International Tables for Crystallography (2006). Vol. A, Section 2.2.11, pp. 27–28.

(i) A symbol denoting the *type* of the symmetry operation (*cf.* Chapter 1.3), 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 given in addition.

Details of this symbolism are presented in Section 11.1.2.

Examples

(1) $a\;\; x,y,\frac{1}{4}$
Glide reflection with glide component $(\frac{1}{2},0,0)$ through the plane $x,y,\frac{1}{4}$, *i.e.* the plane parallel to (001) at $z=\frac{1}{4}$.

(2) $\bar{4}^{+}\;\; \frac{1}{4},\frac{1}{4},z;\;\; \frac{1}{4},\frac{1}{4},\frac{1}{4}$
Fourfold rotoinversion, consisting of a counter clockwise rotation by 90° around the line $\frac{1}{4},\frac{1}{4},z$, followed by an inversion through the point $\frac{1}{4},\frac{1}{4},\frac{1}{4}$.

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

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

(5) 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 $0,\frac{1}{4},z$.

2.2.10. Generators

The line *Generators selected* states the symmetry operations and their sequence, selected to generate all symmetrically 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 2.2.9 [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* 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 8.3.5.1 of Section 8.3.5.

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 symmetrically 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 8.3.5.

For different descriptions of the same space group (settings, cell choices, origin choices), the generating operations are the same. Thus, the transformation relating the two coordinate systems transforms also the generators of one description into those of the other.

From the Fifth Edition onwards, this applies also to the description of the seven rhombohedral (*R*) space groups by means of 'hexagonal' and 'rhombohedral' axes. In previous editions, there was a difference in the *sequence* (not the data) of the 'coordinate triplets' and the 'symmetry operations' in both descriptions (*cf.* Section 2.10 in the First to Fourth Editions).

2.2.11. Positions

The entries under *Positions** (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 M of the Wyckoff position*. This is the number of equivalent points per unit cell. For primitive cells, the multiplicity *M* of the general position is equal to the order of the point group of the space group; for centred cells, *M* 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.

(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 (the theoretical background on Wyckoff positions is given in Section 8.3.2).

(iii) *Site symmetry*. This is explained in Section 2.2.12.

(iv) *Coordinates*. The sequence of the coordinate triplets is based on the *Generators* (*cf.* Section 2.2.10). 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

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

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 *M* coordinate triplets of a position represent the coordinates of the *M* 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 2.2.6.

(v) *Reflection conditions*. These are described in Section 2.2.13.

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

(i) *General position*
A set of symmetrically equivalent points, *i.e.* a 'crystallographic orbit', is said to be in 'general position' if each of its points 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 short-hand form of the matrix representation of the symmetry operations of the space group; this viewpoint is further described in Sections 8.1.6 and 11.1.1.

(ii) *Special position(s)*
A set of symmetrically equivalent points is said to be in 'special position' if each of its points 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 in a space group [up to 26 in *Pmmm* (No. 47)] depends on the number and types of symmetry operations that map a point onto itself.

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 2.2.12. 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.* 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 consequent 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'. The 13 space groups of this kind are listed in Section 8.3.2.

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 entries 'Symmetry operations', 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).

2.2.12. Oriented site-symmetry symbols

The third column of each Wyckoff position gives the *Site symmetry** 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 (symmetrically equivalent) subgroups of the space group. For this reason, all points of one special position are described by the same site-symmetry symbol.

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 2.2.4.1). 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

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