$\frac{1}{2}+$ or $\frac{1}{3}-$, the relative z or y coordinate is $\frac{1}{2}$ *etc.* higher than that of the point with symbol + or −.

Points represented by ◯ and ⊙ are related by inversion, rotoinversion or mirror symmetry and are thus enantiomorphs of each other. If ◯ were to be occupied by the centre of a right-handed molecule, the molecule at ⊙ would be left-handed.

Where a mirror plane exists parallel to the plane of projection, the two positions superimposed in projection are indicated by the use of a ring divided through the centre. The information given on each side refers to one of the two positions related by the mirror plane, as in − ⊕ +.

(ii) *Stereodiagrams for cubic space groups (Fig. 2.2.6.10)*

For each cubic space group, three diagrams are given with the points of the general position as vertices of transparent polyhedra. (The spheres at the vertices are depicted as opaque, however.) For the 'starting point', the same coordinate values, $x = 0.048$, $y = 0.12$, $z = 0.08$, as in the cubic diagrams of *IT* (1935) have been used. The diagram on the left corresponds to that published in *IT* (1935); in this figure, the height h of the centre of each polyhedron is given, if different from zero. For space groups Nos. 198, 199 and 220, h refers to the special point to which the polyhedron (triangle) is connected by dotted lines. In all diagrams, polyhedra with height 1 are omitted. A grid of four squares is drawn to represent the four quarters of the basal plane of the cell.

Of the three diagrams, the image on the left and the central one form a stereopair, as well as the central image and that on the right (Langlet, 1972). The stereoscopic effect is obtained by a 6° tilt between each view. The separation of neighbouring images has the standard value of 55 mm. The presence of the two stereopairs has the advantage that difficulties in seeing the polyhedra due to overlap in one pair do not occur in the other. For space groups Nos. 219, 226 and 228, where the number of points was too large for one set, two sets of three drawings are provided, one for the upper and one for the lower half of the cell.

Notes:

(i) For space group $P4_132$ (213), the coordinates $\bar{x}, \bar{y}, \bar{z}$ have been chosen for the 'starting point' to bring out the enantiomorphism with $P4_332$ (212).

(ii) For the description of a space group with 'Origin choice 2', the coordinates x, y, z of all points have been shifted with the origin to retain the same polyhedra for both origin choices.

Readers who wish to compare other approaches to space-group diagrams and their history are referred to *IT* (1935), *IT* (1952) and the following publications: Astbury & Yardley (1924); Belov *et al.* (1980); Buerger (1956); Fedorov (1895; English translation, 1971); Friedel (1926); Hilton (1903); Niggli (1919); Schiebold (1929).

2.2.7. Origin

The determination and description of crystal structures and particularly the application of direct methods are greatly facilitated by the choice of a suitable origin and its proper identification. This is even more important if related structures are to be compared or if 'chains' of group–subgroup relations are to be constructed. In this volume, as well as in *IT* (1952), the origin of the unit cell has been chosen according to the following conventions (*cf.* Chapter 2.1 and Section 2.2.2):

(i) All centrosymmetric space groups are described with an inversion centre as origin. A further description is given if a centrosymmetric space group contains points of high site symmetry that do not coincide with a centre of symmetry.

Example: $I4_1/amd$ (141).

(ii) For noncentrosymmetric space groups, the origin is at a point of highest site symmetry, as in $P\bar{6}m2$ (187). If no site symmetry is higher than 1, except for the cases listed below under (iii), the origin is placed on a screw axis, or a glide plane, or at the intersection of several such symmetry elements.

Examples: $Pca2_1$ (29); $P6_1$ (169).

(iii) In space group $P2_12_12_1$ (19), the origin is chosen in such a way that it is surrounded symmetrically by three pairs of 2_1 axes. This principle is maintained in the following noncentrosymmetric cubic space groups of classes 23 and 432, which contain $P2_12_12_1$ as subgroup: $P2_13$ (198), $I2_13$ (199), $F4_132$ (210). It has been extended to other noncentrosymmetric orthorhombic and cubic space groups with $P2_12_12_1$ as subgroup, even though in these cases points of higher site symmetry *are* available: $I2_12_12_1$ (24), $P4_332$ (212), $P4_132$ (213), $I4_132$ (214).

There are several ways of determining the location and site symmetry of the origin. First, the origin can be inspected directly in the space-group diagrams (*cf.* Section 2.2.6). This method permits visualization of all symmetry elements that intersect the chosen origin.

