hermann–Mauguin symbol, or by the given list of general positions (see Section 1.2.11). Alternatively, this group is defined by the given diagrams (see Section 1.2.6). The Hermann–Mauguin symbols for the subperiodic group types are distinct except for the rod- and frieze-group types $\mathscr{p}1$ (R1, F1), $\mathscr{p}211$ (R3, F2) and $\mathscr{p}11m$ (R10, F4).

(2) The *short international* (Hermann–Mauguin) *point group symbol* for the geometric class to which the subperiodic group belongs.

(3) The name used in classifying the subperiodic group types. For layer groups this is the combination crystal system/Bravais system classification given in the first two columns of Table 1.2.1.1, and for rod and frieze groups this is the crystal system classification in the first columns of Tables 1.2.1.2 and 1.2.1.3, respectively.

Second line:

(4) The sequential number of the subperiodic group type.

(5) The *full international* (Hermann–Mauguin) *symbol* for the subperiodic group type.

(6) The *Patterson symmetry*.

Third line:

This line is used to indicate the cell choice in the case of layer groups *p*11*a* (L5) and *p*112/*a* (L7), the origin choice for the three layer groups *p*4/*n* (L52), *p*4/*nbm* (L62) and *p*4/*nmm* (L64), and the setting for the 15 rod groups with two distinct Hermann–Mauguin setting symbols (see Table 1.2.6.2).

1.2.4. International (Hermann–Mauguin) symbols for subperiodic groups

Both the short and the full Hermann–Mauguin symbols consist of two parts: (i) a letter indicating the centring type of the conventional cell, and (ii) a set of characters indicating symmetry elements of the subperiodic group.

(i) The letters for the two centring types for layer groups are the lower-case italic letter *p* for a primitive cell and the lower-case 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 $\mathscr{p}$.

(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 $\mathscr{p}4/mcc$ (R40). Crystallographic symmetry directions that carry no symmetry elements are denoted by the symbol '1', *e.g.* *p*3*m*1 (L69) and *p*112 (L2). If no misinterpretation is possible, entries '1' at the end of the symbol are omitted, as in *p*4 (L49) instead of *p*411. Subperiodic groups that have in addition to translations no

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 Orthorhombic	[100]	[010]	[001]
Tetragonal	[001]	[100] [010]	[1$\bar{1}$0] [110]
Trigonal Hexagonal	[001]	[100] [010] [$\bar{1}\bar{1}$0]	[1$\bar{1}$0] [120] [$\bar{2}\bar{1}$0]

(*b*) Frieze groups.

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

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 𝓅1 (R1) and 𝓅$\bar{1}$ (R2), and the frieze group 𝓅1 (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 (1992).] 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.

(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).

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)
$\bar{1}$	𝓅	𝓅$\bar{1}$ (R2)
$2/m11$	𝓅	𝓅$2/m11$ (R6)
$112/m$	𝓅	𝓅$112/m$ (R11)
mmm	𝓅	𝓅mmm (R20)
$4/m$	𝓅	𝓅$4/m$ (R28)
$4/mmm$	𝓅	𝓅$4/mmm$ (R39)
$\bar{3}$	𝓅	𝓅$\bar{3}$ (R48)
$\bar{3}m$	𝓅	𝓅$\bar{3}1m$ (R51)
$6/m$	𝓅	𝓅$6/m$ (R60)
$6/mmm$	𝓅	𝓅$6/mmm$ (R73)

(*c*) Frieze groups.

Laue class	Lattice type	Patterson symmetry (with subperiodic group number)
2	𝓅	𝓅211 (F2)
$2mm$	𝓅	𝓅$2mm$ (F6)

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 $\mathbf{c}_p$. For frieze groups (two-dimensional subperiodic groups), the diagrams are in the plane defined by the frieze group's conventional crystallographic coordinate system (see Table 1.2.1.3).

The graphical symbols for symmetry elements used in the symmetry diagrams are given in Chapter 1.1 and follow those used in *IT* A (1983). For rod groups, the 'heights' h along the projection direction above the plane of the diagram are indicated for symmetry planes and symmetry axes *parallel* to the plane of the diagram, for rotoinversions and for centres of symmetry. The heights are given as fractions of the translation along the projection direction and, if different from zero, are printed next to the graphical symbol.

Schematic representations of the diagrams, displaying their conventional coordinate system, *i.e.* the origin and basis vectors, with the basis vectors labelled in the standard setting, are given below. The general-position diagrams are indicated by the letter G.

(i) *Layer groups*

For the layer groups, all diagrams are orthogonal projections along the basis vector **c**. For the triclinic/oblique layer groups, two diagrams are given: the general-position diagram on the right and the symmetry diagram on the left. These diagrams are illustrated in Fig. 1.2.6.1.

For all monoclinic/oblique layer groups, except groups L5 and L7, two diagrams are given, as shown in Fig. 1.2.6.2. For the layer groups L5 and L7, the descriptions of the three cell choices are

references