

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

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

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

(a) Layer groups and rod groups.

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

(b) Frieze groups.

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

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

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

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

1.2.5. Patterson symmetry

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

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

Table 1.2.5.1. Patterson symmetries for subperiodic groups

(a) Layer groups.

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

(b) Rod groups.

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

(c) Frieze groups.

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

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

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

1.2.6. Subperiodic group diagrams

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

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

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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* (2005). 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

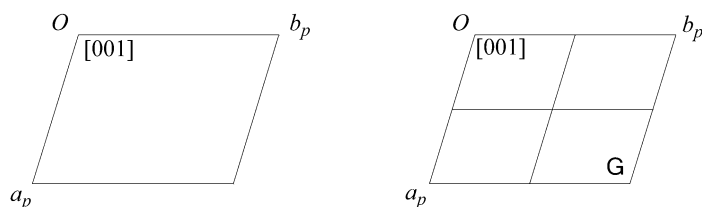


Fig. 1.2.6.1. Diagrams for triclinic/oblique layer groups.

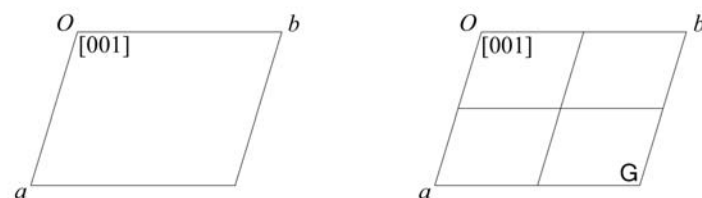


Fig. 1.2.6.2. Diagrams for monoclinic/oblique layer groups.

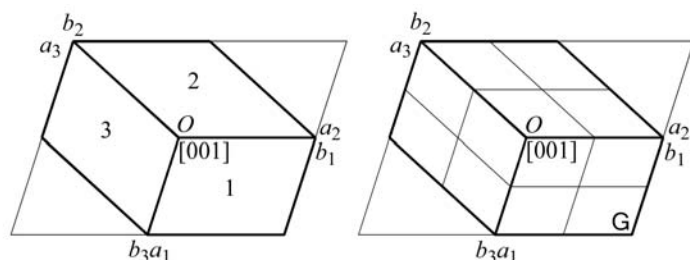


Fig. 1.2.6.3. Monoclinic/oblique layer groups Nos. 5 and 7, cell choices 1, 2, 3. The numbers 1, 2, 3 within the cells and the subscripts of the basis vectors indicate the cell choice.

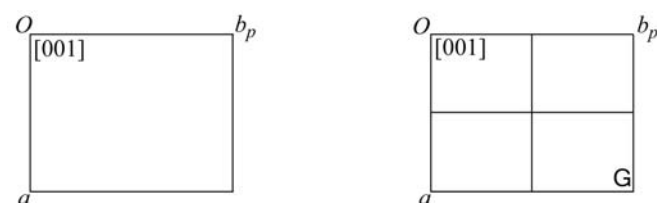


Fig. 1.2.6.4. Diagrams for monoclinic/rectangular layer groups.

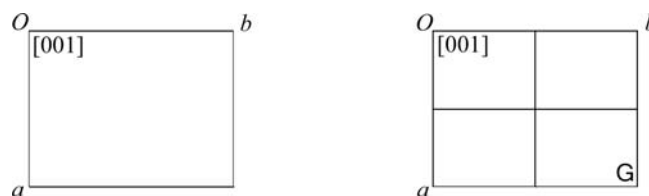


Fig. 1.2.6.5. Diagrams for orthorhombic/rectangular layer groups.

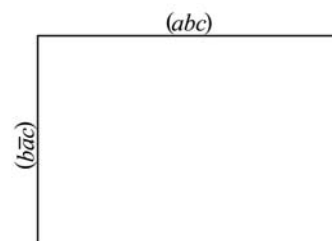


Fig. 1.2.6.6. Monoclinic/rectangular and orthorhombic/rectangular layer groups with two settings. For the second-setting symbol printed vertically, the page must be turned clockwise by 90° or viewed from the right-hand side.

