

1.2. GUIDE TO THE USE OF THE SUBPERIODIC GROUP TABLES

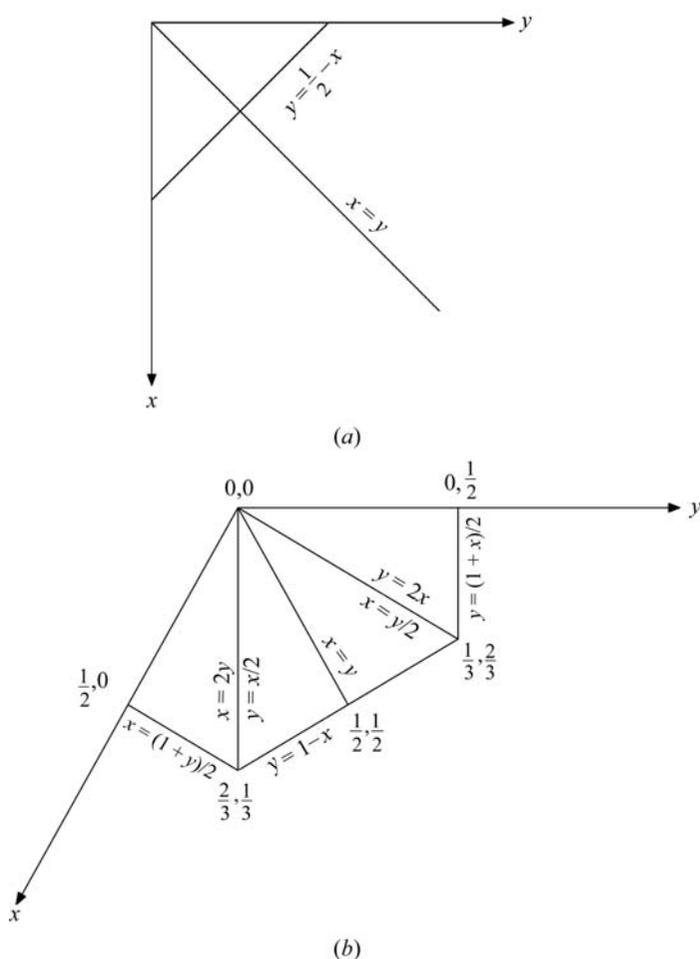


Fig. 1.2.8.2. Boundaries used to define the asymmetric unit for (a) tetragonal/square layer groups and (b) trigonal/hexagonal and hexagonal/hexagonal layer groups. In (b), the coordinates (x, y) of the vertices of the asymmetric unit with the $z = 0$ plane are also given.

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).

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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