International Tables for Crystallography (2016). Vol. A, Section 2.1.3.6, pp. 154–158.

Table 2.1.3.3 (continued)

Space-group types		
Hermann–Mauguin symbols	Nos.	Patterson symmetry
Crystal family cubic, Bravais-lattice type *cF*		
***F*23**	**196**	$Fm\bar{3}$
***Fm*$\bar{3}$**–$Fd\bar{3}$	**202**–203	$Fm\bar{3}$
***F*432**–$F4_132$	**209**–210	$Fm\bar{3}m$
F*$\bar{4}$3*m–$F\bar{4}3c$	**216**, 219	$Fm\bar{3}m$
Fm*$\bar{3}$*m–$Fd\bar{3}c$	**225**–228	$Fm\bar{3}m$
Crystal family cubic, Bravais-lattice type *cI*		
***I*23**, $I2_13$	**197**, 199	$Im\bar{3}$
***Im*$\bar{3}$**, $Ia\bar{3}$	**204**, 206	$Im\bar{3}$
***I*432**, $I4_132$	**211**, 214	$Im\bar{3}m$
I*$\bar{4}$3*m, $I\bar{4}3d$	**217**, 220	$Im\bar{3}m$
Im*$\bar{3}$*m–$Ia\bar{3}d$	**229**–230	$Im\bar{3}m$

(*b*) Plane groups.

Plane-group types		
Hermann–Mauguin symbols	Nos.	Patterson symmetry
Crystal family oblique (monoclinic), Bravais-lattice type *mp*		
***p*1**	**1**	*p*2
***p*2**	**2**	*p*2
Crystal family rectangular (orthorhombic), Bravais-lattice type *op*		
pm–*pg*	**3**–4	*p*2*mm*
p*2*mm–*p*2*gg*	**6**–8	*p*2*mm*
Crystal family rectangular (orthorhombic), Bravais-lattice type *oc*		
cm	**5**	*c*2*mm*
c*2*mm	**9**	*c*2*mm*
Crystal family square (tetragonal), Bravais-lattice type *tp*		
***p*4**	**10**	*p*4
p*4*mm–*p*4*gm*	**11**–12	*p*4*mm*
Crystal family hexagonal, Bravais-lattice type *hp*		
***p*3**	**13**	*p*6
***p*3*m*1**	**14**	*p*6*mm*
p*31*m	**15**	*p*6*mm*
***p*6**	**16**	*p*6
p*6*mm	**17**	*p*6*mm*

(*c*) $P_D(uvw)$: $D(hkl) = |F(hkl)|^2 - |F(\bar{h}\bar{k}\bar{l})|^2$, the difference of the squared structure-factor amplitudes of the pair of Friedel opposites *hkl* and $\bar{h}\bar{k}\bar{l}$. Real $P_D(uvw)$ is the real sine Fourier transform of $D(hkl)$. The crystallographic symmetry of $P_D(uvw)$ is that of the symmorphic space-group representative of the arithmetic crystal class to which the space group belongs (see Table 2.1.3.3). The full symmetry of $P_D(uvw)$ is given by the type-III black-and-white space group generated by the appropriate symmorphic space group and the *centre of antisymmetry*, $P_D(uvw) = -P_D(\bar{u}\bar{v}\bar{w})$ (Fischer & Knof, 1987). Thus $P_D(uvw)$ does not possess the Patterson symmetry.

2.1.3.6. Space-group diagrams

The space-group diagrams serve two purposes: (i) to show the relative locations and orientations of the symmetry elements and (ii) to illustrate the arrangement of a set of symmetry-equivalent points of the general position.

