International Tables for Crystallography (2006). Vol. A, Section 2.2.9.2, pp. 26–27.

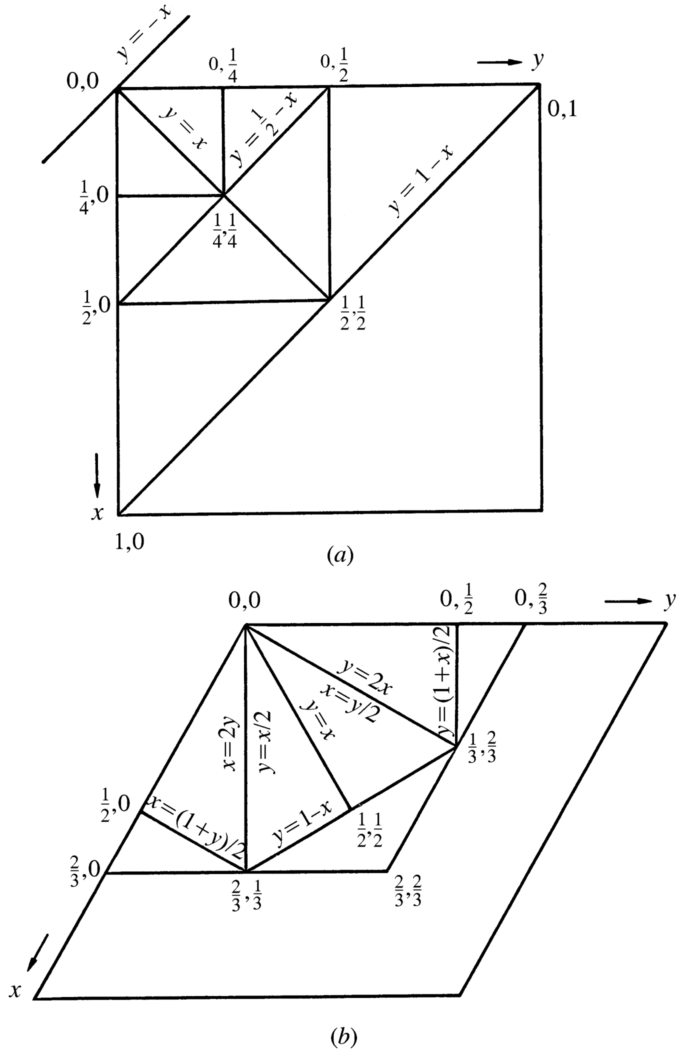

Fig. 2.2.8.1. Boundary planes of asymmetric units occurring in the space-group tables. (*a*) Tetragonal system. (*b*) Trigonal and hexagonal systems. The point coordinates refer to the vertices in the plane $z = 0$.

The asymmetric unit is defined by

$$0 \le x \le \tfrac{2}{3};\quad 0 \le y \le \tfrac{2}{3};\quad 0 \le z \le \tfrac{1}{6};$$
$$x \le (1+y)/2;\quad y \le \min(1-x, (1+x)/2)$$
$$\text{Vertices:}\quad 0,0,0\quad \tfrac{1}{2},0,0\quad \tfrac{2}{3},\tfrac{1}{3},0\quad \tfrac{1}{3},\tfrac{2}{3},0\quad 0,\tfrac{1}{2},0$$
$$0,0,\tfrac{1}{6}\quad \tfrac{1}{2},0,\tfrac{1}{6}\quad \tfrac{2}{3},\tfrac{1}{3},\tfrac{1}{6}\quad \tfrac{1}{3},\tfrac{2}{3},\tfrac{1}{6}\quad 0,\tfrac{1}{2},\tfrac{1}{6}.$$

It is obvious that the indication of the vertices is of great help in drawing the asymmetric unit.

Fourier syntheses

For complicated space groups, the easiest way to calculate Fourier syntheses is to consider the parallelepiped listed, without taking into account the additional boundary planes of the asymmetric unit. These planes should be drawn afterwards in the Fourier synthesis. For the computation of integrated properties from Fourier syntheses, such as the number of electrons for parts of the structure, the values at the boundaries of the asymmetric unit must be applied with a reduced weight if the property is to be obtained as the product of the content of the asymmetric unit and the multiplicity.

Example

In the parallelepiped of space group *Pmmm* (47), the weights for boundary planes, edges and vertices are $\frac{1}{2}$, $\frac{1}{4}$ and $\frac{1}{8}$, respectively.

Asymmetric units of the plane groups have been discussed by Buerger (1949, 1960) in connection with Fourier summations.

2.2.9. Symmetry operations

As explained in Sections 8.1.6 and 11.1.1, the coordinate triplets of the *General position* of a space group may be interpreted as a shorthand description of the symmetry operations in matrix notation. The geometric description of the symmetry operations is found in the space-group tables under the heading *Symmetry operations*.

