2.1.3. Contents and arrangement of the tables

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2.1.3.1. General layout

The presentation of the plane-group and space-group data in Chapters 2.2 and 2.3 follows the style of the previous editions of *International Tables*. The data for most of the space groups are displayed on one page or on two facing pages. A typical distribution of the data is shown below and is illustrated by the example of *Cccm* (66) provided inside the front and back covers.

Left-hand page:

(1) *Headline*
(2) Diagrams for the symmetry elements and the general position (for graphical symbols of symmetry elements see Section 2.1.2)
(3) *Origin*
(4) *Asymmetric unit*
(5) *Symmetry operations*

Right-hand page:

(6) *Headline* in abbreviated form
(7) *Generators selected*; this information is the basis for the order of the entries under *Symmetry operations* and *Positions*
(8) General and special *Positions*, with the following columns:
Multiplicity
Wyckoff letter
Site symmetry, given by the oriented site-symmetry symbol
Coordinates
Reflection conditions
Note: In a few space groups, two special positions with the same reflection conditions are printed on the same line
(9) *Symmetry of special projections* (not given for plane groups)

It is important to note that the symmetry data are displayed in the same sequence for all the space groups. The actual distribution of the data between pages can vary depending on the amount and nature of the data that are shown.

The symmetry data for the ten space groups of the crystal class $m\bar{3}m$ [$Pm\bar{3}m$ (221) to $Ia\bar{3}d$ (230)] are displayed on four pages. Additional general-position diagrams in tilted projection are shown on the fourth page, providing a three-dimensional-style view of these complicated general-position diagrams.

2.1.3.2. Space groups with more than one description

For several space groups, more than one description is available. Three cases occur:

(i) *Two choices of origin (cf. Section 2.1.3.7)*

For all centrosymmetric space groups, the tables contain a description with a centre of symmetry as origin. Some centrosymmetric space groups, however, contain points of high site symmetry that do not coincide with a centre of symmetry. For these 24 cases, a further description (including diagrams) with a high-symmetry point as origin is provided. Neither of the two origin choices is considered standard. Noncentrosymmetric space groups and all plane groups are described with only one choice of origin.

Examples

(1) *Pnnn* (48)
Origin choice 1 at a point with site symmetry 222
Origin choice 2 at a centre with site symmetry $\bar{1}$.
(2) $Fd\bar{3}m$ (227)
Origin choice 1 at a point with site symmetry $\bar{4}3m$
Origin choice 2 at a centre with site symmetry $\bar{3}m$.

(ii) *Monoclinic space groups*

Two complete descriptions are given for each of the 13 monoclinic space groups, one for the setting with 'unique axis *b*', followed by one for the setting with 'unique axis *c*'.

Additional descriptions in synoptic form are provided for the following eight monoclinic space groups with centred lattices or glide planes:

*C*2 (5), *Pc* (7), *Cm* (8), *Cc* (9), *C*2/*m* (12), *P*2/*c* (13), $P2_1/c$ (14), *C*2/*c* (15)

These synoptic descriptions consist of abbreviated treatments for three 'cell choices', here called 'cell choices 1, 2 and 3'. Cell choice 1 corresponds to the complete treatment, mentioned above; for comparative purposes, it is repeated among the synoptic descriptions which, for each setting, are printed on two facing pages. The cell choices and their relations are explained in Section 2.1.3.15.

(iii) *Rhombohedral space groups*

The seven rhombohedral space groups *R*3 (146), $R\bar{3}$ (148), *R*32 (155), *R*3*m* (160), *R*3*c* (161), $R\bar{3}m$ (166) and $R\bar{3}c$ (167) are described with two coordinate systems, first with *hexagonal axes* (triple hexagonal cell) and second with *rhombohedral axes* (primitive rhombohedral cell). The same space-group symbol is used for both descriptions. For convenience, the relations between the cell parameters a, c of the triple hexagonal cell and the cell parameters a' and α' of the primitive rhombohedral cell (*cf.* Table 2.1.1.1) are listed:

$$a = a'\sqrt{2}\sqrt{1-\cos\alpha'} = 2a'\sin\frac{\alpha'}{2}$$

$$c = a'\sqrt{3}\sqrt{1+2\cos\alpha'}$$

$$\frac{c}{a} = \sqrt{\frac{3}{2}}\sqrt{\frac{1+2\cos\alpha'}{1-\cos\alpha'}} = \sqrt{\frac{9}{4\sin^2(\alpha'/2)} - 3}$$

$$a' = \tfrac{1}{3}\sqrt{3a^2 + c^2}$$

$$\sin\frac{\alpha'}{2} = \frac{3}{2\sqrt{3 + (c^2/a^2)}} \text{ or } \cos\alpha' = \frac{(c^2/a^2) - \frac{3}{2}}{(c^2/a^2) + 3}.$$

The hexagonal triple cell is given in the *obverse* setting (centring points $\frac{2}{3},\frac{1}{3},\frac{1}{3}$; $\frac{1}{3},\frac{2}{3},\frac{2}{3}$). In *IT* (1935), the *reverse* setting (centring points $\frac{1}{3},\frac{2}{3},\frac{1}{3}$; $\frac{2}{3},\frac{1}{3},\frac{2}{3}$) was employed; *cf.* Table 2.1.1.2.

Coordinate transformations between different space-group descriptions are treated in detail in Section 1.5.3.

2.1.3.3. Headline

The description of each plane group or space group starts with a headline consisting of two (sometimes three) lines which contain the following information, when read from left to right.

First line

(1) The *short international* (Hermann–Mauguin) *symbol* for the plane or space group. These symbols will be further referred to as Hermann–Mauguin symbols. A detailed discussion of space-group symbols is given in Section 1.4.1 and Chapter 3.3; for convenience, a summary is given in Section 2.1.3.4.

Note on standard monoclinic space-group symbols: In order to facilitate recognition of a monoclinic space-group type, the familiar short symbol for the *b*-axis setting (*e.g.* $P2_1/c$ for No. 14 or $C2/c$ for No. 15) has been adopted as the *standard symbol* for a space-group type. It appears in the headline of *every description of this space group* and thus does not carry any information about the setting or the cell choice of this particular description. No other short symbols for monoclinic space groups are used in this volume (*cf.* Section 2.1.3.15).

(2) The *Schoenflies symbol* for the space group (*cf.* Section 1.4.1).

Note: No Schoenflies symbols exist for the plane groups.

(3) The *short international* (Hermann–Mauguin) *symbol* for the point group to which the plane or space group belongs (*cf.* Section 1.4.1 and Chapter 3.3).

(4) The name of the *crystal system* (*cf.* Table 2.1.1.1).

Second line

(5) The sequential *number of the plane or space group*, as introduced in *IT* (1952).

(6) The *full international* (Hermann–Mauguin) *symbol* for the plane or space group.

For monoclinic space groups, the headline of every description contains the full symbol appropriate to that description.

(7) The *Patterson symmetry* (see Section 2.1.3.5).

Third line

This line is used, where appropriate, to indicate origin choices, settings, cell choices and coordinate axes (see Section 2.1.3.2). For five orthorhombic space groups, an entry 'Former space-group symbol' is given; *cf.* Section 2.1.2.

Table 2.1.3.1
Lattice symmetry directions for two and three dimensions

Directions that belong to the same set of equivalent symmetry directions are collected between braces. The first entry in each set is taken as the representative of that set.

	Symmetry direction (position in Hermann–Mauguin symbol)		
Lattice	Primary	Secondary	Tertiary
Two dimensions			
Oblique	Rotation point in plane		
Rectangular		[10]	[01]
Square		{[10], [01]}	{[1$\bar{1}$], [11]}
Hexagonal		{[10], [01], [1$\bar{1}$]}	{[1$\bar{1}$], [12], [2$\bar{1}$]}
Three dimensions			
Triclinic	None		
Monoclinic†	[010] ('unique axis *b*') [001] ('unique axis *c*')		
Orthorhombic	[100]	[010]	[001]
Tetragonal	[001]	{[100], [010]}	{[1$\bar{1}$0], [110]}
Hexagonal	[001]	{[100], [010], [1$\bar{1}$0]}	{[1$\bar{1}$0], [120], [2$\bar{1}$0]}
Rhombohedral (hexagonal axes)	[001]	{[100], [010], [1$\bar{1}$0]}	
Rhombohedral (rhombohedral axes)	[111]	{[1$\bar{1}$0], [01$\bar{1}$], [$\bar{1}$01]}	
Cubic	{[100], [010], [001]}	{[111], [1$\bar{1}$1], [$\bar{1}$11], [11$\bar{1}$]}	{[1$\bar{1}$0] [110], [01$\bar{1}$] [011], [$\bar{1}$01] [101]}

† For the full Hermann–Mauguin symbols see Sections 2.1.3.4 and 1.4.1.

2.1.3.4. International (Hermann–Mauguin) symbols for plane groups and space groups

(For more details, *cf.* Section 1.4.1 and Chapter 3.3.)

Current symbols. Both the short and the full Hermann–Mauguin symbols consist of two parts: (i) a letter indicating the centring type of the conventional cell, and (ii) a set of characters indicating symmetry elements of the space group (modified point-group symbol).

(i) The letters for the centring types of cells are listed in Table 2.1.1.2. Lower-case letters are used for two dimensions (nets), capital letters for three dimensions (lattices).

(ii) The one, two or three entries after the centring letter refer to the one, two or three kinds of *symmetry directions* of the lattice belonging to the space group. These symmetry directions were called *Blickrichtungen* by Heesch (1929). Symmetry directions occur either as singular directions (as in the monoclinic and orthorhombic crystal systems) or as sets of symmetry-equivalent symmetry directions (as in the higher-symmetry crystal systems). Only one representative of each set is required. The (sets of) symmetry directions and their sequence for the different lattices are summarized in Table 2.1.3.1. According to their position in this sequence, the symmetry directions are referred to as 'primary', 'secondary' and 'tertiary' directions.

This sequence of lattice symmetry directions is transferred to the sequence of positions in the corresponding Hermann–Mauguin space-group symbols. Each position contains one or two characters designating symmetry elements (axes and planes) of the space group (*cf.* Section 2.1.2) that occur for the corresponding lattice symmetry direction. Symmetry planes are represented by their normals; if a symmetry axis and a normal to a symmetry plane are parallel, the two characters (symmetry symbols) are separated by a slash, as in $P6_3/m$ or $P2/m$ ('two over *m*').

Short and *full* Hermann–Mauguin symbols differ only for the plane groups of class *m*, for the monoclinic space groups, and for the space groups of crystal classes *mmm*, $4/mmm$, $\bar{3}m$, $6/mmm$, $m\bar{3}$ and $m\bar{3}m$. In the full symbols, symmetry axes *and* symmetry

Table 2.1.3.2
Changes in Hermann–Mauguin symbols for two-dimensional groups

No.	*IT* (1952)	Present edition
6	*pmm*	*p*2*mm*
7	*pmg*	*p*2*mg*
8	*pgg*	*p*2*gg*
9	*cmm*	*c*2*mm*
11	*p*4*m*	*p*4*mm*
12	*p*4*g*	*p*4*gm*
17	*p*6*m*	*p*6*mm*

planes for each symmetry direction are listed; in the short symbols, symmetry axes are suppressed as much as possible. Thus, for space group No. 62, the full symbol is $P2_1/n\ 2_1/m\ 2_1/a$ and the short symbol is *Pnma*. For No. 194, the full symbol is $P6_3/m\ 2/m\ 2/c$ and the short symbol is $P6_3/mmc$. For No. 230, the full symbol is $I4_1/a\ \bar{3}\ 2/d$ and the short symbol is $Ia\bar{3}d$.

Many space groups contain more kinds of symmetry elements than are indicated in the full symbol ('additional symmetry operations and elements', *cf.* Sections 1.4.2.4 and 1.5.4.1). A listing of additional symmetry operations is given in Tables 1.5.4.3 and 1.5.4.4 under the heading *Extended full symbols*. Note that a centre of symmetry is never explicitly indicated (except for space group $P\bar{1}$); its presence or absence, however, can be readily inferred from the space-group symbol.

Changes in Hermann–Mauguin space-group symbols as compared with the 1952 and 1935 editions of International Tables. Extensive changes in the space-group symbols were applied in *IT* (1952) as compared with the original Hermann–Mauguin symbols of *IT* (1935), especially in the tetragonal, trigonal and hexagonal crystal systems. Moreover, new symbols for the *c*-axis setting of monoclinic space groups were introduced. All these changes are recorded on pp. 51 and 543–544 of *IT* (1952). In the present edition, the symbols of the 1952 edition are retained, except for the following four cases (*cf.* Section 3.3.4).

(i) *Two-dimensional groups*. Short Hermann–Mauguin symbols differing from the corresponding full symbols in *IT* (1952) are replaced by the full symbols for the plane groups listed in Table 2.1.3.2.

For the two-dimensional point group with two mutually perpendicular mirror lines, the symbol *mm* is changed to 2*mm*.

For plane group No. 2, the entries '1' at the end of the full symbol are omitted: No. 2: Change from *p*211 to *p*2.

With these changes, the symbols of the two-dimensional groups follow the rules that were introduced in *IT* (1952) for the space groups.

