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2.2. Contents and arrangement of the tables

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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 ($Cmm2$, 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) $Fd\bar{3}m$ (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 $\frac{2}{3}, \frac{1}{3}, \frac{1}{3}$; $\frac{1}{3}, \frac{2}{3}, \frac{2}{3}$). 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.

(3) The *short international* (Hermann–Mauguin) *symbol* for the point group to which the plane or space group belongs (*cf.* Chapter 12.1).
(4) The name of the *crystal system* (*cf.* Table 2.1.2.1).

Second line
(5) The sequential *number of the plane or space group*, as introduced in *IT* (1952).
(6) The *full international* (Hermann–Mauguin) *symbol* for the plane or space group.
For monoclinic space groups, the headline of every description contains the full symbol appropriate to that description.
(7) The *Patterson symmetry* (see Section 2.2.5).

Third line
This line is used, where appropriate, to indicate origin choices, settings, cell choices and coordinate axes (see Section 2.2.2). For five orthorhombic space groups, an entry 'Former space-group symbol' is given; *cf.* Chapter 1.3, Note (x).

2.2.4. International (Hermann–Mauguin) symbols for plane groups and space groups (*cf.* Chapter 12.2)

2.2.4.1. *Present symbols*

Both the short and the full Hermann–Mauguin symbols consist of two parts: (i) a letter indicating the centring type of the conventional cell, and (ii) a set of characters indicating symmetry elements of the space group (modified point-group symbol).

(i) The letters for the centring types of cells are listed in Chapter 1.2. Lower-case letters are used for two dimensions (nets), capital letters for three dimensions (lattices).

(ii) The one, two or three entries after the centring letter refer to the one, two or three kinds of *symmetry directions* of the lattice belonging to the space group. These symmetry directions were called *blickrichtungen* by Heesch (1929). Symmetry directions occur either as singular directions (as in the monoclinic and orthorhombic crystal systems) or as sets of symmetrically equivalent symmetry directions (as in the higher-symmetrical crystal systems). Only one representative of each set is required. The (sets of) symmetry directions and their sequence for the different lattices are summarized in Table 2.2.4.1. According to their position in this sequence, the symmetry directions are referred to as 'primary', 'secondary' and 'tertiary' directions.

This sequence of lattice symmetry directions is transferred to the sequence of positions in the corresponding Hermann–Mauguin space-group symbols. Each position contains one or two characters designating symmetry elements (axes and planes) of the space group (*cf.* Chapter 1.3) that occur for the corresponding lattice symmetry direction. Symmetry planes are represented by their normals; if a symmetry axis and a normal to a symmetry plane are parallel, the two characters (symmetry symbols) are separated by a slash, as in $P6_3/m$ or $P2/m$ ('two over m').

For the different crystal lattices, the Hermann–Mauguin space-group symbols have the following form:

(i) *Triclinic* lattices have no symmetry direction because they have, in addition to translations, only centres of symmetry, $\bar{1}$. Thus, only two triclinic space groups, $P1$ (1) and $P\bar{1}$ (2), exist.

(ii) *Monoclinic* lattices have one symmetry direction. Thus, for monoclinic space groups, only one position after the centring letter is needed. This is used in the *short* Hermann–Mauguin symbols, as in $P2_1$. Conventionally, the symmetry direction is labelled either b ('unique axis b') or c ('unique axis c').

In order to distinguish between the different settings, the *full* Hermann–Mauguin symbol contains two extra entries '1'. They indicate those two axial directions that are not symmetry directions of the lattice. Thus, the symbols $P121$, $P112$ and $P211$ show that the b axis, c axis and a axis, respectively, is the unique axis. Similar considerations apply to the three *rectangular* plane groups pm, pg and cm (*e.g.* plane group No. 5: short symbol cm, full symbol $c1m1$ or $c11m$).

(iii) *Rhombohedral* lattices have two kinds of symmetry directions. Thus, the symbols of the seven rhombohedral space groups contain only two entries after the letter R, as in $R3m$ or $R3c$.

(iv) *Orthorhombic*, *tetragonal*, *hexagonal* and *cubic* lattices have three kinds of symmetry directions. Hence, the corresponding space-group symbols have three entries after the centring letter, as in $Pmna$, $P3m1$, $P6cc$ or $Ia\bar{3}d$.

Lattice symmetry directions that carry no symmetry elements for the space group under consideration are represented by the symbol '1', as in $P3m1$ and $P31m$. If no misinterpretation is possible, entries '1' at the end of a space-group symbol are omitted, as in $P6$ (instead of $P611$), $R\bar{3}$ (instead of $R\bar{3}1$), $I4_1$ (instead of $I4_111$), $F23$ (instead of $F231$); similarly for the plane groups.

Table 2.2.4.1. *Lattice symmetry directions for two and three dimensions*

Directions that belong to the same set of equivalent symmetry directions are collected between braces. The first entry in each set is taken as the representative of that set.

Lattice	Symmetry direction (position in Hermann–Mauguin symbol)		
	Primary	Secondary	Tertiary
Two dimensions			
Oblique	Rotation point in plane		
Rectangular		[10]	[01]
Square		{[10], [01]}	$\{[1\bar{1}], [11]\}$
Hexagonal		$\{[10], [01], [\bar{1}\bar{1}]\}$	$\{[1\bar{1}], [12], [\bar{2}\bar{1}]\}$
Three dimensions			
Triclinic	None		
Monoclinic*	[010] ('unique axis b') [001] ('unique axis c')		
Orthorhombic	[100]	[010]	[001]
Tetragonal	[001]	{[100], [010]}	$\{[1\bar{1}0], [110]\}$
Hexagonal	[001]	$\{[100], [010], [\bar{1}\bar{1}0]\}$	$\{[1\bar{1}0], [120], [\bar{2}\bar{1}0]\}$
Rhombohedral (hexagonal axes)	[001]	$\{[100], [010], [\bar{1}\bar{1}0]\}$	
Rhombohedral (rhombohedral axes)	[111]	$\{[1\bar{1}0], [01\bar{1}], [\bar{1}01]\}$	
Cubic	{[100], [010], [001]}	$\{[111], [1\bar{1}\bar{1}], [\bar{1}1\bar{1}], [\bar{1}\bar{1}1]\}$	$\{[1\bar{1}0], [110], [01\bar{1}], [011], [\bar{1}01], [101]\}$

* For the full Hermann–Mauguin symbols see Section 2.2.4.1.

references