

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

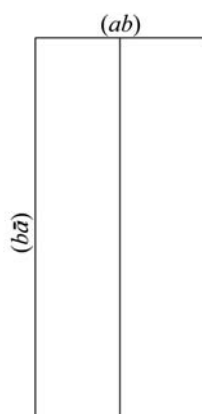


Fig. 1.2.6.18. The two settings for frieze groups. For the second setting, printed vertically, the page must be turned 90° clockwise or viewed from the right-hand side.

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 $\rho 2mm$ (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	$\rho_a 1$	$\rho_b 1$
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	$\rho_a 2mg$	$\rho_b 2gm$

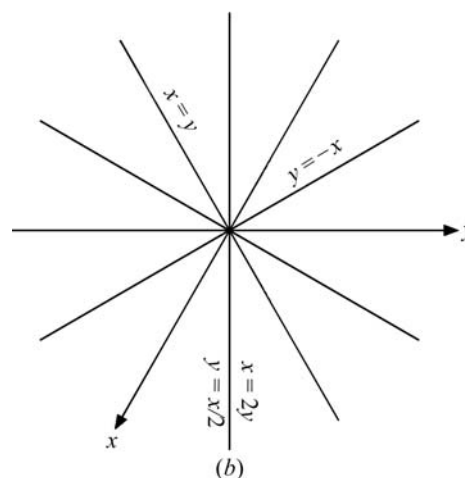
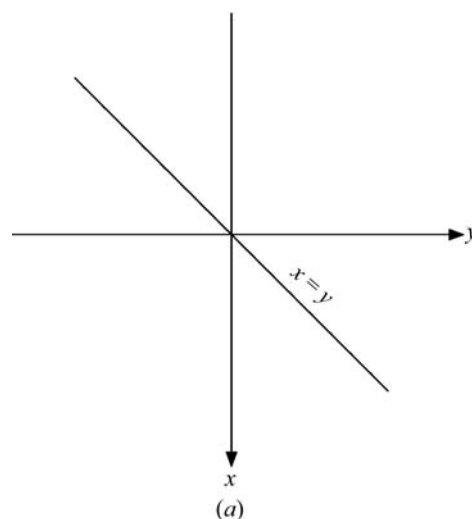


Fig. 1.2.8.1. Boundaries used to define the asymmetric unit for (a) tetragonal rod groups and (b) trigonal and hexagonal rod groups.

Example: The rod group $\rho 6_3mc$ (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

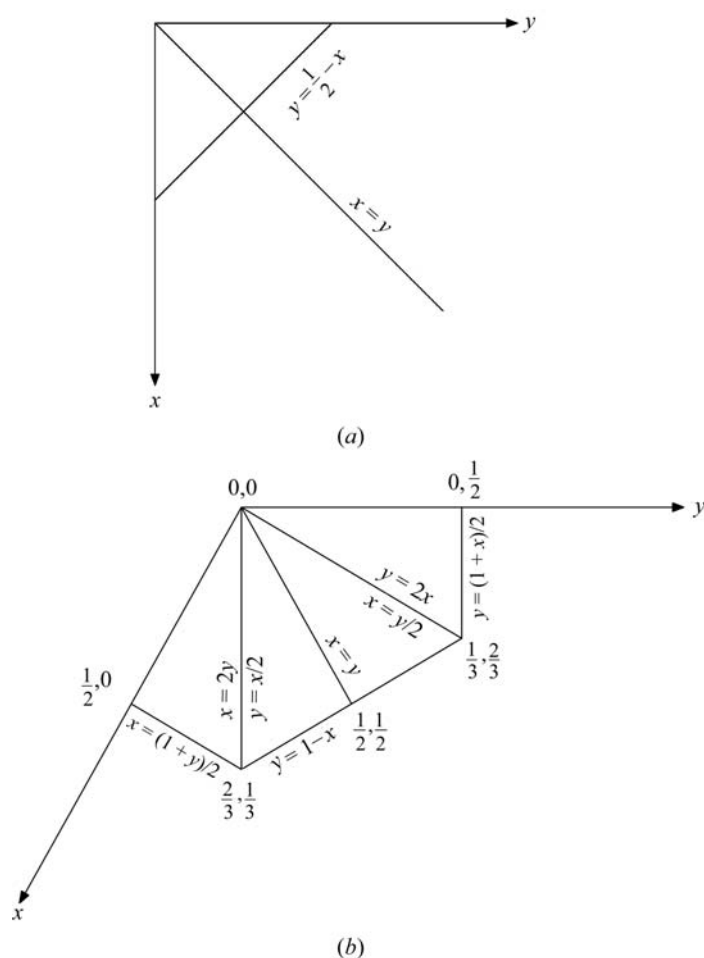


Fig. 1.2.8.2. Boundaries used to define the asymmetric unit for (a) tetragonal/square layer groups and (b) trigonal/hexagonal and hexagonal/hexagonal layer groups. In (b), the coordinates (x, y) of the vertices of the asymmetric unit with the $z = 0$ plane are also given.

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° 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

references