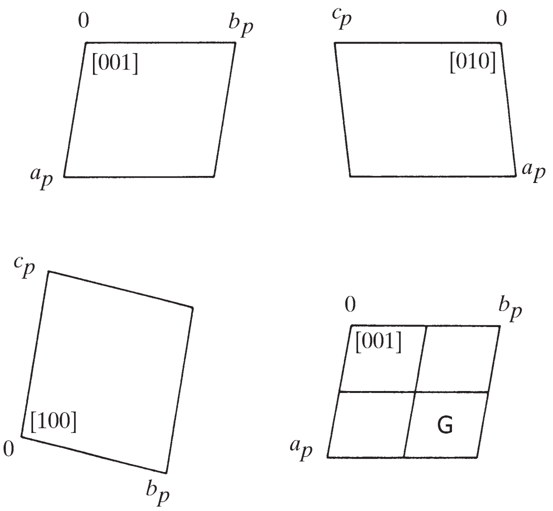

Figure 2.1.3.1
Triclinic space groups (G = general-position diagram).

With the exception of general-position diagrams in perspective projection for some space groups (*cf.* Section 2.1.3.6.8), all of the diagrams are orthogonal projections, *i.e.* the projection direction is perpendicular to the plane of the figure. Apart from the descriptions of the rhombohedral space groups with 'rhombohedral axes' (*cf.* Section 2.1.3.6.6), the projection direction is always a cell axis. If other axes are not parallel to the plane of the figure, they are indicated by the subscript *p*, as a_p, b_p or c_p in the case of one or two axes for monoclinic and triclinic space groups, respectively (*cf.* Figs. 2.1.3.1 to 2.1.3.3), or by the subscript rh for the three rhombohedral axes in Fig. 2.1.3.9.

The graphical symbols for symmetry elements, as used in the drawings, are displayed in Tables 2.1.2.2 to 2.1.2.7.

In the diagrams, 'heights' *h* above the projection plane are indicated for symmetry planes and symmetry axes *parallel* to the projection plane, as well as for centres of symmetry. The heights are given as fractions of the shortest lattice translation normal to the projection plane and, if different from 0, are printed next to the graphical symbols. Each symmetry element at height *h* is accompanied by another symmetry element of the same type at height $h + \frac{1}{2}$ (this does not apply to the horizontal fourfold axes in the diagrams for the cubic space groups). In the space-group diagrams, only the symmetry element at height *h* is indicated (*cf.* Section 2.1.2).

Schematic representations of the diagrams, displaying the origin, the labels of the axes, and the projection direction [*uvw*], are given in Figs. 2.1.3.1 to 2.1.3.10 (except Fig. 2.1.3.6). The general-position diagrams are indicated by the letter G.

2.1.3.6.1. *Plane groups*

Each description of a plane group contains two diagrams, one for the symmetry elements (left) and one for the general position (right). The two axes are labelled *a* and *b*, with *a* pointing downwards and *b* running from left to right.

2.1.3.6.2. *Triclinic space groups*

For each of the two triclinic space groups, three elevations (along *a*, *b* and *c*) are given, in addition to the general-position diagram G (projected along *c*) at the lower right of the set, as illustrated in Fig. 2.1.3.1.

The diagrams represent a reduced cell of type II for which the three interaxial angles are non-acute, *i.e.* $\alpha, \beta, \gamma \geq 90°$. For a cell

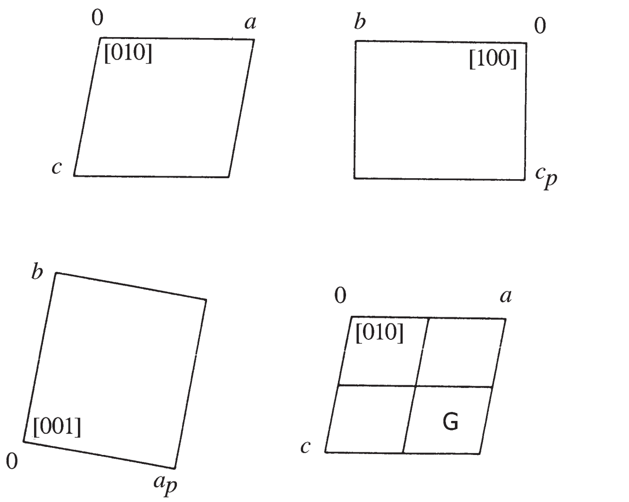

Figure 2.1.3.2
Monoclinic space groups, setting with unique axis *b* (G = general-position diagram).

