Table 1.2.3.1
Symmetry elements in point and space groups

Name of symmetry element	Geometric element	Defining operation (d.o.)	Operations in element set
Mirror plane	Plane *p*	Reflection through *p*	D.o. and its coplanar equivalents†
Glide plane	Plane *p*	Glide reflection through *p*; 2**v** (not **v**) a lattice-translation vector	D.o. and its coplanar equivalents†
Rotation axis	Line *l*	Rotation around *l*, angle $2\pi/N$, $N = 2, 3, 4$ or 6	1st ... $(N-1)$th powers of d.o. and their coaxial equivalents‡
Screw axis	Line *l*	Screw rotation around *l*, angle $2\pi/N$, $u = j/N$ times shortest lattice translation along *l*, right-hand screw, $N = 2, 3, 4$ or 6, $j = 1, \ldots, (N-1)$	1st ... $(N-1)$th powers of d.o. and their coaxial equivalents‡
Rotoinversion axis	Line *l* and point *P* on *l*	Rotoinversion: rotation around *l*, angle $2\pi/N$, followed by inversion through *P*, $N = 3, 4$ or 6	D.o. and its inverse
Centre	Point *P*	Inversion through *P*	D.o. only

† That is, all glide reflections through the same reflection plane, with glide vectors **v** differing from that of the d.o. (taken to be zero for reflections) by a lattice-translation vector. The glide planes *a*, *b*, *c*, *n*, *d* and *e* are distinguished (*cf.* Table 2.1.2.1). ‡ That is, all rotations and screw rotations around the same axis *l*, with the same angle and sense of rotation and the same screw vector **u** (zero for rotation) up to a lattice-translation vector.

In crystallography these group elements, however, were the symmetry operations of the symmetry groups, not the crystallographic symmetry elements. Therefore, the IUCr Commission on Crystallographic Nomenclature appointed an *Ad-hoc* Committee on the Nomenclature of Symmetry with P. M. de Wolff as Chairman to propose definitions for terms of crystallographic symmetry and for several classifications of crystallographic space groups and point groups.

In the reports of the *Ad-hoc* Committee, de Wolff *et al.* (1989) and (1992) with *Addenda*, Flack *et al.* (2000), the results were published. To define the term *symmetry element* for any symmetry operation was more complicated than had been envisaged previously, in particular for unusual screw and glide components.

According to the proposals of the Committee the following procedure has been adopted (*cf.* also Table 1.2.3.1):

(1) No symmetry element is defined for the identity and the (lattice) translations.

(2) For any symmetry operation of point groups and space groups with the exception of the rotoinversions $\bar{3}$, $\bar{4}$ and $\bar{6}$, the *geometric element* is defined as the *set of fixed points* (the second column of Table 1.2.3.1) of the *reduced operation*, *cf.* equation (1.2.2.17). For reflections and glide reflections this is a plane; for rotations and screw rotations it is a line, for the inversion it is a point. For the rotoinversions $\bar{3}$, $\bar{4}$ and $\bar{6}$ the geometric element is a line with a point (the inversion centre) on this line.

(3) The *element set* (*cf.* the last column of Table 1.2.3.1) is defined as a set of operations that share the same geometric element. The element set can consist of symmetry operations of the same type (such as the powers of a rotation) or of different types, *e.g.* by a reflection and a glide reflection through the same plane. The *defining operation* (d.o.) may be any symmetry operation from the element set that suffices to identify the symmetry element. In most cases, the 'simplest' symmetry operation from the element set is chosen as the d.o. (*cf.* the third column of Table 1.2.3.1). For reflections and glide reflections the element set includes the defining operation and all glide reflections through the same reflection plane but with glide vectors differing by a lattice-translation vector, *i.e.* the so-called *coplanar equivalents*. For rotations and screw rotations of angle $2\pi/k$ the element set is the defining operation, its 1st ... $(k-1)$th powers and all rotations and screw rotations with screw vectors differing from that of the defining operation by a lattice-translation vector, known as *coaxial equivalents*. For a rotoinversion the element set includes the defining operation and its inverse.

(4) The combination of the geometric element and its element set is indicated by the name *symmetry element*. The names of the symmetry elements (first column of Table 1.2.3.1) are combinations of the name of the defining operation attached to the name of the corresponding geometric element. Names of symmetry elements are *mirror plane*, *glide plane*, *rotation axis*, *screw axis*, *rotoinversion axis* and *centre*.[2] This allows such statements as *this point lies on a rotation axis* or *these operations belong to a glide plane*.

Examples

(1) *Glide and mirror planes*. The element set of a glide plane with a glide vector **v** consists of infinitely many different glide reflections with glide vectors that are obtained from **v** by adding any lattice-translation vector parallel to the glide plane, including centring translations of centred cells.

(*a*) It is important to note that if among the infinitely many glide reflections of the element set of the same plane there exists one operation with zero glide vector, then this operation is taken as the *defining operation* (d.o). Consider, for example, the symmetry operation $x+1/2, y+1/2, -z+1/2$ of *Cmcm* (63) [*General position* (1/2, 1/2, 0) block]. This is an *n*-glide reflection through the plane $x, y, 1/4$. However, the corresponding symmetry element is a mirror plane, as among the glide reflections of the element set of the plane $x, y, 1/4$ one finds the reflection $x, y, -z+1/2$ [symmetry operation (6) of the *General position* (0, 0, 0) block].

(*b*) The symmetry operation $x+5/2, y-7/2, -z+3$ is a glide reflection. Its geometric element is the plane $x, y, 3/2$. Its symmetry element is a glide plane in space group *Pmmn* (59) because there is no lattice translation by which the glide vector can be changed to **o**. If, however, the same mapping is a symmetry operation of space group *Cmmm* (65), then its symmetry element is a reflection plane because the glide vector with components $5/2, -7/2, 0$ can be cancelled through a translation $(2+\frac{1}{2})\mathbf{a}+(-4+\frac{1}{2})\mathbf{b}$, which is a lattice translation in a *C* lattice. Evidently, the correct specification of the symmetry element is possible only with respect to a specific translation lattice.

[2] The proposal to introduce the symbols for the symmetry elements *Em*, *Eg*, *En*, En_j, $E\bar{n}$ and $E\bar{1}$ was not taken up in practice. The printed and graphical symbols of symmetry elements used throughout the space-group tables of Part 2 are introduced in Section 2.1.2 and listed in Tables 2.1.2.1 to 2.1.2.7.