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 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

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

Layer group	Setting symbol	
	(<i>abc</i>)	($\bar{b}ac$)
	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	$pbma$	$pmab$

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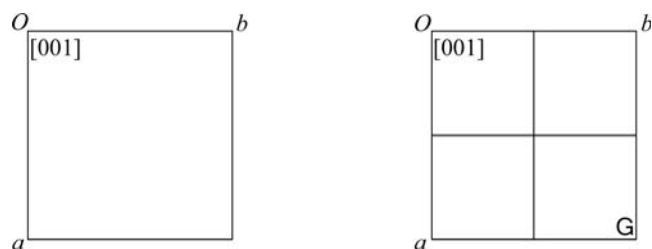


Fig. 1.2.6.7. Diagrams for square/tetragonal layer groups.

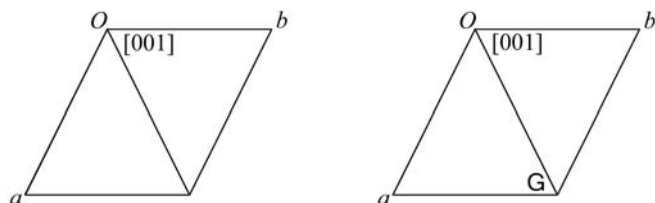


Fig. 1.2.6.8. Diagrams for trigonal/hexagonal and hexagonal/hexagonal layer groups.

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 2.2.6 of *IT A* (2005)].

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 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 the diagram with the $(b\bar{a}c)$ written horizontally, *i.e.* by rotating the page clockwise by 90° 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 pma2 (L24)

In the (abc) setting, the Hermann–Mauguin symbol is $pma2$. In the $(b\bar{a}c)$ setting, the Hermann–Mauguin symbol is $pbm2$.

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.

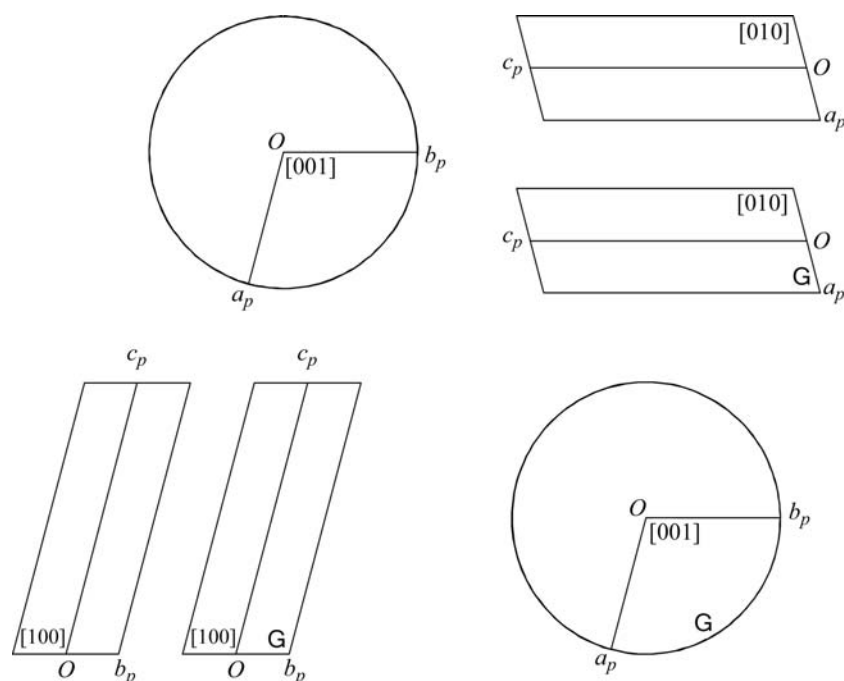


Fig. 1.2.6.9. Diagrams for triclinic rod groups.

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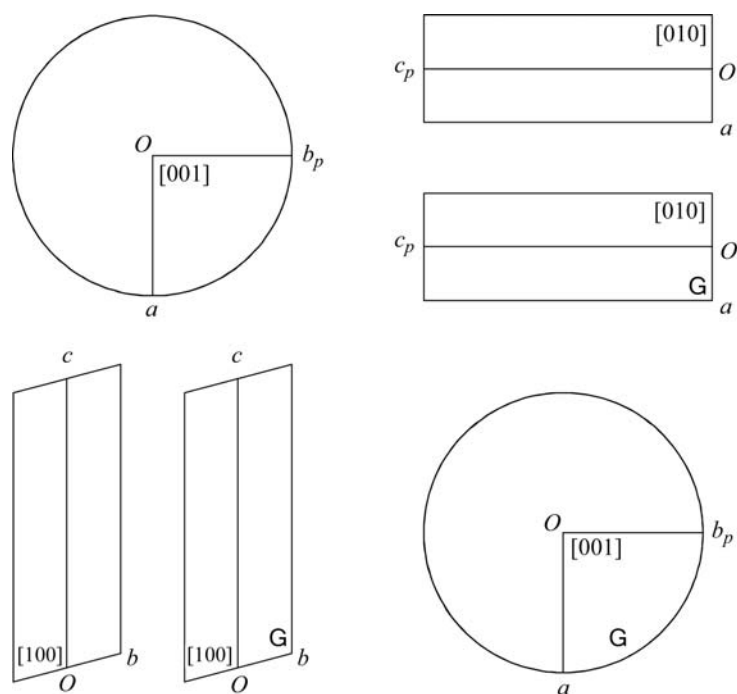


