

## 1.2. Guide to the use of the subperiodic group tables

This present volume is, in part, an extension of *International Tables for Crystallography*, Volume A, *Space-Group Symmetry* (IT A, 1983). Symmetry tables are given in IT A for the 230 three-dimensional crystallographic space-group types (space groups) and the 17 two-dimensional crystallographic space-group types (plane groups). We give in the following three parts of this volume analogous symmetry tables for the two-dimensional and three-dimensional subperiodic group types: the seven crystallographic *frieze-group* types (two-dimensional groups with one-dimensional translations) in Part 2; the 75 crystallographic *rod-group* types (three-dimensional groups with one-dimensional translations) in Part 3; and the 80 crystallographic *layer-group* types (three-dimensional groups with two-dimensional translations) in Part 4. This chapter forms a guide to the entries of the subperiodic group tables given in Parts 2–4.

### 1.2.1. Classification of subperiodic groups

Subperiodic groups can be classified in ways analogous to the space groups. For the mathematical definitions of these classifications and their use for space groups, see Section 8.2 of IT A (1983). Here we shall limit ourselves to those classifications which are explicitly used in the symmetry tables of the subperiodic groups.

#### 1.2.1.1. Subperiodic group types

The subperiodic groups are classified into *affine subperiodic group types*, *i.e.* affine equivalence classes of subperiodic groups. There are 80 affine layer-group types and seven affine frieze-group types. There are 67 crystallographic and an infinity of noncrystallographic affine rod-group types. We shall consider here only rod groups of the 67 crystallographic rod-group types and refer to these crystallographic affine rod-group types simply as affine rod-group types.

The subperiodic groups are also classified into *proper affine subperiodic group types*, *i.e.* proper affine classes of subperiodic groups. For layer and frieze groups, the two classifications are identical. For rod groups, each of eight affine rod-group types splits into a pair of *enantiomorphic crystallographic rod-group types*. Consequently, there are 75 proper affine rod-group types. The eight pairs of enantiomorphic rod-group types are  $\#4_1$  (R24),  $\#4_3$  (R26);  $\#4_122$  (R31),  $\#4_322$  (R33);  $\#3_1$  (R43),  $\#3_2$  (R44);  $\#3_112$  (R47),  $\#3_212$  (R48);  $\#6_1$  (R54),  $\#6_5$  (R58);  $\#6_2$  (R55),  $\#6_4$  (R57);  $\#6_122$  (R63),  $\#6_522$  (R67); and  $\#6_222$  (R64),  $\#6_422$  (R66). (Each subperiodic group is given in the text by its Hermann–Mauguin symbol followed in parenthesis by a letter L, R or F to denote it, respectively, as a layer, rod or frieze group, and its sequential numbering from Parts 2, 3 or 4.) We shall refer to the proper affine subperiodic group types simply as subperiodic group types.

#### 1.2.1.2. Other classifications

There are 27 geometric crystal classes of layer groups and rod groups, and four geometric crystal classes of frieze groups. These are listed, for layer groups, in the fourth column of Table 1.2.1.1, and for the rod and frieze groups in the second columns of Tables 1.2.1.2 and 1.2.1.3, respectively.

We further classify subperiodic groups according to the following classifications of the subperiodic group's point group and lattice group. These classifications are introduced to

emphasize the relationships between subperiodic groups and space groups:

(1) The point group of a layer or rod group is three-dimensional and corresponds to a point group of a three-dimensional space group. The point groups of three-dimensional space groups are classified into the triclinic, monoclinic, orthorhombic, tetragonal, trigonal, hexagonal and cubic crystal systems. We shall use this classification also for subperiodic groups. Consequently, the three-dimensional subperiodic groups are classified, see the third column of Table 1.2.1.1 and the first column of Table 1.2.1.2, into the triclinic, monoclinic, orthorhombic, tetragonal, trigonal and hexagonal crystal systems. The cubic crystal system does not arise for three-dimensional subperiodic groups. Two-dimensional subperiodic groups, *i.e.* frieze groups, are analogously classified, see the first column of Table 1.2.1.3, into the oblique and rectangular crystal systems.

(2) The two-dimensional lattice of a layer group is also a two-dimensional lattice of a plane group. The lattices of plane groups are classified, according to *Bravais (flock) systems*, see IT A (1983), into the oblique, rectangular, square and hexagonal Bravais systems. We shall also use this classification for layer groups, see the first column in Table 1.2.1.1. For rod and frieze groups no lattice classification is used, as all one-dimensional lattices form a single Bravais system.

A subdivision of the monoclinic rod-group category is made into monoclinic/inclined and monoclinic/orthogonal. Two different coordinate systems, see Table 1.2.1.2, are used for the rod groups of these two subdivisions of the monoclinic crystal system. These two coordinate systems differ in the orientation of the plane containing the non-lattice basis vectors relative to the lattice vectors. For the monoclinic/inclined subdivision, the plane containing the non-lattice basis vectors is, see Fig. 1.2.1.1, *inclined* with respect to the lattice basis vector. For the monoclinic/orthogonal subdivision, the plane is, see Fig. 1.2.1.2, *orthogonal*.

##### 1.2.1.2.1. Conventional coordinate systems

The subperiodic groups are described by means of a *crystallographic coordinate system* consisting of a *crystallographic origin*, denoted by *O*, and a *crystallographic basis*. The basis vectors for the three-dimensional layer groups and rod groups are labelled **a**, **b** and **c**. The basis vectors for the two-dimensional frieze groups are labelled **a** and **b**. Unlike space groups, not all basis vectors of the crystallographic basis are lattice vectors. Like space groups, the crystallographic coordinate system is used to define the symmetry operations (see Section 1.2.9) and the Wyckoff positions (see Section 1.2.11). The symmetry operations are defined with respect to the directions of both lattice and non-lattice basis vectors. A Wyckoff position, denoted by a coordinate triplet (*x*, *y*, *z*) for the three-dimensional layer and rod groups, is defined in the crystallographic coordinate system by  $O + \mathbf{r}$ , where  $\mathbf{r} = x\mathbf{a} + y\mathbf{b} + z\mathbf{c}$ . For the two-dimensional frieze groups, a Wyckoff position is denoted by a coordinate doublet (*x*, *y*) and is defined in the crystallographic coordinate system by  $O + \mathbf{r}$ , where  $\mathbf{r} = x\mathbf{a} + y\mathbf{b}$ .

The term *setting* will refer to the assignment of the labels **a**, **b** and **c** (and the corresponding directions [100], [010] and [001], respectively) to the basis vectors of the crystallographic basis (see Section 1.2.6). In the *standard setting*, those basis vectors which are also lattice vectors are labelled as follows: for layer groups with their two-dimensional lattice by **a** and **b**, for rod groups with

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Table 1.2.1.1. *Classification of layer groups*

Bold or bold underlined symbols indicate Laue groups. Bold underlined point groups are also lattice point symmetries (holohedries).

Two-dimensional Bravais system	Symbol	Three-dimensional crystal system	Crystallographic point groups	No. of layer-group types	Restrictions on conventional coordinate system	Cell parameters to be determined	Bravais lattice
Oblique	$m$	Triclinic	1, $\bar{1}$	2	None	$a, b, \gamma^\dagger$	$mp$
		Monoclinic	2, $m$ , $\underline{2/m}$	5	$\alpha = \beta = 90^\circ$		
Rectangular	$o$			11	$\beta = \gamma = 90^\circ$	$a, b$	$op$
		Orthorhombic	222, $2mm$ , $\underline{mmm}$	30	$\alpha = \beta = \gamma = 90^\circ$		$oc$
Square	$t$	Tetragonal	4, $\bar{4}$ , $\underline{4/m}$ 422, $4mm$ , $\bar{4}2m$ , $\underline{4/mmm}$	16	$a = b$ $\alpha = \beta = \gamma = 90^\circ$	$a$	$tp$
Hexagonal	$h$	Trigonal	3, $\bar{3}$ 32, $3m$ , $\bar{3}m$	8	$a = b$	$a$	$hp$
		Hexagonal	6, $\bar{6}$ , $\underline{6/m}$ 622, $6mm$ , $\bar{6}m2$ , $\underline{6/mmm}$	8	$\gamma = 120^\circ$ $\alpha = \beta = 90^\circ$		

† This angle is conventionally taken to be non-acute, i.e.  $\geq 90^\circ$ .

Table 1.2.1.2. *Classification of rod groups*

Bold symbols indicate Laue groups.

Three-dimensional crystal system	Crystallographic point groups	No. of rod-group types	Restrictions on conventional coordinate system
Triclinic	1, $\bar{1}$	2	None
Monoclinic (inclined)	2, $m$ , $\underline{2/m}$	5	$\beta = \gamma = 90^\circ$
Monoclinic (orthogonal)		5	$\alpha = \beta = 90^\circ$
Orthorhombic	222, $2mm$ , $\underline{mmm}$	10	$\alpha = \beta = \gamma = 90^\circ$
Tetragonal	4, $\bar{4}$ , $\underline{4/m}$ 422, $4mm$ , $\bar{4}2m$ , $\underline{4/mmm}$	19	
Trigonal	3, $\bar{3}$ 32, $3m$ , $\bar{3}m$	11	$\alpha = \beta = 90, \gamma = 120^\circ$
Hexagonal	6, $\bar{6}$ , $\underline{6/m}$ 622, $6mm$ , $\bar{6}m2$ , $\underline{6/mmm}$	23	

Table 1.2.1.3. *Classification of frieze groups*

Bold symbols indicate Laue groups.

Two-dimensional crystal system	Crystallographic point groups	No. of frieze-group types	Restrictions on conventional coordinate system
Oblique	1, $\underline{2}$	2	None
Rectangular	$m$ , $\underline{2mm}$	5	$\gamma = 90^\circ$

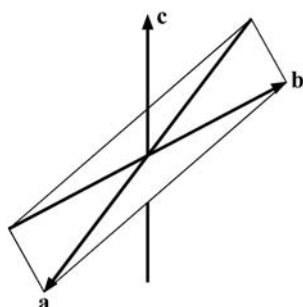


Fig. 1.2.1.1. Monoclinic/inclined basis vectors. For the monoclinic/inclined subdivision,  $\beta = \gamma = 90^\circ$  and the plane containing the  $\mathbf{a}$  and  $\mathbf{b}$  non-lattice basis vectors is *inclined* with respect to the lattice basis vector  $\mathbf{c}$ .

their one-dimensional lattice by  $\mathbf{c}$ , and for frieze groups with their one-dimensional lattice by  $\mathbf{a}$ .

The selection of a crystallographic coordinate system is not unique. Following *IT A* (1983), we choose *conventional crystallographic coordinate systems* which have a right-handed set of basis vectors and such that symmetry of the subperiodic groups is best displayed. The conventional crystallographic coordinate systems used in the standard settings are given in the sixth column of Table 1.2.1.1 for the layer groups, and the fourth columns of Tables 1.2.1.2 and 1.2.1.3 for the rod groups and frieze groups, respectively. The crystallographic origin is conventionally chosen at a centre of symmetry or at a point of high site symmetry (see Section 1.2.7).

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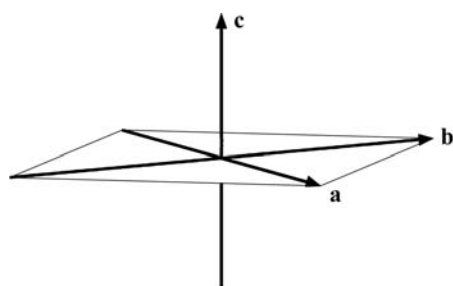


Fig. 1.2.1.2. Monoclinic/orthogonal basis vectors. For the monoclinic/orthogonal subdivision,  $\alpha = \beta = 90^\circ$  and the plane containing the **a** and **b** non-lattice basis vectors is *orthogonal* to the lattice basis vector **c**.

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:  $p11a$  (L5) and  $p112/a$  (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,  $p4/n$  (L52),  $p4/nbm$  (L62) and  $p4/nmm$  (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  $\not{p}1$  (R1, F1),  $\not{p}211$  (R3, F2) and  $\not{p}11m$  (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  $p11a$  (L5) and  $p112/a$  (L7), the origin choice for the three layer groups  $p4/n$  (L52),  $p4/nbm$  (L62) and  $p4/nmm$  (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  $\not{p}$ .

(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  $\not{p}4/mcc$  (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

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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] [1 $\bar{1}$ 0]	[1 $\bar{1}$ 0] [120] [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  $\not\!1$  (R1) and  $\not\!1$  (R2), and the frieze group  $\not\!1$  (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 (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).

## 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

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)
$\bar{1}$	$\not\!$	$\not\!\bar{1}$ (R2)
2/m11	$\not\!$	$\not\!2/m11$ (R6)
112/m	$\not\!$	$\not\!112/m$ (R11)
$mmm$	$\not\!$	$\not\!mmm$ (R20)
4/m	$\not\!$	$\not\!4/m$ (R28)
4/ $mmm$	$\not\!$	$\not\!4/mmm$ (R39)
$\bar{3}$	$\not\!$	$\not\!\bar{3}$ (R48)
$\bar{3}m$	$\not\!$	$\not\!\bar{3}1m$ (R51)
6/m	$\not\!$	$\not\!6/m$ (R60)
6/ $mmm$	$\not\!$	$\not\!6/mmm$ (R73)

(c) Frieze groups.

Laue class	Lattice type	Patterson symmetry (with subperiodic group number)
2	$\not\!$	$\not\!211$ (F2)
2mm	$\not\!$	$\not\!2mm$ (F6)

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  $\mathbf{c}$ . 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

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headed by a pair of diagrams, as illustrated in Fig. 1.2.6.3. Each diagram is a projection of four neighbouring unit cells. The headline of each cell choice contains a small drawing indicating the origin and basis vectors of the cell that apply to that description.

For the monoclinic/rectangular and orthorhombic/rectangular layer groups, two diagrams are given, as illustrated in Figs. 1.2.6.4 and 1.2.6.5, respectively. For these groups, the Hermann–Mauguin symbol for the layer group is given for two settings, *i.e.* for two ways of assigning the labels **a**, **b**, **c** to the basis vectors of the conventional coordinate system.

The symbol for each setting is referred to as a *setting symbol*. The setting symbol for the standard setting is  $(abc)$ . The Hermann–Mauguin symbol of the layer group in the conventional coordinate system, in the standard setting, is the same as the Hermann–Mauguin symbol in the first line of the headline. The setting symbol for all other settings is a shorthand notation for the relabelling of the basis vectors. For example, the setting symbol  $(cab)$  means that the basis vectors relabelled in this setting as **a**, **b** and **c** were in the standard setting labelled **c**, **a** and **b**, respectively [cf. Section 2.6 of *IT A* (1983)].

For these groups, the two settings considered are the standard  $(abc)$  setting and a second  $(b\bar{a}c)$  setting. In Fig. 1.2.6.6, the  $(abc)$  setting symbol is written horizontally across the top of the

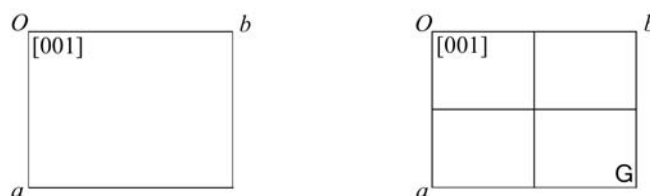


Fig. 1.2.6.5. Diagrams for orthorhombic/rectangular layer groups.

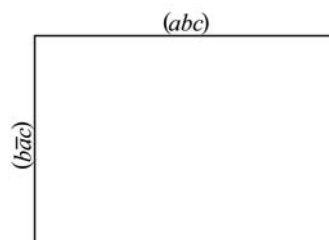


Fig. 1.2.6.6. Monoclinic/rectangular and orthorhombic/rectangular layer groups with two settings. For the second-setting symbol printed vertically, the page must be turned clockwise by 90° or viewed from the right-hand side.

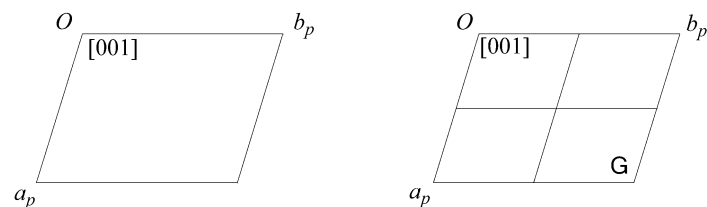


Fig. 1.2.6.1. Diagrams for triclinic/oblique layer groups.

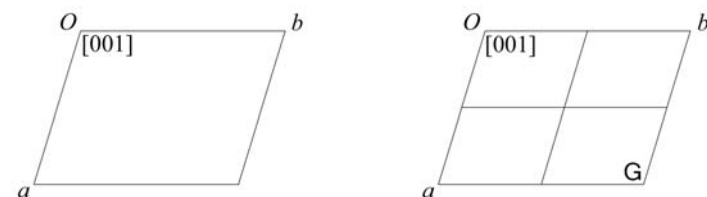


Fig. 1.2.6.2. Diagrams for monoclinic/oblique layer groups.

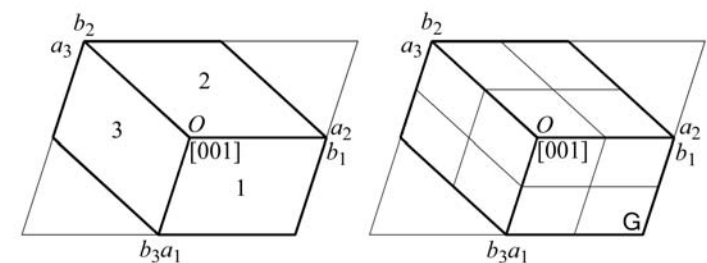


Fig. 1.2.6.3. Monoclinic/oblique layer groups Nos. 5 and 7, cell choices 1, 2, 3. The numbers 1, 2, 3 within the cells and the subscripts of the basis vectors indicate the cell choice.

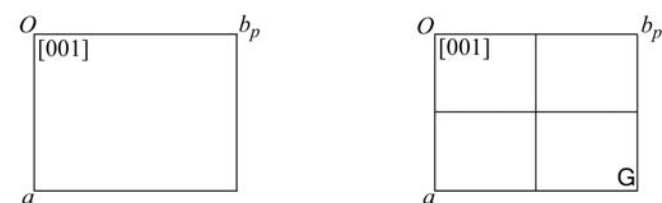


Fig. 1.2.6.4. Diagrams for monoclinic/rectangular layer groups.

diagram and the second  $(b\bar{a}c)$  setting symbol is written vertically on the left-hand side of the diagram. When viewing the diagram with the  $(abc)$  setting symbol written horizontally across the top of the diagram, the origin of the coordinate system is at the upper left-hand corner of the diagram, the basis vector labelled **a** is downward towards the bottom of the page, the basis vector labelled **b** is to the right and the basis vector labelled **c** is upward out of the page (see also Figs. 1.2.6.4 and 1.2.6.5). When viewing

Table 1.2.6.1. Distinct Hermann–Mauguin symbols for monoclinic/rectangular and orthorhombic/rectangular layer groups in different settings

Layer group	Setting symbol	
	$(abc)$	$(b\bar{a}c)$
	Hermann–Mauguin symbol	
L8	$p211$	$p121$
L9	$p2_111$	$p12_11$
L10	$c211$	$c121$
L11	$pm11$	$p1m1$
L12	$pb11$	$p1a1$
L13	$cm11$	$c1m1$
L14	$p2/m11$	$p12/m1$
L15	$p2_1/m11$	$p12_1/m1$
L16	$p2/b11$	$p12/a1$
L17	$p2_1/b11$	$p12_1/a1$
L18	$c2/m11$	$c12/m1$
L20	$p2_122$	$p22_12$
L24	$pma2$	$pbm2$
L27	$pm2m$	$p2mm$
L28	$pm2_1b$	$p2_1ma$
L29	$pb2_1m$	$p2_1am$
L30	$pb2b$	$p2aa$
L31	$pm2a$	$p2mb$
L32	$pm2_1n$	$p2_1mn$
L33	$pb2_1a$	$p2_1ab$
L34	$pb2n$	$p2an$
L35	$cm2m$	$c2mm$
L36	$cm2a$	$c2mb$
L38	$pmaa$	$pbmb$
L40	$pmam$	$pbmm$
L41	$pmma$	$pmmb$
L42	$pman$	$pbmn$
L43	$pbaa$	$pbab$
L45	$pbma$	$pmab$

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

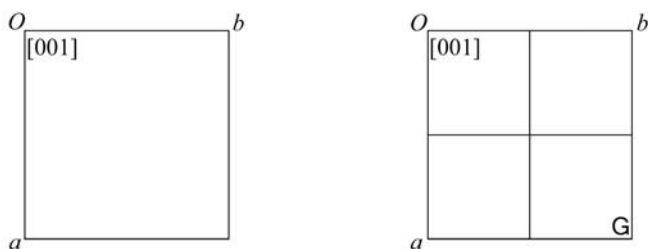


Fig. 1.2.6.7. Diagrams for square/tetragonal layer groups.

