

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

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

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

(a) Layer groups and rod groups.

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

(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  $\not\parallel 1$  (R1) and  $\not\parallel \bar{1}$  (R2), and the frieze group  $\not\parallel 1$  (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 1.2.1.2).

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

(c) Frieze groups.

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

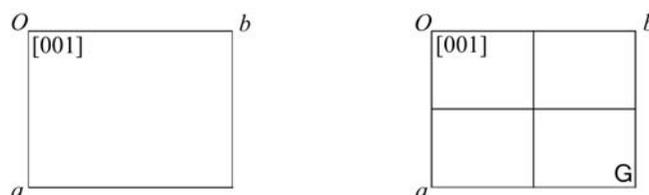


Fig. 1.2.6.5. Diagrams for orthorhombic/rectangular layer groups.

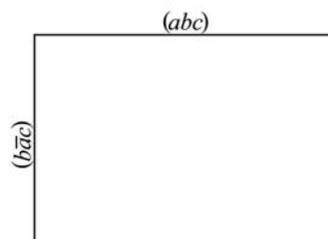


Fig. 1.2.6.6. Monoclinic/rectangular and orthorhombic/rectangular layer groups with two settings. For the second-setting symbol printed vertically, the page must be turned clockwise by 90° or viewed from the right-hand side.

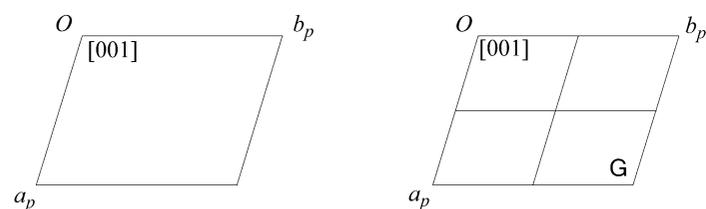


Fig. 1.2.6.1. Diagrams for triclinic/oblique layer groups.

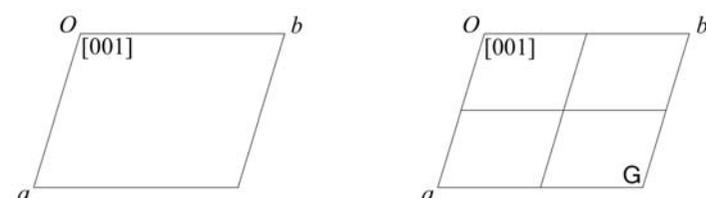


Fig. 1.2.6.2. Diagrams for monoclinic/oblique layer groups.

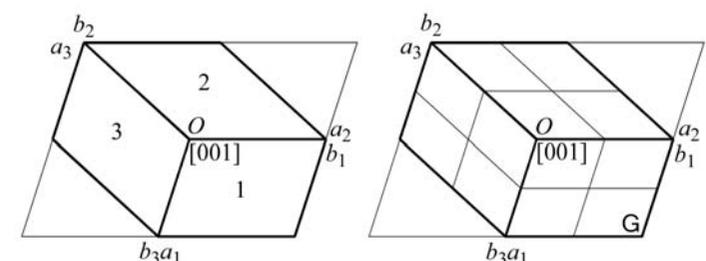


Fig. 1.2.6.3. Monoclinic/oblique layer groups Nos. 5 and 7, cell choices 1, 2, 3. The numbers 1, 2, 3 within the cells and the subscripts of the basis vectors indicate the cell choice.

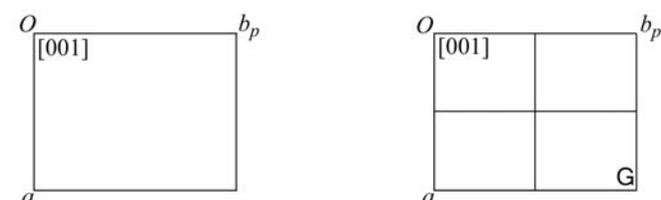


Fig. 1.2.6.4. Diagrams for monoclinic/rectangular layer groups.

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	$p2_1/b11$	$p12_1/a1$
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	$pbma$	$pmab$

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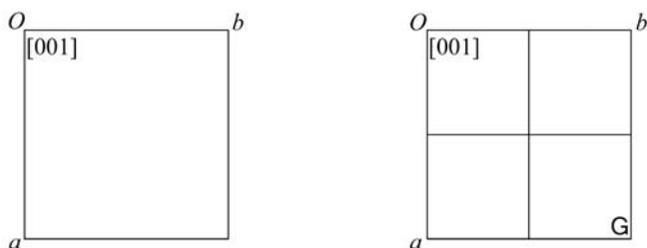


Fig. 1.2.6.7. Diagrams for square/tetragonal layer groups.

