International Tables for Crystallography (2006). Vol. A, Section 2.2.10, p. 27.

(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.

references