(ii) *Monoclinic space groups*. Additional *full* Hermann–Mauguin symbols are introduced for the eight monoclinic space groups with centred lattices or glide planes (Nos. 5, 7–9, 12–15) to indicate the various settings and cell choices. A complete list of symbols, including also the *a*-axis setting, is contained in Table 1.5.4.4; further details are given in Section 2.1.3.15.

For standard *short* monoclinic space-group symbols see Sections 2.1.3.3 and 2.1.3.15.

(iii) *Cubic space groups*. The short symbols for all space groups belonging to the two cubic crystal classes $m\bar{3}$ and $m\bar{3}m$ now contain the symbol $\bar{3}$ instead of 3. This applies to space groups Nos. 200–206 and 221–230, as well as to the two point groups $m\bar{3}$ and $m\bar{3}m$.

Examples

No. 205: Change from $Pa3$ to $Pa\bar{3}$

No. 230: Change from $Ia3d$ to $Ia\bar{3}d$.

With this change, the centrosymmetric nature of these groups is apparent also in the short symbols.

(iv) *Glide-plane symbol e*. For the introduction of the 'double glide plane' *e* into five space-group symbols, see Section 2.1.2.

2.1.3.5. Patterson symmetry

By H. D. Flack

The entry *Patterson symmetry* in the headline gives the symmetry of the 'vector set' generated by the operation of the space group on an arbitrary set of general positions. More prosaically, it may be described as the symmetry of the set of the interatomic vectors of a crystal structure with the selected space group. The Patterson symmetry is a crystallographic space group denoted by its Hermann–Mauguin symbol. It is in fact one of the 24 centrosymmetric symmorphic space groups (see Section 1.3.3.3) in three dimensions and one of 7 in two dimensions. For each of the 230 space groups, the Patterson symmetry has the same Bravais-lattice type as the space group itself and its point group is the lowest-index centrosymmetric supergroup of the point group of the space group. The 'point-group part' of the symbol of the Patterson symmetry represents the Laue class to which the plane group or space group belongs (*cf.* Table 2.1.2.1). By way of examples: space group No. 100, *P*4*bm*, has a Bravais lattice of type *tP* and point group 4*mm*. The centrosymmetric supergroup of 4*mm* (see Fig. 3.2.1.3) is 4/*mmm*, so the Patterson symmetry is *P*4/*mmm*; space group No. 66, *Cccm*, has a Bravais lattice of type *oC* and point group *mmm*. This point group is centrosymmetric, so the Patterson symmetry is *Cmmm*.

Note: For the four space groups *Amm*2 (38), *Aem*2 (39), *Ama*2 (40) and *Aea*2 (41), the standard symbol for their Patterson symmetry, *Cmmm*, is added (between parentheses) after the actual symbol *Ammm* in the space-group tables.

The Patterson symmetry is intimately related to the symmetry of the Patterson function (see Flack, 2015). The latter, $P_{|F|^2}(uvw)$, is the inverse Fourier transform of the squared structure-factor amplitudes. Patterson functions possess the crystallographic symmetry of the symmorphic space-group representative of the arithmetic crystal class (see Section 1.3.4.4.1) to which the space group belongs. Table 2.1.3.3 lists these crystallographic symmetries of the Patterson function and the Patterson symmetries for the space groups and plane groups. However, further symmetry is also present, as desribed below for the three common forms of the Patterson function:

(*a*) $P_{|F|^2}(uvw)$: The most general form of the Patterson function, the complex $P_{|F|^2}(uvw)$, is the complex Fourier transform of $|F(hkl)|^2$. The full symmetry of $P_{|F|^2}(uvw)$ can be described in terms of the 1651 two-colour (Shubnikov) space groups (Fischer & Knof, 1987; Wilson, 1993; Shubnikov & Belov, 1964; *cf.* also Chapter 3.6). The real and imaginary parts of $P_{|F|^2}(uvw)$ have the same symmetry as $P_A(uvw)$ and $P_D(uvw)$, respectively, described below. $P_{|F|^2}(uvw)$ is real for centrosymmetric space groups and noncentrosymmetric ones in the absence of any resonant-scattering contribution.

(*b*) $P_A(uvw)$: $A(hkl) = \frac{1}{2}[|F(hkl)|^2 + |F(\bar{h}\bar{k}\bar{l})|^2]$, the average of the squared structure-factor amplitudes of the pair of Friedel opposites *hkl* and $\bar{h}\bar{k}\bar{l}$. Real $P_A(uvw)$ is the real cosine Fourier

Table 2.1.3.3
Patterson symmetries and symmetries of Patterson functions for space groups and plane groups

The space-group types of each row form an arithmetic crystal class. (In three instances the row is typeset on two lines.) The arithmetic crystal class is identified by its representative symmorphic space group for which both the Hermann–Mauguin symbol and the space-group-type number are shown in bold. A set of space groups with sequential numbers is indicated by the symbols of the first and last space group of the sequence separated by a dash.

The column 'Patterson symmetry' indicates the symmetry of the set of interatomic vectors of crystal structures described in the space groups given in the column 'Space-group types'. The Patterson symmetry is also the symmetry of $P_A(uvw)$ and the real part of the complex $P_{|F|^2}(uvw)$. The Patterson symmetry is given in the headline of each space-group table in Chapter 2.3.

The crystallographic symmetry of both $P_D(uvw)$ and the imaginary part of the complex $P_{|F|^2}(uvw)$ is that of the symmorphic space group of crystal structures described in the space groups given in the column 'Space-group types'. To this crystallographic symmetry, the noncrystallographic operation of a centre of antisymmetry needs to be added to give $P_D(uvw) = -P_D(\bar{u}\bar{v}\bar{w})$. The full symmetry of $P_D(uvw)$ is not shown in this volume.

The setting and origin choice of the chosen space group should also be used for the space group of the Patterson symmetry and the symmorphic space group.

Similar remarks apply to the plane groups listed in part (*b*) of the table.

(*a*) Space groups.

Space-group types		Patterson symmetry
Hermann–Mauguin symbols	Nos.	
Crystal family triclinic (anorthic), Bravais-lattice type *aP*		
***P*1**	**1**	$P\bar{1}$
***P*$\bar{1}$**	**2**	$P\bar{1}$
Crystal family monoclinic, Bravais-lattice type *mP*		
***P*2**–$P2_1$	**3**–4	$P2/m$
Pm–Pc	**6**–7	$P2/m$
P*2/*m–$P2_1/m$, $P2/c$–$P2_1/c$	**10**–11, 13–14	$P2/m$
Crystal family monoclinic, Bravais-lattice type *mS*		
***C*2**	**5**	$C2/m$
Cm–Cc	**8**–9	$C2/m$
C*2/*m, $C2/c$	**12**, 15	$C2/m$
Crystal family orthorhombic, Bravais-lattice type *oP*		
***P*222**–$P2_12_12_1$	**16**–19	$Pmmm$
***Pmm*2**–$Pnn2$	**25**–34	$Pmmm$
Pmmm–$Pnma$	**47**–62	$Pmmm$
Crystal family orthorhombic, Bravais-lattice type *oS*		
$C222_1$, ***C*222**	20, **21**	$Cmmm$
***Cmm*2**–$Ccc2$	**35**–37	$Cmmm$
***Amm*2**–$Aea2$	**38**–41	$Ammm$
$Cmcm$–$Cmce$, ***Cmmm***, $Cccm$–$Ccce$	63–64, **65**, 66–68	$Cmmm$
Crystal family orthorhombic, Bravais-lattice type *oF*		
***F*222**	**22**	$Fmmm$
***Fmm*2**–$Fdd2$	**42**–43	$Fmmm$
Fmmm–$Fddd$	**69**–70	$Fmmm$
Crystal family orthorhombic, Bravais-lattice type *oI*		
***I*222**–$I2_12_12_1$	**23**–24	$Immm$
***Imm*2**–$Ima2$	**44**–46	$Immm$
Immm–$Imma$	**71**–74	$Immm$
Crystal family tetragonal, Bravais-lattice type *tP*		
***P*4**–$P4_3$	**75**–78	$P4/m$
***P*$\bar{4}$**	**81**	$P4/m$
P*4/*m–$P4_2/n$	**83**–86	$P4/m$
***P*422**–$P4_32_12$	**89**–96	$P4/mmm$
P*4*mm–$P4_2bc$	**99**–106	$P4/mmm$
P*$\bar{4}$2*m–$P\bar{4}2_1c$	**111**–114	$P4/mmm$
***P*$\bar{4}$*m*2**–$P\bar{4}n2$	**115**–118	$P4/mmm$
P*4/*mmm–$P4_2/ncm$	**123**–138	$P4/mmm$
Crystal family tetragonal, Bravais-lattice type *tI*		
***I*4**, $I4_1$	**79**–80	$I4/m$
***I*$\bar{4}$**	**82**	$I4/m$
I*4/*m–$I4_1/a$	**87**–88	$I4/m$
***I*422**–$I4_122$	**97**–98	$I4/mmm$
I*4*mm–$I4_1cd$	**107**–110	$I4/mmm$
***I*$\bar{4}$*m*2**–$I\bar{4}c2$	**119**–120	$I4/mmm$
I*$\bar{4}$2*m–$I\bar{4}2d$	**121**–122	$I4/mmm$
I*4/*mmm–$I4_1/acd$	**139**–142	$I4/mmm$
Crystal family hexagonal, Bravais-lattice type *hP*		
***P*3**–$P3_2$	**143**–145	$P\bar{3}$
***P*$\bar{3}$**	**147**	$P\bar{3}$
***P*312**, $P3_112$, $P3_212$	**149**, 151, 153	$P\bar{3}1m$
***P*321**, $P3_121$, $P3_221$	**150**, 152, 154	$P\bar{3}m1$
***P*3*m*1**, $P3c1$	**156**, 158	$P\bar{3}m1$
P*31*m, $P31c$	**157**, 159	$P\bar{3}1m$
P*$\bar{3}$1*m–$P\bar{3}1c$	**162**–163	$P\bar{3}1m$
***P*$\bar{3}$*m*1**–$P\bar{3}c1$	**164**–165	$P\bar{3}m1$
***P*6**–$P6_3$	**168**–173	$P6/m$
***P*$\bar{6}$**	**174**	$P6/m$
P*6/*m–$P6_3/m$	**175**–176	$P6/m$
***P*622**–$P6_322$	**177**–182	$P6/mmm$
P*6*mm–$P6_3mc$	**183**–186	$P6/mmm$
***P*$\bar{6}$*m*2**–$P\bar{6}c2$	**187**–188	$P6/mmm$
P*$\bar{6}$2*m–$P\bar{6}2c$	**189**–190	$P6/mmm$
P*6/*mmm–$P6_3/mmc$	**191**–194	$P6/mmm$
Crystal family hexagonal, Bravais-lattice type *hR*		
***R*3**	**146**	$R\bar{3}$
***R*$\bar{3}$**	**148**	$R\bar{3}$
***R*32**	**155**	$R\bar{3}m$
R*3*m–$R3c$	**160**–161	$R\bar{3}m$
R*$\bar{3}$*m–$R\bar{3}c$	**166**–167	$R\bar{3}m$
Crystal family cubic, Bravais-lattice type *cP*		
***P*23**, $P2_13$	**195**, 198	$Pm\bar{3}$
***Pm*$\bar{3}$**–$Pn\bar{3}$, $Pa\bar{3}$	**200**–201, 205	$Pm\bar{3}$
***P*432**–$P4_232$, $P4_332$–$P4_132$	**207**–208, 212–213	$Pm\bar{3}m$
P*$\bar{4}$3*m, $P\bar{4}3n$	**215**, 218	$Pm\bar{3}m$
Pm*$\bar{3}$*m–$Pn\bar{3}m$	**221**–224	$Pm\bar{3}m$

transform of $A(hkl)$. The symmetry of $P_A(uvw)$ is generated by the symmorphic space-group representative of the arithmetic crystal class to which the space group belongs, combined with a centre of symmetry (inversion centre), *i.e.* $P_A(uvw) = P_A(\bar{u}\bar{v}\bar{w})$. $P_A(uvw)$ thus possesses the Patterson symmetry of the space group whether the latter is centrosymmetric or not, and whether there is any resonant-scattering contribution or not (see Table 2.1.3.3).

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.

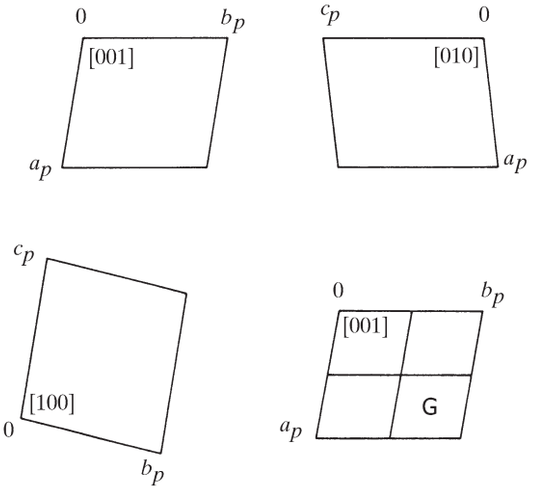

Figure 2.1.3.1
Triclinic space groups (G = general-position diagram).

