

## 2.1. GUIDE TO THE USE OF THE SPACE-GROUP TABLES

(4) *Fmm2* (42)

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

Special position *8b*:  $hkl = 2n$ , 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: *P4̄3n* (218)

Special position *6d*:  $hkl$ :  $h + k + l = 2n$  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	}	[001]	[100]	[010]
Monoclinic				
(both settings)				
Orthorhombic				
Tetragonal		[001]	[100]	[110]
Hexagonal		[001]	[100]	[210]
Rhombohedral		[111]	[1̄10]	[2̄1̄1̄]
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 *p1m1* or as *p11m* (*cf.* Section 1.4.1.5 for explanations of Hermann–Mauguin symbols of plane groups).

(iii) *Relations between the basis vectors a', 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 **a'** and **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.* **a'** and **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 **a<sub>p</sub>, b<sub>p</sub>, c<sub>p</sub>**.

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

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**Table 2.1.3.9**

Cell parameters  $a', b', \gamma'$  of the two-dimensional cell in terms of cell parameters  $a, b, c, \alpha, \beta, \gamma$  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]	$a' = a \sin \beta$ $b' = b \sin \alpha$ $\gamma' = 180^\circ - \gamma^* \dagger$	$a' = a \sin \beta$ $b' = b$ $\gamma' = 90^\circ$	$a' = a$ $b' = b$ $\gamma' = \gamma$	$a' = a$ $b' = b$ $\gamma' = 90^\circ$
[100]	$a' = b \sin \gamma$ $b' = c \sin \beta$ $\gamma' = 180^\circ - \alpha^* \dagger$	$a' = b$ $b' = c \sin \beta$ $\gamma' = 90^\circ$	$a' = b \sin \gamma$ $b' = c$ $\gamma' = 90^\circ$	$a' = b$ $b' = c$ $\gamma' = 90^\circ$
[010]	$a' = c \sin \alpha$ $b' = \alpha \sin \gamma$ $\gamma' = 180^\circ - \beta^* \dagger$	$a' = c$ $b' = a$ $\gamma' = \beta$	$a' = c$ $b' = a \sin \gamma$ $\gamma' = 90^\circ$	$a' = c$ $b' = a$ $\gamma' = 90^\circ$

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]	$a' = a \cos(\alpha/2)$ $b' = a$ $\gamma' = \delta \S$
[ $\bar{2}$ 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]	$a' = (a/2)\sqrt{2}$ $b' = a$ $\gamma' = 90^\circ$

$$\dagger \cos \alpha^* = \frac{\cos \beta \cos \gamma - \cos \alpha}{\sin \beta \sin \gamma}; \quad \cos \beta^* = \frac{\cos \gamma \cos \alpha - \cos \beta}{\sin \gamma \sin \alpha}; \quad \cos \gamma^* = \frac{\cos \alpha \cos \beta - \cos \gamma}{\sin \alpha \sin \beta}$$

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

$$\S \cos \delta = \frac{\cos \alpha}{\cos \alpha/2}$$

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  $[\bar{1}21]$  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.

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**Table 2.1.3.10**

Projections of crystallographic symmetry elements

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

† The term 'with  $\perp$  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 transla-

tion; 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: C12/c1 (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;  $2 \parallel [010]$  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  $c2mm$  (9),  $\mathbf{a}' = \mathbf{a}_p$ ,  $\mathbf{b}' = \mathbf{b}$ .

Projection along  $[100]$ : The periodicity along  $b$  is halved because of the  $C$  centring;  $2 \parallel [010]$  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  $p2gm$  (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  $c$ ;  $2 \parallel [010]$  projects as 2.

*Result:* Plane group  $p2$  (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  $\mathbf{e}$ ,  $\mathbf{f}$  and  $\mathbf{g}$ , in order of increasing length.<sup>5</sup> The two shorter vectors span the 'reduced mesh' (where mesh means a two-dimensional unit cell), here  $\mathbf{e}$  and  $\mathbf{f}$ ; for this mesh, the monoclinic angle is  $\leq 120^\circ$ ,

<sup>5</sup> 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.