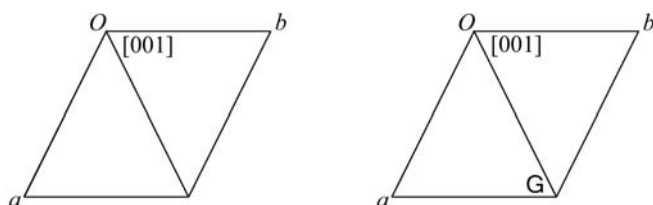


Fig. 1.2.6.8. Diagrams for trigonal/hexagonal and hexagonal/hexagonal layer groups.

the diagram with the  $(b\bar{a}c)$  written horizontally, *i.e.* by rotating the page clockwise by  $90^\circ$  or by viewing the diagram from the right, the position of the origin and the labelling of the basis vectors are as above, *i.e.* the origin is at the upper left-hand corner, the basis vector labelled **a** is downward, the basis vector labelled **b** is to the right and the basis vector labelled **c** is upward out of the page. In the symmetry diagrams of these groups, Part 4, the setting symbols are not given. In their place is given the Hermann–Mauguin symbol of the layer group in the conventional coordinate system in the corresponding setting. The Hermann–Mauguin symbol in the standard setting is given horizontally across the top of the diagram, and in the second setting vertically on the left-hand side.

If the two Hermann–Mauguin symbols are the same (*i.e.* as the Hermann–Mauguin symbol in the first line of the heading), then no symbols are explicitly given. A listing of monoclinic/rectangular and orthorhombic/rectangular layer groups with distinct Hermann–Mauguin symbols in the two settings is given in Table 1.2.6.1.

*Example:* The layer group  $pm\bar{a}2$  (L24)

In the  $(abc)$  setting, the Hermann–Mauguin symbol is  $pm\bar{a}2$ . In the  $(b\bar{a}c)$  setting, the Hermann–Mauguin symbol is  $p\bar{b}m2$ .

For the square/tetragonal, hexagonal/trigonal and hexagonal/hexagonal layer groups, two diagrams are given, as illustrated in Figs. 1.2.6.7 and 1.2.6.8.

(ii) *Rod groups*

For triclinic, monoclinic/inclined, monoclinic/orthogonal and orthorhombic rod groups, six diagrams are given: three symmetry diagrams and three general-position diagrams. These diagrams are orthogonal projections along each of the conventional coordinate system basis vectors. For pictorial clarity, each of the projections contains an area bounded by a circle or a parallelogram. These areas may be considered as the projections of a cylindrical volume, whose axis coincides with the **c** lattice vector, bounded at  $z = 0$  and  $z = 1$  by planes parallel to the plane containing the **a** and **b** basis vectors. The projection of the **c** lattice vector is shown explicitly. Only the *directions* of the projected non-lattice basis vectors **a** and **b** are indicated in the diagrams, denoted by lines from the origin to the boundary of the projected cylinder. These diagrams are illustrated for triclinic rod groups in Fig. 1.2.6.9, for monoclinic/inclined rod groups in Fig. 1.2.6.10, for monoclinic/orthogonal rod groups in Fig. 1.2.6.11 and for orthorhombic rod groups in Fig. 1.2.6.12.

The symmetry diagrams consist of the **c** projection, outlined with a circle at the upper left-hand side, the **a** projection at the lower left-hand side and the **b** projection at the upper right-hand side. The general-position diagrams are the **c** projection, outlined with a circle at the lower right-hand side, and the remaining two general-position diagrams next to the corresponding symmetry diagrams.

Six settings for each of these rod groups are considered and the corresponding setting symbols are shown in Fig. 1.2.6.13. This figure schematically shows the three symmetry diagrams each with two setting symbols, one written horizontally across the top of the diagram and the second written vertically along the left-hand side of the diagram. In the symmetry diagrams of these groups, Part 3, the setting symbols are not given. In their place is given the Hermann–Mauguin symbol of the layer group in the conventional coordinate system in the corresponding setting. As there are only translations in one dimension, it is necessary to add to the translational part of the Hermann–Mauguin symbol a

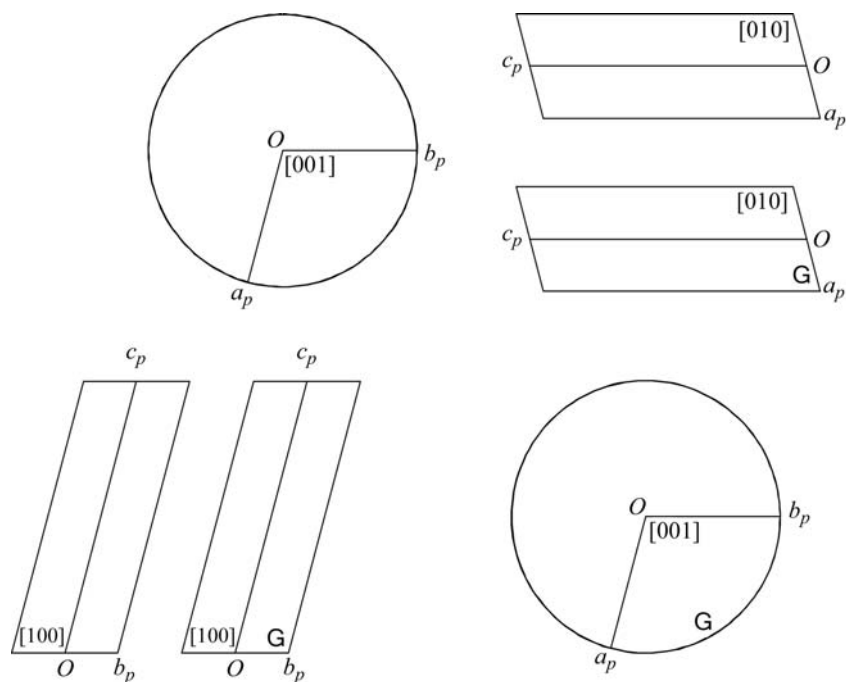


Fig. 1.2.6.9. Diagrams for triclinic rod groups.

## 1.2. GUIDE TO THE USE OF THE SUBPERIODIC GROUP TABLES

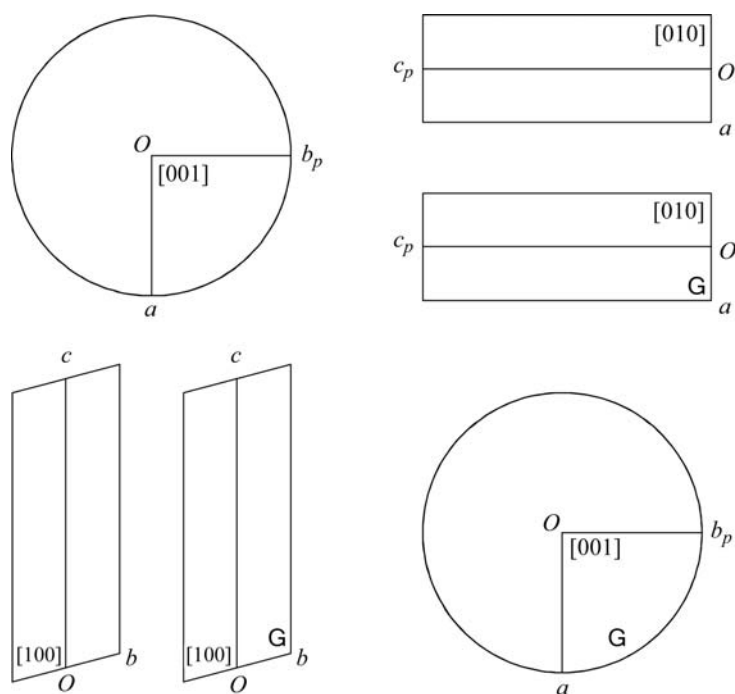


Fig. 1.2.6.10. Diagrams for monoclinic/inclined rod groups.

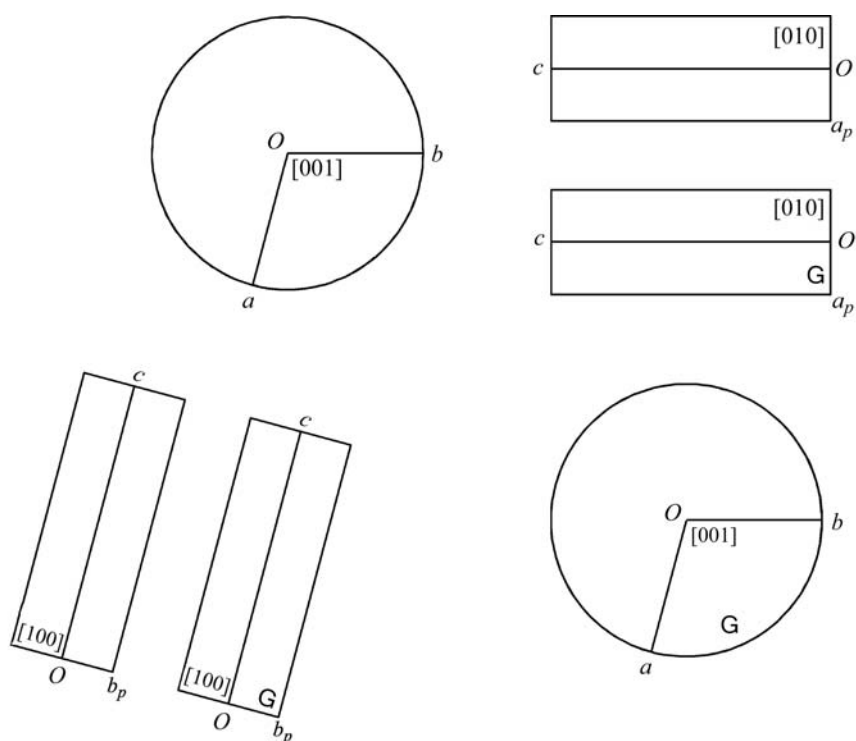


Fig. 1.2.6.11. Diagrams for monoclinic/orthogonal rod groups.

subindex to the lattice symbol to denote the direction of the translations. For example, consider the rod group of the type  $\mu_2 211$  (R3). The Hermann–Mauguin symbol in the conventional coordinate system in the standard  $(abc)$  setting is given by  $\mu_c 211$  as the translations of the rod group in the standard setting are along the direction labelled  $c$ . In the  $(bca)$  setting, the Hermann–Mauguin symbol is  $\mu_b 112$ , where the subindex  $b$  denotes that the translations are, in this setting, along the direction labelled  $b$ . A list of the six Hermann–Mauguin symbols in the six settings for the triclinic, monoclinic/inclined, monoclinic/orthogonal and orthorhombic rod groups is given in Table 1.2.6.2.

*Example:* The rod group  $\mu_c mc 2_1$  (R17)

The Hermann–Mauguin setting symbols for the six settings are:

Setting symbol	Hermann–Mauguin symbol
$(abc)$	$\mu_c mc 2_1$
$(\bar{b}ac)$	$\mu_c cm 2_1$
$(\bar{c}ba)$	$\mu_a 2_1 am$
$(bca)$	$\mu_b b 2_1 m$
$(a\bar{c}b)$	$\mu_b m 2_1 b$
$(\bar{c}\bar{a}b)$	$\mu_a 2_1 ma$

For tetragonal, trigonal and hexagonal rod groups, two diagrams are given: the symmetry diagram and the general-position diagram. These diagrams are illustrated in Figs. 1.2.6.14 and 1.2.6.15. One can consider additional settings for these rod

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

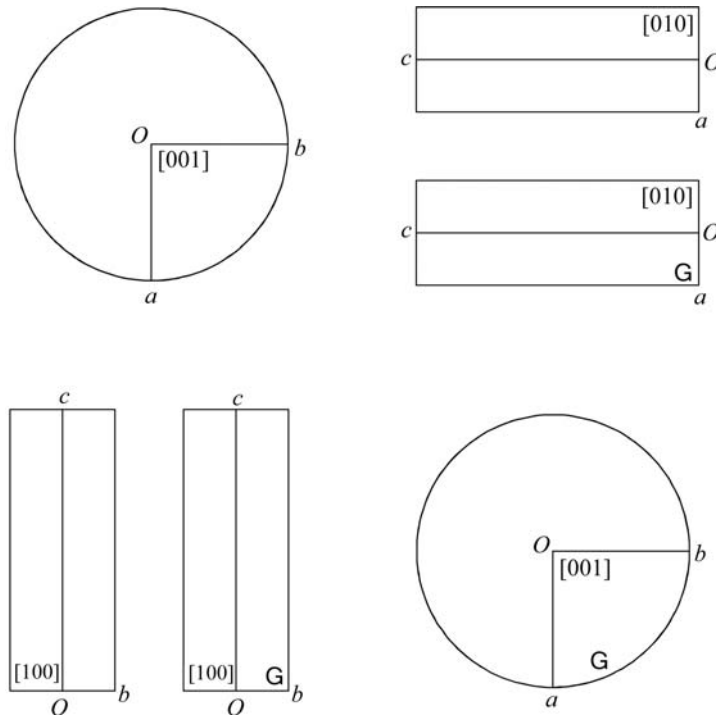


Fig. 1.2.6.12. Diagrams for orthorhombic rod groups.

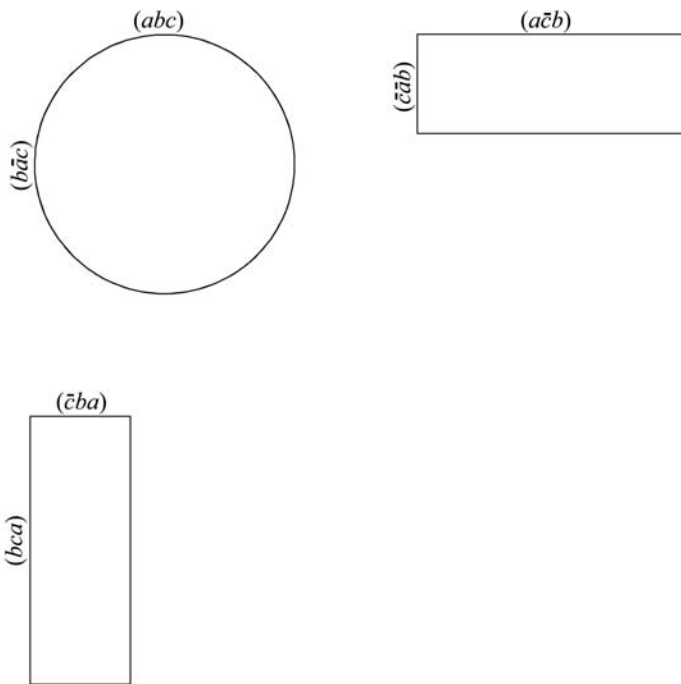


Fig. 1.2.6.13. Setting symbols on symmetry diagrams for the monoclinic/oblique, monoclinic/orthogonal and orthorhombic rod groups.



Fig. 1.2.6.14. Diagrams for tetragonal rod groups.



Fig. 1.2.6.15. Diagrams for trigonal and hexagonal rod groups.

groups: see the setting symbols in Table 1.2.6.3. If the Hermann–Mauguin symbols for the group in these settings are identical, only one tabulation of the group, in the standard setting, is given. If in these settings two distinct Hermann–Mauguin symbols are obtained, a second tabulation for the rod group is given. This second tabulation is in the conventional coordinate system in the  $(a + b \bar{a} + b c)$  setting for tetragonal groups, and in the  $(2a + b \bar{a} + b c)$  setting for trigonal and hexagonal groups. These second tabulations aid in the correlation of Wyckoff positions of space groups and Wyckoff positions of rod groups. For example, the Wyckoff positions of the two space groups types  $P3m1$  and  $P31m$  can be easily correlated with, respectively, the

Wyckoff positions of a rod group of the type R49 in the standard setting where the Hermann–Mauguin symbol is  $\sqrt{3}m1$  and in the second setting where the symbol is  $\sqrt{3}1m$ . In Table 1.2.6.3, we list the tetragonal, trigonal and hexagonal rod groups where in the different settings the two Hermann–Mauguin symbols are distinct.

(iii) Frieze groups

Two diagrams are given for each frieze group: a symmetry diagram and a general-position diagram. These diagrams are illustrated for the oblique and rectangular frieze groups in Figs. 1.2.6.16 and 1.2.6.17, respectively. We consider the two settings  $(ab)$  and  $(b\bar{a})$ , see Fig. 1.2.6.18. In the frieze-group tables, Part 2, we replace the setting symbols with the corresponding Hermann–Mauguin symbols where a subindex is added to the lattice symbol to denote the direction of the translations. A listing of the frieze groups with the Hermann–Mauguin symbols of each group in the two settings is given in Table 1.2.6.4.