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.* $\alpha, \beta, \gamma \geq 90^\circ$. For a cell

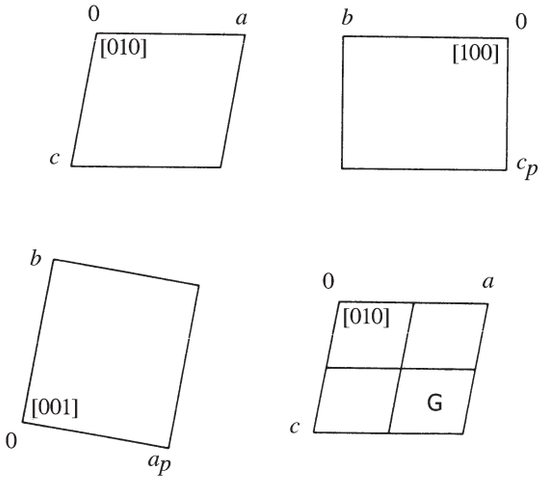

Figure 2.1.3.2
Monoclinic space groups, setting with unique axis *b* (G = general-position diagram).

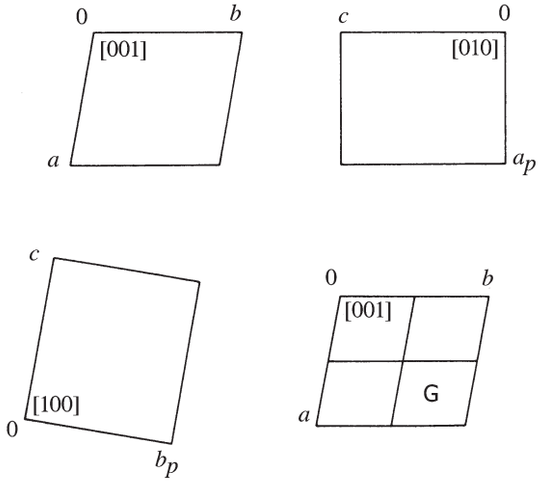

Figure 2.1.3.3
Monoclinic space groups, setting with unique axis *c* (G = general-position diagram).

of type I, all angles are acute, *i.e.* $\alpha, \beta, \gamma < 90°$. 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.

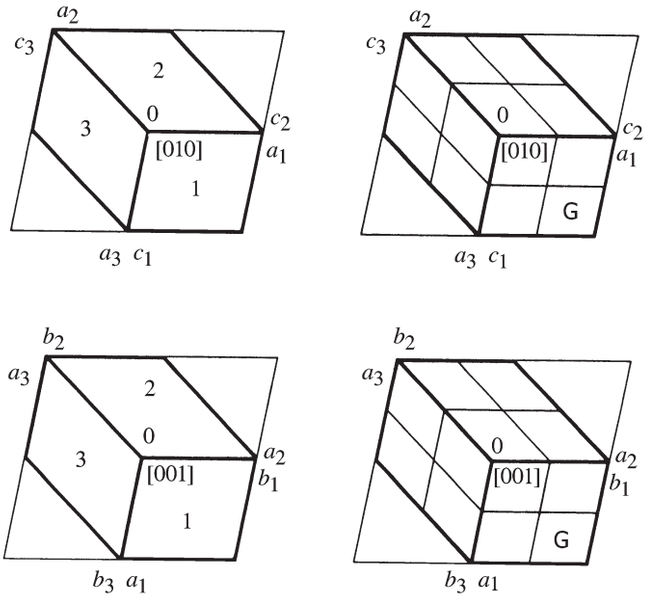

Figure 2.1.3.4
Monoclinic space groups, cell choices 1, 2, 3. Upper pair of diagrams: setting with unique axis *b*. Lower pair of diagrams: setting with unique axis *c*. The numbers 1, 2, 3 within the cells and the subscripts of the labels of the axes indicate the cell choice (*cf.* Section 2.1.3.15).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

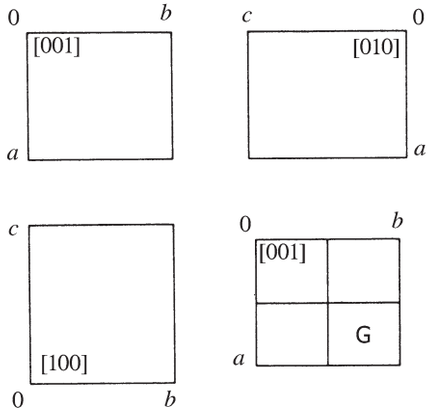

Figure 2.1.3.5
Orthorhombic space groups. Diagrams for the 'standard setting' as described in the space-group tables (G = general-position diagram).

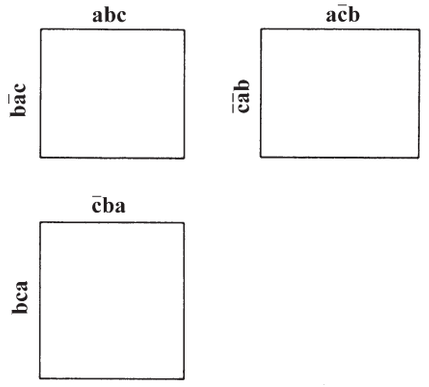

Figure 2.1.3.6
Orthorhombic space groups. The three projections of the symmetry elements with the six setting symbols (see text). For setting symbols printed vertically, the page has to be turned clockwise by 90° or viewed from the side. Note that in the actual space-group tables instead of the setting 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, **a**, **b**, **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, **ba$\bar{\mathbf{c}}$** 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 **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 different projections of a *single* (standard) setting of the space group, with the projected basis vectors **a**, **b**, **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

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	*mm*2	2/*m* 2/*m* 2/*m*
6 (22 space groups)		*Pmc*2_1 (26) *Pma*2 (28) *Pca*2_1 (29) *Pnc*2 (30) *Pna*2_1 (33) *Cmc*2_1 (36) *Amm*2 (38) *Aem*2 (39) *Ama*2 (40) *Aea*2 (41) *Ima*2 (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) *Pmn*2_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)	*P*222$_1$ (17) *P*2_12_12 (18) *C*222$_1$ (20) *C*222 (21)	*Pmm*2 (25) *Pcc*2 (27) *Pba*2 (32) *Pnn*2 (34) *Cmm*2 (35) *Ccc*2 (37) *Fmm*2 (42) *Fdd*2 (43) *Imm*2 (44) *Iba*2 (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)	*P*222 (16) *P*$2_12_12_1$ (19) *F*222 (22) *I*222 (23) *I*$2_12_12_1$ (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

[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 **abc**, **ab$\bar{\mathbf{c}}$**, **$\bar{\mathbf{a}}$b$\bar{\mathbf{c}}$**, **$\bar{\mathbf{a}}\bar{\mathbf{b}}$c** and the left-handed systems **$\bar{\mathbf{a}}\bar{\mathbf{b}}\bar{\mathbf{c}}$**, **$\bar{\mathbf{a}}$bc**, **ab$\bar{\mathbf{c}}$**, **$\bar{\mathbf{a}}\bar{\mathbf{b}}$c**.

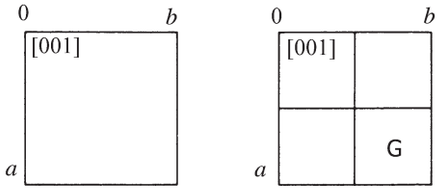

Figure 2.1.3.7
Tetragonal space groups (G = general-position diagram).

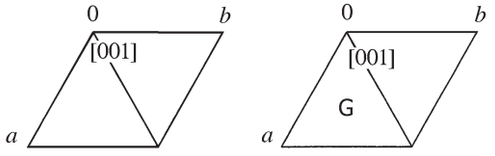

Figure 2.1.3.8
Trigonal *P* and hexagonal *P* space groups (G = general-position diagram).

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 $-z$).

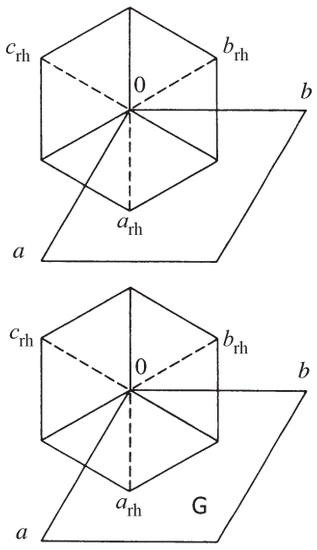

Figure 2.1.3.9
Rhombohedral space groups. Obverse triple hexagonal cell with 'hexagonal axes' *a*, *b* and primitive rhombohedral cell with projections of 'rhombohedral axes' $a_{\rm rh}$, $b_{\rm rh}$, $c_{\rm rh}$. Note: In the actual space-group diagrams the edges of the primitive rhombohedral cell (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).

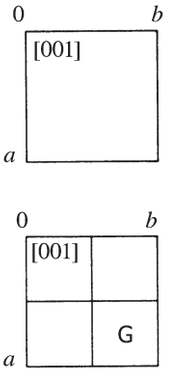

Figure 2.1.3.10
Cubic space groups. G = general-position diagram, in which the equivalent positions are shown as the vertices of polyhedra.

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,

Table 2.1.3.5
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 $\bar{2}\bar{2}\bar{2}$	
*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 $3_11(1, 1, 2)$	$3_1 \parallel [001]$, $2 \parallel [210]$

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 2.1.3.1. 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 *mm*2, 4*mm*, $\bar{4}2m$, 3*m*, 6*mm* and $\bar{6}2m$ if the site symmetry at the origin can be easily recognized from the shortened symbol.

(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 2.1.3.1). 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 2.1.3.1. 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 2.1.3.9 and 1.4.2.1.

(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.

2.1.3.8. 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, following *IT* A (2002), the asymmetric units

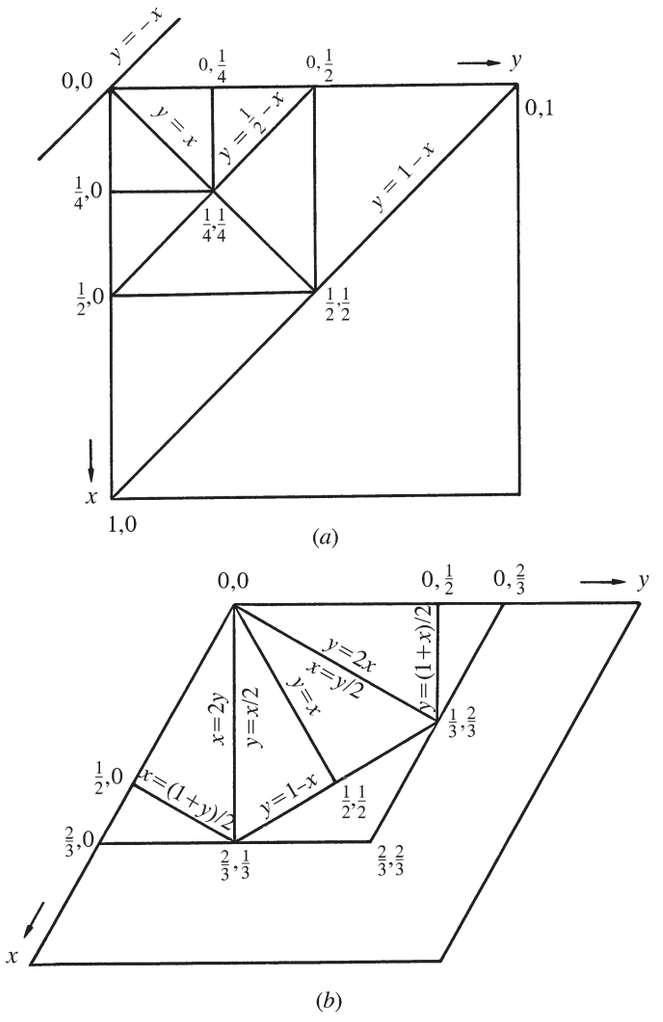

Figure 2.1.3.11
Boundary planes of asymmetric units occurring in the space-group tables. (*a*) Tetragonal system. (*b*) Trigonal and hexagonal systems. The point coordinates refer to the vertices in the plane $z = 0$.

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. 2.1.3.11 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, $x = (1 + y)/2$, $y = 1 - x$, $y = (1 + x)/2$. The asymmetric unit is defined by

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

Vertices: $0,0,0$ $\frac{1}{2},0,0$ $\frac{2}{3},\frac{1}{3},0$ $\frac{1}{3},\frac{2}{3},0$ $0,\frac{1}{2},0$
$0,0,\frac{1}{6}$ $\frac{1}{2},0,\frac{1}{6}$ $\frac{2}{3},\frac{1}{3},\frac{1}{6}$ $\frac{1}{3},\frac{2}{3},\frac{1}{6}$ $0,\frac{1}{2},\frac{1}{6}$.

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.

2.1.3.9. Symmetry operations

As explained in Sections 1.3.3.2 and 1.4.2.3, 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*.

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 space groups with *primitive* cells, the two lists contain the same number of entries.

For space groups with *centred* cells, several (2, 3 or 4) blocks of *Symmetry operations* correspond to the one *General position* block. 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 themselves (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.

The coordinate triplets of the general position represent the symmetry operations chosen as coset representatives of the decomposition of the space group with respect to its translation subgroup (*cf.* Section 1.4.2 for a detailed discussion). In space groups with two origins the origin shift may lead to the choice of symmetry operations of different types as coset representatives of the same coset (*e.g.* mirror *versus* glide plane, rotation *versus* screw axis, see Tables 1.4.2.2 and 1.4.2.3) and designated by the same number (p) in the general-position blocks of the two descriptions. Thus, in $P4/nmm$ (129), (p) = (7) represents a 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.