Fig. 1.2.6.10. Diagrams for monoclinic/inclined rod groups.

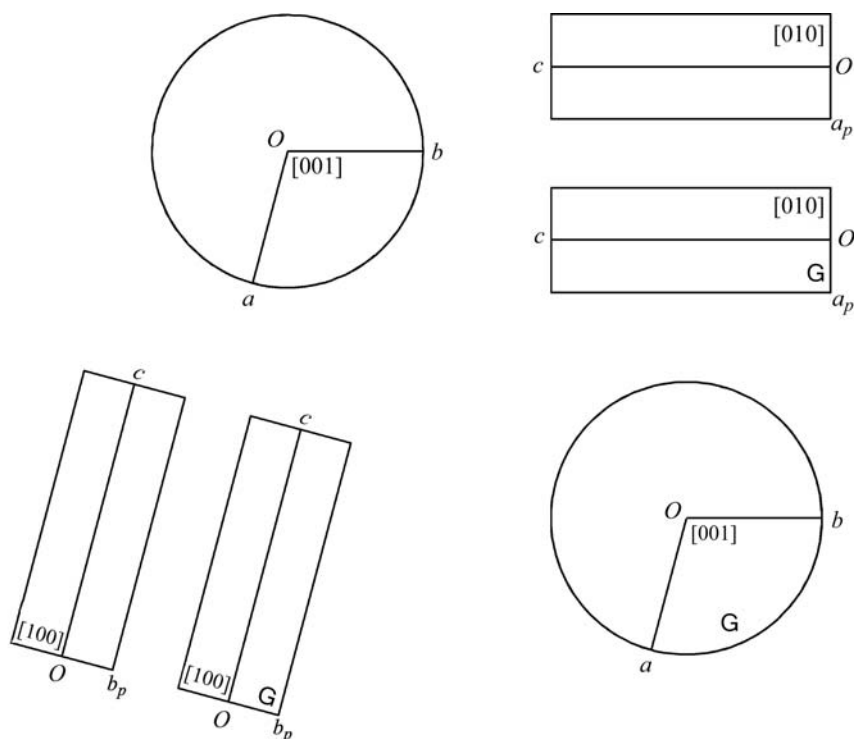


Fig. 1.2.6.11. Diagrams for monoclinic/orthogonal rod groups.

(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 \mathbf{c} lattice vector, bounded at $z=0$ and $z=1$ by planes parallel to the plane containing the \mathbf{a} and \mathbf{b} basis vectors. The projection of the \mathbf{c} lattice vector is shown explicitly. Only the *directions* of the projected non-lattice basis vectors \mathbf{a} and \mathbf{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 \mathbf{c} projection, outlined with a circle at the upper left-hand side, the \mathbf{a} projection at the lower left-hand side and the \mathbf{b} projection at the upper right-hand side. The general-position diagrams are the \mathbf{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.

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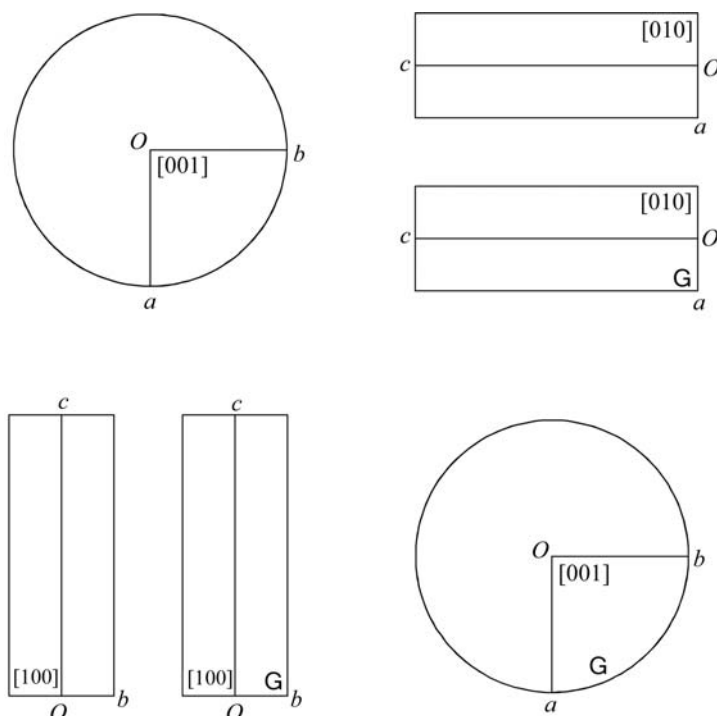


