Table 2.2.14.1. *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 Part 7*

Projection direction	Triclinic	Monoclinic		Orthorhombic	Projection direction	Tetragonal
		Unique axis b	Unique axis c			
[001]	$a' = a\sin\beta$ $b' = b\sin\alpha$ $\gamma' = 180° - \gamma^*$ †	$a' = a\sin\beta$ $b' = b$ $\gamma' = 90°$	$a' = a$ $b' = b$ $\gamma' = \gamma$	$a' = a$ $b' = b$ $\gamma' = 90°$	[001]	$a' = a$ $b' = a$ $\gamma' = 90°$
[100]	$a' = b\sin\gamma$ $b' = c\sin\beta$ $\gamma' = 180° - \alpha^*$ †	$a' = b$ $b' = c\sin\beta$ $\gamma' = 90°$	$a' = b\sin\gamma$ $b' = c$ $\gamma' = 90°$	$a' = b$ $b' = c$ $\gamma' = 90°$	[100]	$a' = a$ $b' = c$ $\gamma' = 90°$
[010]	$a' = c\sin\alpha$ $b' = \alpha\sin\gamma$ $\gamma' = 180° - \beta^*$ †	$a' = c$ $b' = a$ $\gamma' = \beta$	$a' = c$ $b' = a\sin\gamma$ $\gamma' = 90°$	$a' = c$ $b' = a$ $\gamma' = 90°$	[110]	$a' = (a/2)\sqrt{2}$ $b' = c$ $\gamma' = 90°$

Projection direction	Hexagonal	Projection direction	Rhombohedral ‡	Projection direction	Cubic
[001]	$a' = a$ $b' = a$ $\gamma' = 120°$	[111]	$a' = \frac{2}{\sqrt{3}}a\sin(\alpha/2)$ $b' = \frac{2}{\sqrt{3}}a\sin(\alpha/2)$ $\gamma' = 120°$	[001]	$a' = a$ $b' = a$ $\gamma' = 90°$
[100]	$a' = (a/2)\sqrt{3}$ $b' = c$ $\gamma' = 90°$	$[1\bar{1}0]$	$a' = a\cos(\alpha/2)$ $b' = a$ $\gamma' = \delta$ §	[111]	$a' = a\sqrt{2/3}$ $b' = a\sqrt{2/3}$ $\gamma' = 120°$
[210]	$a' = a/2$ $b' = c$ $\gamma' = 90°$	$[\bar{2}11]$	$a' = \frac{1}{\sqrt{3}}a\sqrt{1+2\cos\alpha}$ $b' = a\sin(\alpha/2)$ $\gamma' = 90°$	[110]	$a' = (a/2)\sqrt{2}$ $b' = a$ $\gamma' = 90°$

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

‡ The entry 'Rhombohedral' refers to the primitive rhombohedral cell with $a = b = c, \alpha = \beta = \gamma$ (*cf.* Table 2.1.2.1).

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

2.2.14. 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.

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.

2.2.14.1. *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 2.2.4.1). If a lattice contains less 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*.

(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 Parts 6 and 7. 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 2.2.14.1. 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 2.2.9).

Example

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

2.2.14.2. *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* lattices, the multiplicity is reduced from 4 to 2 because *c*-centred plane 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 $[1\bar{1}1]$, $[\bar{1}1\bar{1}]$, $[1\bar{1}1]$ 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.* Chapter 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.* Chapter 1.2). A simple cell transformation leads to the conventional hexagonal *p* cell.

2.2.14.3. *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 2.2.14.2 for the various crystallographic symmetry elements. From this table the following conclusions can be drawn:

Table 2.2.14.2. *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 $\perp$ component*	Glide line *g*
Glide plane without $\perp$ 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 $\perp$ component' refers to the component of the glide vector normal to the projection direction.

(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 $\bar{2}$. 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