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.* Section 2.1.2), 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 also given.

Examples

(1) $g(\frac{1}{4},\frac{1}{4},\frac{1}{2})$ $\quad x, x, z$
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.

(2) $g(\frac{1}{3},\frac{1}{6},\frac{1}{6})$ $\quad 2x-\frac{1}{2}, x, z$ (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).

(3) 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 $0,\frac{1}{4}, z$.

Details on the symbolism and further illustrative examples are presented in Section 1.4.2.1.

2.1.3.10. Generators

The line *Generators selected* states the symmetry operations and their sequence, selected to generate all symmetry-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 2.1.3.9 [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-centred 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 1.4.3.1.

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 symmetry-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 1.4.3.

The generating operations for different descriptions of the same space group (settings, cell choices, origin choices) are chosen in such a way that the transformation relating the two coordinate systems also transforms the generators of one description into those of the other (*cf.* Section 1.5.3).

2.1.3.11. Positions

The entries under *Positions*[2] (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 of the Wyckoff position*. This is the number of equivalent points per unit cell. For primitive cells, the multiplicity of the general position is equal to the order of the point group of the space group; for centred cells, it 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 and the quotient of the two is equal to the order of the site-symmetry group.

(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.

(iii) *Site symmetry*. This is explained in Section 2.1.3.12.

(iv) *Coordinates*. The sequence of coordinate triplets is produced in the same order as the symmetry operations, generated by the chosen set of generators, omitting duplicates (*cf.* Sections 1.4.3 and 2.1.3.10). 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 these centring translations have to be added to the listed coordinate triplets. Note that not all points of a position always lie within the unit cell; some may be outside since the coordinates are formulated modulo 1; thus, for example, $\bar{x}, \bar{y}, \bar{z}$ is written rather than $\bar{x}+1, \bar{y}+1, \bar{z}+1$.

The coordinate triplets of a position represent the coordinates of the equivalent points (atoms) in the unit cell. A graphic representation of the points of the general position is provided by the general-position diagram; *cf.* Section 2.1.3.6.

(v) *Reflection conditions*. These are described in Section 2.1.3.13.

Detailed treatment of general and special Wyckoff positions, including definitions, theoretical background and examples, is given in Section 1.4.4.

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

(i) *General position*

A point is said to be in general position if it is left invariant only by the identity operation but by no other symmetry operation of the space group. Each space group has only one general position.

The coordinate triplets of a general position (which always start with x, y, z) can also be interpreted as a shorthand form of the matrix representation of the symmetry operations of the space group; this viewpoint is described further in Sections 1.3.3.2 and 1.4.2.3.

(ii) *Special position(s)*

A point is said to be in 'special position' if it is mapped onto itself by the identity and at least one further symmetry operation of the space group. This implies that specific constraints are imposed on the coordinates of each point of a special position; *e.g.* $x=\frac{1}{4}, y=0$, leading to the triplet $\frac{1}{4}, 0, z$; or $y=x+\frac{1}{2}$, leading to the triplet $x, x+\frac{1}{2}, z$. The number of special positions of a space group depends on the space-group type and can vary from 1 to 26 (in *Pmmm*, No. 47).

The set of *all* symmetry operations that map a point onto itself forms a group, known as the 'site-symmetry group' of that point. It is given in the third column by the 'oriented site-symmetry symbol' which is explained in Section 2.1.3.12. General positions always have site symmetry 1, whereas special positions have higher site symmetries, which can differ from one special position to another.

If in a crystal structure the centres of finite objects, such as molecules, are placed at the points of a special position, each such object must display a point symmetry that is at least as high as the site symmetry of the special position. Geometrically, this means that the centres of these objects are located on symmetry elements without translations (centre of symmetry, mirror plane, rotation axis, rotoinversion axis) or at the intersection of several symmetry elements of this kind (*cf.* the space-group diagrams).

Note that the location of an object on a screw axis or on a glide plane does *not* lead to an increase in the site symmetry and to a corresponding reduction of the multiplicity for that object. Accordingly, a space group that contains only symmetry elements *with* translation components does not have any special position. Such a space group is called 'fixed-point-free' (for further discussion, see Section 1.4.4.2).

Example: Space group C12/c1 (15, unique axis b, cell choice 1)

The general position 8*f* of this space 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 coordinates of the other four points are obtained by adding the components $\frac{1}{2}, \frac{1}{2}, 0$ of the *C*-centring translation to the coordinate triplets (1) to (4).

The space group has five special positions with Wyckoff letters *a* to *e*. The positions 4*a* to 4*d* require inversion symmetry, $\bar{1}$, whereas Wyckoff position 4*e* requires twofold rotation symmetry, 2, for any object in such a position. For position 4*e*, for instance, the four equivalent points have the coordinates $0, y, \frac{1}{4}$; $0, \bar{y}, \frac{3}{4}$; $\frac{1}{2}, y+\frac{1}{2}, \frac{1}{4}$; $\frac{1}{2}, \bar{y}+\frac{1}{2}, \frac{3}{4}$. The values of x and z are specified, whereas y may take any value. Since each point of position 4*e* is mapped onto itself by a twofold rotation, the multiplicity of the position is reduced from 8 to 4, whereas the order of the site-symmetry group is increased from 1 to 2.

From the symmetry-element diagram of *C*2/*c*, the locations of the four twofold axes can be deduced as $0, y, \frac{1}{4}$; $0, y, \frac{3}{4}$; $\frac{1}{2}, y, \frac{1}{4}$; $\frac{1}{2}, y, \frac{3}{4}$.

From this example, the general rule is apparent that the product of the position multiplicity and the order of the corresponding site-symmetry group is constant for all Wyckoff positions of a given space group; it is the multiplicity of the general position.

Attention is drawn to ambiguities in the description of crystal structures in a few space groups, depending on whether the coordinate triplets of *IT* (1952) or of this edition are taken. This problem is analysed by Parthé *et al.* (1988).

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

2.1.3.12. Oriented site-symmetry symbols

The third column of each Wyckoff position gives the *Site symmetry*[3] of that position. The site-symmetry group is isomorphic to a (proper or improper) subgroup of the point group to which the space group under consideration belongs. The site-symmetry groups of the different points of the same special position are conjugate (symmetry-equivalent) subgroups of the space group. For this reason, all points of one special position are described by the same site-symmetry symbol. (See Section 1.4.4 for a detailed discussion of site-symmetry groups.)

Oriented site-symmetry symbols (*cf.* Fischer *et al.*, 1973) are employed to show how the symmetry elements at a site are related to the symmetry elements of the crystal lattice. The site-symmetry symbols display the same sequence of symmetry directions as the space-group symbol (*cf.* Table 2.1.3.1). Sets of equivalent symmetry directions that do not contribute any element to the site-symmetry group are represented by a dot. In this way, the orientation of the symmetry elements at the site is emphasized, as illustrated by the following examples.

Examples

(1) In the tetragonal space group $P4_22_12$ (94), Wyckoff position 4*f* has site symmetry ..2 and position 2*b* has site symmetry 2.22. The easiest way to interpret the symbols is to look at the dots first. For position 4*f*, the 2 is preceded by two dots and thus must belong to a tertiary symmetry direction. Only one tertiary direction is used. Consequently, the site symmetry is the monoclinic point group 2 with one of the two tetragonal tertiary directions as twofold axis.
Position *b* has one dot, with one symmetry symbol before and two symmetry symbols after it. The dot corresponds, therefore, to the secondary symmetry directions. The first symbol 2 indicates a twofold axis along the primary symmetry direction (*c* axis). The final symbols 22 indicate two twofold axes along the two mutually perpendicular tertiary directions $[1\bar{1}0]$ and [110]. The site symmetry is thus orthorhombic, 222.

(2) In the cubic space group *I*23 (197), position 6*b* has 222.. as its oriented site-symmetry symbol. The orthorhombic group 222 is completely related to the primary set of cubic symmetry directions, with the three twofold axes parallel to the three equivalent primary directions [100], [010], [001].

(3) In the cubic space group $Pn\bar{3}n$ (222), position 6*b* has 42.2 as its site-symmetry symbol. This 'cubic' site-symmetry symbol displays a tetragonal site symmetry. The position of the dot indicates that there is no symmetry along the four secondary cubic directions. The fourfold axis is connected with one of the three primary cubic symmetry directions and two equivalent twofold axes occur along the remaining two primary directions. Moreover, the group contains two mutually perpendicular (equivalent) twofold axes along those two of the six tertiary cubic directions ⟨110⟩ that are normal to the fourfold axis. Each pair of equivalent twofold axes is given by just one symbol 2. (Note that at the six sites of position 6*b* the fourfold axes are twice oriented along *a*, twice along *b* and twice along *c*.)

(4) In the tetragonal space group $P4_2/nnm$ (134), position 2*a* has site symmetry $\bar{4}2m$. The site has symmetry for all symmetry directions. Because of the presence of the primary $\bar{4}$ axis, only one of the twofold axes along the two secondary directions need be given explicitly and similarly for the mirror planes *m* perpendicular to the two tertiary directions.

The above examples show:

(i) The oriented site-symmetry symbols become identical to Hermann–Mauguin point-group symbols if the dots are omitted.

(ii) Sets of symmetry directions having more than one equivalent direction may require more than one character if the site-symmetry group belongs to a lower crystal system than the space group under consideration.

To show, for the same type of site symmetry, how the oriented site-symmetry symbol depends on the space group under discussion, the site-symmetry group *mm*2 will be considered in orthorhombic and tetragonal space groups. Relevant crystal classes are *mm*2, *mmm*, 4*mm*, $\bar{4}2m$ and $4/mmm$. The site symmetry *mm*2 contains two mutually perpendicular mirror planes intersecting in a twofold axis.

For space groups of crystal class *mm*2, the twofold axis at the site must be parallel to the one direction of the rotation axes of the space group. The site-symmetry group *mm*2, therefore, occurs only in the orientation *mm*2. For space groups of class *mmm* (full symbol $2/m\ 2/m\ 2/m$), the twofold axis at the site may be parallel to *a*, *b* or *c* and the possible orientations of the site symmetry are 2*mm*, *m*2*m* and *mm*2. For space groups of the tetragonal crystal class 4*mm*, the twofold axis of the site-symmetry group *mm*2 must be parallel to the fourfold axis of the crystal. The two mirror planes must belong either to the two secondary or to the two tertiary tetragonal directions so that 2*mm*. and 2.*mm* are possible site-symmetry symbols. Similar considerations apply to class $\bar{4}2m$, which can occur in two settings, $\bar{4}2m$ and $\bar{4}m2$. Finally, for class $4/mmm$ (full symbol $4/m\ 2/m\ 2/m$), the twofold axis of 2*mm* may belong to any of the three kinds of symmetry directions and possible oriented site symmetries are 2*mm*., 2.*mm*, *m*2*m*. and *m*.2*m*. In the first two symbols, the twofold axis extends along the single primary direction and the mirror planes occupy either both secondary or both tertiary directions; in the last two cases, one mirror plane belongs to the primary direction and the second to either one secondary or one tertiary direction (the other equivalent direction in each case being occupied by the twofold axis).

2.1.3.13. Reflection conditions

The *Reflection conditions*[4] are listed in the right-hand column of each Wyckoff position.

These conditions are formulated here, in accordance with general practice, as 'conditions of occurrence' (structure factor not systematically zero) and not as 'extinctions' or 'systematic absences' (structure factor zero). Reflection conditions are listed for *all* those three-, two- and one-dimensional sets of reflections for which extinctions exist; hence, for those nets or rows that are *not* listed, no reflection conditions apply. The theoretical background of reflection conditions and their derivation are discussed in detail in Section 1.6.3.

[3] Often called point symmetry: *Punktsymmetrie* or *Lagesymmetrie* (German): *symétrie ponctuelle* (French).

[4] The reflection conditions were called *Auslöschungen* (German), missing spectra (English) and *extinctions* (French) in *IT* (1935) and 'Conditions limiting possible reflections' in *IT* (1952); they are often referred to as 'Systematic or space-group absences' (*cf.* Section 3.3.3).

There are two types of systematic reflection conditions for diffraction of radiation by crystals:

(1) *General conditions*. They are associated with systematic absences caused by the presence of lattice centrings, screw axes and glide planes. The general conditions are always obeyed, irrespective of which Wyckoff positions are occupied by atoms in a particular crystal structure.
(2) *Special conditions* ('extra' conditions). They apply only to *special* Wyckoff positions and always occur in addition to the general conditions of the space group. Note that each extra condition is valid only for the scattering contribution of those atoms that are located in the relevant special Wyckoff position. If the special position is occupied by atoms whose scattering power is high in comparison with the other atoms in the structure, reflections violating the extra condition will be weak. One should note that the special conditions apply only to isotropic and spherical atoms (*cf.* Section 1.6.3).