Fig. 1.2.6.12. Diagrams for orthorhombic rod groups.

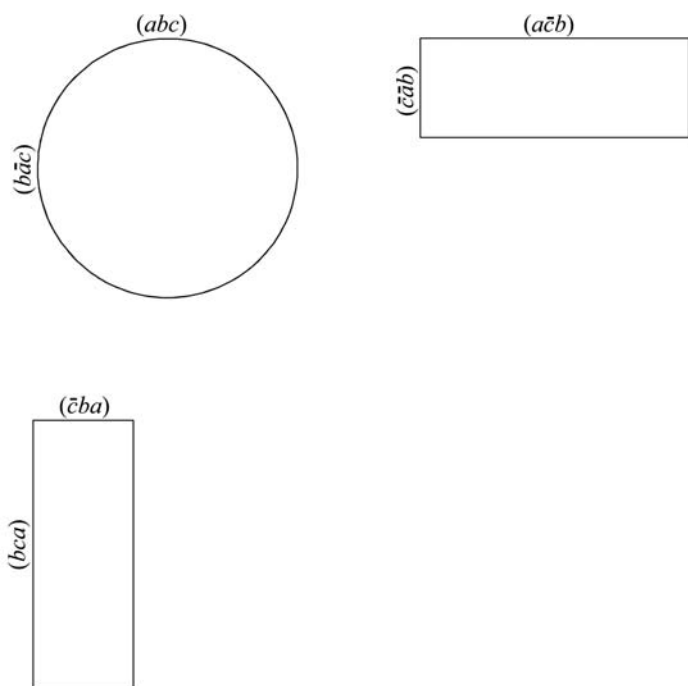


Fig. 1.2.6.13. Setting symbols on symmetry diagrams for the monoclinic/orthorhombic rod groups.

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

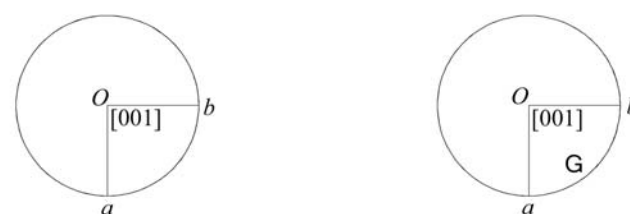


Fig. 1.2.6.14. Diagrams for tetragonal rod groups.

to the translational part of the Hermann–Mauguin symbol a subindex to the lattice symbol to denote the direction of the translations. For example, consider the rod group of the type $\rho_2 211$ (R3). The Hermann–Mauguin symbol in the conventional coordinate system in the standard (abc) setting is given by $\rho_c 211$ 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 $\rho_b 112$, 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 $\rho mc_2 2_1$ (R17)

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

Setting symbol	Hermann–Mauguin symbol
(abc)	$\rho_c mc_2 2_1$
$(\bar{b}ac)$	$\rho_c cm 2_1$
$(\bar{c}ba)$	$\rho_a 2_1 am$
(bca)	$\rho_b b 2_1 m$
$(a\bar{c}b)$	$\rho_b m 2_1 b$
$(\bar{c}ab)$	$\rho_a 2_1 ma$

For tetragonal, trigonal and hexagonal rod groups, two diagrams are given: the symmetry diagram and the general-

