

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

- (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

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
<i>Two dimensions</i>			
Oblique	Rotation point in plane		
Rectangular		[10]	[01]
Square		$\left\{ \begin{matrix} [10] \\ [01] \end{matrix} \right\}$	$\left\{ \begin{matrix} [1\bar{1}] \\ [11] \end{matrix} \right\}$
Hexagonal		$\left\{ \begin{matrix} [10] \\ [01] \\ [1\bar{1}] \end{matrix} \right\}$	$\left\{ \begin{matrix} [1\bar{1}] \\ [12] \\ [2\bar{1}] \end{matrix} \right\}$
<i>Three dimensions</i>			
Triclinic	None		
Monoclinic*	[010] (‘unique axis b ’) [001] (‘unique axis c ’)		
Orthorhombic	[100]	[010]	[001]
Tetragonal	[001]	$\left\{ \begin{matrix} [100] \\ [010] \end{matrix} \right\}$	$\left\{ \begin{matrix} [1\bar{1}0] \\ [110] \end{matrix} \right\}$
Hexagonal	[001]	$\left\{ \begin{matrix} [100] \\ [010] \\ [1\bar{1}0] \end{matrix} \right\}$	$\left\{ \begin{matrix} [1\bar{1}0] \\ [120] \\ [210] \end{matrix} \right\}$
Rhombohedral (hexagonal axes)	[001]	$\left\{ \begin{matrix} [100] \\ [010] \\ [1\bar{1}0] \end{matrix} \right\}$	
Rhombohedral (rhombohedral axes)	[111]	$\left\{ \begin{matrix} [1\bar{1}0] \\ [01\bar{1}] \\ [10\bar{1}] \end{matrix} \right\}$	
Cubic	$\left\{ \begin{matrix} [100] \\ [010] \\ [001] \end{matrix} \right\}$	$\left\{ \begin{matrix} [111] \\ [1\bar{1}\bar{1}] \\ [1\bar{1}1] \\ [\bar{1}\bar{1}1] \end{matrix} \right\}$	$\left\{ \begin{matrix} [1\bar{1}0] [110] \\ [01\bar{1}] [011] \\ [\bar{1}01] [101] \end{matrix} \right\}$

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

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.