Another procedure for finding the site symmetry at the origin is to look for a special position that contains the coordinate triplet 0, 0, 0 or that includes it for special values of the parameters, *e.g.* position 1*a:* 0, 0, z in space group $P4$ (75), or position $3a: x, 0, \frac{1}{3}$; $0, x, \frac{2}{3}$; $\bar{x}, \bar{x}, 0$ in space group $P3_121$ (152). If such a special position occurs, the symmetry at the origin is given by the oriented site-symmetry symbol (see Section 2.2.12) of that special position; if it does not occur, the site symmetry at the origin is 1. For most practical purposes, these two methods are sufficient for the identification of the site symmetry at the origin.

2.2.7.1. *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 (including glide planes and screw axes) that pass through the origin, if any. For space groups with two *origin choices*, for each of the two origins the location relative to the other origin is also given. An example is space group *Ccca* (68).

In order to keep the notation as simple as possible, no rigid rules have been applied in formulating the origin statements. Their meaning is demonstrated by the examples in Table 2.2.7.1, which should be studied together with the appropriate space-group diagrams.

These examples illustrate the following points:

(i) The site symmetry at the origin corresponds to the point group of the space group (examples *E*1–*E*3) or to a subgroup of this point group (*E*4–*E*11).

The presence of a symmetry centre at the origin is always stated explicitly, either by giving the symbol $\bar{1}$ (*E*1 and *E*4) or by the words 'at centre', followed by the full site symmetry between parentheses (*E*2 and *E*5). This completes the origin line, if no further glide planes or screw axes are present at the origin.

(ii) If glide planes or screw axes are present, as in examples *E*4–*E*11, they are given in the order of the symmetry directions listed in Table 2.2.4.1. Such a set of symmetry elements is described here in the form of a 'point-group-like' symbol (although it does not describe a group). With the help of the orthorhombic symmetry directions, the symbols in *E*4–*E*6 can be interpreted easily. The shortened notation of *E*6 and *E*7 is used for space groups of crystal classes $mm2$, $4mm$, $\bar{4}2m$, $3m$, $6mm$ and $\bar{6}2m$ if the site symmetry at the origin can be easily recognized from the shortened symbol.

Table 2.2.7.1. *Examples of origin statements*

Example number	Space group (No.)	Origin statement	Meaning of last symbol in *E*4–*E*11
*E*1	$P\bar{1}$ (2)	at $\bar{1}$	
*E*2	$P2/m$ (10)	at centre $(2/m)$	
*E*3	*P*222 (16)	at 222	
*E*4	*Pcca* (54)	at $\bar{1}$ on 1*ca*	$c \perp [010]$, $a \perp [001]$
*E*5	*Cmcm* (63)	at centre $(2/m)$ at $2/mc2_1$	$2 \parallel [100]$, $m \perp [100]$, $c \perp [010]$, $2_1 \parallel [001]$
*E*6	*Pcc*2 (27)	on *cc*2; short for: on 2 on *cc*2	$c \perp [100]$, $c \perp [010]$, $2 \parallel [001]$
*E*7	*P*4*bm* (100)	on 41*g*; short for: on 4 on 41*g*	$4 \parallel [001]$, $g \perp [1\bar{1}0]$ and $g \perp [110]$
*E*8	$P4_2mc$ (105)	on 2*mm* on 4_2mc	$4_2 \parallel [001]$, $m \perp [100]$ and $m \perp [010]$, $c \perp [1\bar{1}0]$ and $c \perp [110]$
*E*9	$P4_32_12$ (96)	on 2[110] at $2_11(1,2)$	$2_1 \parallel [001]$, 1 in $[1\bar{1}0]$ and $2 \parallel [110]$
*E*10	$P3_121$ (152)	on 2[110] at $3_1(1,1,2)1$	$3_1 \parallel [001]$, $2 \parallel [110]$
*E*11	$P3_112$ (151)	on 2[210] at $3_11(1,1,2)$	$3_1 \parallel [001]$, $2 \parallel [210]$

(iii) For the tetragonal, trigonal and hexagonal space groups, the situation is more complicated than for the orthorhombic groups. The tetragonal space groups have one primary, two secondary and two tertiary symmetry directions. For hexagonal groups, these numbers are one, three and three (Table 2.2.4.1). If the symmetry elements passing through the origin are the same for the two (three) secondary or the two (three) tertiary directions, only one entry is given at the relevant position of the origin statement [example *E*7: 'on 41*g*' instead of 'on 41(*g*, *g*)']. An exception occurs for the site-symmetry group 2*mm* (example *E*8), which is always written in full rather than as 2*m*1.

If the symmetry elements are different, two (three) symbols are placed between parentheses, which stand for the two (three) secondary or tertiary directions. The order of these symbols corresponds to the order of the symmetry directions within the secondary or tertiary set, as listed in Table 2.2.4.1. Directions without symmetry are indicated by the symbol 1. With this rule, the last symbols in the examples *E*9–*E*11 can be interpreted.