## 1.2. GUIDE TO THE USE OF THE SUBPERIODIC GROUP TABLES

Table 1.2.6.2. *Distinct Hermann–Mauguin symbols for monoclinic and orthorhombic rod groups in different settings*

Rod group	Setting symbol					
	$(abc)$	$(b\bar{a}c)$	$(\bar{c}ba)$	$(bca)$	$(a\bar{c}b)$	$(\bar{c}\bar{a}b)$
	Hermann–Mauguin symbol					
R3	$\neq_c 211$	$\neq_c 121$	$\neq_a 112$	$\neq_b 112$	$\neq_b 211$	$\neq_a 121$
R4	$\neq_c m11$	$\neq_c 1m1$	$\neq_a 11m$	$\neq_b 11m$	$\neq_b m11$	$\neq_a 1m1$
R5	$\neq_c c11$	$\neq_c 1c1$	$\neq_a 11a$	$\neq_b 11b$	$\neq_b b11$	$\neq_a 1a1$
R6	$\neq_c 2/m11$	$\neq_c 12/m1$	$\neq_a 112/m$	$\neq_b 112/m$	$\neq_b 2/m11$	$\neq_a 12/m1$
R7	$\neq_c 2/c11$	$\neq_c 12/c1$	$\neq_a 112/a$	$\neq_b 112/b$	$\neq_b 2/b11$	$\neq_a 12/a1$
R8	$\neq_c 112$	$\neq_c 112$	$\neq_a 211$	$\neq_b 121$	$\neq_b 121$	$\neq_a 211$
R9	$\neq_c 112_1$	$\neq_c 112_1$	$\neq_a 2_111$	$\neq_b 12_11$	$\neq_b 12_11$	$\neq_a 2_111$
R10	$\neq_c 11m$	$\neq_c 11m$	$\neq_a m11$	$\neq_b 1m1$	$\neq_b 1m1$	$\neq_a m11$
R11	$\neq_c 112/m$	$\neq_c 112/m$	$\neq_a 2/m11$	$\neq_b 12/m1$	$\neq_b 12/m1$	$\neq_a 2/m11$
R12	$\neq_c 112_1/m$	$\neq_c 112_1/m$	$\neq_a 2_1/m11$	$\neq_b 12_1/m1$	$\neq_b 12_1/m1$	$\neq_a 2_1/m11$
R13	$\neq_c 222$	$\neq_c 222$	$\neq_a 222$	$\neq_b 222$	$\neq_b 222$	$\neq_a 222$
R14	$\neq_c 222_1$	$\neq_c 222_1$	$\neq_a 2_122$	$\neq_b 22_12$	$\neq_b 22_12$	$\neq_a 2_122$
R15	$\neq_c mm2$	$\neq_c mm2$	$\neq_a 2mm$	$\neq_b m2m$	$\neq_b m2m$	$\neq_a 2mm$
R16	$\neq_c cc2$	$\neq_c cc2$	$\neq_a 2aa$	$\neq_b b2b$	$\neq_b b2b$	$\neq_a 2aa$
R17	$\neq_c mc2_1$	$\neq_c cm2_1$	$\neq_a 2_1am$	$\neq_b b2_1m$	$\neq_b m2_1b$	$\neq_a 2_1ma$
R18	$\neq_c 2mm$	$\neq_c m2m$	$\neq_a mm2$	$\neq_b mm2$	$\neq_b 2mm$	$\neq_a m2m$
R19	$\neq_c 2cm$	$\neq_c c2m$	$\neq_a ma2$	$\neq_b bm2$	$\neq_b 2mb$	$\neq_a m2a$
R20	$\neq_c mmm$	$\neq_c mmm$	$\neq_a mmm$	$\neq_b mmm$	$\neq_b mmm$	$\neq_a mmm$
R21	$\neq_c ccm$	$\neq_c ccm$	$\neq_a maa$	$\neq_b bmb$	$\neq_b bmb$	$\neq_a maa$
R22	$\neq_c mcm$	$\neq_c cmm$	$\neq_a mam$	$\neq_b bmm$	$\neq_b mmb$	$\neq_a mma$

Table 1.2.6.3. *Distinct Hermann–Mauguin symbols for tetragonal, trigonal and hexagonal rod groups in different settings*

Rod group	Setting symbol	
	$(abc)$	$(a \pm b \ b \mp a \ c)$
	Hermann–Mauguin symbol	
R35	$\neq_4 2cm$	$\neq_4 2mc$
R37	$\neq_4 \bar{2}m$	$\neq_4 \bar{2}m2$
R38	$\neq_4 \bar{2}c$	$\neq_4 \bar{2}c2$
R41	$\neq_4 2/mmc$	$\neq_4 2/mcm$

Rod group	Setting symbol	
	$(abc)$	$(\pm 2a \pm b \ \mp a \pm b \ c)$ $(\pm a \pm 2b \ \mp 2a \mp b \ c)$ $(\mp a \pm b \ \mp a \mp 2b \ c)$
	Hermann–Mauguin symbol	
R46	$\neq_3 12$	$\neq_3 21$
R47	$\neq_3 112$	$\neq_3 121$
R48	$\neq_3 212$	$\neq_3 212$
R49	$\neq_3 m1$	$\neq_3 1m$
R50	$\neq_3 c1$	$\neq_3 1c$
R51	$\neq_3 \bar{1}m$	$\neq_3 \bar{1}m1$
R52	$\neq_3 \bar{1}c$	$\neq_3 \bar{1}c1$
R70	$\neq_6 3mc$	$\neq_6 3cm$
R71	$\neq_6 \bar{3}m2$	$\neq_6 \bar{3}2m$
R72	$\neq_6 \bar{3}c2$	$\neq_6 \bar{3}2c$
R75	$\neq_6 3/mmc$	$\neq_6 3/mcm$

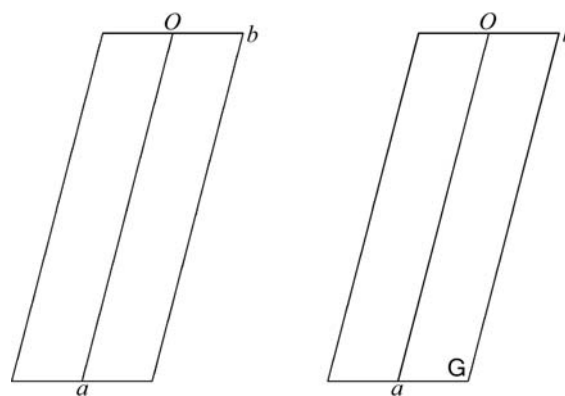


Fig. 1.2.6.16. Diagrams for oblique frieze groups.

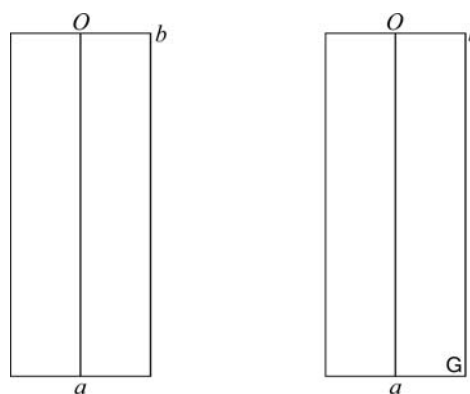


Fig. 1.2.6.17. Diagrams for rectangular frieze groups.

### 1.2.7. Origin

The origin has been chosen according to the following conventions:

(i) If the subperiodic group is centrosymmetric, then the inversion centre is chosen as the origin. For the three layer groups  $p4/n$  (L52),  $p4/nbm$  (L62) and  $p4/nmm$  (L64), we give descriptions for two origins, at the inversion centre and at  $(-\frac{1}{4}, -\frac{1}{4}, 0)$  from the inversion centre. This latter origin is at a position of high site symmetry and is consistent with having the origin on the fourfold axis, as is the case for all other tetragonal layer groups.

The group symbols for the description with the origin at the inversion centre, e.g.  $p4/n(\frac{1}{4}, \frac{1}{4}, 0)$ , are followed by the shift  $(\frac{1}{4}, \frac{1}{4}, 0)$  of the position of the origin used in the description having the origin on the fourfold axis.

(ii) For noncentrosymmetric subperiodic groups, the origin is at a point of highest site symmetry. If no symmetry is higher than 1, the origin is placed on a screw axis, a glide plane or at the intersection of several such symmetry elements.

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

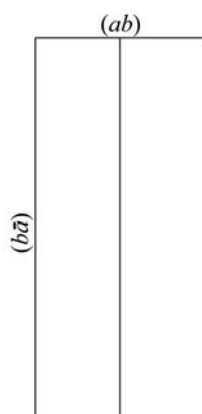


Fig. 1.2.6.18. The two settings for frieze groups. For the second setting, printed vertically, the page must be turned 90° clockwise or viewed from the right-hand side.

*Origin statement:* In the line *Origin* immediately below the diagrams, the site symmetry of the origin is stated if different from the identity. A further symbol indicates all symmetry elements that pass through the origin. For the three layer groups  $p4/n$  (L52),  $p4/nbm$  (L62) and  $p4/nmm$  (L64) where the origin is on the fourfold axis, the statement ‘at  $-\frac{1}{4}, -\frac{1}{4}, 0$  from centre’ is given to denote the position of the origin with respect to an inversion centre.

## 1.2.8. Asymmetric unit

An asymmetric unit of a subperiodic group is a simply connected smallest part of space from which, by application of all symmetry operations of the subperiodic group, the whole space is filled exactly. For three-dimensional (two-dimensional) space groups, because they contain three-dimensional (two-dimensional) translational symmetry, the asymmetric unit is a finite part of space [see Section 2.8 of *IT A* (1983)]. For subperiodic groups, because the translational symmetry is of a lower dimension than that of the space, the asymmetric unit is infinite in size. We define the asymmetric unit for subperiodic groups by setting the limits on the coordinates of points contained in the asymmetric unit.

### 1.2.8.1. Frieze groups

For all frieze groups, a limit is set on the  $x$  coordinate of the asymmetric unit by the inequality

$$0 \leq x \leq \text{upper limit on } x.$$

For the  $y$  coordinate, either there is no limit and nothing further is written, or there is the lower limit of zero, *i.e.*  $0 \leq y$ .

*Example:* The frieze group  $\mu 2mm$  (F6)

**Asymmetric unit**  $0 \leq x \leq 1/2; 0 \leq y$ .

### 1.2.8.2. Rod groups

For all rod groups, a limit is set on the  $z$  coordinate of the asymmetric unit by the inequality

$$0 \leq z \leq \text{upper limit on } z.$$

For each of the  $x$  and  $y$  coordinates, either there is no limit and nothing further is written, or there is the lower limit of zero.

For tetragonal, trigonal and hexagonal rod groups, additional limits are required to define the asymmetric unit. These limits are given by additional inequalities, such as  $x \leq y$  and  $y \leq x/2$ . Fig. 1.2.8.1 schematically shows the boundaries represented by such inequalities.

Table 1.2.6.4. Distinct Hermann–Mauguin symbols for frieze groups in different settings

Frieze group	Setting symbol	
	( $ab$ )	( $b\bar{a}$ )
	Hermann–Mauguin symbol	
F1	$\mu_a 1$	$\mu_b 1$
F2	$\mu_a 211$	$\mu_b 211$
F3	$\mu_a 1m1$	$\mu_b 11m$
F4	$\mu_a 11m$	$\mu_b 1m1$
F5	$\mu_a 11g$	$\mu_b 1g1$
F6	$\mu_a 2mm$	$\mu_b 2mm$
F7	$\mu_a 2mg$	$\mu_b 2gm$

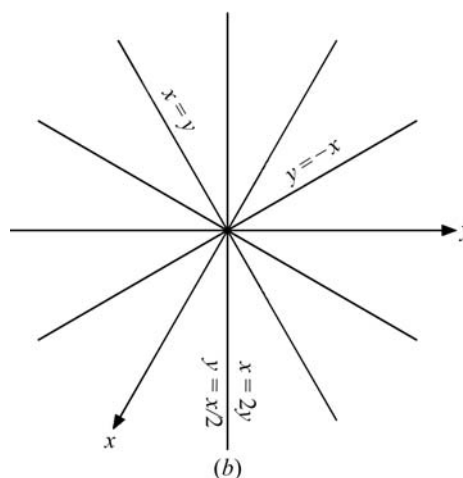
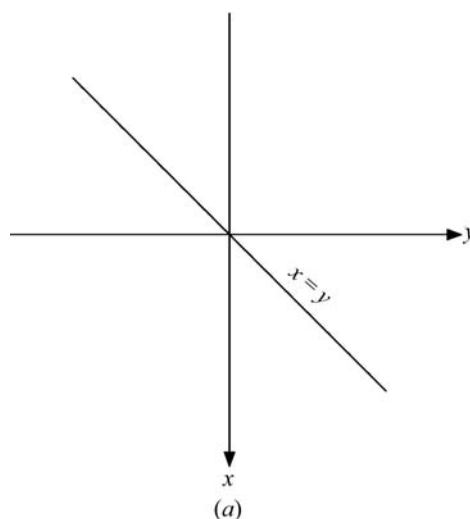


Fig. 1.2.8.1. Boundaries used to define the asymmetric unit for (a) tetragonal rod groups and (b) trigonal and hexagonal rod groups.

*Example:* The rod group  $\mu 6_3mc$  (R70)

**Asymmetric unit**  $0 \leq x; 0 \leq y; 0 \leq z \leq 1; y \leq x/2$ .

### 1.2.8.3. Layer groups

For all layer groups, limits are set on the  $x$  coordinate and  $y$  coordinate of the asymmetric unit by the inequalities

$$0 \leq x \leq \text{upper limit on } x$$

$$0 \leq y \leq \text{upper limit on } y.$$

For the  $z$  coordinate, either there is no limit and nothing further is written, or there is the lower limit of zero.

## 1.2. GUIDE TO THE USE OF THE SUBPERIODIC GROUP TABLES

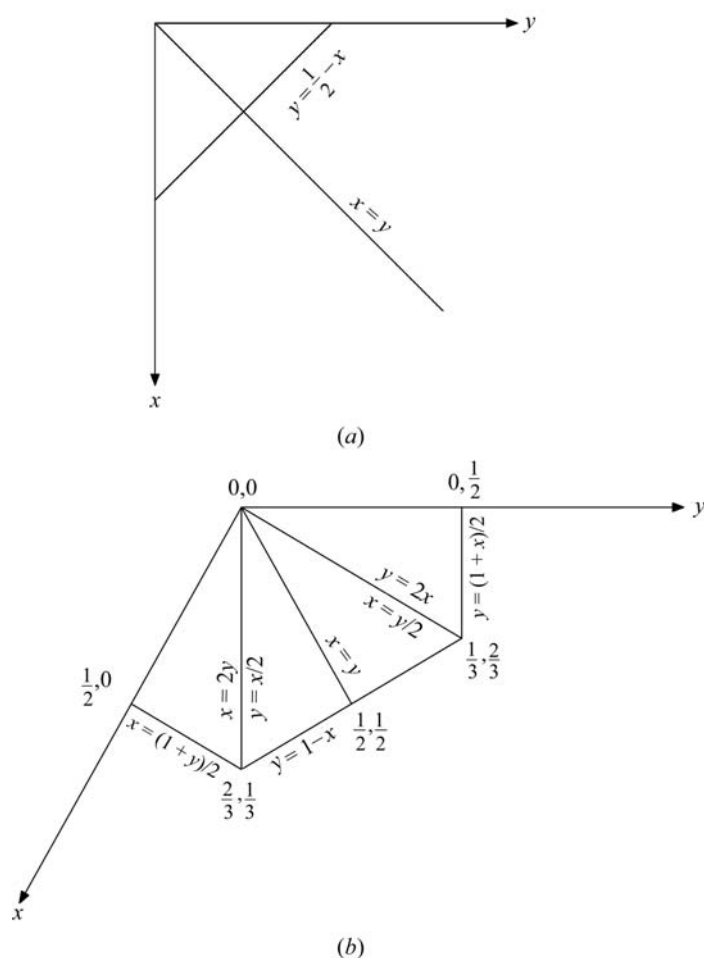


Fig. 1.2.8.2. Boundaries used to define the asymmetric unit for (a) tetragonal/square layer groups and (b) trigonal/hexagonal and hexagonal/hexagonal layer groups. In (b), the coordinates  $(x, y)$  of the vertices of the asymmetric unit with the  $z = 0$  plane are also given.

For tetragonal/square, trigonal/hexagonal and hexagonal/hexagonal layer groups, additional limits are required to define the asymmetric unit. These additional limits are given by additional inequalities. Fig. 1.2.8.2 schematically shows the boundaries represented by these inequalities. For trigonal/hexagonal and hexagonal/hexagonal layer groups, because of the complicated shape of the asymmetric unit, the coordinates  $(x, y)$  of the vertices of the asymmetric unit with the  $z = 0$  plane are given.

*Example:* The layer group  $p3m1$  (L69)

**Asymmetric unit**  $0 \leq x \leq 2/3; 0 \leq y \leq 2/3; x \leq 2y;$   
 $y \leq \min(1-x, 2x)$

**Vertices**  $0, 0; 2/3, 1/3; 1/3, 2/3.$

### 1.2.9. Symmetry operations

The coordinate triplets of the *General position* of a subperiodic group may be interpreted as a shorthand description of the symmetry operations in matrix notation as in the case of space groups [see Sections 2.3, 8.1.5 and 11.1 of *IT A* (1983)]. The geometric description of the symmetry operations is found in the subperiodic group tables under the heading *Symmetry operations*. These data form a link between the subperiodic group diagrams (Section 1.2.6) and the general position (Section 1.2.11).

#### 1.2.9.1. Numbering scheme

The numbering (1) ... (p) ... of the entries in the blocks *Symmetry operations* and *General position* (first block below *Positions*) is the same. Each listed coordinate triplet of the general position is preceded by a number between parentheses (p). The same number (p) precedes the corresponding symmetry operation. For all subperiodic groups with *primitive* lattices, the two lists contain the same number of entries.

For the nine layer groups with *centred* lattices, to the one block of *General positions* correspond two blocks of *Symmetry operations*. The numbering scheme is applied to both blocks. The two blocks correspond to the two centring translations below the subheading *Coordinates*, i.e.  $(0, 0, 0) + (1/2, 1/2, 0) +$ . For the *Positions*, the reader is expected to add these two centring translations to each printed coordinate triplet in order to obtain the complete general position. For the *Symmetry operations*, the corresponding data are listed explicitly with the two blocks having the subheadings 'For  $(0, 0, 0) +$  set' and 'For  $(1/2, 1/2, 0) +$  set', respectively.

#### 1.2.9.2. Designation of symmetry operations

The designation of symmetry operations for the subperiodic groups is the same as for the space groups. An entry in the block *Symmetry operations* is characterized as follows:

(i) A symbol denoting the *type* of the symmetry operation [cf. Section 1.2 of *IT A* (1983)], including its glide or screw part, if present. In most cases, the glide or screw part is given explicitly by fractional coordinates between parentheses. The sense of a rotation is indicated by the superscript + or -. Abbreviated notations are used for the glide reflections  $a(1/2, 0, 0) \equiv a$ ;  $b(0, 1/2, 0) \equiv b$ ;  $c(0, 0, 1/2) \equiv c$ . Glide reflections with complicated and unconventional glide parts are designated by the letter g, followed by the glide part between parentheses.

(ii) A coordinate triplet indicating the *location* and *orientation* of the symmetry element which corresponds to the symmetry operation. For rotoinversions the location of the inversion point is also given.

Details of this symbolism are given in Section 11.2 of *IT A* (1983).

#### *Examples:*

(1)  $m \ x, 0, z$ : a reflection through the plane  $x, 0, z$ , i.e. the plane parallel to (010) containing the point  $(0, 0, 0)$ .

(2)  $m \ x + 1/2, \bar{x}, z$ : a reflection through the plane  $x + 1/2, \bar{x}, z$ , i.e. the plane parallel to (110) containing the point  $(1/2, 0, 0)$ .

(3)  $g(1/2, 1/2, 0) \ x, x, z$ : glide reflection with glide component  $(1/2, 1/2, 0)$  through the plane  $x, x, z$ , i.e. the plane parallel to  $(\bar{1}\bar{1}0)$  containing the point  $(0, 0, 0)$ .

(4)  $2(1/2, 0, 0) \ x, 1/4, 0$ : screw rotation along the (100) direction containing the point  $(0, 1/4, 0)$  with a screw component  $(1/2, 0, 0)$ .

(5)  $4^- \ 1/2, 0, z \ 1/2, 0, 0$ : fourfold rotoinversion consisting of a clockwise rotation by  $90^\circ$  around the line  $1/2, 0, z$  followed by an inversion through the point  $(1/2, 0, 0)$ .

### 1.2.10. Generators

The line *Generators selected* states the symmetry operations and their sequence selected to generate all symmetrically equivalent points of the *General position* from a point with coordinates  $x, y, z$ . The identity operation given by (1) is always selected as the first generator. The generating translations are listed next,  $t(1, 0)$  for frieze groups,  $t(0, 0, 1)$  for rod groups, and  $t(1, 0, 0)$  and  $t(0, 1, 0)$  for layer groups. For centred layer groups, there is the

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additional centring translation  $t(1/2, 1/2, 0)$ . The additional generators are given as numbers ( $p$ ) which refer to the corresponding coordinate triplets of the general position and the corresponding entries under *Symmetry operations*; for centred layer groups, the first block 'For  $(0, 0, 0)^+$  set' must be used.

