

2.2. Contents and arrangement of the tables

BY TH. HAHN AND A. LOOIJENGA-VOS

2.2.1. General layout

The presentation of the plane-group and space-group data in Parts 6 and 7 follows the style of the previous editions of *International Tables*. The entries for a space group are printed on two facing pages as shown below; an example (*Cmm*2, No. 35) is provided inside the front and back covers. Deviations from this standard sequence (mainly for cubic space groups) are indicated on the relevant pages.

Left-hand page:

- (1) *Headline*
- (2) *Diagrams* for the symmetry elements and the general position (for graphical symbols of symmetry elements see Chapter 1.4)
- (3) *Origin*
- (4) *Asymmetric unit*
- (5) *Symmetry operations*

Right-hand page:

- (6) *Headline* in abbreviated form
- (7) *Generators selected*; this information is the basis for the order of the entries under *Symmetry operations* and *Positions*
- (8) General and special *Positions*, with the following columns:
Multiplicity
Wyckoff letter
Site symmetry, given by the oriented site-symmetry symbol
Coordinates
Reflection conditions
Note: In a few space groups, two special positions with the same reflection conditions are printed on the same line
- (9) *Symmetry of special projections* (not given for plane groups)
- (10) *Maximal non-isomorphic subgroups*
- (11) *Maximal isomorphic subgroups of lowest index*
- (12) *Minimal non-isomorphic supergroups*

Note: Symbols for *Lattice complexes* of the plane groups and space groups are given in Tables 14.2.3.1 and 14.2.3.2. Normalizers of space groups are listed in Part 15.

2.2.2. Space groups with more than one description

For several space groups, more than one description is available. Three cases occur:

(i) *Two choices of origin* (cf. Section 2.2.7)

For all centrosymmetric space groups, the tables contain a description with a centre of symmetry as origin. Some centrosymmetric space groups, however, contain points of high site symmetry that do not coincide with a centre of symmetry. For these 24 cases, a further description (including diagrams) with a high-symmetry point as origin is provided. Neither of the two origin choices is considered standard. Noncentrosymmetric space groups and all plane groups are described with only one choice of origin.

Examples

- (1) *Pnnn* (48)
Origin choice 1 at a point with site symmetry 222
Origin choice 2 at a centre with site symmetry $\bar{1}$.
- (2) *Fd3m* (227)
Origin choice 1 at a point with site symmetry $\bar{4}3m$
Origin choice 2 at a centre with site symmetry $\bar{3}m$.

(ii) *Monoclinic space groups*

Two complete descriptions are given for each of the 13 monoclinic space groups, one for the setting with 'unique axis b ', followed by one for the setting with 'unique axis c '.

Additional descriptions in synoptic form are provided for the following eight monoclinic space groups with centred lattices or glide planes:

$C2$ (5), Pc (7), Cm (8), Cc (9), $C2/m$ (12), $P2/c$ (13), $P2_1/c$ (14), $C2/c$ (15).

These synoptic descriptions consist of abbreviated treatments for three 'cell choices', here called 'cell choices 1, 2 and 3'. Cell choice 1 corresponds to the complete treatment, mentioned above; for comparative purposes, it is repeated among the synoptic descriptions which, for each setting, are printed on two facing pages. The cell choices and their relations are explained in Section 2.2.16.

(iii) *Rhombohedral space groups*

The seven rhombohedral space groups $R3$ (146), $R\bar{3}$ (148), $R32$ (155), $R3m$ (160), $R3c$ (161), $R\bar{3}m$ (166), and $R\bar{3}c$ (167) are described with two coordinate systems, first with *hexagonal axes* (triple hexagonal cell) and second with *rhombohedral axes* (primitive rhombohedral cell). For both descriptions, the same space-group symbol is used. The relations between the cell parameters of the two cells are listed in Chapter 2.1.

The hexagonal triple cell is given in the *obverse* setting (centring points $\frac{2}{3}, \frac{1}{3}, \frac{1}{3}; \frac{1}{3}, \frac{1}{3}, \frac{2}{3}; \frac{2}{3}, \frac{1}{3}, \frac{2}{3}$). In *IT* (1935), the *reverse* setting (centring points $\frac{1}{3}, \frac{2}{3}, \frac{1}{3}; \frac{2}{3}, \frac{1}{3}, \frac{2}{3}$) was employed; cf. Chapter 1.2.

2.2.3. Headline

The description of each plane group or space group starts with a headline on a left-hand page, consisting of two (sometimes three) lines which contain the following information, when read from left to right.

First line

- (1) The *short international* (Hermann–Mauguin) *symbol* for the plane or space group. These symbols will be further referred to as Hermann–Mauguin symbols. A detailed discussion of space-group symbols is given in Chapter 12.2, a brief summary in Section 2.2.4.

Note on standard monoclinic space-group symbols: In order to facilitate recognition of a monoclinic space-group type, the familiar short symbol for the b -axis setting (e.g. $P2_1/c$ for No. 14 or $C2/c$ for No. 15) has been adopted as the *standard symbol* for a space-group type. It appears in the headline of *every description of this space group* and thus does not carry any information about the setting or the cell choice of this particular description. No other short symbols for monoclinic space groups are used in this volume (cf. Section 2.2.16).

- (2) The *Schoenflies symbol* for the space group.

Note: No Schoenflies symbols exist for the plane groups.