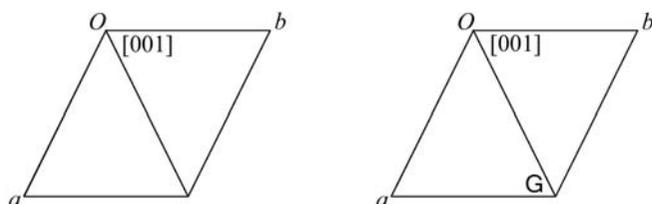


Fig. 1.2.6.8. Diagrams for trigonal/hexagonal and hexagonal/hexagonal layer groups.

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

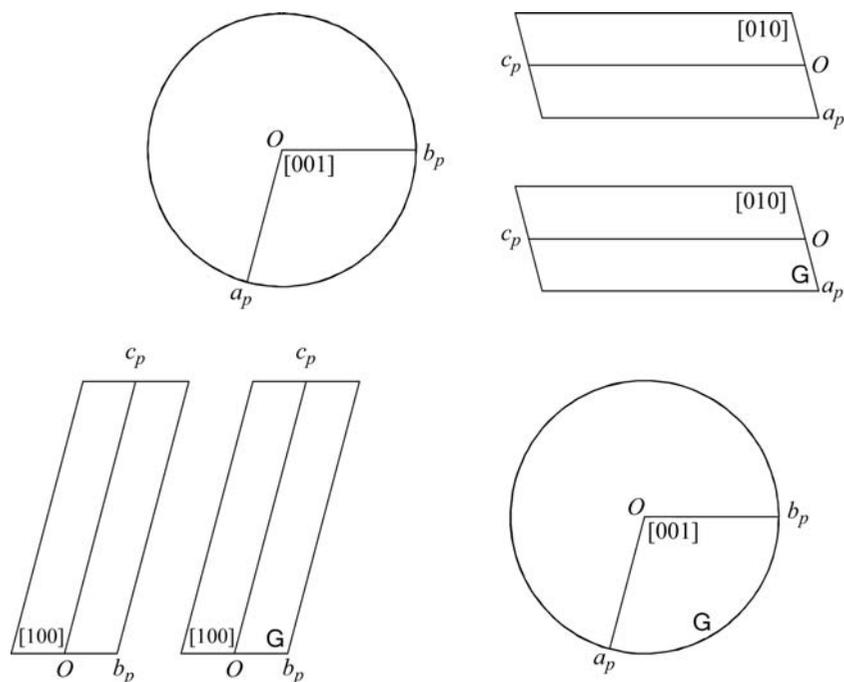


Fig. 1.2.6.9. Diagrams for triclinic rod groups.

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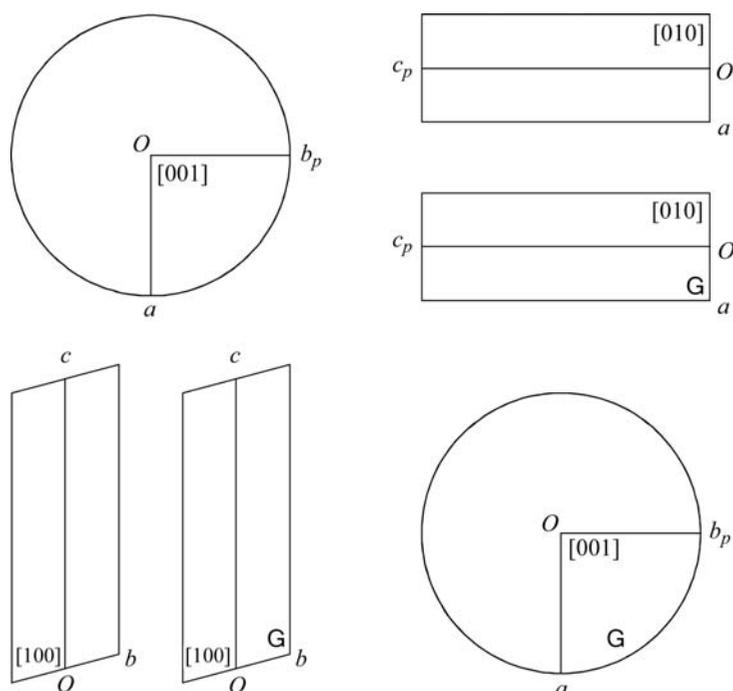


Fig. 1.2.6.10. Diagrams for monoclinic/inclined rod groups.