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

Rod group	Setting symbol					
	(abc)	($\bar{b}ac$)	($\bar{c}ba$)	(bca)	($a\bar{c}b$)	($\bar{c}ab$)
	Hermann–Mauguin symbol					
R3	$\rho_c 211$	$\rho_c 121$	$\rho_a 112$	$\rho_b 112$	$\rho_b 211$	$\rho_a 121$
R4	$\rho_c m11$	$\rho_c 1m1$	$\rho_a 11m$	$\rho_b 11m$	$\rho_b m11$	$\rho_a 1m1$
R5	$\rho_c c11$	$\rho_c 1c1$	$\rho_a 11a$	$\rho_b 11b$	$\rho_b b11$	$\rho_a 1a1$
R6	$\rho_c 2/m11$	$\rho_c 12/m1$	$\rho_a 112/m$	$\rho_b 112/m$	$\rho_b 2/m11$	$\rho_a 12/m1$
R7	$\rho_c 2/c11$	$\rho_c 12/c1$	$\rho_a 112/a$	$\rho_b 112/b$	$\rho_b 2/b11$	$\rho_a 12/a1$
R8	$\rho_c 112$	$\rho_c 112$	$\rho_a 211$	$\rho_b 121$	$\rho_b 121$	$\rho_a 211$
R9	$\rho_c 112_1$	$\rho_c 112_1$	$\rho_a 2_1 11$	$\rho_b 12_1 1$	$\rho_b 12_1 1$	$\rho_a 2_1 11$
R10	$\rho_c 11m$	$\rho_c 11m$	$\rho_a m11$	$\rho_b 1m1$	$\rho_b 1m1$	$\rho_a m11$
R11	$\rho_c 112/m$	$\rho_c 112/m$	$\rho_a 2/m11$	$\rho_b 12/m1$	$\rho_b 12/m1$	$\rho_a 2/m11$
R12	$\rho_c 112_1/m$	$\rho_c 112_1/m$	$\rho_a 2_1/m11$	$\rho_b 12_1/m1$	$\rho_b 12_1/m1$	$\rho_a 2_1/m11$
R13	$\rho_c 222$	$\rho_c 222$	$\rho_a 222$	$\rho_b 222$	$\rho_b 222$	$\rho_a 222$
R14	$\rho_c 222_1$	$\rho_c 222_1$	$\rho_a 2_1 22$	$\rho_b 22_1 2$	$\rho_b 22_1 2$	$\rho_a 2_1 22$
R15	$\rho_c mm2$	$\rho_c mm2$	$\rho_a 2mm$	$\rho_b m2m$	$\rho_b m2m$	$\rho_a 2mm$
R16	$\rho_c cc2$	$\rho_c cc2$	$\rho_a 2aa$	$\rho_b b2b$	$\rho_b b2b$	$\rho_a 2aa$
R17	$\rho_c mc2_1$	$\rho_c cm2_1$	$\rho_a 2_1 am$	$\rho_b b2_1 m$	$\rho_b m2_1 b$	$\rho_a 2_1 ma$
R18	$\rho_c 2mm$	$\rho_c m2m$	$\rho_a mm2$	$\rho_b mm2$	$\rho_b 2mm$	$\rho_a m2m$
R19	$\rho_c 2cm$	$\rho_c c2m$	$\rho_a ma2$	$\rho_b bm2$	$\rho_b 2mb$	$\rho_a m2a$
R20	$\rho_c mmm$	$\rho_c mmm$	$\rho_a mmm$	$\rho_b mmm$	$\rho_b mmm$	$\rho_a mmm$
R21	$\rho_c ccm$	$\rho_c ccm$	$\rho_a maa$	$\rho_b bmb$	$\rho_b bmb$	$\rho_a maa$
R22	$\rho_c mcm$	$\rho_c cmm$	$\rho_a mam$	$\rho_b bmm$	$\rho_b mmb$	$\rho_a mma$

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	$\rho_4 2cm$	$\rho_4 2mc$
R37	$\rho_4 2m$	$\rho_4 2m$
R38	$\rho_4 2c$	$\rho_4 2c$
R41	$\rho_4 2/mmc$	$\rho_4 2/mcm$



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

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	$\rho_3 312$	$\rho_3 321$
R47	$\rho_3 1,12$	$\rho_3 1,21$
R48	$\rho_3 2,12$	$\rho_3 2,21$
R49	$\rho_3 m1$	$\rho_3 31m$
R50	$\rho_3 c1$	$\rho_3 31c$
R51	$\rho_3 \bar{3}1m$	$\rho_3 \bar{3}m1$
R52	$\rho_3 \bar{3}1c$	$\rho_3 \bar{3}c1$
R70	$\rho_6 3mc$	$\rho_6 3cm$
R71	$\rho_6 \bar{6}m2$	$\rho_6 \bar{6}2m$
R72	$\rho_6 \bar{6}c2$	$\rho_6 \bar{6}2c$
R75	$\rho_6 3/mmc$	$\rho_6 3/mcm$