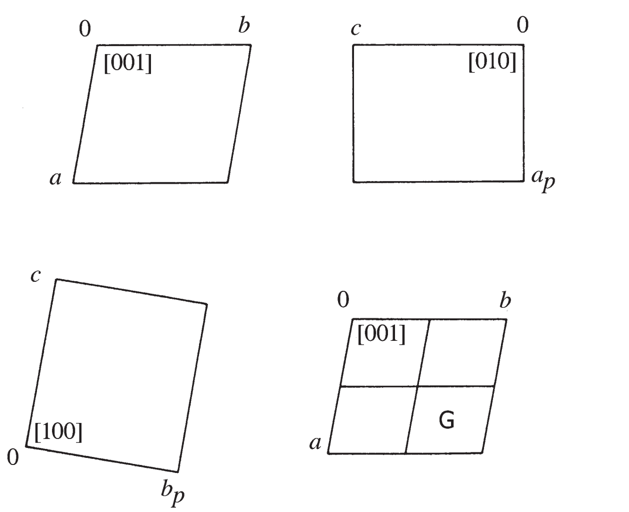

Figure 2.1.3.3
Monoclinic space groups, setting with unique axis *c* (G = general-position diagram).

of type I, all angles are acute, *i.e.* α, β, $\gamma < 90^\circ$. For a discussion of the two types of reduced cells, see Section 3.1.3.

2.1.3.6.3. Monoclinic space groups (cf. Sections 2.1.3.2 and 2.1.3.15)

The 'complete treatment' of each of the two settings contains four diagrams (Figs. 2.1.3.2 and 2.1.3.3). Three of them are projections of the symmetry elements, taken along the unique axis (upper left) and along the other two axes (lower left and upper right). For the general position, only the projection along the unique axis is given (lower right).

The 'synoptic descriptions' of the three cell choices (for each setting) are headed by a pair of diagrams, as illustrated in Fig. 2.1.3.4. The drawings on the left display the symmetry elements and the ones on the right the general position (labelled G). Each diagram is a projection of four neighbouring unit cells along the unique axis. It contains the outlines of the three cell choices drawn as heavy lines. For the labelling of the axes, see Fig. 2.1.3.4. The headline of the description of each cell choice contains a small-scale drawing, indicating the basis vectors and the cell that apply to that description.

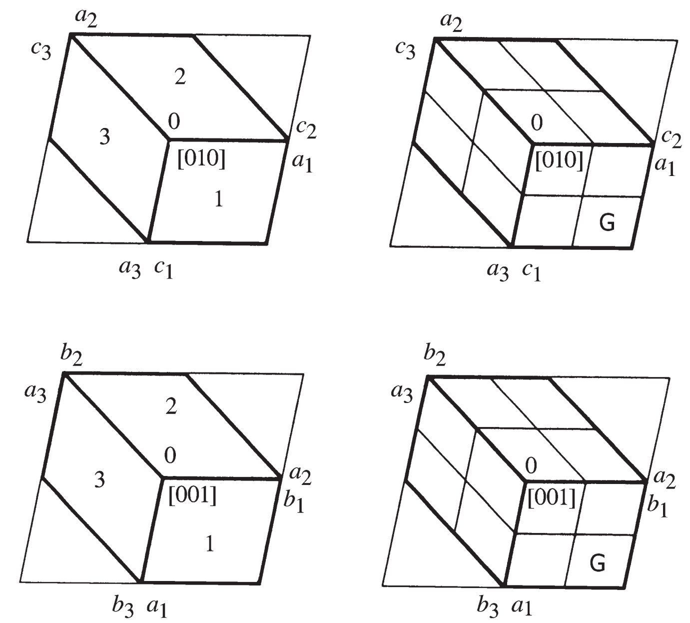

Figure 2.1.3.4
Monoclinic space groups, cell choices 1, 2, 3. Upper pair of diagrams: setting with unique axis *b*. Lower pair of diagrams: setting with unique axis *c*. The numbers 1, 2, 3 within the cells and the subscripts of the labels of the axes indicate the cell choice (*cf.* Section 2.1.3.15). The unique axis points upwards from the page. G = general-position diagram.