Note that for some tetragonal space groups (Nos. 100, 113, 125, 127, 129, 134, 138, 141, 142) the glide-plane symbol *g* is used in the origin statement. This symbol occurs also in the block *Symmetry operations* of these space groups; it is explained in Sections 2.2.9 and 11.1.2.

(iv) To emphasize the orientation of the site-symmetry elements at the origin, examples *E*9 and *E*10 start with 'on 2[110]' and *E*11 with 'on 2[210]'. In *E*8, the site-symmetry group is 2*mm*. Together with the space-group symbol this indicates that 2 is along the primary tetragonal direction, that the two symbols *m* refer to the two secondary symmetry directions [100] and [010], and that the tertiary set of directions does not contribute to the site symmetry.

For monoclinic space groups, an indication of the orientation of the symmetry elements is not necessary; hence, the site symmetry at the origin is given by non-oriented symbols. For orthorhombic space groups, the orientation is obvious from the symbol of the space group.

(v) The extensive description of the symmetry elements passing through the origin is not retained for the cubic space groups, as this would have led to very complicated notations for some of the groups.

2.2.8. Asymmetric unit

An asymmetric unit of a space group is a (simply connected) smallest closed part of space from which, by application of all symmetry operations of the space group, the whole of space is filled. This implies that mirror planes and rotation axes must form boundary planes and boundary edges of the asymmetric unit. A twofold rotation axis may bisect a boundary plane. Centres of inversion must either form vertices of the asymmetric unit or be located at the midpoints of boundary planes or boundary edges. For glide planes and screw axes, these simple restrictions do not hold. An asymmetric unit contains all the information necessary for the complete description of the crystal structure. In mathematics, an asymmetric unit is called 'fundamental region' or 'fundamental domain'.

Example

The boundary planes of the asymmetric unit in space group *Pmmm* (47) are fixed by the six mirror planes x, y, 0; $x, y, \frac{1}{2}$; x, 0, z; $x, \frac{1}{2}, z$; 0, y, z; and $\frac{1}{2}, y, z$. For space group $P2_12_12_1$ (19), on the other hand, a large number of connected regions, each with a volume of $\frac{1}{4}V$(cell), may be chosen as asymmetric unit.

In cases where the asymmetric unit is not uniquely determined by symmetry, its choice may depend on the purpose of its application. For the description of the structures of molecular crystals, for instance, it is advantageous to select asymmetric units that contain one or more complete molecules. In the space-group tables of this volume, the asymmetric units are chosen in such a way that Fourier summations can be performed conveniently.

For all triclinic, monoclinic and orthorhombic space groups, the asymmetric unit is chosen as a parallelepiped with one vertex at the origin of the cell and with boundary planes parallel to the faces of the cell. It is given by the notation

$$0 \le x_i \le \text{upper limit of } x_i,$$

where x_i stands for x, y or z.

For space groups with higher symmetry, cases occur where the origin does not coincide with a vertex of the asymmetric unit or where not all boundary planes of the asymmetric unit are parallel to those of the cell. In all these cases, parallelepipeds

$$\text{lower limit of } x_i \le x_i \le \text{upper limit of } x_i$$

are given that are equal to or larger than the asymmetric unit. Where necessary, the boundary planes lying within these parallelepipeds are given by additional inequalities, such as $x \le y$, $y \le \frac{1}{2} - x$ *etc.*

In the trigonal, hexagonal and especially the cubic crystal systems, the asymmetric units have complicated shapes. For this reason, they are also specified by the coordinates of their vertices. Drawings of asymmetric units for cubic space groups have been published by Koch & Fischer (1974). Fig. 2.2.8.1 shows the boundary planes occurring in the tetragonal, trigonal and hexagonal systems, together with their algebraic equations.

Examples

(1) In space group *P*4*mm* (99), the boundary plane $y = x$ occurs in addition to planes parallel to the unit-cell faces; the asymmetric unit is given by

$$0 \le x \le \tfrac{1}{2}; \quad 0 \le y \le \tfrac{1}{2}; \quad 0 \le z \le 1; \quad x \le y.$$

(2) In *P*4*bm* (100), one of the boundary planes is $y = \frac{1}{2} - x$. The asymmetric unit is given by

$$0 \le x \le \tfrac{1}{2}; \quad 0 \le y \le \tfrac{1}{2}; \quad 0 \le z \le 1; \quad y \le \tfrac{1}{2} - x.$$

(3) In space group *R*32 (155; hexagonal axes), the boundary planes are, among others, $x = (1 + y)/2$, $y = 1 - x$, $y = (1 + x)/2$.