Examples

(1) $P4_2/mbc$ (135). From the full symbol, the *first* maximal t subgroup is found to be $P2_1/b\ 2_1/a\ 2/m$ (*Pbam*). The C-cell symbol is $C4_2/m\ cg_1$ and gives rise to the *second* maximal orthorhombic t subgroup *Cccm*, cell $\mathbf{a}', \mathbf{b}', \mathbf{c}'$.

(2) $I4/m\ cm$ (140). Similarly, the *first* orthorhombic maximal t subgroup is *Iccm* (*Ibam*); the *second* maximal orthorhombic t subgroup is obtained from the F-cell symbol as $Fc\ c\ m$ / mmn (*Fmmm*), cell $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$.

These examples show that P- and C-cell, as well as I- and F-cell descriptions of tetragonal groups have to be considered together.

(iii) *Monoclinic subgroups*

Only space groups of classes 4, $\bar{4}$ and $4/m$ have maximal monoclinic t subgroups.

Examples

(1) $P4_1$ (76) has the subgroup $P112_1$ ($P2_1$). The C-cell description does not add new features: $C112_1$ is reducible to $P2_1$.

(2) $I4_1/a$ (88) has the subgroup $I112_1/a$, equivalent to $I112/a$ ($C2/c$). The F-cell description yields the same subgroup $F11\ 2/d$, again reducible to $C2/c$.

4.3.5. Trigonal and hexagonal systems

The trigonal and hexagonal crystal systems are considered together, because they form the hexagonal 'crystal family', as explained in Chapter 2.1. Hexagonal lattices occur in both systems, whereas rhombohedral lattices occur only in the trigonal system.

4.3.5.1. *Historical note*

The 1935 edition of *International Tables* contains the symbols C and H for the *hexagonal lattice* and R for the *rhombohedral lattice*. C recalls that the hexagonal lattice can be described by a double rectangular C-centred cell (orthohexagonal axes); H was used for a hexagonal triple cell (see below); R designates the rhombohedral lattice and is used for both the rhombohedral description (primitive cell) and the hexagonal description (triple cell).

In the 1952 edition the following changes took place (*cf.* pages x, 51 and 544 of *IT* 1952): The lattice symbol C was replaced by P for reasons of consistency; the H description was dropped. The symbol R was kept for both descriptions, rhombohedral and hexagonal. The tertiary symmetry element in the short Hermann–Mauguin symbols of class 622, which was omitted in *IT* (1935), was re-established.

In the present volume, the use of P and R is the same as in *IT* (1952). The H cell, however, reappears in the sub- and supergroup data of Part 7 and in Table 4.3.2.1 of this section, where short symbols for the H description of trigonal and hexagonal space groups are given. The C cell reappears in the subgroup data for all trigonal and hexagonal space groups having symmetry elements orthogonal to the main axis.

4.3.5.2. *Primitive cells*

The primitive cells of the hexagonal and the rhombohedral lattice, hP and hR, are defined in Table 2.1.2.1 In Part 7, the 'rhombohedral' description of the hR lattice is designated by 'rhombohedral axes'; *cf.* Chapter 1.2.

4.3.5.3. *Multiple cells*

Multiple cells are frequently used to describe both the hexagonal and the rhombohedral lattice.

(i) *The triple hexagonal R cell; cf. Chapters 1.2 and 2.1*

When the lattice is *rhombohedral hR* (primitive cell **a**, **b**, **c**), the triple R cell $\mathbf{a}', \mathbf{b}', \mathbf{c}'$ corresponds to the 'hexagonal description' of the rhombohedral lattice. There are three right-handed *obverse R* cells:

$$\begin{array}{lllll} R_1: & \mathbf{a}' = \mathbf{a} - \mathbf{b}; & \mathbf{b}' = \mathbf{b} - \mathbf{c}; & \mathbf{c}' = \mathbf{a} + \mathbf{b} + \mathbf{c}; \\ R_2: & \mathbf{a}' = \mathbf{b} - \mathbf{c}; & \mathbf{b}' = \mathbf{c} - \mathbf{a}; & \mathbf{c}' = \mathbf{a} + \mathbf{b} + \mathbf{c}; \\ R_3: & \mathbf{a}' = \mathbf{c} - \mathbf{a}; & \mathbf{b}' = \mathbf{a} - \mathbf{b}; & \mathbf{c}' = \mathbf{a} + \mathbf{b} + \mathbf{c}. \end{array}$$

Three further right-handed R cells are obtained by changing $\mathbf{a}'$ and $\mathbf{b}'$ to $-\mathbf{a}'$ and $-\mathbf{b}'$, *i.e.* by a 180° rotation around $\mathbf{c}'$. These cells are *reverse*. The transformations between the triple R cells and the primitive rhombohedral cell are given in Table 5.1.3.1 and Fig. 5.1.3.6.