General reflection conditions. These are due to one of three effects:

(i) *Centred cells*. The resulting conditions apply to the whole three-dimensional set of reflections *hkl*. Accordingly, they are called *integral reflection conditions*. They are given in Table 2.1.3.6. These conditions result from the centring vectors of centred cells. They disappear if a primitive cell is chosen instead of a centred cell. Note that the centring symbol and the corresponding integral reflection condition may change with a change of the basis vectors (*e.g.* monoclinic: $C \rightarrow A \rightarrow I$).
(ii) *Glide planes*. The resulting conditions apply only to two-dimensional sets of reflections, *i.e.* to reciprocal-lattice nets containing the origin (such as *hk*0, *h*0*l*, 0*kl, hhl*). For this reason, they are called *zonal reflection conditions*. The indices *hkl* of these 'zonal reflections' obey the relation $hu + kv + lw = 0$, where $[uvw]$, the direction of the zone axis, is normal to the reciprocal-lattice net. Note that the symbol of a glide plane and the corresponding zonal reflection condition may change with a change of the basis vectors (*e.g.* monoclinic: $c \rightarrow n \rightarrow a$).
(iii) *Screw axes*. The resulting conditions apply only to one-dimensional sets of reflections, *i.e.* reciprocal-lattice rows containing the origin (such as *h*00, 0*k*0, 00*l*). They are called *serial reflection conditions*. It is interesting to note that some diagonal screw axes do not give rise to systematic absences (*cf.* Section 1.6.3 for more details).

Reflection conditions of types (ii) and (iii) are listed in Table 2.1.3.7. They can be understood as follows: Zonal and serial reflections form two- or one-dimensional sections through the origin of reciprocal space. In direct space, they correspond to projections of a crystal structure onto a plane or onto a line. Glide planes or screw axes may reduce the translation periods in these projections (*cf.* Section 2.1.3.14) and thus decrease the size of the projected cell. As a consequence, the cells in the corresponding reciprocal-lattice sections are increased, which means that systematic absences of reflections occur.

For the two-dimensional groups, the reasoning is analogous. The reflection conditions for the plane groups are assembled in Table 2.1.3.8.

For the *interpretation of observed reflections*, the general reflection conditions must be studied in the order (i) to (iii), as conditions of type (ii) may be included in those of type (i), while conditions of type (iii) may be included in those of types (i) or (ii). This is shown in the example below.

Table 2.1.3.6
Integral reflection conditions for centred cells (lattices)

Reflection condition	Centring type of cell	Centring symbol
None	Primitive	P
		R† (rhombohedral axes)
$h + k = 2n$	C-face centred	C
$k + l = 2n$	A-face centred	A
$h + l = 2n$	B-face centred	B
$h + k + l = 2n$	Body centred	I
$h + k$, $h + l$ and $k + l = 2n$ or: h, k, l all odd or all even ('unmixed')	All-face centred	F
$-h + k + l = 3n$	Rhombohedrally centred, obverse setting (standard)	R† (hexagonal axes)
$h - k + l = 3n$	Rhombohedrally centred, reverse setting	R† (hexagonal axes)
$h - k = 3n$	Hexagonally centred	H‡

† For further explanations see Section 2.1.1 and Table 2.1.1.2.
‡ For the use of the unconventional H cell, see Section 1.5.4 and Table 2.1.1.2.

In the *space-group tables*, the reflection conditions are given according to the following rules:

(i) for a given space group, all reflection conditions [up to symmetry equivalence, *cf.* rule (v)] are listed; hence for those nets or rows that are *not* listed no conditions apply. No distinction is made between 'independent' and 'included' conditions, as was done in *IT* (1952), where 'included' conditions were placed in parentheses;
(ii) the integral condition, if present, is always listed first, followed by the zonal and serial conditions;
(iii) conditions that have to be satisfied simultaneously are separated by a comma or by 'AND'. Thus, if two indices must be even, say h and l, the condition is written $h, l = 2n$ rather than $h = 2n$ and $l = 2n$. The same applies to sums of indices. Thus, there are several different ways to express the integral conditions for an F-centred lattice: '$h + k, h + l, k + l = 2n$' or '$h + k, h + l = 2n$ and $k + l = 2n$' or '$h + k = 2n$ and $h + l, k + l = 2n$' (*cf.* Table 2.1.3.6);
(iv) conditions separated by 'OR' are alternative conditions. For example, '*hkl*: $h = 2n + 1$ or $h + k + l = 4n$' means that *hkl* is 'present' if either the condition $h = 2n + 1$ *or* the alternative condition $h + k + l = 4n$ is fulfilled. Obviously, *hkl* is also a 'present' reflection if both conditions are satisfied. Note that 'or' conditions occur only for the *special conditions* described below;
(v) in crystal systems with two or more symmetry-equivalent nets or rows (tetragonal and higher), only *one* representative set (the first one in Table 2.1.3.7) is listed; *e.g.* tetragonal: only the first members of the equivalent sets 0*kl* and *h*0*l* or *h*00 and 0*k*0 are listed;
(vi) for cubic space groups, it is stated that the indices *hkl* are 'cyclically permutable' or 'permutable'. The cyclic permutability of h, k and l in all rhombohedral space groups, described with 'rhombohedral axes', and of h and k in some tetragonal space groups are not stated;

Table 2.1.3.7
Zonal and serial reflection conditions for glide planes and screw axes (*cf.* Table 2.1.2.1)

(*a*) Glide planes

Type of reflections	Reflection condition	Glide plane: Orientation of plane	Glide plane: Glide vector	Glide plane: Symbol	Crystallographic coordinate system to which condition applies	
$0kl$	$k = 2n$	(100)	$\mathbf{b}/2$	b	Monoclinic (a unique), Tetragonal	Orthorhombic, Cubic
	$l = 2n$		$\mathbf{c}/2$	c		
	$k + l = 2n$		$\mathbf{b}/2 + \mathbf{c}/2$	n		
	$k + l = 4n$ $(k, l = 2n)$ †		$\mathbf{b}/4 \pm \mathbf{c}/4$	d		
$h0l$	$l = 2n$	(010)	$\mathbf{c}/2$	c	Monoclinic (b unique), Tetragonal	Orthorhombic, Cubic
	$h = 2n$		$\mathbf{a}/2$	a		
	$l + h = 2n$		$\mathbf{c}/2 + \mathbf{a}/2$	n		
	$l + h = 4n$ $(l, h = 2n)$ †		$\mathbf{c}/4 \pm \mathbf{a}/4$	d		
$hk0$	$h = 2n$	(001)	$\mathbf{a}/2$	a	Monoclinic (c unique), Tetragonal	Orthorhombic, Cubic
	$k = 2n$		$\mathbf{b}/2$	b		
	$h + k = 2n$		$\mathbf{a}/2 + \mathbf{b}/2$	n		
	$h + k = 4n$ $(h, k = 2n)$ †		$\mathbf{a}/4 \pm \mathbf{b}/4$	d		
$h\bar{h}0l$ $0k\bar{k}l$ $\bar{h}0hl$	$l = 2n$	$(11\bar{2}0)$ $(\bar{2}110)$ $(1\bar{2}10)$ } $\{11\bar{2}0\}$	$\mathbf{c}/2$	c	Hexagonal	
$hh.\overline{2h}.l$ $\overline{2h}.hhl$ $h.\overline{2h}.hl$	$l = 2n$	$(1\bar{1}00)$ $(01\bar{1}0)$ $(\bar{1}010)$ } $\{1\bar{1}00\}$	$\mathbf{c}/2$	c	Hexagonal	
hhl	$l = 2n$	$(1\bar{1}0)$ } $\{1\bar{1}0\}$	$\mathbf{c}/2$	c, n	Rhombohedral‡	
hkk	$h = 2n$	$(01\bar{1})$	$\mathbf{a}/2$	a, n		
hkh	$k = 2n$	$(\bar{1}01)$	$\mathbf{b}/2$	b, n		
$hhl, h\bar{h}l$	$l = 2n$	$(1\bar{1}0), (110)$	$\mathbf{c}/2$	c, n	Tetragonal§	Cubic¶
	$2h + l = 4n$		$\mathbf{a}/4 \pm \mathbf{b}/4 \pm \mathbf{c}/4$	d		
$hkk, hk\bar{k}$	$h = 2n$	$(01\bar{1}), (011)$	$\mathbf{a}/2$	a, n		
	$2k + h = 4n$		$\pm\mathbf{a}/4 + \mathbf{b}/4 \pm \mathbf{c}/4$	d		
$hkh, \bar{h}kh$	$k = 2n$	$(\bar{1}01), (101)$	$\mathbf{b}/2$	b, n		
	$2h + k = 4n$		$\pm\mathbf{a}/4 \pm \mathbf{b}/4 + \mathbf{c}/4$	d		

† Glide planes *d* with orientations (100), (010) and (001) occur only in orthorhombic and cubic *F* space groups. Combination of the integral reflection condition (*hkl:* all odd or all even) with the zonal conditions for the *d* glide planes leads to the further conditions given between parentheses.
‡ For rhombohedral space groups described with 'rhombohedral axes', the three reflection conditions ($l = 2n, h = 2n, k = 2n$) imply interleaving of *c* and *n* glides, *a* and *n* glides, and *b* and *n* glides, respectively. In the Hermann–Mauguin space-group symbols, *c* is always used, as in $R3c$ (161) and $R\bar{3}c$ (167), because *c* glides also occur in the hexagonal description of these space groups.
§ For tetragonal *P* space groups, the two reflection conditions (*hhl* and $h\bar{h}l$ with $l = 2n$) imply interleaving of *c* and *n* glides. In the Hermann–Mauguin space-group symbols, *c* is always used, irrespective of which glide planes contain the origin: *cf.* $P4cc$ (103), $P\bar{4}2c$ (112) and $P4/nnc$ (126).
¶ For cubic space groups, the three reflection conditions ($l = 2n, h = 2n, k = 2n$) imply interleaving of *c* and *n* glides, *a* and *n* glides, and *b* and *n* glides, respectively. In the Hermann–Mauguin space-group symbols, either *c* or *n* is used, depending upon which glide plane contains the origin, *cf.* $P\bar{4}3n$ (218), $Pn\bar{3}n$ (222), $Pm\bar{3}n$ (223) *versus* $F\bar{4}3c$ (219), $Fm\bar{3}c$ (226), $Fd\bar{3}c$ (228).

(vii) in the 'hexagonal-axes' descriptions of trigonal and hexagonal space groups, Bravais–Miller indices *hkil* are used. They obey two conditions:

(*a*) $h + k + i = 0$, *i.e.* $i = -(h + k)$;
(*b*) the indices h, k, i are cyclically permutable; this is not stated. Further details can be found in textbooks of crystallography.

Note that the integral reflection conditions for a rhombohedral lattice, described with 'hexagonal axes', permit the presence of only one member of the pair *hkil* and $\bar{h}\bar{k}\bar{i}l$ for $l \neq 3n$ (*cf.* Table 2.1.3.6). This applies also to the zonal reflections $h\bar{h}0l$ and $\bar{h}h0l$, which for the rhombohedral space groups must be considered separately.

Example

For a monoclinic crystal (*b* unique), the following reflection conditions have been observed:

(1) hkl: $h + k = 2n$;
(2) $0kl$: $k = 2n$; $h0l$: $h, l = 2n$; $hk0$: $h + k = 2n$;
(3) $h00$: $h = 2n$; $0k0$: $k = 2n$; $00l$: $l = 2n$.

Line (1) states that the cell used for the description of the space group is *C* centred. In line (2), the conditions $0kl$ with $k = 2n$, $h0l$ with $h = 2n$ and $hk0$ with $h + k = 2n$ are a consequence of the integral condition (1), leaving only $h0l$ with $l = 2n$ as a new condition. This indicates a glide plane *c*. Line (3) presents no new condition, since $h00$ with $h = 2n$ and $0k0$ with $k = 2n$ follow from the integral condition (1), whereas $00l$

Table 2.1.3.7 (continued)

(*b*) Screw axes

Type of reflections	Reflection conditions	Screw axis			Crystallographic coordinate system to which condition applies
		Direction of axis	Screw vector	Symbol	
*h*00	$h = 2n$	[100]	**a**/2	2_1	Monoclinic (*a* unique), Orthorhombic, Tetragonal; Cubic
				4_2	
	$h = 4n$		**a**/4	$4_1, 4_3$	
0*k*0	$k = 2n$	[010]	**b**/2	2_1	Monoclinic (*b* unique), Orthorhombic, Tetragonal; Cubic
				4_2	
	$k = 4n$		**b**/4	$4_1, 4_3$	
00*l*	$l = 2n$	[001]	**c**/2	2_1	Monoclinic (*c* unique), Orthorhombic; Tetragonal; Cubic
				4_2	
	$l = 4n$		**c**/4	$4_1, 4_3$	
000*l*	$l = 2n$	[001]	**c**/2	6_3	Hexagonal
	$l = 3n$		**c**/3	$3_1, 3_2, 6_2, 6_4$	
	$l = 6n$		**c**/6	$6_1, 6_5$	

with $l = 2n$ is a consequence of a zonal condition (2). Accordingly, there need not be a twofold screw axis along [010]. Space groups obeying the conditions are *Cc* (9, *b* unique, cell choice 1) and *C*2/*c* (15, *b* unique, cell choice 1). Under certain conditions, using methods based on resonant scattering, it is possible to determine whether the structure space group is centrosymmetric or not (*cf.* Section 1.6.5.1).

For a different choice of the basis vectors, the reflection conditions would appear in a different form owing to the transformation of the reflection indices (*cf.* cell choices 2 and 3 for space groups *Cc* and *C*2/*c* in Chapter 2.3). The transformations of reflection conditions under coordinate transformations are discussed and illustrated in Sections 1.5.2 and 1.5.3.