2.1.3.6.4. Orthorhombic space groups and orthorhombic settings

The space-group tables contain a set of four diagrams for each orthorhombic space group. The set consists of three projections of the symmetry elements [along the *c* axis (upper left), the *a* axis (lower left) and the *b* axis (upper right)] in addition to the general-position diagram, which is given only in the projection along *c* (lower right). The projected axes, the origins and the projection directions of these diagrams are illustrated in Fig. 2.1.3.5. They refer to the so-called 'standard setting' of the space group, *i.e.* the setting described in the space-group tables and indicated by the 'standard Hermann–Mauguin symbol' in the headline.

For each orthorhombic space group, *six settings* exist, *i.e.* six different ways of assigning the labels *a*, *b*, *c* to the three orthorhombic symmetry directions; thus the shape and orientation of the cell are the same for each setting. These settings correspond

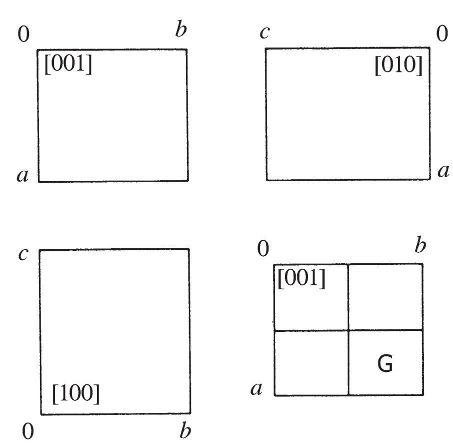

Figure 2.1.3.5
Orthorhombic space groups. Diagrams for the 'standard setting' as described in the space-group tables (G = general-position diagram).

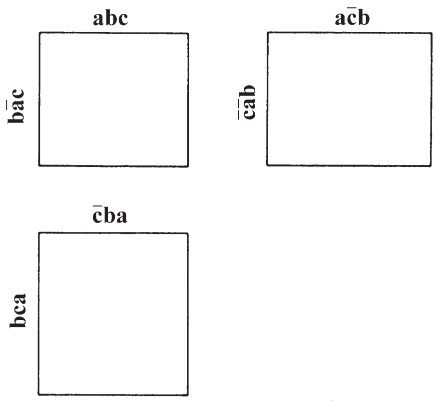

Figure 2.1.3.6
Orthorhombic space groups. The three projections of the symmetry elements with the six setting symbols (see text). For setting symbols printed vertically, the page has to be turned clockwise by 90° or viewed from the side. Note that in the actual space-group tables instead of the setting symbols the corresponding full Hermann–Mauguin space-group symbols are printed.

to the six permutations of the labels of the axes (including the identity permutation); *cf.* Section 1.5.4.3:

$$\mathbf{abc} \quad \mathbf{ba\bar{c}} \quad \mathbf{cab} \quad \mathbf{\bar{c}ba} \quad \mathbf{bca} \quad \mathbf{a\bar{c}b}.$$

The symbol for each setting, here called 'setting symbol', is a shorthand notation for the (3×3) transformation matrix $\boldsymbol{P}$ of the basis vectors of the standard setting, $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$, into those of the setting considered (*cf.* Chapter 1.5 for a detailed discussion of coordinate transformations). For instance, the setting symbol **cab** stands for the cyclic permutation

$$\mathbf{a}' = \mathbf{c}, \quad \mathbf{b}' = \mathbf{a}, \quad \mathbf{c}' = \mathbf{b}$$

or

$$(\mathbf{a}', \mathbf{b}', \mathbf{c}') = (\mathbf{a}, \mathbf{b}, \mathbf{c})\boldsymbol{P} = (\mathbf{a}, \mathbf{b}, \mathbf{c})\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} = (\mathbf{c}, \mathbf{a}, \mathbf{b}),$$

where $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$ is the new set of basis vectors. An interchange of two axes reverses the handedness of the coordinate system; in order to keep the system right-handed, each interchange is accompanied by the reversal of the sense of one axis, *i.e.* by an element $\bar{1}$ in the transformation matrix. Thus, $\mathbf{ba\bar{c}}$ denotes the transformation

$$(\mathbf{a}', \mathbf{b}', \mathbf{c}') = (\mathbf{a}, \mathbf{b}, \mathbf{c})\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix} = (\mathbf{b}, \mathbf{a}, \bar{\mathbf{c}}).$$