### 1.2.11. Positions

The entries under *Positions* (more explicitly called *Wyckoff positions*) consist of the *General position* (upper block) and the *Special positions* (blocks below). The columns in each block, from left to right, contain the following information for each Wyckoff position.

(i) *Multiplicity M* of the Wyckoff position. This is the number of equivalent points per conventional cell. The multiplicity  $M$  of the general position is equal to the order of the point group of the subperiodic group, except in the case of centred layer groups when it is twice the order of the point group. The multiplicity  $M$  of a special position is equal to the order of the point group of the subperiodic group divided by the order of the site-symmetry group (see Section 1.2.12).

(ii) *Wyckoff letter*. This letter is a coding scheme for the Wyckoff positions, starting with  $a$  at the bottom position and continuing upwards in alphabetical order.

(iii) *Site symmetry*. This is explained in Section 1.2.12.

(iv) *Coordinates*. The sequence of the coordinate triplets is based on the *Generators*. For the centred layer groups, the centring translations  $(0, 0, 0)^+$  and  $(1/2, 1/2, 0)^+$  are listed above the coordinate triplets. The symbol '+' indicates that in order to obtain a complete Wyckoff position, the components of these centring translations have to be added to the listed coordinate triplets.

(v) *Reflection conditions*. These are described in Section 1.2.13.

The two types of positions, general and special, are characterized as follows:

(i) *General position*. A set of symmetrically equivalent points is said to be in a 'general position' if each of its points is left invariant only by the identity operation but by no other symmetry operation of the subperiodic group.

(ii) *Special position(s)*. A set of symmetrically equivalent points is said to be in a 'special position' if each of its points is mapped onto itself by at least one additional operation in addition to the identity operation.

*Example:* Layer group  $c2/m11$  (L18)

The general position  $8f$  of this layer group contains eight equivalent points per cell each with site symmetry 1. The coordinate triplets of four points (1) to (4) are given explicitly, the coordinate triplets of the other four points are obtained by adding the components  $(1/2, 1/2, 0)$  of the  $c$ -centring translation to the coordinate triplets (1) to (4).

This layer group has five special positions with the Wyckoff letters  $a$  to  $e$ . The product of the multiplicity and the order of the site-symmetry group is the multiplicity of the general position. For position  $4d$ , for example, the four equivalent points have the coordinates  $x, 0, 0$ ,  $\bar{x}, 0, 0$ ,  $x + 1/2, 1/2, 0$  and  $\bar{x} + 1/2, 1/2, 0$ . Since each point of position  $4d$  is mapped onto itself by a twofold rotation, the multiplicity of the position is reduced from eight to four, whereas the order of the site symmetry is increased from one to two.

### 1.2.12. Oriented site-symmetry symbols

The third column of each Wyckoff position gives the *site symmetry* of that position. The site-symmetry group is isomorphic to a proper or improper subgroup of the point group to which the subperiodic group under consideration belongs. *Oriented site-symmetry symbols* are used to show how the symmetry elements

at a site are related to the conventional crystallographic basis. The site-symmetry symbols display the same sequence of symmetry directions as the subperiodic group symbol (*cf.* Table 1.2.4.1). Sets of equivalent symmetry directions that do not contribute any element to the site-symmetry group are represented by a dot. Sets of symmetry directions having more than one equivalent direction may require more than one character if the site-symmetry group belongs to a lower crystal system. For example, for the  $2c$  position of tetragonal layer group  $p4mm$  (L55), the site-symmetry group is the orthorhombic group ' $2mm$ '. The two characters ' $mm$ ' represent the secondary set of tetragonal symmetry directions, whereas the dot represents the tertiary tetragonal symmetry direction.

### 1.2.13. Reflection conditions

The *Reflection conditions* are listed in the right-hand column of each Wyckoff position. There are two types of reflection conditions:

(i) *General conditions*. These conditions apply to *all* Wyckoff positions of the subperiodic group.

(ii) *Special conditions* ('extra' conditions). These conditions apply only to *special* Wyckoff positions and must always be added to the general conditions of the subperiodic group.

The *general reflection conditions* are the result of three effects: centred lattices, glide planes and screw axes. For the nine layer groups with *centred* lattices, the corresponding general reflection condition is  $h + k = 2n$ . The general reflection conditions due to glide planes and screw axes for the subperiodic groups are given in Table 1.2.13.1.

*Example:* The layer group  $p4bm$  (L56)

General position  $8d$ :  $0k$ :  $k = 2n$  and  $h0$ :  $h = 2n$  due respectively to the glide planes  $b$  and  $a$ . The projections along  $[100]$  and  $[010]$  of any crystal structure with this layer-group symmetry have, respectively, periodicity  $\mathbf{b}/2$  and  $\mathbf{a}/2$ .

Special positions  $2a$  and  $2b$ :  $hk$ :  $h + k = 2n$ . Any set of equivalent atoms in either of these positions displays additional  $c$ -centring.

### 1.2.14. Symmetry of special projections

#### 1.2.14.1. Data listed in the subperiodic group tables

Under the heading *Symmetry of special projections*, the following data are listed for three orthogonal projections of each layer group and rod group and two orthogonal projections of each frieze group:

(i) For layer and rod groups, each projection is made onto a plane normal to the projection direction. If there are three kinds of symmetry directions (*cf.* Table 1.2.4.1), the three projection directions correspond to the primary, secondary and tertiary symmetry directions. If there are fewer than three symmetry directions, the additional projection direction(s) are taken along coordinate axes.

For frieze groups, each projection is made on a line normal to the projection direction.

The directions for which data are listed are as follows:

(a) *Layer groups:*

Triclinic/oblique	}	[001][100][010]
Monoclinic/oblique		
Monoclinic/rectangular		
Orthorhombic/rectangular		
Tetragonal/square	}	[001][100][110]
Trigonal/hexagonal		
Hexagonal/hexagonal		

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(b) Rod groups:

Triclinic	}	[001][100][010]
Monoclinic/inclined		
Monoclinic/orthogonal		
Orthorhombic		
Tetragonal	}	[001][100][110]
Trigonal		
Hexagonal		
		[001][100][210]

(c) Frieze groups:

Oblique	}	[10][01]
Rectangular		

(ii) *The Hermann–Mauguin symbol.* For the [001] projection of a layer group, the Hermann–Mauguin symbol for the plane group resulting from the projection of the layer group is given. For the [001] projection of a rod group, the Hermann–Mauguin symbol for the resulting two-dimensional point group is given. For the remainder of the projections, in the case of both layer groups and rod groups, the Hermann–Mauguin symbol is given for the resulting frieze group. For the [10] projection of a frieze group, the Hermann–Mauguin symbol of the resulting one-dimensional point group, *i.e.* 1 or  $m$ , is given. For the [01] projection, the Hermann–Mauguin symbol of the resulting one-dimensional space group, *i.e.*  $p1$  or  $pm$ , is given.

(iii) For layer groups, the basis vectors  $\mathbf{a}'$ ,  $\mathbf{b}'$  of the plane group resulting from the [001] projection and the basis vector  $\mathbf{a}'$  of the frieze groups resulting from the additional two projections are given as linear combinations of the basis vectors  $\mathbf{a}$ ,  $\mathbf{b}$  of the layer group. Basis vectors  $\mathbf{a}$ ,  $\mathbf{b}$  inclined to the plane of projection are replaced by the projected vectors  $\mathbf{a}_p$ ,  $\mathbf{b}_p$ . For the two projections of a rod group resulting in a frieze group, the basis vector  $\mathbf{a}'$  of the resulting frieze group is given in terms of the basis vector  $\mathbf{c}$  of the rod group. For the [01] projection of a frieze group, the basis vector  $\mathbf{a}'$  of the resulting one-dimensional space group is given in terms of the basis vector  $\mathbf{a}$  of the frieze group.

For rod groups and layer groups, the relations between  $\mathbf{a}'$ ,  $\mathbf{b}'$  and  $\gamma'$  of the projected conventional basis vectors and  $a$ ,  $b$ ,  $c$ ,  $\alpha$ ,  $\beta$  and  $\gamma$  of the conventional basis vectors of the subperiodic group are given in Table 1.2.14.1. We also give in this table the relations between  $\mathbf{a}'$  of the projected conventional basis and  $a$ ,  $b$  and  $\gamma$  of the conventional basis of the frieze group.

(iv) *Location of the origin* of the plane group, frieze group and one-dimensional space group is given with respect to the conventional lattice of the subperiodic group. The same description is used as for the location of symmetry elements (see Section 1.2.9). *Example:* ‘Origin at  $x$ , 0, 0’ or ‘Origin at  $x$ , 1/4, 0’.

### 1.2.14.2. Projections of centred subperiodic groups

The only centred subperiodic groups are the nine types of centred layer groups. For the [100] and [010] projection directions, because of the centred layer-group lattice, the basis vectors of the resulting frieze groups are  $\mathbf{a}' = \mathbf{b}/2$  and  $\mathbf{a}' = \mathbf{a}/2$ , respectively.

### 1.2.14.3. Projection of symmetry elements

A symmetry element of a subperiodic group projects as a symmetry element only if its orientation bears a special relationship to the projection direction. In Table 1.2.14.2, the three-dimensional symmetry elements of the layer and rod groups and in Table 1.2.14.3 the two-dimensional symmetry elements of the frieze groups are listed along with the corresponding symmetry element in projection.

Table 1.2.13.1. General reflection conditions due to glide planes and screw axes

(a) Layer groups.

(1) Glide planes.

Reflection condition	Orientation of plane	Glide vector	Symbol
$hk: h = 2n$	(001)	$\mathbf{a}/2$	$a$
$hk: k = 2n$	(001)	$\mathbf{b}/2$	$b$
$hk: h + k = 2n$	(001)	$\mathbf{a}/2 + \mathbf{b}/2$	$n$
$0k: k = 2n$	(100)	$\mathbf{b}/2$	$b$
$h0: h = 2n$	(010)	$\mathbf{a}/2$	$a$

(2) Screw axes.

Reflection condition	Direction of axis	Screw vector	Symbol
$h0: h = 2n$	[100]	$\mathbf{a}/2$	$2_1$
$0k: k = 2n$	[010]	$\mathbf{b}/2$	$2_1$

(b) Rod groups.

(1) Glide planes.

Reflection condition	Orientation of plane	Glide vector	Symbol
$l: l = 2n$	Any orientation parallel to the $c$ axis	$\mathbf{c}/2$	$c$

(2) Screw axes.

Reflection condition	Direction of axis	Screw vector	Symbol
$l: l = 2n$	[001]	$\mathbf{c}/2$	$2_1, 4_2, 6_3$
$l: l = 3n$	[001]	$\mathbf{c}/3$	$3_1, 3_2, 6_2, 6_4$
$l: l = 4n$	[001]	$\mathbf{c}/4$	$4_1, 4_3$
$l: l = 6n$	[001]	$\mathbf{c}/6$	$6_1, 6_5$

(c) Frieze groups, glide plane.

Reflection condition	Orientation of plane	Glide vector	Symbol
$h: h = 2n$	(10)	$\mathbf{a}/2$	$g$

*Example:* Layer group  $cm2m$  (L35)

Projection along [001]: This orthorhombic/rectangular plane group is centred;  $m$  perpendicular to [100] is projected as a reflection line, 2 parallel to [010] is projected as the same reflection line and  $m$  perpendicular to [001] gives rise to no symmetry element in projection, but to an overlap of atoms. *Result:* Plane group  $c1m1$  (5) with  $\mathbf{a}' = \mathbf{a}$  and  $\mathbf{b}' = \mathbf{b}$ .

Projection along [100]: The frieze group has the basis vector  $\mathbf{a}' = \mathbf{b}/2$  due to the centred lattice of the layer group.  $m$  perpendicular to [100] gives rise only to an overlap of atoms, 2 parallel to [010] is projected as a reflection line and  $m$  perpendicular to [001] is projected as the same reflection line. *Result:* Frieze group  $\neq 11m$  (F4) with  $\mathbf{a}' = \mathbf{b}/2$ .

Projection along [010]: The frieze group has the basis vector  $\mathbf{a}' = \mathbf{a}/2$  due to the centred lattice of the layer group. The two reflection planes project as perpendicular reflection lines and 2 parallel to [010] projects as the rotation point 2. *Result:* Frieze group  $\neq 2mm$  (F6) with  $\mathbf{a}' = \mathbf{a}/2$ .

## 1.2.15. Maximal subgroups and minimal supergroups

In *IT A* (1983), for the representative space group of each space-group type the following information is given:

(i) maximal non-isomorphic subgroups,

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Table 1.2.14.1.  $a', b', \gamma'$  ( $a'$ ) of the projected conventional coordinate system in terms of  $a, b, c, \alpha, \beta, \gamma$  ( $a, b, \gamma$ ) of the conventional coordinate system of the layer and rod groups (frieze groups)

(a) Layer groups.

Projection direction	Triclinic/oblique	Monoclinic/oblique
[001]	$a' = a \sin \beta$ $b' = b \sin \alpha$ $\gamma' = 180^\circ - \gamma^{*\dagger}$	$a' = a$ $b' = b$ $\gamma' = \gamma$
[100]	$a' = b \sin \gamma$ $b' = c \sin \beta$ $\gamma' = 180^\circ - \alpha^{*\dagger}$	$a' = b \sin \gamma$ $b' = c$ $\gamma' = 90^\circ$
[010]	$a' = a \sin \gamma$ $b' = c \sin \alpha$ $\gamma' = 180^\circ - \beta^{*\dagger}$	$a' = a \sin \gamma$ $b' = c$ $\gamma' = 90^\circ$
	Monoclinic/ rectangular	Orthorhombic/ rectangular
[001]	$a' = a$ $b' = b \sin \alpha$ $\gamma' = 90^\circ$	$a' = a$ $b' = b$ $\gamma' = 90^\circ$
[100]	$a' = b$ $b' = c$ $\gamma' = \alpha$	$a' = b$ $b' = c$ $\gamma' = 90^\circ$
[010]	$a' = a$ $b' = c \sin \alpha$ $\gamma' = 90^\circ$	$a' = a$ $b' = c$ $\gamma' = 90^\circ$
	Tetragonal/square	
[001]	$a' = a$ $b' = a$ $\gamma' = 90^\circ$	
[100]	$a' = a$ $b' = c$ $\gamma' = 90^\circ$	
[110]	$a' = (a/2)(2)^{1/2}$ $b' = c$ $\gamma' = 90^\circ$	
	Trigonal/hexagonal, hexagonal/hexagonal	
[001]	$a' = a$ $b' = a$ $\gamma' = 120^\circ$	
[100]	$a' = [(3)^{1/2}/2]a$ $b' = c$ $\gamma' = 90^\circ$	
[210]	$a' = a/2$ $b' = c$ $\gamma' = 90^\circ$	

$\dagger \cos \alpha^* = (\cos \beta \cos \gamma - \cos \alpha)/(\sin \beta \sin \gamma)$ ,  
 $\cos \beta^* = (\cos \gamma \cos \alpha - \cos \beta)/(\sin \gamma \sin \alpha)$ ,  
 $\cos \gamma^* = (\cos \alpha \cos \beta - \cos \gamma)/(\sin \alpha \sin \beta)$ .

(b) Rod groups.

Projection direction	Triclinic	Monoclinic/inclined
[001]	$a' = a \sin \beta$ $b' = b \sin \alpha$ $\gamma' = 180^\circ - \gamma^{*\dagger}$	$a' = a$ $b' = b \sin \alpha$ $\gamma' = 90^\circ$
[100]	$a' = c \sin \beta$ $b' = b \sin \gamma$ $\gamma' = 180^\circ - \alpha^{*\dagger}$	$a' = c$ $b' = b$ $\gamma' = \alpha$
[010]	$a' = c \sin \alpha$ $b' = a \sin \gamma$ $\gamma' = 180^\circ - \beta^{*\dagger}$	$a' = c \sin \alpha$ $b' = a$ $\gamma' = 90^\circ$
	Monoclinic/ orthogonal	Orthorhombic
[001]	$a' = a$ $b' = b$ $\gamma' = \gamma$	$a' = a$ $b' = b$ $\gamma' = 90^\circ$
[100]	$a' = c$ $b' = b \sin \gamma$ $\gamma' = 90^\circ$	$a' = c$ $b' = b$ $\gamma' = 90^\circ$
[010]	$a' = c$ $b' = a \sin \gamma$ $\gamma' = 90^\circ$	$a' = c$ $b' = a$ $\gamma' = 90^\circ$
	Tetragonal	
[001]	$a' = a$ $b' = a$ $\gamma' = 90^\circ$	
[100]	$a' = c$ $b' = a$ $\gamma' = 90^\circ$	
[110]	$a' = c$ $b' = (a/2)(2)^{1/2}$ $\gamma' = 90^\circ$	
	Trigonal, hexagonal	
[001]	$a' = a$ $b' = a$ $\gamma' = 120^\circ$	
[100]	$a' = c$ $b' = [(3)^{1/2}/2]a$ $\gamma' = 90^\circ$	
[210]	$a' = c$ $b' = a/2$ $\gamma' = 90^\circ$	

(c) Frieze groups.

Projection direction	Oblique	Rectangular
[10]	$a' = b \sin \gamma$	$a' = b$
[01]	$a' = a \sin \gamma$	$a' = a$

- (ii) maximal isomorphic subgroups of lowest index,
- (iii) minimal non-isomorphic supergroups and
- (iv) minimal isomorphic supergroups of lowest index.

However, Bieberbach's theorem for space groups, *i.e.* the classification into isomorphism classes is identical with the classification into affine equivalence classes, is not valid for subperiodic groups. Consequently, to obtain analogous tables for the subperiodic groups, we provide the following information for each representative subperiodic group:

- (i) maximal non-isotypic non-enantiomorphic subgroups,
- (ii) maximal isotypic subgroups and enantiomorphic subgroups of lowest index,

- (iii) minimal non-isotypic non-enantiomorphic supergroups and

(iv) minimal isotypic supergroups and enantiomorphic supergroups of lowest index, where *isotypic* means 'belonging to the same subperiodic group type'. The cases of maximal enantiomorphic subgroups of lowest index and minimal enantiomorphic supergroups of lowest index arise only in the case of rod groups.

## 1.2.15.1. Maximal non-isotypic non-enantiomorphic subgroups

The maximal non-isotypic non-enantiomorphic subgroups  $\mathbf{S}$  of a subperiodic group  $\mathbf{G}$  are divided into two types:

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Table 1.2.14.2. *Projection of three-dimensional symmetry elements (layer and rod groups)*

Symmetry element in three dimensions		Symmetry element in projection	
<i>Arbitrary orientation</i>			
Symmetry centre $\bar{1}$		Rotation point 2 at projection of centre	
<i>Parallel to projection direction</i>			
Rotation axis	2, 3, 4, 6	Rotation point	2, 3, 4, 6
Screw axis	$2_1$	Rotation point	2
	$3_1, 3_2$		3
	$4_1, 4_2, 4_3$		4
	$6_1, 6_2, 6_3, 6_4, 6_5$		6
Rotoinversion axis	$\bar{4}$	Rotation point	4
	$\bar{6} \equiv 3/m$		3 (with overlap of atoms)
	$\bar{3} \equiv 3 \times \bar{1}$		6
Reflection plane $m$		Reflection line $m$	
Glide plane with $\perp$ component <sup>†</sup>		Glide line $g$	
Glide plane without $\perp$ component <sup>†</sup>		Reflection line $m$	
<i>Normal to projection direction</i>			
Rotation axis	2, 4, 6	Reflection line $m$	
	3	None	
Screw axis	$4_2, 6_2, 6_4$	Reflection line $m$	
	$2_1, 4_1, 4_3, 6_1, 6_3, 6_5$	Glide line $g$	
	$3_1, 3_2$	None	
Rotoinversion axis	$\bar{4}$	Reflection line $m$ parallel to axis	
	$\bar{6} \equiv 3/m$	Reflection line $m$ perpendicular to axis	
	$\bar{3} \equiv 3 \times \bar{1}$	Rotation point 2 (at projection of centre)	
Reflection plane $m$		None, but overlap of atoms	
Glide plane with glide component $t$		Translation $t$	

<sup>†</sup> The term 'with  $\perp$  component' refers to the component of the glide vector normal to the projection direction.

