

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

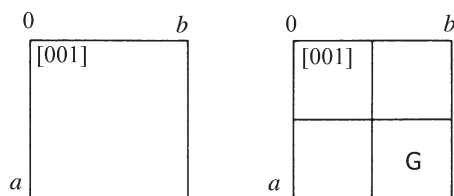


Figure 2.1.3.7
Tetragonal space groups (G = general-position diagram).

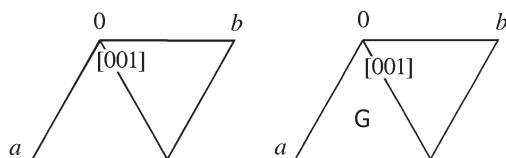


Figure 2.1.3.8
Trigonal *P* and hexagonal *P* space groups (G = general-position diagram).

symbol can easily be deduced by comparing Fig. 2.1.3.6 with the diagrams for the space group under consideration.

Not all of the 59 orthorhombic space groups have all six projections distinct, *i.e.* have different Hermann–Mauguin symbols for the six settings. This aspect is treated in Table 2.1.3.4. Only 22 space groups have six, 25 have three, 2 have two different symbols, while 10 have all symbols the same. This information can be of help in the early stages of a crystal-structure analysis.

The six setting symbols, *i.e.* the six permutations of the labels of the axes, form the column headings of the orthorhombic entries in Table 1.5.4.4, which contains the extended Hermann–Mauguin symbols for the six settings of each orthorhombic space group. Note that some of these setting symbols exhibit different sign changes compared with those in Fig. 2.1.3.6.

2.1.3.6.5. Tetragonal, trigonal *P* and hexagonal *P* space groups

The pairs of diagrams for these space groups are similar to those in the previous editions of *IT*. Each pair consists of a general-position diagram (right) and a diagram of the symmetry elements (left), both projected along *c*, as illustrated in Figs. 2.1.3.7 and 2.1.3.8.

2.1.3.6.6. Trigonal *R* (rhombohedral) space groups

The seven rhombohedral space groups are treated in two versions, the first based on ‘hexagonal axes’ (obverse setting), the second on ‘rhombohedral axes’ (*cf.* Sections 2.1.1.2 and 2.1.3.2). The pairs of diagrams are similar to those in *IT* (1952) and *IT A* (2002); the left or top one displays the symmetry elements, the right or bottom one the general position. This is illustrated in Fig. 2.1.3.9, which gives the axes *a* and *b* of the triple hexagonal cell and the projections of the axes of the primitive rhombohedral cell, labelled a_{rh} , b_{rh} and c_{rh} . For convenience, all ‘heights’ in the space-group diagrams are fractions of the hexagonal *c* axis. For ‘hexagonal axes’, the projection direction is [001], for ‘rhombohedral axes’ it is [111]. In the general-position diagrams, the circles drawn in heavier lines represent atoms that lie within the primitive rhombohedral cell (provided the symbol ‘–’ is read as $1 - z$ rather than as $-z$).

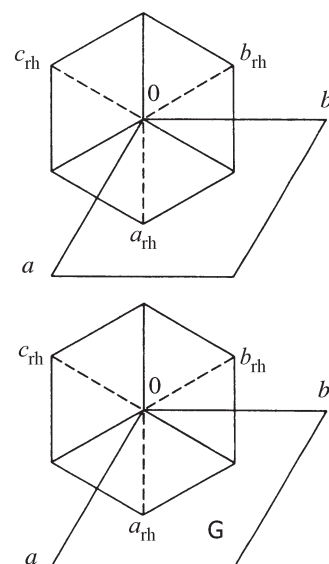


Figure 2.1.3.9
Rhombohedral space groups. Obverse triple hexagonal cell with ‘hexagonal axes’ *a*, *b* and primitive rhombohedral cell with projections of ‘rhombohedral axes’ a_{rh} , b_{rh} , c_{rh} . Note: In the actual space-group diagrams the edges of the primitive rhombohedral cell (dashed lines) are only indicated in the general-position diagram of the rhombohedral-axes description (G = general-position diagram).

The symmetry-element diagrams for the hexagonal and the rhombohedral descriptions of a space group are the same. The edges of the primitive rhombohedral cell (*cf.* Fig. 2.1.3.9) are only indicated in the general-position diagram of the rhombohedral description.

2.1.3.6.7. Cubic space groups

For each cubic space group, one projection of the symmetry elements along [001] is given, Fig. 2.1.3.10; for details of the diagrams, see Section 2.1.2 and Buerger (1956). For face-centred lattices *F*, only a quarter of the unit cell is shown; this is sufficient since the projected arrangement of the symmetry elements is translation-equivalent in the four quarters of an *F* cell. It is important to note that symmetry axes inclined to the projection plane are indicated where they intersect the plane of projection. Symmetry planes inclined to the projection plane that occur in classes $\bar{4}3m$ and $m\bar{3}m$ are shown as ‘inserts’ around the high-symmetry points, such as $0, 0, 0$; $\frac{1}{2}, 0, 0$; *etc.*

The cubic diagrams given in *IT* (1935) are different from the ones used here. No drawings for cubic space groups were provided in *IT* (1952).

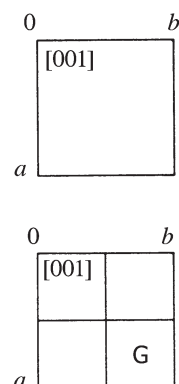


Figure 2.1.3.10
Cubic space groups. G = general-position diagram, in which the equivalent positions are shown as the vertices of polyhedra.