The six orthorhombic settings correspond to six Hermann–Mauguin symbols which, however, need not all be different; *cf.* Table 2.1.3.4.[1]

In the earlier (1935 and 1952) editions of *International Tables*, only one setting was illustrated, in a projection along $\mathbf{c}$, so that it was usual to consider it as the 'standard setting' and to accept its cell edges as crystal axes and its space-group symbol as the 'standard Hermann–Mauguin symbol'. In the present edition, following *IT* A (2002), however, *all six* orthorhombic settings are illustrated, as explained below.

The three projections of the symmetry elements can be interpreted in two ways. First, in the sense indicated above, that is, as

[1] A space-group symbol is invariant under sign changes of the axes; *i.e.* the same symbol applies to the right-handed coordinate systems $\mathbf{abc}$, $\mathbf{a\bar{b}\bar{c}}$, $\mathbf{\bar{a}b\bar{c}}$, $\mathbf{\bar{a}\bar{b}c}$ and the left-handed systems $\mathbf{\bar{a}bc}$, $\mathbf{a\bar{b}c}$, $\mathbf{ab\bar{c}}$, $\mathbf{\bar{a}\bar{b}\bar{c}}$.

Table 2.1.3.4
Numbers of distinct projections and different Hermann–Mauguin symbols for the orthorhombic space groups

The space-group numbers are given in parentheses. The space groups are listed according to point group as indicated in the column headings.

Number of distinct projections	222	$mm2$	$2/m\,2/m\,2/m$
6 (22 space groups)		$Pmc2_1$ (26) $Pma2$ (28) $Pca2_1$ (29) $Pnc2$ (30) $Pna2_1$ (33) $Cmc2_1$ (36) $Amm2$ (38) $Aem2$ (39) $Ama2$ (40) $Aea2$ (41) $Ima2$ (46)	$P\,2_1/m\,2/m\,2/a$ (51) $P\,2/n\,2_1/n\,2/a$ (52) $P\,2/m\,2/n\,2_1/a$ (53) $P\,2_1/c\,2/c\,2/a$ (54) $Pmn2_1$ (31) $P\,2/b\,2_1/c\,2_1/m$ (57) $P\,2_1/b\,2/c\,2_1/n$ (60) $P\,2_1/n\,2_1/m\,2_1/a$ (62) $C\,2/m\,2/c\,2_1/m$ (63) $C\,2/m\,2/c\,2_1/e$ (64) $I\,2_1/m\,2_1/m\,2_1/a$ (74)
3 (25 space groups)	$P222_1$ (17) $P2_12_12$ (18) $C222_1$ (20) $C222$ (21)	$Pmm2$ (25) $Pcc2$ (27) $Pba2$ (32) $Pnn2$ (34) $Cmm2$ (35) $Ccc2$ (37) $Fmm2$ (42) $Fdd2$ (43) $Imm2$ (44) $Iba2$ (45)	$P\,2/c\,2/c\,2/m$ (49) $P\,2/b\,2/a\,2/n$ (50) $P\,2_1/b\,2_1/a\,2/m$ (55) $P\,2_1/c\,2_1/c\,2/n$ (56) $P\,2_1/n\,2_1/n\,2/m$ (58) $P\,2_1/m\,2_1/m\,2/n$ (59) $C\,2/m\,2/m\,2/m$ (65) $C\,2/c\,2/c\,2/m$ (66) $C\,2/m\,2/m\,2/e$ (67) $C\,2/c\,2/c\,2/e$ (68) $I\,2/b\,2/a\,2/m$ (72)
2 (2 space groups)			$P\,2_1/b\,2_1/c\,2_1/a$ (61) $I\,2_1/b\,2_1/c\,2_1/a$ (73)
1 (10 space groups)	$P222$ (16) $P2_12_12_1$ (19) $F222$ (22) $I222$ (23) $I2_12_12_1$ (24)		$P\,2/m\,2/m\,2/m$ (47) $P\,2/n\,2/n\,2/n$ (48) $F\,2/m\,2/m\,2/m$ (69) $F\,2/d\,2/d\,2/d$ (70) $I\,2/m\,2/m\,2/m$ (71)
Total: 59	9	22	28