Table 1.2.14.3. *Projection of two-dimensional symmetry elements (frieze groups)*

Symmetry element in two dimensions		Symmetry element in projection	
Rotation point 2		Reflection point $m$	
<i>Parallel to projection direction</i>			
Reflection line $m$		Reflection point $m$	
Glide line $g$		Reflection point $m$	
<i>Normal to projection direction</i>			
Reflection line $m$		None (with overlap of atoms)	
Glide line $g$ with glide component $t$		Translation $t$	

**I** *translationengleiche* or  $t$  subgroups and

**II** *klassengleiche* or  $k$  subgroups.

Type **II** is subdivided again into two blocks:

**IIa**: the conventional cells of **G** and **S** are the same, and

**IIb**: the conventional cell of **S** is larger than that of **G**.

Block **IIa** has no entries for subperiodic groups with a primitive cell. Only in the case of the nine centred layer groups are there entries, when it contains those maximal subgroups **S** which have lost all the centring translations of **G** but none of the integral translations.

### 1.2.15.1.1. Blocks **I** and **IIa**

In blocks **I** and **IIa**, every maximal subgroup **S** of a subperiodic group **G** is listed with the following information:

[ $i$ ] HMS1 (HMS2) Sequence of numbers

The symbols have the following meaning:

[ $i$ ]: index of **S** in **G**.

HMS1: short Hermann–Mauguin symbol of **S**, referred to the coordinate system and setting of **G**; this symbol may be unconventional.

(HMS2): conventional short Hermann–Mauguin symbol of **S**, given only if HMS1 is not in conventional short form.

Sequence of numbers: coordinate triplets of **G** retained in **S**. The numbers refer to the numbering scheme of the coordinate triplets of the general position. For the centred layer groups the following abbreviations are used:

**Block I** (all translations retained). *Number* +: coordinate triplet given by *Number*, plus that obtained by adding the centring translation  $(1/2, 1/2, 0)$  of **G**. (*Numbers*) +: the same as above, but applied to all *Numbers* between parentheses.

**Block IIa** (not all translations retained). *Number* +  $(1/2, 1/2, 0)$ : coordinate triplet obtained by adding the translation  $(1/2, 1/2, 0)$  to the triplet given by *Number*. (*Numbers*) +  $(1/2, 1/2, 0)$ : the same as above, but applied to all *Numbers* between parentheses.

*Examples*

(1) **G**: Layer group  $c211$  (L10)

**I** [2]  $c1$  ( $p1$ )  $1+$   
**IIa** [2]  $p2_111$   $1; 2 + (1/2, 1/2, 0)$   
[2]  $p211$   $1; 2$

where the numbers have the following meaning:

$1+$   $x, y, z$   $x + 1/2, y + 1/2, z$   
 $1; 2$   $x, y, z$   $x, \bar{y}, \bar{z}$   
 $1; 2+$   $x, y, z$   $x + 1/2, \bar{y} + 1/2, \bar{z}$

(2) **G**: Rod group  $\#422$  (R30)

**I** [2]  $\#411$  ( $\#4$ )  $1; 2; 3; 4$   
[2]  $\#221$  ( $\#222$ )  $1; 2; 5; 6$   
[2]  $\#212$  ( $\#222$ )  $1; 2; 7; 8$

The HMS1 symbol in each of the three subgroups **S** is given in the tetragonal coordinate system of the group **G**. In the first case,

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Table 1.2.17.1. *Frieze-group symbols*

	1	2	3	4	5	6	7	8	9	10	11
Oblique	1	$\neq 1$	$r1$	$r1$	$r111$	$(a)$	$t$	1	$p[1](1)1$	$r1$	$\neq 1$
	2	$\neq 211$	$r\bar{1}'$	$r112$	$r112$	$(a) : 2$	$t : 2$	5	$p[2](1)1$	$r2$	$\neq 112$
Rectangular	3	$\neq 1m1$	$r\bar{1}$	$r1m$	$rm11$	$(a) : m$	$t : m$	3	$p[1](1)m$	$r1m$	$\neq m11$
	4	$\neq 11m$	$r11'$	$rm$	$r1m1$	$(a) \cdot m$	$t \cdot m$	2	$p[1](m)1$	$r11m$	$\neq 1m1$
	5	$\neq 11g$	$r_21$	$rg$	$r1c1$	$(a) \cdot \bar{a}$	$t \cdot a$	4	$p[1](c)1$	$r11g$	$\neq 1a1$
	6	$\neq 2mm$	$r\bar{1}1'$	$rm2$	$rm2$	$(a) : 2 \cdot m$	$t : 2 \cdot m$	6	$p[2](m)m$	$r2mm$	$\neq mm2$
	7	$\neq 2mg$	$r_2\bar{1}$	$rgm2$	$rmc2$	$(a) : 2 \cdot \bar{a}$	$t : 2 \cdot a$	7	$p[2](c)m$	$r2mg$	$\neq ma2$

$\neq 411$  is not the conventional short Hermann–Mauguin symbol and a second conventional symbol  $\neq 4$  is given. In the latter two cases, since the subgroups are orthorhombic rod groups, a second conventional symbol of the subgroup in an orthorhombic coordinate system is given.

## 1.2.15.1.2. Block **IIb**

Whereas in blocks **I** and **IIa** every maximal subgroup **S** of **G** is listed, *this is no longer the case* for the entries of block **IIb**. The information given in this block is

[i] HMS1 (Vectors) (HMS2)

The symbols have the following meaning:

[i]: index of **S** in **G**.

HMS1: Hermann–Mauguin symbol of **S**, referred to the coordinate system and setting of **G**; this symbol may be unconventional.

(Vectors): basis vectors of **S** in terms of the basis vectors of **G**. No relations are given for basis vectors which are unchanged.

(HMS2): conventional short Hermann–Mauguin symbol, given only if HMS1 is not in conventional short form.

### Examples

(1) **G**: Rod group  $\neq 222$  (R13)

**IIb** [2]  $\neq 222_1$  ( $\mathbf{c}' = 2\mathbf{c}$ )

There are two subgroups which obey the same basis-vector relation. Apart from the translations of the enlarged cell, the generators of the subgroups, referred to the basis vectors of the enlarged cell, are

$$\begin{array}{lll} x, y, z & x, \bar{y}, \bar{z} + 1/2 & \bar{x}, y, \bar{z} \\ x, y, z & x, \bar{y}, \bar{z} & \bar{x}, y, \bar{z} + 1/2. \end{array}$$

(2) **G**: Layer group  $pm2_1b$  (L28)

**IIb** [2]  $pm2_1n$  ( $\mathbf{a}' = 2\mathbf{a}$ )

This entry represents two subgroups whose generators, apart from the translations of the enlarged cell, are

$$\begin{array}{lll} x, y, z & \bar{x} + 1/2, y, z & \bar{x}, y + 1/2, \bar{z} \\ x, y, z & \bar{x}, y, z & \bar{x} + 1/2, y + 1/2, \bar{z}. \end{array}$$

The difference between the two subgroups represented by the one entry is due to the different sets of symmetry operations of **G** which are retained in **S**. This can also be expressed as different conventional origins of **S** with respect to **G**: the two subgroups in the first example above are related by a translation  $\mathbf{c}/4$  of the origin, and the two subgroups in the second example by  $\mathbf{a}/4$ .

## 1.2.15.2. Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

Another set of *klassengleiche* subgroups is that listed under **IIc**, i.e. the subgroups **S** which are of the same or of the enantio-

morphic subperiodic group type as **G**. Again, one entry may correspond to more than one isotypic subgroup:

(a) As in block **IIb**, one entry may correspond to two isotypic subgroups whose difference can be expressed as different conventional origins of **S** with respect to **G**.

(b) One entry may correspond to two isotypic subgroups of equal index but with cell enlargements in different directions which are conjugate subgroups in the affine normalizer of **G**. The different vector relationships are given, separated by ‘or’ and placed within one pair of parentheses; cf. example (2).

### Examples

(1) **G**: Rod group  $\neq 222$  (R13)

**IIc** [2]  $\neq 222$  ( $\mathbf{c}' = 2\mathbf{c}$ )

This entry corresponds to two isotypic subgroups. Apart from the translations of the enlarged cell, the generators of the subgroups are

$$\begin{array}{lll} x, y, z & x, \bar{y}, \bar{z} & \bar{x}, y, \bar{z} \\ x, y, z & x, \bar{y}, \bar{z} + 1/2 & \bar{x}, y, \bar{z} + 1/2 \end{array}$$

(2) **G**: Layer group  $pmm2$  (L23)

**IIc** [2]  $pmm2$  ( $\mathbf{a}' = 2\mathbf{a}$  or  $\mathbf{b}' = 2\mathbf{b}$ )

This entry corresponds to four isotypic subgroups, two with the enlarged cell with  $\mathbf{a}' = 2\mathbf{a}$  and two with the enlarged cell with  $\mathbf{b}' = 2\mathbf{b}$ . The generators of these subgroups are

$$\begin{array}{llll} \mathbf{a}' = 2\mathbf{a} & \mathbf{b}' = \mathbf{b} & x, y, z & \bar{x}, y, z & x, \bar{y}, z \\ \mathbf{a}' = 2\mathbf{a} & \mathbf{b}' = \mathbf{b} & x, y, z & \bar{x} + 1/2, y, z & x, \bar{y}, z \\ \mathbf{a}' = \mathbf{a} & \mathbf{b}' = 2\mathbf{b} & x, y, z & \bar{x}, y, z & x, \bar{y}, z \\ \mathbf{a}' = \mathbf{a} & \mathbf{b}' = 2\mathbf{b} & x, y, z & \bar{x}, y + 1/2, z & x, \bar{y}, z \end{array}$$

(3) **G**: Rod group  $\neq 4_1$  (R24)

**IIc** [3]  $\neq 4_3$  ( $\mathbf{c}' = 3\mathbf{c}$ )

[5]  $\neq 4_1$  ( $\mathbf{c}' = 5\mathbf{c}$ )

Listed here are both the maximal isotypic subgroup  $\neq 4_1$  and the maximal enantiomorphic subgroup  $\neq 4_3$ , each of lowest index.

## 1.2.15.3. Minimal non-isotypic non-enantiomorphic supergroups

If **G** is a maximal subgroup of a group **H**, then **H** is called a minimal supergroup of **G**. Minimal supergroups are again subdivided into two types, the *translationengleiche* or *t* supergroups **I** and the *klassengleiche* or *k* supergroups **II**. For the *t* supergroups **I** of **G**, the listing contains the index [i] of **G** in **H** and the *conventional* Hermann–Mauguin symbol of **H**. For the *k* supergroups **II**, the subdivision between **IIa** and **IIb** is not made. The information given is similar to that for the subgroups **IIb**, i.e. the relations between the basis vectors of group and supergroup are given, in addition to the Hermann–Mauguin symbols of **H**. Note that either the conventional cell of the *k* supergroup **H** is smaller than that of the subperiodic group **G**, or **H** contains additional centring translations.



1.2. GUIDE TO THE USE OF THE SUBPERIODIC GROUP TABLES

Table 1.2.17.2. Rod-group symbols

	1	2	3	4	5	6	7	8	9
Triclinic	1	$\bar{1}$	1	$P(11)1$	1	$(a) \cdot 1$	$p1$	$r1$	$1P1$
	2	$\bar{1}$	2	$P(\bar{1}\bar{1})\bar{1}$	7	$(a) \cdot \bar{1}$	$p\bar{1}$	$r\bar{1}$	$1P\bar{1}$
Monoclinic/inclined	3	$\bar{2}11$	6	$P(12)1$	2	$(a) : 2$	$p112$	$r112$	$1P2$
	4	$\bar{m}11$	3	$P(1m)1$	22	$(a) \cdot m$	$p11m$	$r1m1$	$mP1$
	5	$\bar{c}11$	5	$P(1c)1$	24	$(a) \cdot \bar{a}$	$p11a$	$r1c1$	$gP1$
	6	$\bar{2}/m11$	9	$P(12/m)1$	25	$(a) : 2 : m$	$p112/m$	$r12/m1$	$mP2$
	7	$\bar{2}/c11$	12	$P(12/c)1$	28	$(a) : 2 : \bar{a}$	$p112/a$	$r12/c1$	$gP2$
Monoclinic/orthogonal	8	$\bar{1}112$	7	$P(11)2$	3	$(a) \cdot 2$	$p211$	$r211$	$2P1$
	9	$\bar{1}112_1$	8	$P(11)2_1$	8	$(a) \cdot 2_1$	$p2_1$	$r2_1$	$2_1P1$
	10	$\bar{1}11m$	4	$P(11)m$	23	$(a) : m$	$pm11$	$rm11$	$1Pm$
	11	$\bar{1}112/m$	10	$P(11)2/m$	26	$(a) \cdot 2 : m$	$p2/m11$	$r2/m11$	$2Pm$
	12	$\bar{1}112_1/m$	11	$P(11)2_1/m$	27	$(a) \cdot 2_1 : m$	$p2_1/m11$	$r2_1/m11$	$2_1Pm$
Orthorhombic	13	$\bar{2}22$	18	$P(22)2$	61	$(a) \cdot 2 : 2$	$p222$	$r222$	$2P22$
	14	$\bar{2}22_1$	19	$P(22)2_1$	62	$(a) \cdot 2_1 : 2$	$p2_122$	$r2_122$	$2_1P22$
	15	$\bar{m}m2$	13	$P(mm)2$	34	$(a) \cdot 2 \cdot m$	$p2mm$	$r2mm$	$2mmP1$
	16	$\bar{c}c2$	16	$P(cc)2$	35	$(a) \cdot 2 \cdot \bar{a}$	$p2aa$	$r2cc$	$2ggP1$
	17	$\bar{m}c2_1$	15	$P(mc)2_1$	36	$(a) \cdot 2_1 \cdot m$	$p2_1ma$	$r2_1mc$	$2_1mgP1$
	18	$\bar{2}m2$	14	$P(2m)m$	33	$(a) : 2 \cdot m$	$pmma$	$rm2$	$mPm2$
	19	$\bar{2}c2$	17	$P(2c)m$	37	$(a) : 2 \cdot \bar{a}$	$pma2$	$rmc2$	$gPm2$
	20	$\bar{m}m2$	20	$P(2/m2/m)2/m$	46	$(a) \cdot m \cdot 2 : m$	$pmmm$	$r2/m2/m2/m$	$mmPm$
	21	$\bar{c}ccm$	21	$P(2/c2/c)2/m$	47	$(a) \cdot \bar{a} \cdot 2 : m$	$pmaa$	$r2/m2/c2/c$	$ggPm$
	22	$\bar{m}c2$	22	$P(2/m2/c)2_1/m$	48	$(a) \cdot m \cdot 2_1 : m$	$pmma$	$r2_1/m2/m2/c$	$mgPm$
Tetragonal	23	$\bar{4}$	26	$P4(11)$	5	$(a) \cdot 4$	$p4$	$r4$	$4P1$
	24	$\bar{4}_1$	27	$P4_1(11)$	11	$(a) \cdot 4_1$	$p4_1$	$r4_1$	$4_1P1$
	25	$\bar{4}_2$	28	$P4_2(11)$	12	$(a) \cdot 4_2$	$p4_2$	$r4_2$	$4_2P1$
	26	$\bar{4}_3$	29	$P4_3(11)$	13	$(a) \cdot 4_3$	$p4_3$	$r4_3$	$4_3P1$
	27	$\bar{4}$	23	$P\bar{4}(11)$	20	$(a) \cdot \bar{4}$	$p\bar{4}$	$r\bar{4}$	$1P\bar{4}$
	28	$\bar{4}/m$	30	$P4/m(11)$	29	$(a) \cdot 4 : m$	$p4/m$	$r4/m$	$4Pm$
	29	$\bar{4}_2/m$	31	$P4_2/m(11)$	30	$(a) \cdot 4_2 : m$	$p4_2/m$	$r4_2/m$	$4_2Pm$
	30	$\bar{4}22$	35	$P4(22)$	66	$(a) \cdot 4 : 2$	$p422$	$r422$	$4P22$
	31	$\bar{4}_122$	36	$P4_1(22)$	67	$(a) \cdot 4_1 : 2$	$p4_122$	$r4_122$	$4_1P22$
	32	$\bar{4}_222$	37	$P4_2(22)$	68	$(a) \cdot 4_2 : 2$	$p4_222$	$r4_222$	$4_2P22$
	33	$\bar{4}_322$	38	$P4_3(22)$	69	$(a) \cdot 4_3 : 2$	$p4_322$	$r4_322$	$4_3P22$
	34	$\bar{4}mm$	32	$P4(mm)$	40	$(a) \cdot 4 \cdot m$	$p4mm$	$r4mm$	$4mmP1$
	35	$\bar{4}_2cm$	33	$P4_2(cm)$	42	$(a) \cdot 4_2 \cdot m$	$p4_2ma$	$r4_2mc$	$4_2mgP1$
	36	$\bar{4}cc$	34	$P4(cc)$	41	$(a) \cdot 4 \cdot \bar{a}$	$p4aa$	$r4cc$	$4ggP1$
	37	$\bar{4}2m$	24	$P\bar{4}(2m)$	49	$(a) \cdot \bar{4} \cdot m$	$p\bar{4}2m$	$r\bar{4}m2$	$mP\bar{4}2$
	38	$\bar{4}2c$	25	$P\bar{4}(2c)$	50	$(a) \cdot \bar{4} \cdot \bar{a}$	$p\bar{4}2a$	$r\bar{4}c2$	$gP\bar{4}2$
	39	$\bar{4}/mmm$	39	$P4/m(2/m2/m)$	53	$(a) \cdot m \cdot 4 : m$	$p4/mmm$	$r4/m2/m2/m$	$4mmPm$
	40	$\bar{4}/mnc$	40	$P4/m(2/c2/c)$	54	$(a) \cdot \bar{a} \cdot 4 : m$	$p4/maa$	$r4/m2/c2/c$	$4ggPm$
41	$\bar{4}_2/mmc$	41	$P4_2/m(2/m2/c)$	55	$(a) \cdot m \cdot 4_2 : m$	$p4_2/mma$	$r4_2/m2/m2/c$	$4_2mgPm$	
Trigonal	42	$\bar{3}$	42	$P3(11)$	4	$(a) \cdot 3$	$p3$	$r3$	$3P1$
	43	$\bar{3}_1$	43	$P3_1(11)$	9	$(a) \cdot 3_1$	$p3_1$	$r3_1$	$3_1P1$
	44	$\bar{3}_2$	44	$P3_2(11)$	10	$(a) \cdot 3_2$	$p3_2$	$r3_2$	$3_2P1$
	45	$\bar{3}$	45	$P\bar{3}(11)$	19	$(a) \cdot \bar{3}$	$p\bar{3}$	$r\bar{3}$	$3P\bar{1}$
	46	$\bar{3}12$	48	$P3(21)$	63	$(a) \cdot 3 : 2$	$p32$	$r32$	$3P2$
	47	$\bar{3}_112$	49	$P3_1(21)$	64	$(a) \cdot 3_1 : 2$	$p3_12$	$r3_12$	$3_1P2$
	48	$\bar{3}_212$	50	$P3_2(21)$	65	$(a) \cdot 3_2 : 2$	$p3_22$	$r3_22$	$3_2P2$
	49	$\bar{3}m1$	46	$P3(m1)$	38	$(a) \cdot 3 \cdot m$	$p3m$	$r3m$	$3mP1$
	50	$\bar{3}c1$	47	$P3(c1)$	39	$(a) \cdot 3 \cdot \bar{a}$	$p3a$	$r3c$	$3gP1$
	51	$\bar{3}1m$	51	$P\bar{3}(m1)$	59	$(a) \cdot \bar{3} \cdot m$	$p\bar{3}m$	$r\bar{3}2/m$	$3mP\bar{1}2$
Hexagonal	52	$\bar{3}1c$	52	$P\bar{3}(c1)$	60	$(a) \cdot \bar{3} \cdot \bar{a}$	$p\bar{3}a$	$r\bar{3}2/c$	$3gP\bar{1}2$
	53	$\bar{6}$	56	$P6(11)$	6	$(a) \cdot 6$	$p6$	$r6$	$6P1$
	54	$\bar{6}_1$	57	$P6_1(11)$	14	$(a) \cdot 6_1$	$p6_1$	$r6_1$	$6_1P1$
	55	$\bar{6}_2$	59	$P6_2(11)$	15	$(a) \cdot 6_2$	$p6_2$	$r6_2$	$6_2P1$
	56	$\bar{6}_3$	61	$P6_3(11)$	16	$(a) \cdot 6_3$	$p6_3$	$r6_3$	$6_3P1$
	57	$\bar{6}_4$	60	$P6_4(11)$	17	$(a) \cdot 6_4$	$p6_4$	$r6_4$	$6_4P1$
	58	$\bar{6}_5$	58	$P6_5(11)$	18	$(a) \cdot 6_5$	$p6_5$	$r6_5$	$6_5P1$
	59	$\bar{6}$	53	$P\bar{6}(11)$	21	$(a) \cdot 3 : m$	$p\bar{6}$	$r\bar{6}$	$3Pm$
	60	$\bar{6}/m$	62	$P6/m(11)$	31	$(a) \cdot 6 : m$	$p6/m$	$r6/m$	$6Pm$
	61	$\bar{6}_3/m$	63	$P6_3/m(11)$	32	$(a) \cdot 6_3 : m$	$p6_3/m$	$r6_3/m$	$6_3Pm$
	62	$\bar{6}22$	67	$P6(22)$	70	$(a) \cdot 6 : 2$	$p622$	$r622$	$6P22$
	63	$\bar{6}_122$	68	$P6_1(22)$	71	$(a) \cdot 6_1 : 2$	$p6_122$	$r6_122$	$6_1P22$
	64	$\bar{6}_222$	70	$P6_2(22)$	72	$(a) \cdot 6_2 : 2$	$p6_222$	$r6_222$	$6_2P22$
	65	$\bar{6}_322$	72	$P6_3(22)$	73	$(a) \cdot 6_3 : 2$	$p6_322$	$r6_322$	$6_3P22$
	66	$\bar{6}_422$	71	$P6_4(22)$	74	$(a) \cdot 6_4 : 2$	$p6_422$	$r6_422$	$6_4P22$