2.2.9.1. *Numbering scheme*

The numbering $(1)\ldots(p)\ldots$ 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 space groups with *primitive* cells, both lists contain the same number of entries.

For space groups with *centred* cells, to the one block *General position* several (2, 3 or 4) blocks *Symmetry operations* correspond. The numbering scheme of the general position is applied to each one of these blocks. The number of blocks equals the multiplicity of the centred cell, *i.e.* the number of centring translations below the subheading *Coordinates*, such as $(0,0,0)+$, $(\frac{2}{3},\frac{1}{3},\frac{1}{3})+$, $(\frac{1}{3},\frac{2}{3},\frac{2}{3})+$.

Whereas for the *Positions* the reader is expected to add these centring translations to each printed coordinate triplet himself (in order to obtain the complete general position), for the *Symmetry operations* the corresponding data are listed explicitly. The different blocks have the subheadings 'For (0,0,0)+ set', 'For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set', *etc.* Thus, an obvious one-to-one correspondence exists between the analytical description of a symmetry operation in the form of its general-position coordinate triplet and the geometrical description under *Symmetry operations*. Note that the coordinates are reduced modulo 1, where applicable, as shown in the example below.

Example: Ibca (73)

The centring translation is $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$. Accordingly, above the general position one finds $(0,0,0)+$ and $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$. In the block *Symmetry operations*, under the subheading 'For $(0,0,0)+$ set', entry (2) refers to the coordinate triplet $\bar{x}+\frac{1}{2},\ \bar{y},\ z+\frac{1}{2}$. Under the subheading 'For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set', however, entry (2) refers to $\bar{x},\ \bar{y}+\frac{1}{2},\ z$. The triplet $\bar{x},\ \bar{y}+\frac{1}{2},\ z$ is selected rather than $\bar{x}+1,\ \bar{y}+\frac{1}{2},\ z+1$, because the coordinates are reduced modulo 1.

In space groups with two origins where a 'symmetry element' and an 'additional symmetry element' are of different type (*e.g.* mirror *versus* glide plane, rotation *versus* screw axis, Tables 4.1.2.2 and 4.1.2.3), the origin shift may interchange the two *different* types in the *same* location (referred to the appropriate origin) under the same number (*p*). Thus, in $P4/nmm$ (129), (*p*) = (7) represents a $\bar{2}$ and a 2_1 axis, both in $x,x,0$, whereas (*p*) = (16) represents a *g* and an *m* plane, both in x,x,z.

2.2.9.2. *Designation of symmetry operations*

An entry in the block *Symmetry operations* is characterized as follows.

(i) A symbol denoting the *type* of the symmetry operation (*cf.* Chapter 1.3), 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 $a(\frac{1}{2},0,0) \equiv a$; $b(0,\frac{1}{2},0) \equiv b$; $c(0,0,\frac{1}{2}) \equiv c$. 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 given in addition.

Details of this symbolism are presented in Section 11.1.2.

Examples

(1) $a\ \ x,y,\frac{1}{4}$
Glide reflection with glide component $(\frac{1}{2},0,0)$ through the plane $x,y,\frac{1}{4}$, *i.e.* the plane parallel to (001) at $z=\frac{1}{4}$.

(2) $\bar{4}^{+}\ \ \frac{1}{4},\frac{1}{4},z;\ \ \frac{1}{4},\frac{1}{4},\frac{1}{4}$
Fourfold rotoinversion, consisting of a counter clockwise rotation by 90° around the line $\frac{1}{4},\frac{1}{4},z$, followed by an inversion through the point $\frac{1}{4},\frac{1}{4},\frac{1}{4}$.

(3) $g(\frac{1}{4},\frac{1}{4},\frac{1}{2})\ \ x,x,z$
Glide reflection with glide component $(\frac{1}{4},\frac{1}{4},\frac{1}{2})$ through the plane x,x,z, *i.e.* the plane parallel to $(1\bar{1}0)$ containing the point 0, 0, 0.

(4) $g(\frac{1}{3},\frac{1}{6},\frac{1}{6})\ \ 2x-\frac{1}{2},x,z$ (hexagonal axes)
Glide reflection with glide component $(\frac{1}{3},\frac{1}{6},\frac{1}{6})$ through the plane $2x-\frac{1}{2},x,z$, *i.e.* the plane parallel to $(1\bar{2}10)$, which intersects the *a* axis at $-\frac{1}{2}$ and the *b* axis at $\frac{1}{4}$; this operation occurs in $R\bar{3}c$ (167, hexagonal axes).

