

## 2.2. CONTENTS AND ARRANGEMENT OF THE TABLES

associated with a particular setting symbol can easily be deduced by comparing Fig. 2.2.6.6 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 2.2.6.1. 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 listed in the second paragraph of this section form the column headings of the orthorhombic entries in Table 4.3.2.1, 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. 2.2.6.6.

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

The pairs of diagrams for these space groups are similar to those in *IT* (1935) and *IT* (1952). 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. 2.2.6.7 and 2.2.6.8.

 2.2.6.6. Rhombohedral (trigonal *R*) space groups

The seven rhombohedral *R* space groups are treated in two versions, the first based on ‘hexagonal axes’ (obverse setting), the second on ‘rhombohedral axes’ (*cf.* Sections 2.1.3 and 2.2.2). The pairs of diagrams are similar to those in *IT* (1952); the left or top one displays the symmetry elements, the right or bottom one the general position. This is illustrated in Fig. 2.2.6.9, 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<sub>p</sub>*, *b<sub>p</sub>* and *c<sub>p</sub>*. 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  $-z$ ).

The pairs of drawings for the hexagonal and the rhombohedral descriptions of a space group are the same. In the rhombohedral descriptions of space groups Nos. 166 and 167,  $R\bar{3}m$  and  $R\bar{3}c$ , the diagrams are omitted for reasons of space, and the reader is referred to the drawings in the hexagonal descriptions.

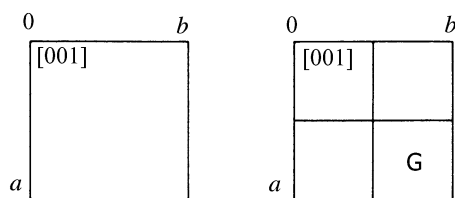


Fig. 2.2.6.7. Tetragonal space groups (G = general-position diagram).

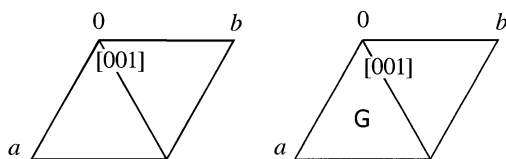
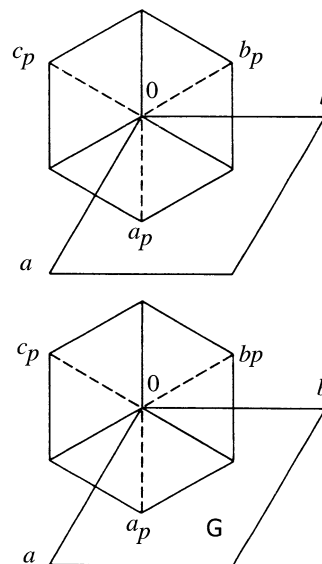

 Fig. 2.2.6.8. Trigonal *P* and hexagonal *P* space groups (G = general-position diagram).


Fig. 2.2.6.9. Rhombohedral *R* space groups. Obverse triple hexagonal cell with ‘hexagonal axes’ *a*, *b* and primitive rhombohedral cell with projections of ‘rhombohedral axes’ *a<sub>p</sub>*, *b<sub>p</sub>*, *c<sub>p</sub>*. Note: In the actual space-group diagrams only the upper edges (full lines), not the lower edges (dashed lines) of the primitive rhombohedral cell are shown (G = general-position diagram).

## 2.2.6.7. Cubic space groups

For each cubic space group, one projection of the symmetry elements along [001] is given, Fig. 2.2.6.10; for details of the diagrams, see Chapter 1.4 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. The three stereoscopic general-position diagrams in the lower part of the page are explained below.

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

## 2.2.6.8. Diagrams of the general position

## (i) Non-cubic space groups

In these diagrams, the ‘heights’ of the points are *z* coordinates, except for monoclinic space groups with unique axis *b* where they are *y* coordinates. For rhombohedral space groups, the heights are always fractions of the hexagonal *c* axis. The symbols + and – stand for +*z* and –*z* (or +*y* and –*y*) in which *z* or *y* can assume any value. For points with symbols + or – preceded by a fraction, *e.g.*

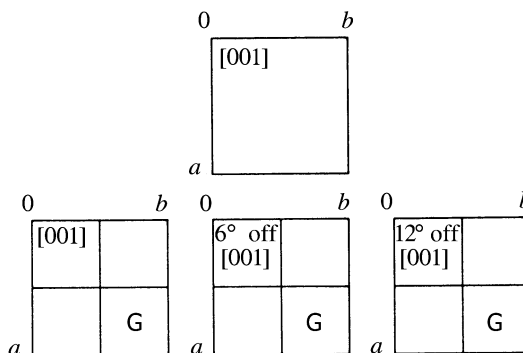


Fig. 2.2.6.10. Cubic space groups (G = general-position stereodiagrams).