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

Table 1.2.17.2. Rod-group symbols (cont.)

	1	2	3	4	5	6	7	8	9
	67	$\mu 6_5 22$	69	$P6_5(22)$	75	$(a) \cdot 6_5 : 2$	$p6_5 22$	$r6_5 22$	$6_5 P22$
	68	$\mu 6 mm$	64	$P6(mm)$	43	$(a) \cdot 6 \cdot m$	$p6 mm$	$r6 mm$	$6 mm P1$
	69	$\mu 6 cc$	65	$P6(cc)$	44	$(a) \cdot 6 \cdot \bar{a}$	$p6 a a$	$r6 cc$	$6 gg P1$
	70	$\mu 6_3 mc$	66	$P6_3(cm)$	45	$(a) \cdot 6_3 \cdot m$	$p6_3 ma$	$r6_3 mc$	$6_3 mg P1$
	71	$\mu 6 m 2$	54	$P\bar{6}(m2)$	51	$(a) \cdot m \cdot 3 : m$	$p\bar{6} m 2$	$r\bar{6} m 2$	$3 m P m 2$
	72	$\mu 6 c 2$	55	$P\bar{6}(c2)$	52	$(a) \cdot \bar{a} \cdot 3 : m$	$p\bar{6} a 2$	$r\bar{6} c 2$	$3 g P m 2$
	73	$\mu 6 / m m m$	73	$P6/m(2/m2/m)$	56	$(a) \cdot m \cdot 6 : m$	$p6 / m m m$	$r6 / m 2 / m 2 / m$	$6 m m P m$
	74	$\mu 6 / m c c$	74	$P6/m(2/c2/c)$	57	$(a) \cdot \bar{a} \cdot 6 : m$	$p6 / m a a$	$r6 / m 2 / c 2 / c$	$6 g g P m$
	75	$\mu 6_3 / m m c$	75	$P6_3/m(2/c2/m)$	58	$(a) \cdot m \cdot 6_3 : m$	$p6_3 / m m a$	$r6_3 / m 2 / m 2 / c$	$6_3 m g P m$

Example: **G**: Layer group  $p2_1/m11$  (L15)

Minimal non-isotypic non-enantiomorphic supergroups:

**I** [2]  $pmam$ ; [2]  $pmma$ ; [2]  $pbma$ ; [2]  $pmmn$

**II** [2]  $c2/m11$ ; [2]  $p2/m11$  ( $2a' = a$ )

Block **I** lists [2]  $pmam$ , [2]  $pmma$  and [2]  $pmmn$ . Looking up the subgroup data of these three groups one finds [2]  $p2_1/m11$ . Block **I** also lists [2]  $pbma$ . Looking up the subgroup data of this group one finds [2]  $p12_1/m1$  ( $p2_1/m11$ ). This shows that the setting of  $pbma$  does not correspond to that of  $p2_1/m11$  but rather to  $p12_1/m1$ . To obtain the supergroup **H** referred to the basis of  $p2_1/m11$ , the basis vectors **a** and **b** must be interchanged. This changes  $pbma$  to  $pmba$ , which is the correct symbol of the supergroup of  $p2_1/m11$ .

Block **II** contains two entries: the first where the conventional cells are the same with the supergroup having additional centring translations, and the second where the conventional cell of the supergroup is smaller than that of the original subperiodic group.

## 1.2.15.4. Minimal isotypic supergroups and enantiomorphic supergroups of lowest index

No data are listed for supergroups **IIc**, because they can be derived directly from the corresponding data of subgroups **IIc**.

Example: **G**: Rod group  $\mu 4_2/m$  (R29)

The maximal isotypic subgroup of lowest index of  $\mu 4_2/m$  is found in block **IIc**: [3]  $\mu 4_2/m$  ( $c' = 3c$ ). By interchanging  $c'$  and **c**, one obtains the minimal isotypic supergroup of lowest index, i.e. [3]  $\mu 4_2/m$  ( $3c' = c$ ).

## 1.2.16. Nomenclature

There exists a wide variety of nomenclature for layer, rod and frieze groups (Holser, 1961). Layer-group nomenclature includes *zweidimensionale Raumgruppen* (Alexander & Herrmann, 1929a,b), *Ebenengruppen* (Weber, 1929), *Netzgruppen* (Hermann, 1929a), *net groups* (IT, 1952; Opechowski, 1986), *reversal space groups in two dimensions* (Cochran, 1952), *plane groups in three dimensions* (Dornberger-Schiff, 1956, 1959; Belov, 1959), *black and white space groups in two dimensions* (Mackay, 1957), *(two-sided) plane groups* (Holser, 1958), *Schichtgruppen* (Niggli, 1959; Chapuis, 1966), *diperiodic groups in three dimensions* (Wood, 1964a,b), *layer space groups* (Shubnikov & Koptsik, 1974), *layer groups* (Köhler, 1977; Koch & Fischer, 1978; Vainshtein, 1981; Goodman, 1984; Litvin, 1989), *two-dimensional (subperiodic) groups in three-dimensional space* (Brown et al., 1978) and *plane space groups in three dimensions* (Grell et al., 1989).

Rod-group nomenclature includes *Kettengruppen* (Hermann, 1929a,b), *eindimensionalen Raumgruppen* (Alexander, 1929, 1934), *(crystallographic) line groups in three dimensions* (IT, 1952; Opechowski, 1986), *rod groups* (Belov, 1956; Vujicic et al., 1977; Köhler, 1977; Koch & Fischer, 1978), *Balkengruppen*

(Niggli, 1959; Chapuis, 1966), *stem groups* (Galyarskii & Zamorzaev, 1965), *linear space groups* (Bohm & Dornberger-Schiff, 1966) and *one-dimensional (subperiodic) groups in three dimensions* (Brown et al., 1978).

Frieze-group nomenclature includes *Bortenornamente* (Speiser, 1927), *Bandgruppen* (Niggli, 1959), *line groups (borders) in two dimensions* (IT, 1952), *line groups in a plane* (Belov, 1956), *eindimensionale 'zweifarbige' Gruppen* (Nowacki, 1960), *groups of one-sided bands* (Shubnikov & Koptsik, 1974), *ribbon groups* (Köhler, 1977), *one-dimensional (subperiodic) groups in two-dimensional space* (Brown et al., 1978) and *groups of borders* (Vainshtein, 1981).

## 1.2.17. Symbols

The following general criterion was used in selecting the sets of symbols for the subperiodic groups: *consistency with the symbols used for the space groups given in IT A* (1983). Specific criteria following from this general criterion are as follows:

(1) The symbols of subperiodic groups are to be of the Hermann-Mauguin (international) type. This is the type of symbol used for space groups in IT A (1983).

(2) A symbol of a subperiodic group is to consist of a letter indicating the lattice centring type followed by a set of characters indicating symmetry elements. This is the format of the Hermann-Mauguin (international) space-group symbols in IT A (1983).

(3) The sets of symmetry directions and their sequences in the symbols of the subperiodic groups are those of the corresponding space groups. Layer and rod groups are three-dimensional subperiodic groups of the three-dimensional space groups, and frieze groups are two-dimensional subperiodic groups of the two-dimensional space groups. Consequently, the symmetry directions and sequence of the characters indicating symmetry elements in layer and rod groups are those of the three-dimensional space groups; in frieze groups, they are those of the two-dimensional space groups, see Table 1.2.4.1 above and Table 2.4.1 of IT A (1983). Layer groups appear as subgroups of three-dimensional space groups, as factor groups of three-dimensional reducible space groups (Kopský, 1986, 1988, 1989a,b, 1993; Fuksa & Kopský, 1993) and as the symmetries of planes which transect a crystal of a given three-dimensional space-group symmetry. For example, the layer group  $pmm2$  is a subgroup of the three-dimensional space group  $Pmm2$ ; is isomorphic to the factor group  $Pmm2/T_z$  of the three-dimensional space group  $Pmm2$ , where  $T_z$  is the translational subgroup of all translations along the  $z$  axis; and is the symmetry of the plane transecting a crystal of three-dimensional space-group symmetry  $Pmm2$ , perpendicular to the  $z$  axis, at  $z = 0$ . In these examples, the symbols for the three-dimensional space group and the related subperiodic layer group differ only in the letter indicating the lattice type.

A survey of sets of symbols that have been used for the subperiodic groups is given below. Considering these sets of

1.2. GUIDE TO THE USE OF THE SUBPERIODIC GROUP TABLES

Table 1.2.17.3. Layer-group symbols

(a) Columns 1–9.

	1	2	3	4	5	6	7	8	9	
Triclinic/oblique	1	$p1$	1	$P1$	1	$P11(1)$	1	$p1$	$p1$	
	2	$p\bar{1}$	2	$P\bar{1}$	2	$P\bar{1}\bar{1}(\bar{1})$	3	$p\bar{1}$	$p\bar{1}$	
Monoclinic/oblique	3	$p112$	3	$P211$	9	$P11(2)$	5	$p112$	$p21$	
	4	$p11m$	4	$Pm11$	4	$P11(m)$	2	$p11m$	$pm1$	
	5	$p11a$	5	$Pb11$	5	$P11(b)$	4	$p11b$	$pa1$	
	6	$p112/m$	6	$P2/m11$	13	$P11(2/m)$	6	$p112/m$	$p2/m1$	
	7	$p112/a$	7	$P2/b11$	17	$P11(2/b)$	7	$p112/b$	$p2/a1$	
	8	$p211$	8	$P112$	8	$P12(1)$	14	$p121$	$p12$	
Monoclinic/rectangular	9	$p2_111$	9	$P112_1$	10	$P12_1(1)$	15	$p12_11$	$p12_1$	
	10	$c211$	10	$C121$	11	$C12(1)$	16	$c121$	$c12$	
	11	$pm11$	11	$P11m$	3	$P1m(1)$	8	$p1m1$	$p1m$	
	12	$pb11$	12	$P11a$	5	$P1a(1)$	10	$p1a1$	$p1b$	
	13	$cm11$	13	$C11m$	7	$C1m(1)$	12	$c1m1$	$c1m$	
	14	$p2/m11$	14	$P112/m$	12	$P12/m(1)$	17	$p12/m1$	$p12/m$	
	15	$p2_1/m11$	15	$P112_1/m$	14	$P12_1/m(1)$	18	$p12_1/m1$	$p12_1/m$	
	16	$p2/b11$	17	$P112/a$	16	$P12/a(1)$	20	$p12/a1$	$p12/b$	
	17	$p2_1/b11$	18	$P112_1/a$	18	$P12_1/a(1)$	21	$p12_1/a1$	$p12_1/b$	
	18	$c2/m11$	16	$C112/m$	15	$C12/m(1)$	19	$c12/m1$	$c12/m$	
	Orthorhombic/rectangular	19	$p222$	19	$P222$	33	$P22(2)$	37	$p222$	$p222$
		20	$p2_122$	20	$P222_1$	34	$P2_12(2)$	38	$p2_122$	$p222_1$
		21	$p2_12_12$	21	$P22_12_1$	35	$P2_12_1(2)$	39	$p2_12_12$	$p22_12_1$
		22	$c222$	22	$C222$	36	$C22(2)$	40	$c222$	$c222$
		23	$pmm2$	23	$P2mm$	19	$Pmm(2)$	22	$pmm2$	$p2mm$
		24	$pma2$	28	$P2ma$	24	$Pma(2)$	24	$pbm2$	$p2ma$
		25	$pba2$	33	$P2ba$	29	$Pba(2)$	26	$pba2$	$p2ba$
		26	$cmm2$	34	$C2mm$	30	$Cmm(2)$	28	$cmm2$	$c2mm$
27		$pm2m$	24	$Pmm2$	20	$P2m(m)$	9	$p2mm$	$pm2m$	
28		$pm2_1b$	26	$Pbm2_1$	21	$P2_1m(a)$	30	$p2_1ma$	$pa2_1m$	
29		$pb2_1m$	25	$Pm2_1a$	22	$P2_1a(m)$	11	$p2_1am$	$pm2_1a$	
30		$pb2b$	27	$Pbb2$	23	$P2a(a)$	31	$p2aa$	$pa2a$	
31		$pm2a$	29	$Pam2$	25	$P2m(b)$	32	$p2mb$	$pb2m$	
32		$pm2_1n$	32	$Pnm2_1$	28	$P2_1m(n)$	35	$p2_1mn$	$pn2_1m$	
33		$pb2_1a$	30	$Pab2_1$	26	$P2_1a(b)$	33	$p2_1ab$	$pb2_1a$	
34		$pb2n$	31	$Pnb2$	27	$P2a(n)$	34	$p2an$	$pn2a$	
35		$cm2m$	35	$Cmm2$	31	$C2m(m)$	13	$c2mn$	$cm2m$	
36		$cm2e$	36	$Cam2$	32	$Cm2(a)$	36	$c2mb$	$cb2m$	
37		$pmmm$	37	$P2/m2/m2/m$	37	$P2/m2/m(2/m)$	23	$pmmm$	$p2/m2/m2/m$	
38		$pmaa$	38	$P2/a2/m2/a$	38	$P2/m2/a(2/a)$	41	$pmaa$	$p2/a2/m2/a$	
39		$pban$	39	$P2/n2/b2/a$	39	$P2/b2/a(2/n)$	42	$pban$	$p2/n2/b2/a$	
40		$pmam$	40	$P2/m2_1/m2/a$	41	$P2/b2_1/m(2/m)$	25	$pmmm$	$p2/m2_1/m2/a$	
41		$pmma$	41	$P2/a2_1/m2/m$	40	$P2_1/m2/m(2/a)$	43	$pmma$	$p2/a2_1/m2/m$	
42		$pman$	42	$P2/n2/m2_1/a$	42	$P2_1/b2/m(2/n)$	44	$pbnm$	$p2/n2/m2_1/a$	
43		$pbaa$	43	$P2/a2/b2_1/a$	43	$P2/b2_1/a(2/a)$	45	$pbaa$	$p2/a2/b2_1/a$	
44		$pbam$	44	$P2/m2_1/b2_1/a$	44	$P2_1/b2_1/a(2/m)$	27	$pbam$	$p2/m2_1/b2_1/a$	
45		$pbma$	45	$P2/a2_1/b2_1/m$	45	$P2_1/m2_1/a(2/b)$	46	$pbma$	$p2/a2_1/b2_1/m$	
46		$pmmn$	46	$P2/n2_1/m2_1/m$	46	$P2_1/m2_1/m(2/n)$	47	$pmmn$	$p2/n2_1/m2_1/m$	
47		$cnmm$	47	$C2/m2/m2/m$	47	$C2/m2/m(2/m)$	29	$cnmm$	$c2/m2/m2/m$	
48		$cmme$	48	$C2/a2/m2/m$	48	$C2/m2/m(2/a)$	48	$cmma$	$c2/a2/m2/m$	
49		$p4$	49	$P4$	54	$P(4)11$	50	$p4$	$p4$	
50		$p\bar{4}$	50	$P\bar{4}$	49	$P(\bar{4})11$	49	$p\bar{4}$	$p\bar{4}$	
51		$p4/m$	51	$P4/m$	55	$P(4/m)11$	51	$p4/m$	$p4/m$	
52		$p4/n$	52	$P4/n$	56	$P(4/n)11$	57	$p4/n$	$p4/n$	
53	$p422$	53	$P422$	59	$P(4)22$	55	$p422$	$p422$		
54	$p42_12$	54	$P42_12$	60	$P(4)2_12$	56	$p42_12$	$p42_12$		
55	$p4mm$	55	$P4mm$	57	$P(4)mm$	52	$p4mm$	$p4mm$		
56	$p4bm$	56	$P4bm$	58	$P(4)bm$	59	$p4bm$	$p4bm$		
57	$p\bar{4}2m$	57	$P\bar{4}2m$	50	$P(\bar{4})2m$	54	$p\bar{4}2m$	$p\bar{4}2m$		
58	$p\bar{4}2_1m$	58	$P\bar{4}2_1m$	51	$P(\bar{4})2_1m$	60	$p\bar{4}2_1m$	$p\bar{4}2_1m$		
59	$p4m2$	59	$P4m2$	52	$P(4)m2$	61	$p4m2$	$p4m2$		
60	$p\bar{4}b2$	60	$P\bar{4}b2$	53	$P(\bar{4})b2$	64	$p\bar{4}b2$	$p\bar{4}b2$		
61	$p4/mmm$	61	$P4/m2/m2/m$	61	$P(4/m)2/m2/m$	53	$p4/mmm$	$p4/m2/m2/m$		
62	$p4/nbm$	62	$P4/n2/b2/m$	62	$P(4/n)2/b2/m$	62	$p4/nbm$	$p4/n2/b2/m$		
63	$p4/mbm$	63	$P4/m2_1/b2/m$	63	$P(4/m)2_1/b2/m$	58	$p4/mbm$	$p4/m2_1/b2/m$		
64	$p4/nmm$	64	$P4/n2_1/m2/m$	64	$P(4/n)2_1/m2/m$	63	$p4/nmm$	$p4/n2_1/m2/m$		

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

Table 1.2.17.3. Layer-group symbols (cont.)