different projections of a *single* (standard) setting of the space group, with the projected basis vectors $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ labelled as in Fig. 2.1.3.5. Second, each one of the three diagrams can be considered as the projection along $\mathbf{c}'$ of either one of *two different* settings: one setting in which $\mathbf{b}'$ is horizontal and one in which $\mathbf{b}'$ is vertical ($\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$ refer to the setting under consideration). This second interpretation is used to illustrate in the same figure the space-group symbols corresponding to these two settings. In order to view these projections in conventional orientation ($\mathbf{b}'$ horizontal, $\mathbf{a}'$ vertical, origin in the upper left corner, projection down the positive $\mathbf{c}'$ axis), the setting with $\mathbf{b}'$ horizontal can be inspected directly with the figure upright; hence, the corresponding space-group symbol is printed above the projection. The other setting with $\mathbf{b}'$ vertical and $\mathbf{a}'$ horizontal, however, requires turning the figure by 90°, or looking at it from the side; thus, the space-group symbol is printed at the left, and it runs upwards.

The 'setting symbols' for the six settings are attached to the three diagrams of Fig. 2.1.3.6, which correspond to those of Fig. 2.1.3.5. In the orientation of the diagram where the setting symbol is read in the usual way, $\mathbf{a}'$ is vertical pointing downwards, $\mathbf{b}'$ is horizontal pointing to the right, and $\mathbf{c}'$ is pointing upwards from the page. Each setting symbol is printed in the position that in the space-group tables is actually occupied by the corresponding full Hermann–Mauguin symbol. The changes in the space-group symbol that are associated with a particular setting

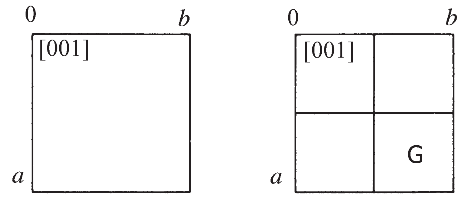

Figure 2.1.3.7
Tetragonal space groups (G = general-position diagram).

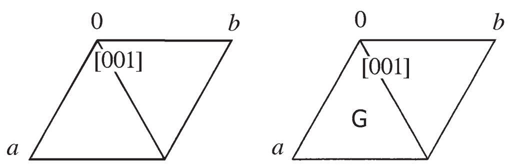

Figure 2.1.3.8
Trigonal *P* and hexagonal *P* space groups (G = general-position diagram).

symbol can easily be deduced by comparing Fig. 2.1.3.6 with the diagrams for the space group under consideration.

Not all of the 59 orthorhombic space groups have all six projections distinct, *i.e.* have different Hermann–Mauguin symbols for the six settings. This aspect is treated in Table 2.1.3.4. Only 22 space groups have six, 25 have three, 2 have two different symbols, while 10 have all symbols the same. This information can be of help in the early stages of a crystal-structure analysis.

The six setting symbols, *i.e.* the six permutations of the labels of the axes, form the column headings of the orthorhombic entries in Table 1.5.4.4, which contains the extended Hermann–Mauguin symbols for the six settings of each orthorhombic space group. Note that some of these setting symbols exhibit different sign changes compared with those in Fig. 2.1.3.6.

