

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

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:

- 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 ($\bar{6} \equiv 3/m$).
- 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 .
- 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.

- 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.
- 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:

- the unit cell chosen, here called 'cell choice';
- 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.⁵ 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 $\leq 120^\circ$,

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.