(a) Columns 1–9 (cont.).

	1	2	3	4	5	6	7	8	9
	65	$p\bar{3}$	65	$P\bar{3}$	65	$P(3)11$	65	$p\bar{3}$	$p\bar{3}$
	66	$p\bar{3}12$	66	$P\bar{3}12$	66	$P(\bar{3})11$	67	$p\bar{3}$	$p\bar{3}$
	67	$p312$	67	$P312$	70	$P(3)12$	72	$p312$	$p312$
	68	$p321$	68	$P321$	69	$P(3)21$	73	$p321$	$p321$
	69	$p3m1$	69	$P3m1$	67	$P(3)m1$	68	$p3m1$	$p3m1$
	70	$p\bar{3}1m$	70	$P\bar{3}1m$	68	$P(3)1m$	70	$p\bar{3}1m$	$p\bar{3}1m$
	71	$p\bar{3}m1$	71	$P\bar{3}12/m$	72	$P(\bar{3})1m$	74	$p\bar{3}1m$	$p\bar{3}12/m$
	72	$p\bar{6}$	72	$P\bar{6}$	71	$P(\bar{3})m1$	75	$p\bar{3}m1$	$p\bar{3}2/m1$
	73	$p6$	73	$P6$	76	$P(6)11$	76	$p6$	$p6$
	74	$p\bar{6}m2$	74	$P\bar{6}m2$	73	$P(\bar{6})11$	66	$p\bar{6}$	$p\bar{6}$
	75	$p6/m$	75	$P6/m$	77	$P(6/m)11$	77	$p6/m$	$p6/m$
	76	$p622$	76	$P622$	79	$P(6)22$	80	$p622$	$p622$
	77	$p6mm$	77	$P6mm$	78	$P(6)mm$	78	$p6mm$	$p6mm$
	78	$p\bar{6}m2$	78	$P\bar{6}m2$	74	$P(\bar{6})m2$	69	$p\bar{6}m2$	$p\bar{6}m2$
	79	$p\bar{6}2m$	79	$P\bar{6}2m$	75	$P(\bar{6})2m$	71	$p\bar{6}2m$	$p\bar{6}2m$
	80	$p6/mmm$	80	$P6/m2/m2/m$	80	$P(6/m)2/m2/m$	79	$p6/mmm$	$p6/m2/m2/m$

(b) Columns 10–17.

	10	11	12	13	14	15	16	17
Triclinic/oblique	1	$C_1\bar{p}$	$C_1^1$	1P1	$(a/b) \cdot 1$	1p1	p1	p1
	2	$S_2\bar{p}$	$C_1^1$	1P $\bar{1}$	$(a/b) \cdot \bar{1}$	1p $\bar{1}$	p2'	p2'
Monoclinic/oblique	8	$C_2\bar{p}$	$C_2^1$	1P2	$(a/b) : 2$	1p112	p2	p2
	3	$C_{1h}\bar{p}\mu$	$C_{1h}^1$	mP1	$(a/b) \cdot m$	mp1	p*1	
	4	$C_{1h}\bar{p}\alpha$	$C_{1h}^2$	aP1	$(a/b) \cdot \bar{b}$	bp1	p'_b1	p'_b1
	12	$C_{2h}\bar{p}\mu$	$C_{2h}^1$	mP2	$(a/b) \cdot m : 2$	mp112	p*2	
	13	$C_{2h}\bar{p}\alpha$	$C_{2h}^2$	aP2	$(a/b) \cdot \bar{b} : 2$	bp112	p'_b2	p'_b2
Monoclinic/rectangular	9	$D_1\bar{p}1$	$C_2^2$	1P12	$(a : b) \cdot 2$	1p12	p1m'1	pm'
	10	$D_1\bar{p}2$	$C_2^3$	1P12 $_1$	$(a : b) \cdot 2_1$	1p12 $_1$	p1g'1	pg'
	11	$D_1\bar{c}1$	$C_2^4$	1C12	$(\frac{a+b}{2}/a : b) \cdot 2$	1c12	c1m'1	cm'
	5	$C_{1v}\bar{p}\mu$	$C_{1h}^3$	1P1m	$(a : b) : m$	1p1m	p11m	pm
	6	$C_{1v}\bar{p}\beta$	$C_{1h}^4$	1P1g	$(a : b) : \bar{a}$	1p1a	p11g	pg
	7	$C_{1v}\bar{c}\mu$	$C_{1h}^5$	1C1m	$(\frac{a+b}{2}/a : b) : m$	1c1m	c11m	cm
	14	$D_{1d}\bar{p}\mu1$	$C_{2h}^3$	1P12/m	$(a : b) \cdot 2 : m$	1p12/m	p2'm'm	pm'm
	15	$D_{1d}\bar{p}\mu2$	$C_{2h}^5$	1P12 $_1/m$	$(a : b) \cdot 2_1 : m$	1p12 $_1/m$	p2'g'm	pg'm
	18	$D_{1d}\bar{p}\beta2$	$C_{2h}^6$	1P12/g	$(a : b) \cdot 2 \cdot \bar{a}$	1p12 $_1/a$	p2'g'g	pg'g
	17	$D_{1d}\bar{p}\beta1$	$C_{2h}^4$	1P12 $_1/g$	$(a : b) \cdot 2_1 : \bar{a}$	1p12/a	p2'm'g	pm'g
	16	$D_{1d}\bar{c}\mu1$	$C_{2h}^7$	1C12/m	$(\frac{a+b}{2}/a : b) \cdot 2 : m$	1c12/m	c2'm'm	cm'm
Orthorhombic/rectangular	33	$D_2\bar{p}11$	$V^1$	1P222	$(a : b) : 2 : 2$	1p222	p2m'm'	pm'm'
	34	$D_2\bar{p}12$	$V^3$	1P222 $_1$	$(a : b) : 2 : 2_1$	1p22 $_1$	p2g'm'	pg'm'
	35	$D_2\bar{p}22$	$V^2$	1P22 $_1$ 2 $_1$	$(a : b) \cdot 2_1 : 2_1$	1p2 $_1$ 2 $_1$	p2g'g'	pg'g'
	36	$D_2\bar{c}11$	$V^4$	1C222	$(\frac{a+b}{2}/a : b) : 2 : 2$	1c222	c2m'm'	cm'm'
	19	$C_{2v}\bar{p}\mu\mu$	$C_{2v}^1$	1P2mm	$(a : b) : 2 \cdot m$	1pmm2	p2mm	pmm
	20	$C_{2v}\bar{p}\mu\alpha$	$C_{2v}^2$	1P2mg	$(a : b) : 2 \cdot \bar{b}$	1pma2	p2mg	pmg
	21	$C_{2v}\bar{p}\beta\alpha$	$C_{2v}^{10}$	1P2gg	$(a : b) : \bar{a} : \bar{b}$	1pba2	p2gg	pgg
	22	$C_{2v}\bar{c}\mu\mu$	$C_{2v}^3$	1C2mm	$(\frac{a+b}{2}/a : b) : m \cdot 2$	1cmm2	c2mm	cmm
	23	$D_{1h}\bar{p}\mu\mu$	$C_{2v}^4$	mP12m	$(a : b) \cdot m \cdot 2$	mpm2	p*1m1	
	25	$D_{1h}\bar{p}\beta\mu$	$C_{2v}^5$	aP12 $_1$ m	$(a : b) : m \cdot 2_1$	bp $_1$ m $_1$	p'_b1m1	p'_a1m
	24	$D_{1h}\bar{p}\mu\beta$	$C_{2v}^7$	mP12 $_1$ g	$(a : b) \cdot m \cdot 2_1$	mp $_1$ b $_1$	p*1g1	
	26	$D_{1h}\bar{p}\beta\beta$	$C_{2v}^6$	aP12g	$(a : b) \cdot \bar{a} \cdot 2$	bp $_1$ b $_1$	p'_b1m'1	p'_a1g
	27	$D_{1h}\bar{p}\alpha\mu$	$C_{2v}^{11}$	bP12m	$(a : b) \cdot \bar{b} \cdot 2$	ap $_1$ m $_1$	p'_a1m1	p'_b1m
	30	$D_{1h}\bar{p}\nu\mu$	$C_{2v}^{13}$	nP12 $_1$ m	$(a : b) \cdot ab \cdot 2_1$	np $_1$ m $_1$	c'1m1	p'_c1m
	28	$D_{1h}\bar{p}\alpha\beta$	$C_{2v}^{14}$	bP12 $_1$ g	$(a : b) \cdot \bar{b} : \bar{a}$	ap $_1$ b $_1$	p'_a1g1	p'_b1g
	29	$D_{1h}\bar{p}\nu\beta$	$C_{2v}^{12}$	nP12g	$(a : b) \cdot ab \cdot 2$	np $_1$ b $_1$	c'1m'1	p'_c1m'
	31	$D_{1h}\bar{c}\mu\mu$	$C_{2v}^8$	mC12m	$(\frac{a+b}{2}/a : b) \cdot m \cdot 2$	mcm2	c*1m1	
	32	$D_{1h}\bar{c}\alpha\mu$	$C_{2v}^9$	aC12m	$(\frac{a+b}{2}/a : b) \cdot \bar{b} \cdot 2$	acm2	p'_a1m1	c'1m
	37	$D_{2h}\bar{p}\mu\mu\mu$	$V_h^1$	mP2mm	$(a : b) \cdot m : 2 \cdot m$	mp2/m2/m2	p*2mm	
	38	$D_{2h}\bar{p}\alpha\mu\alpha$	$V_h^5$	aP2mg	$(a : b) \cdot \bar{a} : 2 \cdot \bar{a}$	ip2/m2/a2	p'_a2mg	p'_a'mg
	39	$D_{2h}\bar{p}\nu\beta\alpha$	$V_h^6$	nP2gg	$(a : b) \cdot ab : 2 \cdot a$	np2/b2/a2	c'2m'm'	p'_c'm'm'
	40	$D_{2h}\bar{p}\mu\mu\alpha$	$V_h^3$	mP2mg	$(a : b) \cdot m : 2 \cdot \bar{b}$	np2 $_1$ /m2/a2	p*2mg	
	41	$D_{2h}\bar{p}\alpha\mu\mu$	$V_h^9$	aP2mm	$(a : b) \cdot \bar{a} : 2 \cdot m$	ap2 $_1$ /m2/m2	p'_a2mm	p'_b'mm
	42	$D_{2h}\bar{p}\nu\mu\alpha$	$V_h^{11}$	nP2mg	$(a : b) \cdot ab : 2 \cdot b$	np2/m2 $_1$ /a2	c'2mm'	p'_c'm'm
	43	$D_{2h}\bar{p}\alpha\beta\alpha$	$V_h^{10}$	aP2gg	$(a : b) \cdot \bar{a} : 2 : \bar{b}$	ap2/b2 $_1$ /a2	p'_a2gg	p'_b'sg
	44	$D_{2h}\bar{p}\mu\beta\alpha$	$V_h^2$	mP2gg	$(a : b) \cdot m : \bar{a} : \bar{b}$	np2 $_1$ /b2 $_1$ /a2	p*2gg	

1.2. GUIDE TO THE USE OF THE SUBPERIODIC GROUP TABLES

Table 1.2.17.3. Layer-group symbols (cont.)

(a) Columns 10–17 (cont.).

	10	11	12	13	14	15	16	17
	45	$D_{2h}\bar{p}\alpha\beta\mu$	$V_h^7$	$aP2gm$	$(a : b) \cdot \bar{b} : 2 \cdot \bar{a}$	$ap2_1/b2_1/m2$	$p'_a2gm$	$p'_bmg$
	46	$D_{2h}\bar{p}\nu\mu\mu$	$V_h^8$	$nP2mm$	$(a : b) \cdot ab : 2 \cdot m$	$np2_1/m2_1/m2$	$c'2mm$	$p'_cmm$
	47	$D_{2h}\bar{c}\mu\mu\mu$	$V_h^4$	$mC2mm$	$(\frac{a+b}{2}/a : b) \cdot m : 2 \cdot m$	$mc2/m2/m2$	$c^*2mm$	
	48	$D_{2h}\bar{c}\alpha\mu\mu$	$V_h^{12}$	$aC2mm$	$(\frac{a+b}{2}/a : b) \cdot \bar{a} : 2 \cdot m$	$ac2/m2/m2$	$p'_{a'b'}2mm$	$c'mm$
	58	$C_4\bar{p}$	$C_4^1$	$1P4$	$(a : a) : 4$	$1p4$	$p4$	$p4$
	57	$S_4\bar{p}$	$S_4^1$	$1P\bar{4}$	$(a : a) : \bar{4}$	$1p\bar{4}$	$p4'$	$p4'$
	61	$C_{4h}\bar{p}\mu$	$C_{4h}^1$	$mP4$	$(a : a) : 4 : m$	$mp4$	$p^*4$	
	62	$C_{4h}\bar{p}\nu$	$C_{4h}^2$	$nP4$	$(a : a) : 4 : ab$	$np4$	$c'4$	$p'4$
	67	$D_4\bar{p}11$	$D_4^1$	$1P422$	$(a : a) : 4 : 2$	$1p422$	$p4m'm'$	$p4m'm'$
	68	$D_4\bar{p}21$	$D_4^2$	$1P42_12$	$(a : a) : 4 : 2_1$	$1p42_12$	$p4g'm'$	$p4g'm'$
	59	$C_{4v}\bar{p}\mu\mu$	$C_{4v}^1$	$1P4mm$	$(a : a) : 4 \cdot m$	$1p4mm$	$p4mm$	$p4mm$
	60	$C_{4v}\bar{p}\beta\mu$	$C_{4v}^2$	$1P4gm$	$(a : a) : 4 \odot b$	$1p4bm$	$p4gm$	$p4gm$
	63	$D_{2d}\bar{p}\mu 1$	$V_d^1$	$1P\bar{4}2m$	$(a : a) : \bar{4} : 2$	$1p\bar{4}2m$	$p4'm'm'$	$p4'm'm'$
	64	$D_{2d}\bar{p}\mu 2$	$V_d^2$	$1P\bar{4}2_1m$	$(a : a) : \bar{4} \odot 2_1$	$1p\bar{4}2_1m$	$p4'g'm'$	$p4'g'm'$
	65	$D_{2d}\bar{c}\mu 1$	$V_d^3$	$1P4m2$	$(a : a) : 4 \cdot m$	$1p4m2$	$p4'mm'$	$p4'mm'$
	66	$D_{2d}\bar{c}\beta 1$	$V_d^4$	$1P4g2$	$(a : a) : \bar{4} \odot \bar{b}$	$1p4b2$	$p4'gm'$	$p4'gm'$
	69	$D_{4h}\bar{p}\mu\mu\mu$	$D_{4h}^1$	$mP4mm$	$(a : a) \cdot m : 4 \cdot m$	$mp42/m2/m$	$p^*4mm$	
	70	$D_{4h}\bar{p}\nu\beta\mu$	$D_{4h}^2$	$nP4gm$	$(a : a) : ab : 4 \odot b$	$np42/b2/m$	$c'4m'm$	$p'4gm$
	71	$D_{4h}\bar{p}\mu\beta\mu$	$D_{4h}^3$	$mP4gm$	$(a : a) \cdot m : 4 \odot b$	$mp42_1/b2/m$	$p^*4gm$	
	72	$D_{4h}\bar{p}\nu\mu\mu$	$D_{4h}^4$	$nP4mm$	$(a : a) \cdot ab : 4 \cdot m$	$np42_1/m2/m$	$c'4mm$	$p'4mm$
	49	$C_3\bar{c}$	$C_3^1$	$1P3$	$(a/a) : 3$	$1p3$	$p3$	$p3$
	50	$S_6\bar{p}$	$C_{3i}^1$	$1P\bar{3}$	$(a/a) : \bar{3}$	$1p\bar{3}$	$p6'$	$p6'$
	54	$D_3\bar{c}1$	$D_3^1$	$1P312$	$(a/a) : 2 : 3$	$1p312$	$p3m'1$	$p3m'1$
	53	$D_3\bar{h}1$	$D_3^2$	$1P321$	$(a/a) \cdot 2 : 3$	$1p321$	$p31m'$	$p31m'$
	51	$C_{3v}\bar{c}\mu$	$C_{3v}^2$	$1P3m1$	$(a/a) : m \cdot 3$	$1p3m1$	$p3m1$	$p3m1$
	52	$C_{3v}\bar{h}\mu$	$C_{3v}^1$	$1P31m$	$(a/a) \cdot m \cdot 3$	$1p31m$	$p31m$	$p31m$
	55	$D_{3d}\bar{c}\mu 1$	$D_{3d}^2$	$1P\bar{3}1m$	$(a/a) \cdot m \cdot \bar{6}$	$1p\bar{3}12/m$	$p6'm'm'$	$p6'm'm'$
	56	$D_{3d}\bar{h}\mu 1$	$D_{3d}^1$	$1P\bar{3}m1$	$(a/a) : m \cdot \bar{6}$	$1p\bar{3}2/m1$	$p6'mm'$	$p6'mm'$
	76	$C_6\bar{c}$	$C_6^1$	$1P6$	$(a/a) : 6$	$1p6$	$p6$	$p6$
	73	$C_{3h}\bar{c}\mu$	$C_{3h}^1$	$mP3$	$(a/a) : 3 : m$	$mp3$	$p^*3$	
	78	$C_{6h}\bar{c}\mu$	$C_{6h}^1$	$mP6$	$(a/a) \cdot m : 6$	$mp6$	$p^*6$	
	79	$D_6\bar{c}11$	$D_6^1$	$1P622$	$(a/a) \cdot 2 : 6$	$1p622$	$p6m'm'$	$p6m'm'$
	77	$C_{6v}\bar{c}\mu\mu$	$C_{6v}^1$	$1P6mm$	$(a/a) : m \cdot 6$	$1p6mm$	$p6mm$	$p6mm$
	74	$D_{3h}\bar{c}\mu\mu$	$D_{3h}^1$	$mP3m2$	$(a/a) : m \cdot 3 : m$	$mp3m2$	$p^*3m1$	
	75	$D_{3h}\bar{h}\mu\mu$	$D_{3h}^2$	$mP32m$	$(a/a) \cdot m : 3 \cdot m$	$mp32m$	$p^*31m$	
	80	$D_{6h}\bar{c}\mu\mu\mu$	$D_{6h}^1$	$mP6mm$	$(a/a) \cdot m : 6 \cdot m$	$mp6mm$	$p^*6mm$	

(c) Columns 18–25.