2.1.3.6.5. *Tetragonal, trigonal P and hexagonal P space groups*

The pairs of diagrams for these space groups are similar to those in the previous editions of *IT*. Each pair consists of a general-position diagram (right) and a diagram of the symmetry elements (left), both projected along **c**, as illustrated in Figs. 2.1.3.7 and 2.1.3.8.

2.1.3.6.6. *Trigonal R (rhombohedral) space groups*

The seven rhombohedral space groups are treated in two versions, the first based on 'hexagonal axes' (obverse setting), the second on 'rhombohedral axes' (*cf.* Sections 2.1.1.2 and 2.1.3.2). The pairs of diagrams are similar to those in *IT* (1952) and *IT* A (2002); the left or top one displays the symmetry elements, the right or bottom one the general position. This is illustrated in Fig. 2.1.3.9, which gives the axes *a* and *b* of the triple hexagonal cell and the projections of the axes of the primitive rhombohedral cell, labelled $a_{\rm rh}$, $b_{\rm rh}$ and $c_{\rm rh}$. For convenience, all 'heights' in the space-group diagrams are fractions of the hexagonal *c* axis. For 'hexagonal axes', the projection direction is [001], for 'rhombohedral axes' it is [111]. In the general-position diagrams, the circles drawn in heavier lines represent atoms that lie within the primitive rhombohedral cell (provided the symbol '−' is read as $1 - z$ rather than as $-z$).

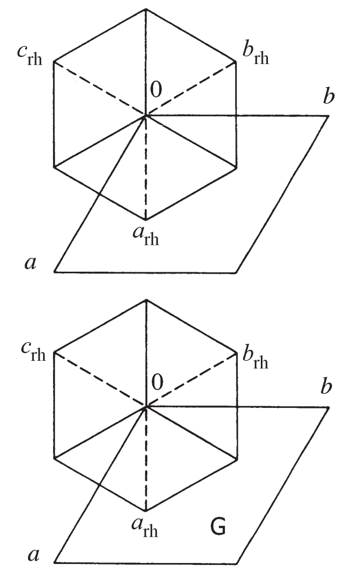

Figure 2.1.3.9
Rhombohedral space groups. Obverse triple hexagonal cell with 'hexagonal axes' *a*, *b* and primitive rhombohedral cell with projections of 'rhombohedral axes' $a_{\rm rh}$, $b_{\rm rh}$, $c_{\rm rh}$. Note: In the actual space-group diagrams the edges of the primitive rhombohedral cell (dashed lines) are only indicated in the general-position diagram of the rhombohedral-axes description (G = general-position diagram).

The symmetry-element diagrams for the hexagonal and the rhombohedral descriptions of a space group are the same. The edges of the primitive rhombohedral cell (*cf.* Fig. 2.1.3.9) are only indicated in the general-position diagram of the rhombohedral description.

2.1.3.6.7. *Cubic space groups*

For each cubic space group, one projection of the symmetry elements along [001] is given, Fig. 2.1.3.10; for details of the diagrams, see Section 2.1.2 and Buerger (1956). For face-centred lattices *F*, only a quarter of the unit cell is shown; this is sufficient since the projected arrangement of the symmetry elements is translation-equivalent in the four quarters of an *F* cell. It is important to note that symmetry axes inclined to the projection plane are indicated where they intersect the plane of projection. Symmetry planes inclined to the projection plane that occur in classes $\bar{4}3m$ and $m\bar{3}m$ are shown as 'inserts' around the high-symmetry points, such as 0, 0, 0; $\frac{1}{2}$, 0, 0; *etc.*

The cubic diagrams given in *IT* (1935) are different from the ones used here. No drawings for cubic space groups were provided in *IT* (1952).

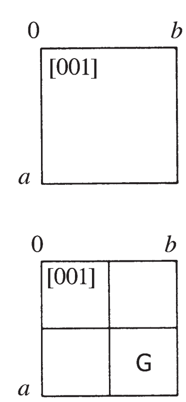

Figure 2.1.3.10
Cubic space groups. G = general-position diagram, in which the equivalent positions are shown as the vertices of polyhedra.