(5) Symmetry operations in *Ibca* (73)
Under the subheading 'For (0, 0, 0)+ set', the operation generating the coordinate triplet (2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$ from (1) *x*, *y*, *z* is symbolized by $2(0,0,\frac{1}{2})\ \ \frac{1}{4},0,z$. This indicates a twofold screw rotation with screw part $(0,0,\frac{1}{2})$ for which the corresponding screw axis coincides with the line $\frac{1}{4},0,z$, *i.e.* runs parallel to [001] through the point $\frac{1}{4},0,0$. Under the subheading 'For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$+ set', the operation generating the coordinate triplet (2) $\bar{x},\bar{y}+\frac{1}{2},z$ from (1) *x*, *y*, *z* is symbolized by $2\ \ 0,\frac{1}{4},z$. It is thus a twofold rotation (without screw part) around the line $0,\frac{1}{4},z$.

2.2.10. 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*. Generating translations are listed as *t*(1, 0, 0), *t*(0, 1, 0), *t*(0, 0, 1); likewise for additional centring translations. The other symmetry operations are given as numbers (*p*) that refer to the corresponding coordinate triplets of the general position and the corresponding entries under *Symmetry operations*, as explained in Section 2.2.9 [for centred space groups the first block 'For (0, 0, 0)+ set' must be used].

For all space groups, the identity operation given by (1) is selected as the first generator. It is followed by the generators *t*(1, 0, 0), *t*(0, 1, 0), *t*(0, 0, 1) of the integral lattice translations and, if necessary, by those of the centring translations, *e.g.* $t(\frac{1}{2},\frac{1}{2},0)$ for a *C* lattice. In this way, point *x, y, z* and all its translationally equivalent points are generated. (The remark 'and its translationally equivalent points' will hereafter be omitted.) The sequence chosen for the generators following the translations depends on the crystal class of the space group and is set out in Table 8.3.5.1 of Section 8.3.5.

Example: $P12_1/c1$ (14, unique axis *b*, cell choice 1)
After the generation of (1) *x*, *y*, *z*, the operation (2) which stands for a twofold screw rotation around the axis $0,y,\frac{1}{4}$ generates point (2) of the general position with coordinate triplet $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$. Finally, the inversion (3) generates point (3) $\bar{x},\bar{y},\bar{z}$ from point (1), and point (4′) $x,\bar{y}-\frac{1}{2},z-\frac{1}{2}$ from point (2). Instead of (4′), however, the coordinate triplet (4) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$ is listed, because the coordinates are reduced modulo 1.

The example shows that for the space group $P12_1/c1$ two operations, apart from the identity and the generating translations, are sufficient to generate all symmetrically equivalent points. Alternatively, the inversion (3) plus the glide reflection (4), or the glide reflection (4) plus the twofold screw rotation (2), might have been chosen as generators. The process of generation and the selection of the generators for the space-group tables, as well as the resulting sequence of the symmetry operations, are discussed in Section 8.3.5.

For different descriptions of the same space group (settings, cell choices, origin choices), the generating operations are the same. Thus, the transformation relating the two coordinate systems transforms also the generators of one description into those of the other.

From the Fifth Edition onwards, this applies also to the description of the seven rhombohedral (*R*) space groups by means of 'hexagonal' and 'rhombohedral' axes. In previous editions, there was a difference in the *sequence* (not the data) of the 'coordinate triplets' and the 'symmetry operations' in both descriptions (*cf.* Section 2.10 in the First to Fourth Editions).

2.2.11. Positions

The entries under *Positions** (more explicitly called *Wyckoff positions*) consist of the one *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 unit cell. For primitive cells, the multiplicity *M* of the general position is equal to the order of the point group of the space group; for centred cells, *M* is the product of the order of the point group and the number (2, 3 or 4) of lattice points per cell. The multiplicity of a special position is always a divisor of the multiplicity of the general position.

(ii) *Wyckoff letter*. This letter is merely a coding scheme for the Wyckoff positions, starting with *a* at the bottom position and continuing upwards in alphabetical order (the theoretical background on Wyckoff positions is given in Section 8.3.2).

(iii) *Site symmetry*. This is explained in Section 2.2.12.

(iv) *Coordinates*. The sequence of the coordinate triplets is based on the *Generators* (*cf.* Section 2.2.10). For centred space groups, the centring translations, for instance $(0,0,0)+\ (\frac{1}{2},\frac{1}{2},\frac{1}{2})+$, are listed above the coordinate triplets. The symbol '+' indicates that, in order to obtain a complete Wyckoff position, the components of

* The term *Position* (singular) is defined as a *set* of symmetrically equivalent points, in agreement with *IT* (1935): Point position; *Punktlage* (German); *Position* (French). Note that in *IT* (1952) the plural, equivalent positions, was used.

references