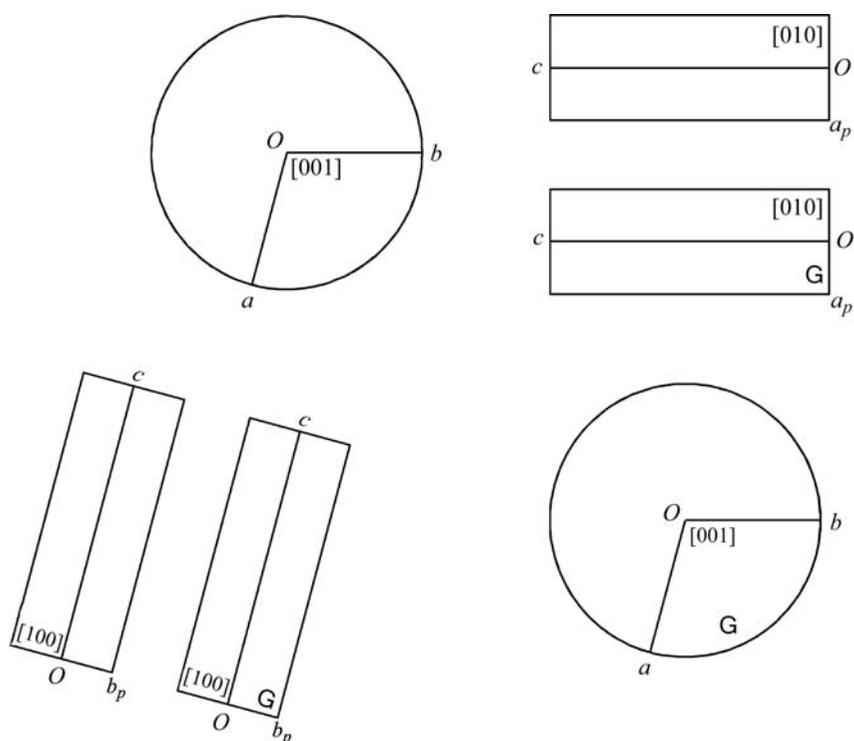


Fig. 1.2.6.11. Diagrams for monoclinic/orthogonal rod groups.

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

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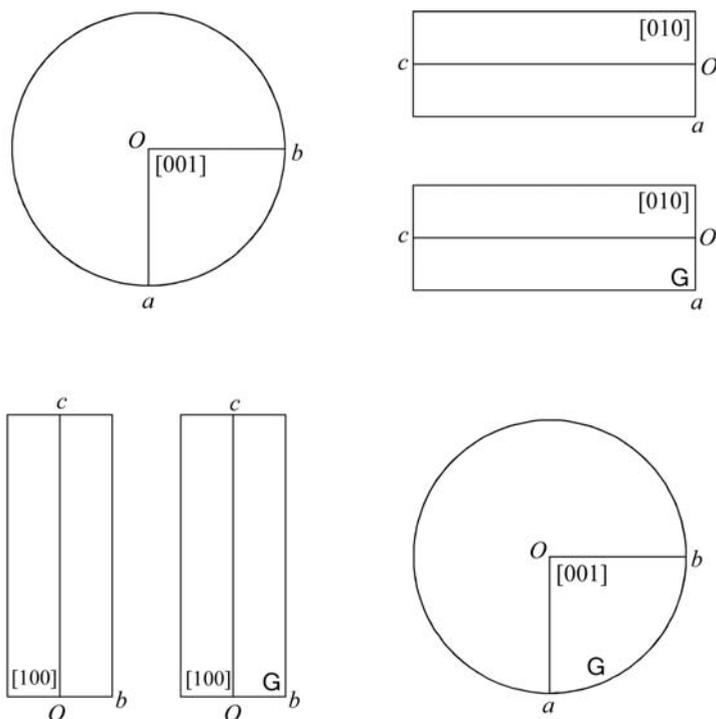


Fig. 1.2.6.12. Diagrams for orthorhombic rod groups.

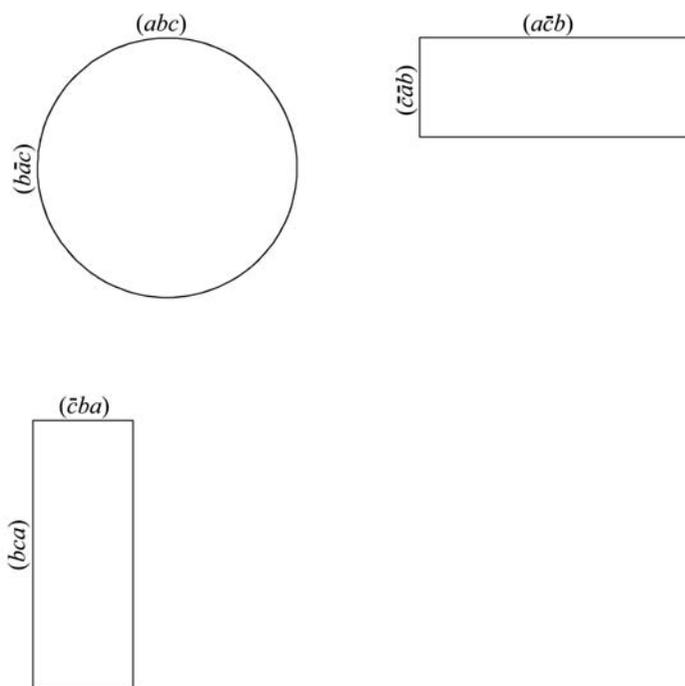


Fig. 1.2.6.13. Setting symbols on symmetry diagrams for the monoclinic/oblique, monoclinic/orthogonal and orthorhombic rod groups.

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



Fig. 1.2.6.14. Diagrams for tetragonal rod groups.



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

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.

references