2.1.3.6.8. Diagrams of the general position (by K. Momma and M. I. Aroyo)

Non-cubic space groups. In these diagrams, the 'heights' of the points are z coordinates, except for monoclinic space groups with unique axis b where they are y coordinates. For rhombohedral space groups, the heights are always fractions of the hexagonal c axis. The symbols $+$ and $-$ stand for $+z$ and $-z$ (or $+y$ and $-y$) in which z or y can assume any value. For points with symbols $+$ or $-$ preceded by a fraction, *e.g.* $\frac{1}{2}+$ or $\frac{1}{3}-$, the relative z or y coordinate is $\frac{1}{2}$ *etc.* higher than that of the point with symbol $+$ or $-$.

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 $-$ ⦶ $+$.

Diagrams for cubic space groups (Fig. 2.1.3.10). Following the approach of *IT* (1935), for each cubic space group a diagram showing the points of the general position as the vertices of polyhedra is given. In these diagrams, the polyhedra are transparent, but the spheres at the vertices are opaque. For most of the space groups, 'starting points' with the same coordinate values, $x = 0.048$, $y = 0.12$, $z = 0.089$, have been used. The origins of the polyhedra are chosen at special points of highest site symmetry, which for most space groups coincide with the origin (and its equivalent points in the unit cell). Polyhedra with origins at sites $(\frac{1}{8}, \frac{1}{8}, \frac{1}{8})$ have been chosen for the space groups $P4_332$ (212) and $I4_132$ (214), and $(\frac{3}{8}, \frac{3}{8}, \frac{3}{8})$ for $P4_132$ (213). The two diagrams shown for the space groups $I\bar{4}3d$ (220) and $Ia\bar{3}d$ (230) correspond to polyhedra with origins chosen at two different special sites with site-symmetry groups of equal (32 *versus* $\bar{3}$ in $Ia\bar{3}d$) or nearly equal order (3 *versus* $\bar{4}$ in $I\bar{4}3d$). The height h of the centre of each polyhedron is given on the diagram, if different from zero. For space-group Nos. 198, 199 and 220, h refers to the special point to which the polyhedron (triangle) is connected. Polyhedra with height 1 are omitted in all the diagrams. A grid of four squares is drawn to represent the four quarters of the basal plane of the cell. For space groups $F\bar{4}3c$ (219), $Fm\bar{3}c$ (226) and $Fd\bar{3}c$ (228), where the number of points is too large for one diagram, two diagrams are provided, one for the upper half 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 show 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.

An additional general-position diagram is shown on the fourth page for each of the ten space groups of the $m\bar{3}m$ crystal class. To provide a clearer three-dimensional-style overview of the arrangements of the polyhedra, these general-position diagrams are shown in tilted projection (in contrast to the orthogonal-projection diagrams described above).

The general-position diagrams of the cubic groups in both orthogonal and tilted projections were generated using the program *VESTA* (Momma & Izumi, 2011).

Readers who wish to compare other approaches to space-group diagrams and their history are referred to *IT* (1935), *IT* (1952), the fifth edition of *IT* A (2002) (where general-position stereodiagrams of the cubic space groups are shown) and the following publications: Astbury & Yardley (1924), Belov *et al.* (1980), Buerger (1956), Fedorov (1895; English translation, 1971), Friedel (1926), Hilton (1903), Niggli (1919) and Schiebold (1929).

2.1.3.7. 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) and *IT* A (2002), the origin of the unit cell has been chosen according to the following conventions (*cf.* Sections 2.1.1 and 2.1.3.2):

(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. As an example, study the origin choice 1 and origin choice 2 descriptions of $I4_1/amd$ (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, see for example space groups $Pca2_1$ (29) and $P6_1$ (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 2.1.3.6). 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 3*a*: $x, 0, \frac{1}{3}$; $0, x, \frac{2}{3}$; $\bar{x}, \bar{x}, 0$ 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 2.1.3.12) 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.

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 *Ccce* (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 2.1.3.5,