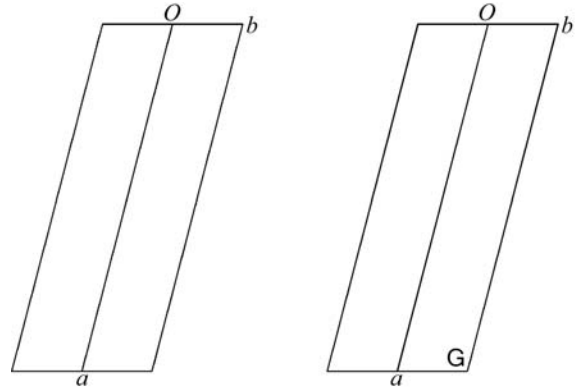


Fig. 1.2.6.16. Diagrams for oblique frieze groups.

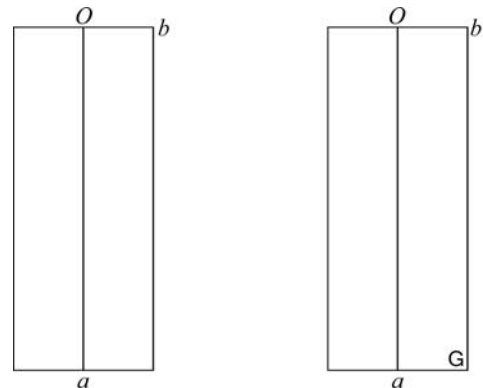


Fig. 1.2.6.17. Diagrams for rectangular frieze groups.

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 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

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

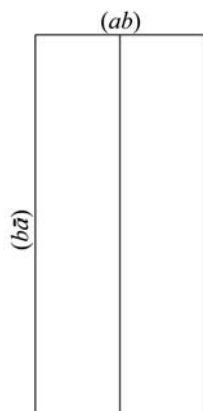


Fig. 1.2.6.18. The two settings for frieze groups. For the second setting, printed vertically, the page must be turned 90° clockwise or viewed from the right-hand side.

($2a + b \bar{a} + b c$) 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 $\rho 3m1$ and in the second setting where the symbol is $\rho 31m$. 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.

1.2.7. 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.

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

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	$\rho_a 1$	$\rho_b 1$
F2	$\rho_a 211$	$\rho_b 211$
F3	$\rho_a 1m1$	$\rho_b 11m$
F4	$\rho_a 11m$	$\rho_b 1m1$
F5	$\rho_a 11g$	$\rho_b 1g1$
F6	$\rho_a 2mm$	$\rho_b 2mm$
F7	$\rho_a 2mg$	$\rho_b 2gm$

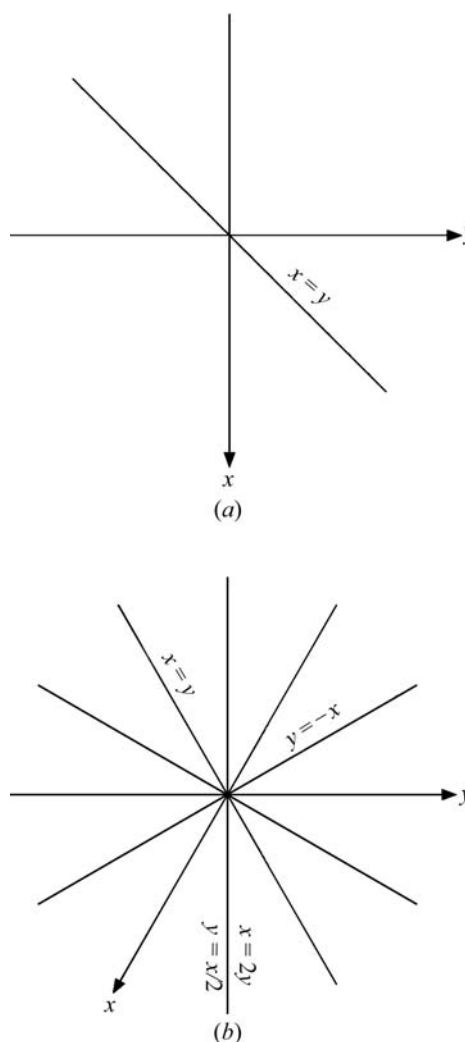


Fig. 1.2.8.1. Boundaries used to define the asymmetric unit for (a) tetragonal rod groups and (b) trigonal and hexagonal rod groups.

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,