Special or 'extra' reflection conditions. These apply either to the integral reflections *hkl* or to particular sets of zonal or serial reflections. In the space-group tables, the minimal special conditions are listed that, on combination with the general conditions, are sufficient to generate the complete set of conditions. This will be apparent from the examples below.

Examples

(1) $P4_222$ (93)

General position 8*p*: 00*l*: $l = 2n$, due to 4_2; the projection on [001] of any crystal structure with this space group has periodicity $\frac{1}{2}c$.

Special position 4*i*: *hkl*: $h + k + l = 2n$; any set of symmetry-equivalent atoms in this position displays additional *I* centring.

Special position 4*n*: 0*kl*: $l = 2n$; any set of equivalent atoms in this position displays a glide plane $c \perp [100]$. Projection of this set along [100] results in a halving of the original *c* axis, hence the special condition. Analogously for *h*0*l*: $l = 2n$.

(2) *C*12/*c*1 (15, unique axis *b*, cell choice 1)

General position 8*f*: *hkl*: $h + k = 2n$, due to the *C*-centred cell.

Special position 4*d*: *hkl*: $k + l = 2n$, due to additional *A* and *B* centring for atoms in this position. Combination with the general condition results in *hkl*: $h + k, h + l$, $k + l = 2n$ or *hkl* all odd or all even; this corresponds to an *F*-centred arrangement of atoms in this position.

Special position 4*b*: *hkl*: $l = 2n$, due to additional halving of the *c* axis for atoms in this position. Combination with the general condition results in *hkl*: $h + k, l = 2n$; this corresponds to a *C*-centred arrangement in a cell with half the original *c* axis. No further condition results from the combination.

(3) *I*12/*a*1 (15, unique axis *b*, cell choice 3)

For the description of space group No. 15 with cell choice 3 (see Section 2.1.3.15 and the space-group tables), the reflection conditions appear as follows:

General position 8*f*: *hkl*: $h + k + l = 2n$, due to the *I*-centred cell.

Special position 4*b*: *hkl*: $h = 2n$, due to additional halving of the *a* axis. Combination gives *hkl*: $h, k + l = 2n$, *i.e.* an *A*-centred arrangement of atoms in a cell with half the original *a* axis.

An analogous result is obtained for position 4*d*.

Table 2.1.3.8
Reflection conditions for the plane groups

Type of reflections	Reflection condition	Centring type of plane cell; or glide line with glide vector	Coordinate system to which condition applies
hk	None	Primitive *p*	All systems
	$h + k = 2n$	Centred *c*	Rectangular
	$h - k = 3n$	Hexagonally centred *h*†	Hexagonal
*h*0	$h = 2n$	Glide line *g* normal to *b* axis; glide vector $\frac{1}{2}\mathbf{a}$	Rectangular, Square
0*k*	$k = 2n$	Glide line *g* normal to *a* axis; glide vector $\frac{1}{2}\mathbf{b}$	

† For the use of the unconventional *h* cell see Table 2.1.1.2.

(4) *Fmm*2 (42)

General position 16*e*: *hkl*: $h + k, h + l, k + l = 2n$, due to the *F*-centred cell.

Special position 8*b*: *hkl*: $= 2n$, due to additional halving of the *a* axis. Combination results in *hkl*: $h, k, l = 2n$, *i.e.* all indices even; the atoms in this position are arranged in a primitive lattice with axes $\frac{1}{2}a$, $\frac{1}{2}b$ and $\frac{1}{2}c$.

For the cases where the special reflection conditions are described by means of combinations of 'OR' and 'AND' instructions, the 'AND' condition always has to be evaluated with priority, as shown by the following example.

Example: P$\bar{4}$3*n (218)*

Special position 6*d*: *hkl*: $h + k + l = 2n$ or $h = 2n + 1, k = 4n$ and $l = 4n + 2$.

This expression contains the following two conditions:

(*a*) *hkl*: $h + k + l = 2n$;

(*b*) $h = 2n + 1$ and $k = 4n$ and $l = 4n + 2$.

A reflection is 'present' (occurring) if either condition (*a*) is satisfied or if a permutation of the three conditions in (*b*) are simultaneously fulfilled.

Structural or non-space-group absences. Note that in addition *non-space-group absences* may occur that are not due to the symmetry of the space group (*i.e.* centred cells, glide planes or screw axes). Atoms in general or special positions may cause additional systematic absences if their coordinates assume special values [*e.g.* 'noncharacteristic orbits'; *cf.* Section 1.4.4.4 and Engel *et al.* (1984)]. Non-space-group absences may also occur for special arrangements of atoms ('false symmetry') in a crystal structure (*cf.* Templeton, 1956; Sadanaga *et al.*, 1978). Non-space-group absences may occur also for polytypic structures; this is briefly discussed by Durovič in Section 9.2.2.2.5 of *International Tables for Crystallography* (2004), Vol. C. Even though all these 'structural absences' are fortuitous and due to the special arrangements of atoms in a particular crystal structure, they have the appearance of space-group absences. Occurrence of structural absences thus may lead to an *incorrect assignment of the space group*. Accordingly, the reflection conditions in the space-group tables must be considered as a minimal set of conditions.

The use of reflection conditions and of the symmetry of reflection intensities for space-group determination is described in Chapter 1.6.

2.1.3.14. Symmetry of special projections

Projections of crystal structures are used by crystallographers in special cases. Use of so-called 'two-dimensional data' (zero-layer intensities) results in the projection of a crystal structure along the normal to the reciprocal-lattice net. A detailed treatment of projections of space groups, including basic definitions and illustrative examples, is given in Section 1.4.5.3.

Even though the projection of a finite object along *any* direction may be useful, the projection of a *periodic* object such as a crystal structure is only sensible along a rational lattice direction (lattice row). Projection along a nonrational direction results in a constant density in at least one direction.

Data listed in the space-group tables. Under the heading *Symmetry of special projections*, the following data are listed for three projections of each space group; no projection data are given for the plane groups.

(i) *The projection direction*. All projections are orthogonal, *i.e.* the projection is made onto a plane normal to the projection direction. This ensures that spherical atoms appear as circles in the projection. For each space group, three projections are listed. If a lattice has three kinds of symmetry directions, the three projection directions correspond to the primary, secondary and tertiary symmetry directions of the lattice (*cf.* Table 2.1.3.1). If a lattice contains fewer than three kinds of symmetry directions, as in the triclinic, monoclinic and rhombohedral cases, the additional projection direction(s) are taken along coordinate axes, *i.e.* lattice rows lacking symmetry.

The directions for which projection data are listed are as follows:

Triclinic Monoclinic (both settings) Orthorhombic	[001]	[100]	[010]
Tetragonal	[001]	[100]	[110]
Hexagonal	[001]	[100]	[210]
Rhombohedral	[111]	[1$\bar{1}$0]	[2$\bar{1}\bar{1}$]
Cubic	[001]	[111]	[110]

(ii) *The Hermann–Mauguin symbol of the plane group* resulting from the projection of the space group. If necessary, the symbols are given in oriented form; for example, plane group *pm* is expressed either as *p*1*m*1 or as *p*11*m* (*cf.* Section 1.4.1.5 for explanations of Hermann–Mauguin symbols of plane groups).

(iii) *Relations between the basis vectors* $\mathbf{a}'$, $\mathbf{b}'$ of the plane group and the basis vectors **a**, **b**, **c** of the space group. Each set of basis vectors refers to the conventional coordinate system of the plane group or space group, as employed in Chapters 2.2 and 2.3. The basis vectors of the two-dimensional cell are always called $\mathbf{a}'$ and $\mathbf{b}'$ irrespective of which two of the basis vectors **a**, **b**, **c** of the three-dimensional cell are projected to form the plane cell. All relations between the basis vectors of the two cells are expressed as vector equations, *i.e.* $\mathbf{a}'$ and $\mathbf{b}'$ are given as linear combinations of **a**, **b** and **c**. For the triclinic or monoclinic space groups, basis vectors **a**, **b** or **c** inclined to the plane of projection are replaced by the projected vectors $\mathbf{a}_p$, $\mathbf{b}_p$, $\mathbf{c}_p$.

For primitive three-dimensional cells, the *metrical* relations between the lattice parameters of the space group and the plane group are collected in Table 2.1.3.9. The additional relations for centred cells can be derived easily from the table.

(iv) *Location of the origin* of the plane group with respect to the unit cell of the space group. The same description is used as for the location of symmetry elements (*cf.* Section 2.1.3.9).

Example

'Origin at *x*, 0, 0' or 'Origin at $\frac{1}{4}, \frac{1}{4}, z$'.

Projections of centred cells (lattices). For centred lattices, two different cases may occur:

(i) The projection direction is parallel to a lattice-centring vector. In this case, the projected plane cell is primitive for the centring types *A*, *B*, *C*, *I* and *R*. For *F*-centred lattices, the multiplicity is reduced from 4 to 2 because *c*-centred plane

Table 2.1.3.9
Cell parameters a', b', γ' of the two-dimensional cell in terms of cell parameters a, b, c, α, β, γ of the three-dimensional cell for the projections listed in the space-group tables of Chapter 2.3

Projection direction	Triclinic	Monoclinic		Orthorhombic
		Unique axis b	Unique axis c	
[001]	$a' = a \sin\beta$ $b' = b \sin\alpha$ $\gamma' = 180^\circ - \gamma^*$†	$a' = a \sin\beta$ $b' = b$ $\gamma' = 90^\circ$	$a' = a$ $b' = b$ $\gamma' = \gamma$	$a' = a$ $b' = b$ $\gamma' = 90^\circ$
[100]	$a' = b \sin\gamma$ $b' = c \sin\beta$ $\gamma' = 180^\circ - \alpha^*$†	$a' = b$ $b' = c \sin\beta$ $\gamma' = 90^\circ$	$a' = b \sin\gamma$ $b' = c$ $\gamma' = 90^\circ$	$a' = b$ $b' = c$ $\gamma' = 90^\circ$
[010]	$a' = c \sin\alpha$ $b' = \alpha \sin\gamma$ $\gamma' = 180^\circ - \beta^*$†	$a' = c$ $b' = a$ $\gamma' = \beta$	$a' = c$ $b' = a \sin\gamma$ $\gamma' = 90^\circ$	$a' = c$ $b' = a$ $\gamma' = 90^\circ$

Projection direction	Tetragonal
[001]	$a' = a$ $b' = a$ $\gamma' = 90^\circ$
[100]	$a' = a$ $b' = c$ $\gamma' = 90^\circ$
[110]	$a' = (a/2)\sqrt{2}$ $b' = c$ $\gamma' = 90^\circ$

Projection direction	Hexagonal
[001]	$a' = a$ $b' = a$ $\gamma' = 120^\circ$
[100]	$a' = (a/2)\sqrt{3}$ $b' = c$ $\gamma' = 90^\circ$
[210]	$a' = a/2$ $b' = c$ $\gamma' = 90^\circ$

Projection direction	Rhombohedral‡
[111]	$a' = \frac{2}{\sqrt{3}} a \sin(\alpha/2)$ $b' = \frac{2}{\sqrt{3}} a \sin(\alpha/2)$ $\gamma' = 120^\circ$
$[1\bar{1}0]$	$a' = a \cos(\alpha/2)$ $b' = a$ $\gamma' = \delta$§
$[\bar{2}11]$	$a' = \frac{1}{\sqrt{3}} a\sqrt{1 + 2\cos\alpha}$ $b' = a \sin(\alpha/2)$ $\gamma' = 90^\circ$

Projection direction	Cubic
[001]	$a' = a$ $b' = a$ $\gamma' = 90^\circ$
[111]	$a' = a\sqrt{2/3}$ $b' = a\sqrt{2/3}$ $\gamma' = 120^\circ$
[110]	$a' = (a/2)\sqrt{2}$ $b' = a$ $\gamma' = 90^\circ$

† $\cos\alpha^* = \dfrac{\cos\beta\cos\gamma - \cos\alpha}{\sin\beta\sin\gamma}$; $\cos\beta^* = \dfrac{\cos\gamma\cos\alpha - \cos\beta}{\sin\gamma\sin\alpha}$; $\cos\gamma^* = \dfrac{\cos\alpha\cos\beta - \cos\gamma}{\sin\alpha\sin\beta}$.

‡ The entry 'Rhombohedral' refers to the primitive rhombohedral cell with $a = b = c$, $\alpha = \beta = \gamma$ (*cf.* Table 2.1.1.1).

§ $\cos\delta = \dfrac{\cos\alpha}{\cos\alpha/2}$.

cells result from projections along face diagonals of three-dimensional F cells.

Examples

(1) A body-centred lattice with centring vector $\frac{1}{2}(\mathbf{a} + \mathbf{b} + \mathbf{c})$ gives a primitive net if projected along [111], $[\bar{1}11]$, $[1\bar{1}1]$ or $[11\bar{1}]$.
(2) A C-centred lattice projects to a primitive net along the directions [110] and $[1\bar{1}0]$.
(3) An R-centred lattice described with 'hexagonal axes' (triple cell) results in a primitive net if projected along $[\bar{1}11]$, [211] or $[\bar{1}\bar{2}1]$ for the obverse setting. For the reverse setting, the corresponding directions are $[1\bar{1}1]$, $[\bar{2}\bar{1}1]$, [121]; *cf.* Table 2.1.1.2.

