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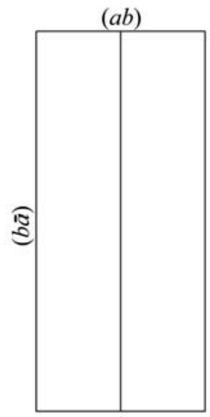

Fig. 1.2.6.18. The two settings for frieze groups. For the second setting, printed vertically, the page must be turned 90° clockwise or viewed from the right-hand side.

$(2a+b\ \bar{a}+b\ c)$ 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 $\not{p}3m1$ and in the second setting where the symbol is $\not{p}31m$. 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.

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

Frieze group	Setting symbol (ab)	Setting symbol $(b\bar{a})$
	Hermann–Mauguin symbol	
F1	$\not{p}_a1$	$\not{p}_b1$
F2	$\not{p}_a211$	$\not{p}_b211$
F3	$\not{p}_a1m1$	$\not{p}_b11m$
F4	$\not{p}_a11m$	$\not{p}_b1m1$
F5	$\not{p}_a11g$	$\not{p}_b1g1$
F6	$\not{p}_a2mm$	$\not{p}_b2mm$
F7	$\not{p}_a2mg$	$\not{p}_b2gm$

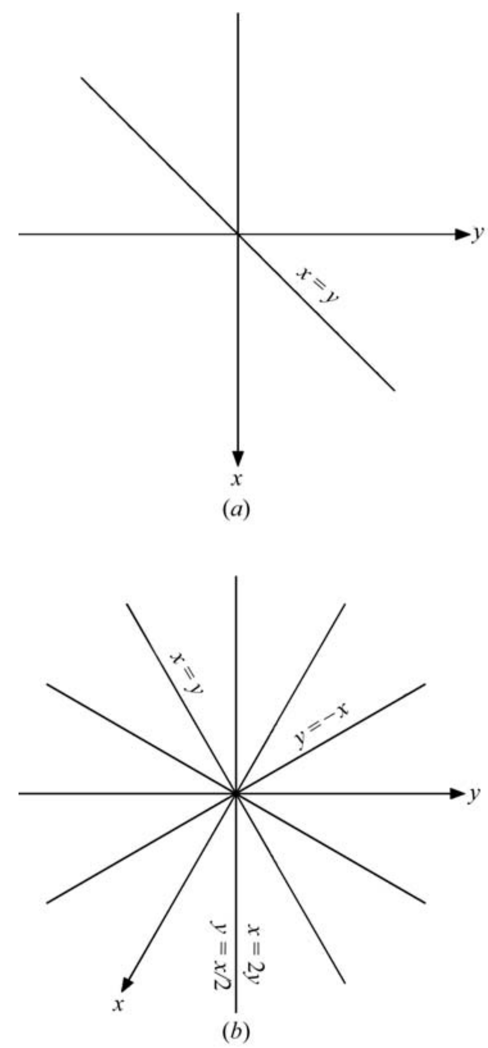

Fig. 1.2.8.1. Boundaries used to define the asymmetric unit for (a) tetragonal rod groups and (b) trigonal and hexagonal rod groups.

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.

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,

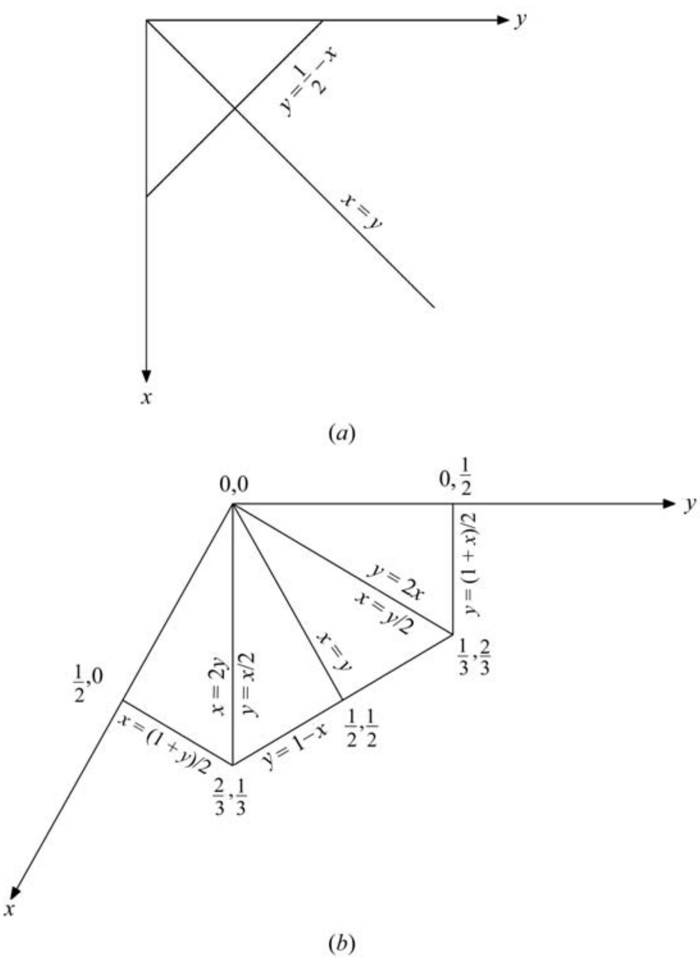

Fig. 1.2.8.2. Boundaries used to define the asymmetric unit for (*a*) tetragonal/square layer groups and (*b*) trigonal/hexagonal and hexagonal/hexagonal layer groups. In (*b*), the coordinates (x, y) of the vertices of the asymmetric unit with the $z = 0$ plane are also given.

because they contain three-dimensional (two-dimensional) translational symmetry, the asymmetric unit is a finite part of space [see Section 2.2.8 of *IT* A (2005)]. 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

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

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

Example: The frieze group $\not{p}2mm$ *(F6)*

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

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

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

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 $x \le y$ and $y \le x/2$. Fig. 1.2.8.1 schematically shows the boundaries represented by such inequalities.

Example: The rod group $\not{p}6_3mc$ *(R70)*

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

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

$$0 \le x \le \text{upper limit on } x$$
$$0 \le y \le \text{upper limit on } y.$$

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

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 $0 \le x \le 2/3;\ 0 \le y \le 2/3;\ x \le 2y;$
$y \le \min(1 - x, 2x)$

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 2.2.3, 8.1.5 and 11.1.1 of *IT* A (2005)]. 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). Below the geometric description we give the Seitz notation (Burns & Glazer, 1990) of each symmetry operation using the subindex notation of Zak *et al.* (1969).

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