	18	19	20	21	22	23	24	25
Triclinic/oblique	$p1$	47			$p1$			
Monoclinic/oblique	$p2'$	1	$p2'$	$p2^-$	$p2'$	$p2[2]_1$	$2'11$	$p2/p1$
	$p2$	48			$p2$			
Monoclinic/rectangular	$p1'$	64			$p11'$			
	$p'_b1$	2	$pt'$	$pt^-$	$p_{2b}1$	$p1[2]$	$b11$	$p1/p1$
	$p21'$	65			$p21'$			
	$p'_b2$	3	$p2t'$	$p2t^-$	$p_{2b}2$	$p2[2]_2$	$2/b11$	$p2/p2$
	$pm'$	4	$pm'$	$pm^-$	$pm'$	$pm[2]_4$	$12'1$	$pm/p1$
	$pg'$	5	$pg'$	$pg^-$	$pg'$	$pg[2]_1$	$112'_1$	$pg/p1$
	$cm'$	6	$cm'$	$cm^-$	$cm'$	$cm[2]_1$	$c112'$	$cm/p1$
	$pm$	49			$pm$			
	$pg$	50			$pg$			
	$cm$	51			$cm$			
Orthorhombic/rectangular	$pmm'$	14	$pmm'$	$pmm^-$	$pm'm$	$pmm[2]_2$	$2'2'2$	$pmm/pm$
	$pmg'$	17	$pmg'$	$pmg^-$	$pmg'$	$pmg[2]_4$	$2'2'_12$	$pmg/pm$
	$pgg'$	18	$pgg'$	$pgg^-$	$pgg'$	$pgg[2]_1$	$2'2'_12_1$	$pgg/pg$
	$pm'g$	16	$pm'g$	$pm^-g$	$pm'g$	$pmg[2]_2$	$2'2'_12'$	$pmg/pg$
	$cmm'$	21	$cmm'$	$cmm^-$	$cmm'$	$cmm[2]_2$	$c2'22'$	$cmm/cm$
	$pm'm'$	15	$pm'm'$	$pm^-m^-$	$pm'm'$	$pmm[2]_5$	$22'2'$	$pmm/p2$
	$pm'g'$	20	$pm'g'$	$pm^-g^-$	$pm'g'$	$pmg[2]_5$	$22'_1$	$pmg/p2$
	$pg'g'$	19	$pg'g'$	$pg^-g^-$	$pg'g'$	$pgg[2]_5$	$22'_12_1$	$pgg/p2$
	$cm'm'$	22	$cm'm'$	$cm^-m^-$	$cm'm'$	$cmm[2]_4$	$c22'2'$	$cmm/p2$
	$pmm2$	52			$pmm$			
$pmg2$	53			$pmg$				

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

Table 1.2.17.3. Layer-group symbols (cont.)

(a) Columns 18–25 (cont.).

	18	19	20	21	22	23	24	25
	<i>pgg2</i>	54			<i>pgg</i>			
	<i>cmm2</i>	55			<i>cmm</i>			
	<i>pm1'</i>	66			<i>pm1'</i>			
	<i>p'<sub>b</sub>m</i>	7	<i>pm + t'</i>	<i>pm + t<sup>-</sup></i>	<i>p<sub>2b</sub>m</i>	<i>pm[2]<sub>3</sub></i>	<i>b12</i>	<i>pm/pm(m)</i>
	<i>pg1'</i>	67			<i>pg1'</i>			
	<i>p'<sub>b</sub>g</i>	8	<i>pg + t'</i>	<i>pg + t<sup>-</sup></i>	<i>p<sub>2b</sub>m'</i>	<i>pm[2]<sub>1</sub></i>	<i>b12<sub>1</sub></i>	<i>pm/pg</i>
	<i>p'<sub>b</sub>1m</i>	9	<i>pm + m'</i>	<i>pm + m<sup>-</sup></i>	<i>p<sub>2a</sub>m</i>	<i>pm[2]<sub>5</sub></i>	<i>b'1m</i>	<i>pm/pm(m')</i>
	<i>p'<sub>c</sub>m</i>	11	<i>pm + g'</i>	<i>pm + g<sup>-</sup></i>	<i>c<sub>p</sub>m</i>	<i>cm[2]<sub>3</sub></i>	<i>n12</i>	<i>cm/pm</i>
	<i>p'<sub>b</sub>1g</i>	10	<i>pg + g'</i>	<i>pg + g<sup>-</sup></i>	<i>p<sub>2a</sub>g</i>	<i>pg[2]<sub>2</sub></i>	<i>b2<sub>1</sub>1</i>	<i>pg/pg</i>
	<i>p'<sub>c</sub>g</i>	12	<i>pg + m'</i>	<i>pg + m<sup>-</sup></i>	<i>c<sub>p</sub>m'</i>	<i>cm[2]<sub>2</sub></i>	<i>n12<sub>1</sub></i>	<i>cm/pg</i>
	<i>cm1'</i>	68			<i>cm1'</i>			
	<i>c'm</i>	13	<i>cm + m'</i>	<i>cm + m<sup>-</sup></i>	<i>p<sub>c</sub>m</i>	<i>pm[2]<sub>2</sub></i>	<i>ca12</i>	<i>pm/cm</i>
	<i>pmm21'</i>	69			<i>pmm1'</i>			
	<i>p'<sub>b</sub>gm</i>	25	<i>pg, m + m'</i>	<i>pg, m + m<sup>-</sup></i>	<i>p<sub>2a</sub>mm'</i>	<i>pmm[2]<sub>4</sub></i>	<i>a2<sub>1</sub>2</i>	<i>pmm/pmg</i>
	<i>p'<sub>c</sub>gg</i>	29	<i>pg + m', g + m'</i>	<i>pg + m<sup>-</sup>, g + m<sup>-</sup></i>	<i>c<sub>p</sub>m'm'</i>	<i>cmm[2]<sub>1</sub></i>	<i>n2<sub>1</sub>2<sub>1</sub></i>	<i>cmm/pgg</i>
	<i>pmg21'</i>	70			<i>pmg1'</i>			
	<i>p'<sub>b</sub>mm</i>	23	<i>pm, m + m'</i>	<i>pm, m + m<sup>-</sup></i>	<i>p<sub>2a</sub>mm</i>	<i>pmm[2]<sub>1</sub></i>	<i>a22</i>	<i>pmm/pmm</i>
	<i>p'<sub>c</sub>mg</i>	28	<i>pm + g', g + m'</i>	<i>pm + g<sup>-</sup>, g + m<sup>-</sup></i>	<i>c<sub>p</sub>mm'</i>	<i>cmm[2]<sub>3</sub></i>	<i>n22<sub>1</sub></i>	<i>cmm/pmg</i>
	<i>p'<sub>b</sub>gg</i>	26	<i>pg, g + g'</i>	<i>pg, g + g<sup>-</sup></i>	<i>p<sub>2b</sub>m'g</i>	<i>pmg[2]<sub>3</sub></i>	<i>a2<sub>1</sub>2<sub>1</sub></i>	<i>pmg/pgg</i>
	<i>pgg21'</i>	71			<i>pgg1'</i>			
	<i>p'<sub>b</sub>mg</i>	24	<i>pm, g + g'</i>	<i>pm, g + g<sup>-</sup></i>	<i>p<sub>2b</sub>mg</i>	<i>pmg[2]<sub>1</sub></i>	<i>b2<sub>1</sub>2</i>	<i>pmg/pmg</i>
	<i>p'<sub>c</sub>mm</i>	27	<i>pm + g', m + g'</i>	<i>pm + g<sup>-</sup>, m + g<sup>-</sup></i>	<i>c<sub>p</sub>mm</i>	<i>cmm[2]<sub>5</sub></i>	<i>n22</i>	<i>cmm/pmm</i>
	<i>cmm21'</i>	72			<i>cmm1'</i>			
	<i>c'nm</i>	30	<i>cm + m', m + m'</i>	<i>cm + m<sup>-</sup>, m + m<sup>-</sup></i>	<i>p<sub>c</sub>mm</i>	<i>pmm[2]<sub>3</sub></i>	<i>ca22</i>	<i>pmm/cmm</i>
	<i>p4</i>	56			<i>p4</i>			
	<i>p4'</i>	31	<i>p4'</i>	<i>p4<sup>-</sup></i>	<i>p4'</i>	<i>p4[2]<sub>2</sub></i>	<i>4'11</i>	<i>p4/p2</i>
	<i>p41'</i>	73			<i>p41'</i>			
	<i>p'<sub>c</sub>4</i>	32	<i>p4t'</i>	<i>p4t<sup>-</sup></i>	<i>p<sub>p</sub>4</i>	<i>p4[2]<sub>1</sub></i>	<i>4/n11</i>	<i>p4/p4</i>
	<i>p4m'm'</i>	35	<i>p4m'm'</i>	<i>p4m<sup>-</sup>m<sup>-</sup></i>	<i>p4m'</i>	<i>pm4[2]<sub>2</sub></i>	<i>42'2'</i>	<i>p4m/p4</i>
	<i>p4g'm'</i>	38	<i>p4g'm'</i>	<i>p4g<sup>-</sup>m<sup>-</sup></i>	<i>p4g'</i>	<i>p4g[2]<sub>1</sub></i>	<i>42'<sub>1</sub>2'</i>	<i>p4g/p4</i>
	<i>p4mm</i>	57			<i>p4m</i>			
	<i>p4gm</i>	58			<i>p4g</i>			
	<i>p4'm'm</i>	34	<i>p4'm'm</i>	<i>p4<sup>-</sup>m<sup>-</sup>m</i>	<i>p4'm'</i>	<i>p4m[2]<sub>3</sub></i>	<i>4'2'2</i>	<i>p4m/cmm</i>
	<i>p4'g'm</i>	37	<i>p4'g'm</i>	<i>p4<sup>-</sup>g<sup>-</sup>m</i>	<i>p4'g'</i>	<i>p4g[2]<sub>2</sub></i>	<i>4'2'<sub>1</sub>2</i>	<i>p4g/cmm</i>
	<i>p4'nm'</i>	33	<i>p4'nm'</i>	<i>p4<sup>-</sup>mm<sup>-</sup></i>	<i>p4'm</i>	<i>p4m[2]<sub>4</sub></i>	<i>4'22'</i>	<i>p4m/pmm</i>
	<i>p4'gm'</i>	36	<i>p4'gm'</i>	<i>p4<sup>-</sup>gm<sup>-</sup></i>	<i>p4'g</i>	<i>p4g[2]<sub>3</sub></i>	<i>4'2<sub>1</sub>2'</i>	<i>p4g/pgg</i>
	<i>p4mm1'</i>	74			<i>p4m1'</i>			
	<i>p'<sub>c</sub>4gm</i>	40	<i>p4g + m', m + m'</i>	<i>p4g + m<sup>-</sup>, m + m<sup>-</sup></i>	<i>p<sub>p</sub>4m'</i>	<i>p4m[2]<sub>1</sub></i>	<i>4/n2<sub>1</sub>2</i>	<i>p4m/p4g</i>
	<i>p4gm1'</i>	75			<i>p4g1'</i>			
	<i>p'<sub>c</sub>4mm</i>	39	<i>p4m + g', m + m'</i>	<i>p4m + g<sup>-</sup>, m + m<sup>-</sup></i>	<i>p<sub>p</sub>4m</i>	<i>p4m[2]<sub>5</sub></i>	<i>4/n22</i>	<i>p4m/p4m</i>
	<i>p3</i>	59			<i>p3</i>			
	<i>p6'</i>	43	<i>p6'</i>	<i>p6<sup>-</sup></i>	<i>p6'</i>	<i>p6[2]</i>	<i>6'</i>	<i>p6/p3</i>
	<i>p3m'</i>	41	<i>p3m'1</i>	<i>p3m<sup>-</sup>1</i>	<i>p3m'1</i>	<i>p3m1[2]</i>	<i>312'</i>	<i>p3m1/p3</i>
	<i>p31m'</i>	42	<i>p31m'</i>	<i>p31m<sup>-</sup></i>	<i>p31m'</i>	<i>p31m[2]</i>	<i>32'1</i>	<i>p31m/p3</i>
	<i>p3m</i>	60			<i>p3m1</i>			
	<i>p31m</i>	61			<i>p31m</i>			
	<i>p6'm'm</i>	44	<i>p6'm'm</i>	<i>p6<sup>-</sup>m<sup>-</sup>m</i>	<i>p6'm'</i>	<i>p6m[2]<sub>1</sub></i>	<i>6'22'</i>	<i>p6m/p31m</i>
	<i>p6'nm'</i>	45	<i>p6'nm'</i>	<i>p6<sup>-</sup>mm<sup>-</sup></i>	<i>p6'm</i>	<i>p6m[2]<sub>2</sub></i>	<i>6'2'2</i>	<i>p6m/p3m1</i>
	<i>p6</i>	62			<i>p6</i>			
	<i>p3'</i>	76			<i>p31'</i>			
	<i>p61'</i>	79			<i>p61'</i>			
	<i>p6m'm'</i>	46	<i>p6m'm'</i>	<i>p6m<sup>-</sup>m<sup>-</sup></i>	<i>p6m'</i>	<i>p6m[2]<sub>3</sub></i>	<i>62'2'</i>	<i>p6m/p6</i>
	<i>p6mm</i>	63			<i>p6m</i>			
	<i>p3'm</i>	77			<i>p3m11'</i>			
	<i>p3'1m</i>	78			<i>p31m1'</i>			
	<i>p6mm1'</i>	80			<i>p6m1'</i>			

symbols in relation to the above criteria leads to the sets of symbols for subperiodic groups used in Parts 2, 3 and 4.

1.2.17.1. Frieze groups

A list of sets of symbols for the frieze groups is given in Table 1.2.17.1. The information provided in this table is as follows:

Columns 1 and 2: sequential numbering and symbols used in Part 2.

Columns 3, 4 and 5: symbols listed by Opechowski (1986).

Column 6: symbols listed by Shubnikov & Koptsik (1974).

Column 7: symbols listed by Vainshtein (1981).

Columns 8 and 9: sequential numbering and symbols listed by Bohm & Dornberger-Schiff (1967).

## 1.2. GUIDE TO THE USE OF THE SUBPERIODIC GROUP TABLES

Column 10: symbols listed by Lockwood & Macmillan (1978).

Column 11: symbols listed by Shubnikov & Koptsik (1974).

Sets of symbols which are of a non-Hermann–Mauguin (international) type are the set of symbols of the ‘black and white’ symmetry type (column 3) and the sets of symbols in columns 6 and 7. The sets of symbols in columns 4, 5 and 11 do not follow the sequence of symmetry directions used for two-dimensional space groups. The sets of symbols in columns 3, 4, 5 and 10 do not use a lower-case script  $\rho$  to denote a one-dimensional lattice. The set of symbols in column 9 uses parentheses and square brackets to denote specific symmetry directions. The symbol  $g$  is used in Part 1 to denote a glide line, a standard symbol for two-dimensional space groups (*IT A*, 1983). A letter identical with a basis-vector symbol, e.g.  $a$  or  $c$ , is not used to denote a glide line, as is done in the symbols of columns 5, 6, 7, 9 and 11, as such a letter is a standard notation for a three-dimensional glide plane (*IT A*, 1983).

Columns 2 and 3 show the isomorphism between frieze groups and one-dimensional magnetic space groups. The one-dimensional space groups are denoted by  $\rho 1$  and  $\rho \bar{1}$ . The list of symbols in column 3, on replacing  $r$  with  $\rho$ , is the list of one-dimensional magnetic space groups. The isomorphism between these two sets of groups interchanges the elements  $\bar{1}$  and  $1'$  of the one-dimensional magnetic space groups and, respectively, the elements  $m_x$  and  $m_y$ , mirror lines perpendicular to the  $[10]$  and  $[01]$  directions, of the frieze groups.

### 1.2.17.2. Rod groups

A list of sets of symbols for the rod groups is given in Table 1.2.17.2. The information provided in the columns of this table is as follows:

Columns 1 and 2: sequential numbering and symbols used in Part 3.

Columns 3 and 4: sequential numbering and symbols listed by Bohm & Dornberger-Schiff (1966, 1967).

Columns 5, 6 and 7: sequential numbering and two sets of symbols listed by Shubnikov & Koptsik (1974).

Column 8: symbols listed by Opechowski (1986).

Column 9: symbols listed by Niggli (Chapuis, 1966).

Sets of symbols which are of a non-Hermann–Mauguin (international) type are the set of symbols in column 6 and the Niggli-type set of symbols in column 9. The set of symbols in column 8 does not use the lower-case script letter  $\rho$ , as does *IT A* (1983), to denote a one-dimensional lattice. The order of the characters indicating symmetry elements in the set of symbols in column 7 does not follow the sequence of symmetry directions used for three-dimensional space groups. The set of symbols in column 4 have the characters indicating symmetry elements along non-lattice directions enclosed in parentheses, and do not use a lower-case script letter to denote the one-dimensional lattice. Lastly, the set of symbols in column 4, without the parentheses and with the one-dimensional lattice denoted by a lower-case script  $\rho$ , are identical with the symbols in Part 3, or in some cases are the second setting of rod groups whose symbols are given in Part 3. These second-setting symbols are included in the symmetry diagrams of the rod groups.

### 1.2.17.3. Layer groups

A list of sets of symbols for the layer groups is given in Table 1.2.17.3. The information provided in the columns of this table is as follows:

Columns 1 and 2: sequential numbering and symbols used in Part 4.

Columns 3 and 4: sequential numbering and symbols listed by Wood (1964*a,b*) and Litvin & Wike (1991).

Columns 5 and 6: sequential numbering and symbols listed by Bohm & Dornberger-Schiff (1966, 1967).

Columns 7 and 8: sequential numbering and symbols listed by Shubnikov & Koptsik (1974) and Vainshtein (1981).

Column 9: symbols listed by Holser (1958).

Column 10: sequential numbering listed by Weber (1929).

Column 11: symbols listed by Hermann (1929*a,b*).

Column 12: symbols listed by Alexander & Herrmann (1929*a,b*).

Column 13: symbols listed by Niggli (Wood, 1964*a,b*).

Column 14: symbols listed by Shubnikov & Koptsik (1974).

Columns 15 and 16: symbols listed by Aroyo & Wondratschek (1987).

Column 17: symbols listed by Belov *et al.* (1957).

Columns 18 and 19: symbols and sequential numbering listed by Belov & Tarkhova (1956*a,b*).

Columns 20 and 21: symbols listed by Cochran as listed, respectively, by Cochran (1952) and Belov & Tarkhova (1956*a,b*).

Column 22: symbols listed by Opechowski (1986).

Column 23: symbols listed by Grunbaum & Shephard (1987).

Column 24: symbols listed by Woods (1935*a,b,c*, 1936).

Column 25: symbols listed by Coxeter (1986).

There is also a notation for layer groups, introduced by Janovec (1981), in which all elements in the group symbol which change the direction of the normal to the plane containing the translations are underlined, e.g.  $p4/\underline{m}$ . However, we know of no listing of all layer-group types in this notation.

Sets of symbols which are of a non-Hermann–Mauguin (international) type are the sets of symbols of the Schoenflies type (columns 11 and 12) and symbols of the ‘black and white’ symmetry type (columns 16, 17, 18, 20, 21, 22, 24 and 25). Additional non-Hermann–Mauguin (international) type sets of symbols are those in columns 14 and 23.

Sets of symbols which do not begin with a letter indicating the lattice centring type are the sets of symbols of the Niggli type (columns 13 and 15). The order of the characters indicating symmetry elements in the sets of symbols in columns 4 and 9 does not follow the sequence of symmetry directions used for three-dimensional space groups. The set of symbols in column 6 uses parentheses to denote a symmetry direction which is not a lattice direction. In addition, the set of symbols in column 6 uses upper-case letters to denote the two-dimensional lattice of the layer group, where as in *IT A* (1983) upper-case letters denote three-dimensional lattices.

The symbols in column 8 are either identical with or, in some monoclinic and orthorhombic cases, are the second-setting or alternative-cell-choice symbols of the layer groups whose symbols are given in Part 4. These second-setting and alternative-cell-choice symbols are included in the symmetry diagrams of the layer groups.

The isomorphism between layer groups and two-dimensional magnetic space groups can be seen in Table 1.2.17.3. The set of symbols which we use for layer groups is given in column 2. The sets of symbols in columns 16, 17 and 22 are sets of symbols for the two-dimensional magnetic space groups. The basic relationship between these two sets of groups is the interchanging of the magnetic symmetry element  $1'$  and the layer symmetry element  $m_z$ . A detailed discussion of the relationship between these two sets of groups has been given by Opechowski (1986).

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

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