(ii) The projection direction is not parallel to a lattice-centring vector (general projection direction). In this case, the plane cell has the same multiplicity as the three-dimensional cell. Usually, however, this centred plane cell is unconventional and a transformation is required to obtain the conventional plane cell. This transformation has been carried out for the projection data in this volume.

Examples

(1) Projection along [010] of a cubic I-centred cell leads to an unconventional quadratic c-centred plane cell. A simple cell transformation leads to the conventional quadratic p cell.
(2) Projection along [010] of an orthorhombic I-centred cell leads to a rectangular c-centred plane cell, which is conventional.
(3) Projection along [001] of an R-centred cell (both in obverse and reverse setting) results in a triple hexagonal plane cell h (the two-dimensional analogue of the H cell, *cf.* Table 2.1.1.2). A simple cell transformation leads to the conventional hexagonal p cell.

Table 2.1.3.10
Projections of crystallographic symmetry elements

Symmetry element in three dimensions	Symmetry element in projection
Arbitrary orientation	
Symmetry centre $\bar{1}$ Rotoinversion axis $\bar{3} \equiv 3 \times \bar{1}$	Rotation point 2 (at projection of centre)
Parallel to projection direction	
Rotation axis 2; 3; 4; 6	Rotation point 2; 3; 4; 6
Screw axis 2_1	Rotation point 2
$3_1, 3_2$	3
$4_1, 4_2, 4_3$	4
$6_1, 6_2, 6_3, 6_4, 6_5$	6
Rotoinversion axis $\bar{4}$	Rotation point 4
$\bar{6} \equiv 3/m$	3, with overlap of atoms
$\bar{3} \equiv 3 \times \bar{1}$	6
Reflection plane *m*	Reflection line *m*
Glide plane with ⊥ component†	Glide line *g*
Glide plane without ⊥ component†	Reflection line *m*
Normal to projection direction	
Rotation axis 2;4;6	Reflection line *m*
3	None
Screw axis 4_2; $6_2, 6_4$	Reflection line *m*
2_1; $4_1, 4_3$; $6_1, 6_3, 6_5$	Glide line *g*
$3_1, 3_2$	None
Rotoinversion axis $\bar{4}$	Reflection line *m* parallel to axis
$\bar{6} \equiv 3/m$	Reflection line *m* perpendicular to axis (through projection of inversion point)
$\bar{3} \equiv 3 \times \bar{1}$	Rotation point 2 (at projection of centre)
Reflection plane *m*	None, but overlap of atoms
Glide plane with glide vector **t**	Translation with translation vector **t**

† The term 'with ⊥ component' refers to the component of the glide vector normal to the projection direction.

Projections of symmetry elements. A symmetry element of a space group does not project as a symmetry element unless its orientation bears a special relation to the projection direction; all translation components of a symmetry operation along the projection direction vanish, whereas those perpendicular to the projection direction (*i.e.* parallel to the plane of projection) may be retained. This is summarized in Table 2.1.3.10 for the various crystallographic symmetry elements. From this table the following conclusions can be drawn:

(i) *n*-fold rotation axes and *n*-fold screw axes, as well as rotoinversion axes $\bar{4}$, *parallel to the projection direction* project as *n*-fold rotation points; a $\bar{3}$ axis projects as a sixfold, a $\bar{6}$ axis as a threefold rotation point. For the latter, a doubling of the projected electron density occurs owing to the mirror plane normal to the projection direction ($\bar{6} \equiv 3/m$).

(ii) *n*-fold rotation axes and *n*-fold screw axes *normal to the projection direction* (*i.e.* parallel to the plane of projection) do not project as symmetry elements if *n* is odd. If *n* is even, all rotation and rotoinversion axes project as mirror lines: the same applies to the screw axes 4_2, 6_2 and 6_4 because they contain an axis 2. Screw axes 2_1, 4_1, 4_3, 6_1, 6_3 and 6_5 project as glide lines because they contain 2_1.

(iii) Reflection planes *normal* to the projection direction do not project as symmetry elements but lead to a doubling of the projected electron density owing to overlap of atoms. Projection of a glide plane results in an additional translation; the new translation vector is equal to the glide vector of the glide plane. Thus, a reduction of the translation period in that particular direction takes place.

(iv) Reflection planes *parallel* to the projection direction project as reflection lines. Glide planes project as glide lines or as reflection lines, depending upon whether the glide vector has or does not have a component parallel to the projection plane.

(v) Centres of symmetry, as well as $\bar{3}$ axes in *arbitrary* orientation, project as twofold rotation points.

A detailed discussion of the correspondence between the symmetry elements and their projections is given in Section 1.4.5.3.

*Example: C*12/*c*1 *(15, b unique, cell choice 1)*

The *C*-centred cell has lattice points at 0, 0, 0 and $\frac{1}{2}, \frac{1}{2}, 0$. In all projections, the centre $\bar{1}$ projects as a twofold rotation point.

Projection along [001]: The plane cell is centred; 2 ∥ [010] projects as *m*; the glide component $(0, 0, \frac{1}{2})$ of glide plane *c* vanishes and thus *c* projects as *m*.

Result: Plane group *c*2*mm* (9), $\mathbf{a}' = \mathbf{a}_p$, $\mathbf{b}' = \mathbf{b}$.

Projection along [100]: The periodicity along *b* is halved because of the *C* centring; 2 ∥ [010] projects as *m*; the glide component $(0, 0, \frac{1}{2})$ of glide plane *c* is retained and thus *c* projects as *g*.

Result: Plane group *p*2*gm* (7), $\mathbf{a}' = \mathbf{b}/2$, $\mathbf{b}' = \mathbf{c}_p$.

Projection along [010]: The periodicity along *a* is halved because of the *C* centring; that along *c* is halved owing to the glide component $(0, 0, \frac{1}{2})$ of glide plane *c*; 2 ∥ [010] projects as 2.

Result: Plane group *p*2 (2), $\mathbf{a}' = \mathbf{c}/2$, $\mathbf{b}' = \mathbf{a}/2$.

Further details about the geometry of projections can be found in publications by Buerger (1965) and Biedl (1966).

2.1.3.15. Monoclinic space groups

In this volume, space groups are described by one (or at most two) conventional coordinate systems (*cf.* Sections 2.1.1.2 and 2.1.3.2). Eight monoclinic space groups, however, are treated more extensively. In order to provide descriptions for frequently encountered cases, they are given in six versions.

The description of a monoclinic crystal structure in this volume, including its Hermann–Mauguin space-group symbol, depends upon two choices:

(i) the unit cell chosen, here called 'cell choice';

(ii) the labelling of the edges of this cell, especially of the monoclinic symmetry direction ('unique axis'), here called 'setting'.

Cell choices. One edge of the cell, *i.e.* one crystal axis, is always chosen along the monoclinic symmetry direction. The other two edges are located in the plane perpendicular to this direction and coincide with translation vectors in this 'monoclinic plane'. It is sensible and common practice (see below) to choose these two basis vectors from the *shortest three* translation vectors in that plane. They are shown in Fig. 2.1.3.12 and labelled **e**, **f** and **g**, in order of increasing length.[5] The two shorter vectors span the 'reduced mesh' (where mesh means a two-dimensional unit cell), here **e** and **f**; for this mesh, the monoclinic angle is $\leq 120°$,

[5] These three vectors obey the 'closed-triangle' condition $\mathbf{e} + \mathbf{f} + \mathbf{g} = \mathbf{0}$; they can be considered as two-dimensional homogeneous axes.

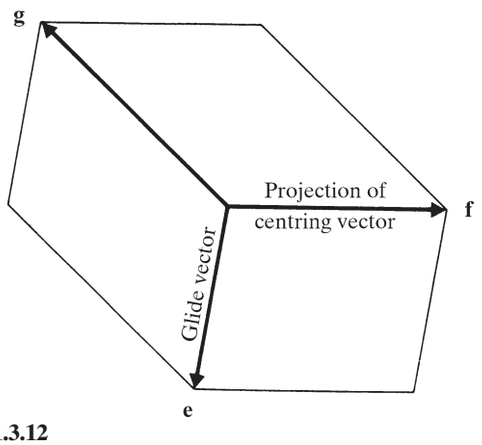

Figure 2.1.3.12
The three primitive two-dimensional cells which are spanned by the shortest three translation vectors **e**, **f**, **g** in the monoclinic plane. For the present discussion, the glide vector is considered to be along **e** and the projection of the centring vector along **f**.

whereas for the other two primitive meshes larger angles are possible.

Other choices of the basis vectors in the monoclinic plane are possible, provided they span a primitive mesh. It turns out, however, that the space-group symbol for any of these (non-reduced) meshes already occurs among the symbols for the three meshes formed by **e**, **f**, **g** in Fig. 2.1.3.12; hence only these cases need be considered. They are designated in this volume as 'cell choice 1, 2 or 3' and are depicted in Fig. 2.1.3.4. The transformation matrices for the three cell choices are listed in Table 1.5.1.1.

Settings. The term *setting* of a cell or of a space group refers to the assignment of labels (a, b, c) and directions to the edges of a given unit cell, resulting in a set of basis vectors **a**, **b**, **c**. (For orthorhombic space groups, the six settings are described and illustrated in Section 2.1.3.6.4.)

The symbol for each setting is a shorthand notation for the transformation of a given starting set **abc** into the setting considered. It is called here 'setting symbol'. For instance, the setting symbol **bca** stands for

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

or

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

where $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$ is the new set of basis vectors. [Note that the setting symbol **bca** means that the 'old' vector **a** changes its label to $\mathbf{c}'$ (and not to $\mathbf{b}'$), that the 'old' vector **b** changes its label to $\mathbf{a}'$ (and not to $\mathbf{c}'$) and that the 'old' vector **c** changes its label to $\mathbf{b}'$ (and not to $\mathbf{a}'$).] Transformation of one setting into another preserves the shape of the cell and its orientation relative to the lattice. The matrices of these transformations have *one* entry +1 or −1 in each row and column; all other entries are 0.

In monoclinic space groups, one axis, the monoclinic symmetry direction, is unique. Its label must be chosen first and, depending upon this choice, one speaks of 'unique axis b', 'unique axis c' or 'unique axis a'.[6] Conventionally, the positive directions of the two further ('oblique') axes are oriented so as to make the monoclinic angle non-acute, *i.e.* $\geq 90°$, and the coordinate system right-handed. For the three cell choices, settings obeying this condition and having the same label and direction of the unique axis are considered as one setting; this is illustrated in Fig. 2.1.3.4.

Note: These three cases of labelling the monoclinic axis are often called somewhat loosely b-axis, c-axis and a-axis 'settings'. It must be realized, however, that the choice of the 'unique axis' alone does *not* define a *single* setting but only a *pair*, as for each cell the labels of the two oblique axes can be interchanged.

Table 2.1.3.11
Monoclinic setting symbols

The settings are distributed between three sets (with two columns in each set) depending on the choice of unique axis. The unique axis is underlined. The setting symbol is a shorthand notation for the transformation of the corresponding starting setting (first row **abc**; second row **abc**; third row **abc**). For example, the symbol **cab** represents a transformation of the starting setting **abc** such that $\mathbf{a}' = \mathbf{c}$, $\mathbf{b}' = \mathbf{a}$, $\mathbf{c}' = \mathbf{b}$.

Starting setting	Unique axis b		Unique axis c		Unique axis a	
abc	**abc**	**cba**	**cab**	**acb**	**bca**	**bac**
abc	**bca**	**acb**	**abc**	**bac**	**cab**	**cba**
abc	**cab**	**bac**	**bca**	**cba**	**abc**	**acb**

Note: An interchange of two axes involves a change of the handedness of the coordinate system. In order to keep the system right-handed, one sign reversal is necessary.

Table 2.1.3.11 lists the setting symbols for the six monoclinic settings in three equivalent forms, starting with the symbols **abc** (first line), **abc** (second line) and **abc** (third line); the unique axis is underlined. These symbols are also found in the headline of the synoptic Table 1.5.4.4, which lists the space-group symbols for all monoclinic settings and cell choices. Again, the corresponding transformation matrices are listed in Table 1.5.1.1.

In the space-group tables, only the settings with b and c unique are treated and for these only the left-hand members of the double entries in Table 2.1.3.11. This implies, for instance, that the c-axis setting is obtained from the b-axis setting by cyclic permutation of the labels, *i.e.* by the transformation

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

The setting with a unique is also included in the present discussion, as this setting occurs in Table 1.5.4.4. The a-axis setting $\underline{\mathbf{a}}'\mathbf{b}'\mathbf{c}' = \underline{\mathbf{c}}\mathbf{ab}$ (*i.e.* $\underline{\mathbf{a}}' = \underline{\mathbf{c}}, \mathbf{b}' = \mathbf{a}, \mathbf{c}' = \mathbf{b}$) is obtained from the c-axis setting also by cyclic permutation of the labels and from the b-axis setting by the reverse cyclic permutation: $\underline{\mathbf{a}}'\mathbf{b}'\mathbf{c}' = \underline{\mathbf{b}}\mathbf{ca}$.