The obverse triple R cell has 'centring points' at

$$0,0,0; \quad \tfrac{2}{3},\tfrac{1}{3},\tfrac{1}{3}; \quad \tfrac{1}{3},\tfrac{2}{3},\tfrac{2}{3},$$

whereas the reverse R cell has 'centring points' at

$$0,0,0; \quad \tfrac{1}{3},\tfrac{2}{3},\tfrac{1}{3}; \quad \tfrac{2}{3},\tfrac{1}{3},\tfrac{2}{3}.$$

In the space-group tables of Part 7, the obverse R_1 cell is used, as illustrated in Fig. 2.2.6.9. This 'hexagonal description' is designated by 'hexagonal axes'.

(ii) *The triple rhombohedral D cell*

Parallel to the 'hexagonal description of the rhombohedral lattice' there exists a 'rhombohedral description of the hexagonal lattice'. Six right-handed rhombohedral cells (here denoted by D) with cell vectors $\mathbf{a}', \mathbf{b}', \mathbf{c}'$ of equal lengths are obtained from the hexagonal P cell **a**, **b**, **c** by the following transformations and by cyclic permutations of $\mathbf{a}', \mathbf{b}', \mathbf{c}'$:

$$\begin{array}{lllll} D_1: & \mathbf{a}' = & \mathbf{a} + \mathbf{c}; & \mathbf{b}' = & \mathbf{b} + \mathbf{c}; \quad \mathbf{c}' = -(\mathbf{a} + \mathbf{b}) + \mathbf{c} \\ D_2: & \mathbf{a}' = -\mathbf{a} + \mathbf{c}; & & \mathbf{b}' = -\mathbf{b} + \mathbf{c}; & \mathbf{c}' = \mathbf{a} + \mathbf{b} + \mathbf{c}. \end{array}$$

The transformation matrices are listed in Table 5.1.3.1. D_2 follows from D_1 by a 180° rotation around [111]. The D cells are triple rhombohedral cells with 'centring' points at

$$0,0,0; \quad \tfrac{1}{3},\tfrac{1}{3},\tfrac{1}{3}; \quad \tfrac{2}{3},\tfrac{2}{3},\tfrac{2}{3}.$$

The D cell, not used in practice and not considered explicitly in the present volume, is useful for a deeper understanding of the relations between hexagonal and rhombohedral lattices.

(iii) *The triple hexagonal H cell; cf. Chapter 1.2*

Generally, a hexagonal lattice hP is described by means of the smallest hexagonal P cell. An alternative description employs a larger hexagonal H-centred cell of three times the volume of the P cell; this cell was extensively used in *IT* (1935), see *Historical note* above.

There are three right-handed orientations of the H cell (basis vectors $\mathbf{a}', \mathbf{b}', \mathbf{c}'$) with respect to the basis vectors **a**, **b**, **c** of the P cell:

$$\begin{array}{lllll} H_1: & \mathbf{a}' = & \mathbf{a} - & \mathbf{b}; & \mathbf{b}' = & \mathbf{a} + 2\mathbf{b}; & \mathbf{c}' = \mathbf{c} \\ H_2: & \mathbf{a}' = 2\mathbf{a} + & \mathbf{b}; & \mathbf{b}' = - & \mathbf{a} + \mathbf{b}; & \mathbf{c}' = \mathbf{c} \\ H_3: & \mathbf{a}' = & \mathbf{a} + 2\mathbf{b}; & \mathbf{b}' = -2\mathbf{a} - & \mathbf{b}; & \mathbf{c}' = \mathbf{c}. \end{array}$$

The transformations are given in Table 5.1.3.1 and Fig. 5.1.3.8. The new vectors $\mathbf{a}'$ and $\mathbf{b}'$ are rotated in the *ab* plane by $-30°(H_1)$, $+30°(H_2)$, $+90°(H_3)$ with respect to the old vectors **a** and **b**. Three further right-handed H cells are obtained by changing $\mathbf{a}'$ and $\mathbf{b}'$ to $-\mathbf{a}'$ and $-\mathbf{b}'$, *i.e.* by a rotation of 180° around $\mathbf{c}'$.

The H cell has 'centring' points at

$$0,0,0; \quad \tfrac{2}{3},\tfrac{1}{3},0; \quad \tfrac{1}{3},\tfrac{2}{3},0.$$

references