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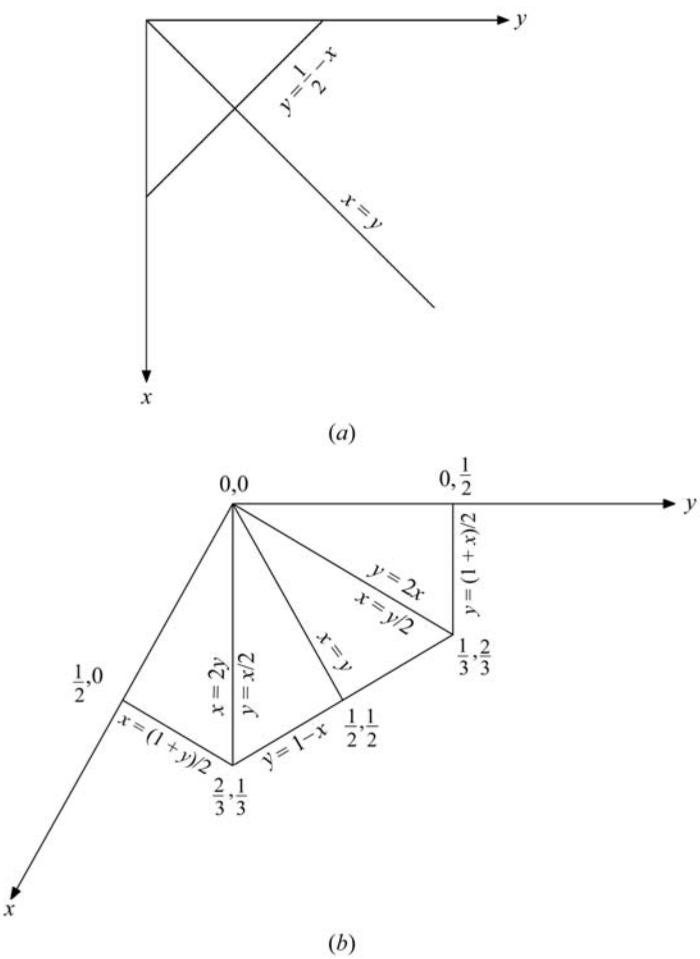

Fig. 1.2.8.2. Boundaries used to define the asymmetric unit for (*a*) tetragonal/square layer groups and (*b*) trigonal/hexagonal and hexagonal/hexagonal layer groups. In (*b*), the coordinates (x, y) of the vertices of the asymmetric unit with the $z = 0$ plane are also given.

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 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.* Chapter 1.2 of *IT* A (2005)], 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 11.1.2 of *IT* A (2005).

Examples

(1) $m \quad x, 0, z$: a reflection through the plane $x, 0, z$, *i.e.* the plane parallel to (010) containing the point (0, 0, 0).

(2) $m \quad x + 1/2, \bar{x}, z$: 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) $g(1/2, 1/2, 0) \quad x, x, z$: glide reflection with glide component (1/2, 1/2, 0) through the plane x, x, z, *i.e.* the plane parallel to $(1\bar{1}0)$ containing the point (0, 0, 0).

(4) $2(1/2, 0, 0) \quad x, 1/4, 0$: screw rotation along the (100) direction containing the point (0, 1/4, 0) with a screw component (1/2, 0, 0).

(5) $\bar{4}^{-} \quad 1/2, 0, z \quad 1/2, 0, 0$: 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 additional centring translation $t(1/2, 1/2, 0)$. The additional generators are given as numbers (p) which refer to the corresponding coordinate triplets of the general position and the corresponding entries under *Symmetry operations*; for centred layer groups, the first block 'For (0, 0, 0)+ set' must be used.

1.2.11. Positions

The entries under *Positions* (more explicitly called *Wyckoff positions*) consist of the *General position* (upper block) and the *Special positions* (blocks below). The columns in each block, from left to right, contain the following information for each Wyckoff position.

(i) *Multiplicity M* of the Wyckoff position. This is the number of equivalent points per conventional cell. The multiplicity M of the general position is equal to the order of the point group of the subperiodic group, except in the case of centred layer groups when it is twice the order of the point group. The multiplicity M of a special position is equal to the order of the point group of the subperiodic group divided by the order of the site-symmetry group (see Section 1.2.12).

(ii) *Wyckoff letter*. This letter is a coding scheme for the Wyckoff positions, starting with a at the bottom position and continuing upwards in alphabetical order.

(iii) *Site symmetry*. This is explained in Section 1.2.12.

(iv) *Coordinates*. The sequence of the coordinate triplets is based on the *Generators*. For the centred layer groups, the centring translations (0, 0, 0)+ and (1/2, 1/2, 0)+ are listed above the coordinate triplets. The symbol '+' indicates that in order to obtain a complete Wyckoff position, the components of these centring translations have to be added to the listed coordinate triplets.

(v) *Reflection conditions*. These are described in Section 1.2.13.

The two types of positions, general and special, are characterized as follows:

(i) *General position*. A set of symmetrically equivalent points is said to be in a 'general position' if each of its points is left invariant only by the identity operation but by no other symmetry operation of the subperiodic group.

(ii) *Special position(s)*. A set of symmetrically equivalent points is said to be in a 'special position' if each of its points is mapped onto itself by at least one additional operation in addition to the identity operation.

Example: Layer group $c2/m11$ (L18)

The general position $8f$ of this layer group contains eight equivalent points per cell each with site symmetry 1. The coordinate triplets of four points (1) to (4) are given explicitly, the coordinate triplets of the other four points are obtained by adding the components (1/2, 1/2, 0) of the c-centring translation to the coordinate triplets (1) to (4).

This layer group has five special positions with the Wyckoff letters a to e. The product of the multiplicity and the order of the site-symmetry group is the multiplicity of the general position. For position $4d$, for example, the four equivalent points have the coordinates $x, 0, 0$, $\bar{x}, 0, 0$, $x + 1/2, 1/2, 0$ and $\bar{x} + 1/2, 1/2, 0$. Since each point of position $4d$ is mapped onto itself by a twofold rotation, the multiplicity of the position is reduced from eight to four, whereas the order of the site symmetry is increased from one to two.

1.2.12. Oriented site-symmetry symbols

The third column of each Wyckoff position gives the *site symmetry* of that position. The site-symmetry group is isomorphic to a proper or improper subgroup of the point group to which the subperiodic group under consideration belongs. *Oriented site-symmetry symbols* are used to show how the symmetry elements at a site are related to the conventional crystallographic basis. The site-symmetry symbols display the same sequence of symmetry directions as the subperiodic group symbol (*cf.* Table 1.2.4.1). Sets of equivalent symmetry directions that do not contribute any element to the site-symmetry group are represented by a dot. Sets of symmetry directions having more than one equivalent direction may require more than one character if

references