By the conventions described above, the setting of each of the cell choices 1, 2 and 3 is determined once the label and the direction of the unique-axis vector have been selected. Six of the nine resulting possibilities are illustrated in Fig. 2.1.3.4.

Cell choices and settings in the present tables. There are five monoclinic space groups for which the Hermann–Mauguin symbols are independent of the cell choice, *viz* those space groups that do *not* contain centred lattices or glide planes:

$$P2\ (3),\ P2_1\ (4),\ Pm\ (6),\ P2/m\ (10),\ P2_1/m\ (11).$$

In these cases, description of the space group by one cell choice is sufficient.

For the eight monoclinic space groups *with centred lattices or glide planes*, the Hermann–Mauguin symbol depends on the

[6] In *IT* (1952), the terms '1st setting' and '2nd setting' were used for 'unique axis c' and 'unique axis b'. In the present volume, as in the previous editions of this series, these terms have been dropped in favour of the latter names, which are unambiguous.

Table 2.1.3.12
Symbols for centring types and glide planes of monoclinic space groups

Setting		Cell choice		
		1	2	3
Unique axis *b*	Centring type Glide planes	*C* *c*, *n*	*A* *n*, *a*	*I* *a*, *c*
Unique axis *c*	Centring type Glide planes	*A* *a*, *n*	*B* *n*, *b*	*I* *b*, *a*
Unique axis *a*	Centring type Glide planes	*B* *b*, *n*	*C* *n*, *c*	*I* *c*, *b*

choice of the oblique axes with respect to the glide vector and/or the centring vector. These eight space groups are:

*C*2 (5), *Pc* (7), *Cm* (8), *Cc* (9), *C*2/*m* (12), *P*2/*c* (13), $P2_1/c$ (14), *C*2/*c* (15).

Here, the glide vector or the projection of the centring vector onto the monoclinic plane is always directed along *one* of the vectors **e**, **f** or **g** in Fig. 2.1.3.12, *i.e.* is parallel to the shortest, the second-shortest or the third-shortest translation vector in the monoclinic plane (note that a glide vector and the projection of a centring vector cannot be parallel). This results in three possible orientations of the glide vector or the centring vector with respect to these crystal axes, and thus in three different full Hermann–Mauguin symbols (*cf.* Section 2.1.3.4) for each setting of a space group.

Table 2.1.3.12 lists the symbols for centring types and glide planes for the cell choices 1, 2, 3. The order of the three cell choices is defined as follows: The symbols occurring in the familiar 'standard short monoclinic space-group symbols' (see Section 2.1.3.3) define cell choice 1; for 'unique axis *b*', this applies to the centring type *C* and the glide plane *c*, as in *Cm* (8) and $P2_1/c$ (14). Cell choices 2 and 3 follow from the anticlockwise order 1–2–3 in Fig. 2.1.3.4 and their space-group symbols can be obtained from Table 2.1.3.12. The *c*-axis and the *a*-axis settings then are derived from the *b*-axis setting by cyclic permutations of the axial labels, as described in this section.

In the two space groups *Cc* (9) and *C*2/*c* (15), glide planes occur in pairs, *i.e.* each vector **e**, **f**, **g** is associated either with a glide vector or with the centring vector of the cell. For *Pc* (7), *P*2/*c* (13) and $P2_1/c$ (14), which contain only one type of glide plane, the left-hand member of each pair of glide planes in Table 2.1.3.12 applies.

In the space-group tables of this volume, the following treatments of monoclinic space groups are given:

(1) *Two complete descriptions* for each of the five monoclinic space groups with primitive lattices and without glide planes, one for 'unique axis *b*' and one for 'unique axis *c*', similar to the treatment in *IT* (1952).

(2) A total of *six descriptions* for each of the eight space groups with centred lattices or glide planes, as follows:

(*a*) *One complete* description for 'unique axis *b*' and 'cell choice' 1. This is considered the standard description of the space group, and its *short* Hermann–Mauguin symbol is used as the *standard* symbol of the space group.

This standard short symbol corresponds to the one symbol of *IT* (1935) and to that of the *b*-axis setting in *IT* (1952), *e.g.* $P2_1/c$ or *C*2/*c*. It serves only to identify the space-group type but carries no information about the setting or cell choice of a particular description. The *standard short symbol* is given in the headline of every description of a monoclinic space group; *cf.* Section 2.1.3.3.

(*b*) *Three condensed* (synoptic) descriptions for 'unique axis *b*' and the three 'cell choices' 1, 2, 3. Cell choice 1 is repeated to facilitate comparison with the other cell choices. Diagrams are provided to illustrate the three cell choices: *cf.* Section 2.1.3.6.

(*c*) *One complete* description for 'unique axis *c*' and 'cell choice' 1.

(*d*) *Three condensed* (synoptic) descriptions for 'unique axis *c*' and the three 'cell choices' 1, 2, 3. Again cell choice 1 is repeated and appropriate diagrams are provided.

All settings and cell choices are identified by the appropriate *full* Hermann–Mauguin symbols (*cf.* Section 2.1.3.4), *e.g.* *C*12/*c*1 or *I*112/*b*. For the two space groups *Cc* (9) and *C*2/*c* (15) with pairs of different glide planes, the 'simplest operation rule' for reflections ($m > a$, b, $c > n$) is not followed (*cf.* Section 1.4.1). Instead, in order to bring out the relations between the various settings and cell choices, the glide-plane symbol always refers to that glide plane which intersects the conventional origin.

*Example: No. 15, standard short symbol C*2/*c*

The full symbols for the three cell choices (rows) and the three unique axes (columns) read

*C*12/*c*1	*A*12/*n*1	*I*12/*a*1
*A*112/*a*	*B*112/*n*	*I*112/*b*
*B*2/*b*11	*C*2/*n*11	*I*2/*c*11.

Application of the priority rule would have resulted in the following symbols:

*C*12/*c*1	*A*12/*a*1	*I*12/*a*1
*A*112/*a*	*B*112/*b*	*I*112/*a*
*B*2/*b*11	*C*2/*c*11	*I*2/*b*11.

Here, the transformation properties are obscured.

Comparison with earlier editions of International Tables. In *IT* (1935), each monoclinic space group was presented in one description only, with *b* as the unique axis. Hence, only one short Hermann–Mauguin symbol was needed.

In *IT* (1952), the *c*-axis setting (first setting) was newly introduced, in addition to the *b*-axis setting (second setting). This extension was based on a decision of the Stockholm General Assembly of the International Union of Crystallography in 1951 [*cf. Acta Cryst.* (1951), **4**, 569 and *Preface* to *IT* (1952)]. According to this decision, the *b*-axis setting should continue to be accepted as standard for morphological and structural studies. The two settings led to the introduction of *full* Hermann–Mauguin symbols for *all* 13 monoclinic space groups (*e.g.* $P12_1/c1$ and $P112_1/b$) and of two different *standard short* symbols (*e.g.* $P2_1/c$ and $P2_1/b$) for the *eight* space groups with centred lattices or glide planes [*cf.* p. 545 of *IT* (1952)]. In the present volume (as in the previous editions of this series), only one of these standard short symbols is retained (see above and Section 2.1.3.3).

The *c*-axis setting (primed labels) was obtained from the *b*-axis setting (unprimed labels) by the following transformation:

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

This corresponds to an interchange of two labels and not to the more logical cyclic permutation, as used in all editions of this series. The reason for this particular transformation was to obtain short space-group symbols that indicate the setting unambiguously; thus the lattice letters were chosen as C (b-axis setting) and B (c-axis setting). The use of A in either case would not have distinguished between the two settings [*cf.* pp. 7, 55 and 543 of *IT* (1952); see also Table 2.1.3.12].

As a consequence of the different transformations between b- and c-axis settings in *IT* (1952) and in this volume (and all editions of this series), some space-group symbols have changed. This is apparent from a comparison of pairs such as $P12_1/c1$ & $P112_1/b$ and $C12/c1$ & $B112/b$ in *IT* (1952) with the corresponding pairs in this volume, $P12_1/c1$ & $P112_1/a$ and $C12/c1$ & $A112/a$. The symbols with B-centred cells appear now for cell choice 2, as can be seen from Table 2.1.3.12.

Selection of monoclinic cell. In practice, the selection of the (right-handed) unit cell of a monoclinic crystal can be approached in three ways, whereby the axes refer to the b-unique setting; for c unique similar considerations apply:

(i) Irrespective of their lengths, the basis vectors are chosen such that, in Fig. 2.1.3.12, one obtains $\mathbf{c} = \mathbf{e}$, $\mathbf{a} = \mathbf{f}$ and $\mathbf{b}$ normal to $\mathbf{a}$ and $\mathbf{c}$ pointing upwards. This corresponds to a selection of cell choice 1. It ensures that the crystal structure can always be referred directly to the description and the space-group symbol in *IT* (1935) and *IT* (1952). However, this is at the expense of possibly using a non-reduced and, in many cases, even a very awkward cell.

(ii) Selection of the reduced mesh, *i.e.* the shortest two translation vectors in the monoclinic plane are taken as axes and labelled $\mathbf{a}$ and $\mathbf{c}$, with either $a < c$ or $c < a$. This results with equal probability in one of the three cell choices described in the present volume.

(iii) Selection of the cell on special grounds, *e.g.* to compare the structure under consideration with another related crystal structure. This may result again in a non-reduced cell and it may even necessitate use of the a-axis setting. In all these cases, the coordinate system chosen should be carefully explained in the description of the structure.

2.1.3.16. Crystallographic groups in one dimension

In one dimension, only one crystal family, one crystal system and one Bravais lattice exist. No name or common symbol is required for any of them. All one-dimensional lattices are primitive, which is symbolized by the script letter $\mathscr{p}$; *cf.* Table 2.1.1.1.

There occur two types of one-dimensional point groups, 1 and $m \equiv \bar{1}$. The latter contains reflections through a point (reflection point or mirror point). This operation can also be described as inversion through a point, thus $m \equiv \bar{1}$ for one dimension; *cf.* Section 2.1.2.

Two types of line groups (one-dimensional space groups) exist, with Hermann–Mauguin symbols $\mathscr{p}1$ and $\mathscr{p}m \equiv \mathscr{p}\bar{1}$, which are illustrated in Fig. 2.1.3.13. Line group $\mathscr{p}1$, which consists of one-dimensional translations only, has merely one (general) position with coordinate x. Line group $\mathscr{p}m$ consists of one-dimensional translations and reflections through points. It has one general and two special positions. The coordinates of the general position are x and $\bar{x}$; the coordinate of one special position is 0, that of the other $\frac{1}{2}$. The site symmetries of both special positions are $m \equiv \bar{1}$. For $\mathscr{p}1$, the origin is arbitrary, for $\mathscr{p}m$ it is at a reflection point.

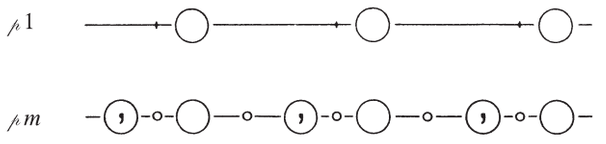

Figure 2.1.3.13
The two line groups (one-dimensional space groups). Small circles are reflection points; large circles represent the general position; in line group $\mathscr{p}1$, the vertical bars are the origins of the unit cells.

The one-dimensional *point groups* are of interest as 'edge symmetries' of two-dimensional 'edge forms'; they are listed in Table 3.2.3.1. The one-dimensional *space groups* occur as projection and section symmetries of crystal structures.

2.1.4. Computer production of the space-group tables

By P. Konstantinov and K. Momma

The space-group tables for the first (1983) edition of Volume A were produced and typeset by a computer-aided process as described by Fokkema (1983). However, the computer programs used and the data files were then lost. All corrections in the subsequent three editions were done by photocopying and 'cut-and-paste' work based on the printed version of the book.

Hence, in October 1997, a new project for the electronic production of the fifth edition of Volume A of *International Tables for Crystallography* was started. Part of this project concerned the computer generation of the plane- and space-group tables [Parts 6 and 7 of *IT* A (2002)], excluding the space-group diagrams. The aim was to be able to produce PostScript and Portable Document Format (PDF) documents that could be used for printing and displaying the tables. The layout of the tables had to follow exactly that of the previous editions of Volume A. Having the space-group tables in electronic form opened the way for easy corrections and modifications of later editions and made possible the online edition of Volume A in 2006 (http://it.iucr.org/A/). Although the plane- and space-group data were encoded in a format designed for printing, they were later machine-read and transformed to other electronic formats, and were incorporated into the data files on which the Symmetry Database in the online version of *International Tables for Crystallography* (http://it.iucr.org/resources/symmetrydatabase/) and the online services offered by the Bilbao Crystallographic Server (http://www.cryst.ehu.es/) are based.

The LaTeX document preparation system (Lamport, 1994), which is based on the TeX typesetting software, was used for the preparation of these tables. It was chosen because of its high versatility and general availability on almost any computer platform. It is also worth noting the longevity of the system. Even though the hardware and operating system software used almost 20 years ago, when the project began, are now obsolete, the software is still available on all major modern computer systems. All the material – LaTeX code and data – created for the fifth edition of 2002 was re-used in the preparation of the current edition with only small changes concerning the presentation.

A separate file was created for each plane and space group and each setting. These data files contain the information listed in the plane- and space-group tables and are encoded using standard LaTeX constructs. As is customary, these specially designed commands and environments are defined in a separate package