(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, P*3*m*1, *P*6*cc* 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], [1$\bar{1}$]}	{[1$\bar{1}$], [12], [$\bar{2}$1]}
Three dimensions			
Triclinic	None		
Monoclinic*	[010] ('unique axis b') [001] ('unique axis c')		
Orthorhombic	[100]	[010]	[001]
Tetragonal	[001]	{[100], [010]}	{[1$\bar{1}$0], [110]}
Hexagonal	[001]	{[100], [010], [1$\bar{1}$0]}	{[1$\bar{1}$0], [120], [$\bar{2}$10]}
Rhombohedral (hexagonal axes)	[001]	{[100], [010], [1$\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}$1], [11$\bar{1}$], [$\bar{1}$11]}	{[1$\bar{1}$0] [110], [01$\bar{1}$] [011], [$\bar{1}$01] [101]}

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

Short and *full* Hermann–Mauguin symbols differ only for the plane groups of class *m*, for the monoclinic space groups, and for the space groups of crystal classes *mmm*, $4/mmm$, $\bar{3}m$, $6/mmm$, $m\bar{3}$ and $m\bar{3}m$. In the full symbols, symmetry axes *and* symmetry planes for each symmetry direction are listed; in the short symbols, symmetry axes are suppressed as much as possible. Thus, for space group No. 62, the full symbol is $P2_1/n\ 2_1/m\ 2_1/a$ and the short symbol is *Pnma*. For No. 194, the full symbol is $P6_3/m\ 2/m\ 2/c$ and the short symbol is $P6_3/mmc$. For No. 230, the two symbols are $I4_1/a\ \bar{3}\ 2/d$ and $Ia\bar{3}d$.

Many space groups contain more kinds of symmetry elements than are indicated in the full symbol ('additional symmetry elements', *cf.* Chapter 4.1). A complete listing of the symmetry elements is given in Tables 4.2.1.1 and 4.3.2.1 under the heading *Extended full symbols*. Note that a centre of symmetry is never explicitly indicated (except for space group $P\bar{1}$); its presence or absence, however, can be readily inferred from the space-group symbol.

2.2.4.2. *Changes in Hermann–Mauguin space-group symbols as compared with the 1952 and 1935 editions of International Tables*

Extensive changes in the space-group symbols were applied in *IT* (1952) as compared with the original Hermann–Mauguin symbols of *IT* (1935), especially in the tetragonal, trigonal and hexagonal crystal systems. Moreover, new symbols for the *c*-axis setting of monoclinic space groups were introduced. All these changes are recorded on pp. 51 and 543–544 of *IT* (1952). In the present edition, the symbols of the 1952 edition are retained, except for the following four cases (*cf.* Chapter 12.4).

(i) *Two-dimensional groups*

Short Hermann–Mauguin symbols differing from the corresponding full symbols in *IT* (1952) are replaced by the full symbols for the listed plane groups in Table 2.2.4.2.

For the two-dimensional point group with two mutually perpendicular mirror lines, the symbol *mm* is changed to 2*mm*.

For plane group No. 2, the entries '1' at the end of the full symbol are omitted:

No. 2: Change from *p*211 to *p*2.

With these changes, the symbols of the two-dimensional groups follow the rules that were introduced in *IT* (1952) for the space groups.

(ii) *Monoclinic space groups*

Additional *full* Hermann–Mauguin symbols are introduced for the eight monoclinic space groups with centred lattices or glide planes (Nos. 5, 7–9, 12–15) to indicate the various settings and cell choices. A complete list of symbols, including also the *a*-axis setting, is contained in Table 4.3.2.1; further details are given in Section 2.2.16.

For standard *short* monoclinic space-group symbols see Sections 2.2.3 and 2.2.16.

(iii) *Cubic groups*

The short symbols for all space groups belonging to the two cubic crystal classes $m\bar{3}$ and $m\bar{3}m$ now contain the symbol $\bar{3}$ instead of 3. This applies to space groups Nos. 200–206 and 221–230, as well as to the two point groups $m\bar{3}$ and $m\bar{3}m$.

Examples

No. 205: Change from $Pa3$ to $Pa\bar{3}$

No. 230: Change from $Ia3d$ to $Ia\bar{3}d$.

With this change, the centrosymmetric nature of these groups is apparent also in the short symbols.

(iv) *Glide-plane symbol e*

For the recent introduction of the 'double glide plane' *e* into five space-group symbols, see Chapter 1.3, Note (x).

Table 2.2.4.2. *Changes in Hermann–Mauguin symbols for two-dimensional groups*

No.	*IT* (1952)	Present edition
6	*pmm*	*p*2*mm*
7	*pmg*	*p*2*mg*
8	*pgg*	*p*2*gg*
9	*cmm*	*c*2*mm*
11	*p*4*m*	*p*4*mm*
12	*p*4*g*	*p*4*gm*
17	*p*6*m*	*p*6*mm*

2.2.5. Patterson symmetry

The entry *Patterson symmetry* in the headline gives the space group of the *Patterson function* $P(x, y, z)$. With neglect of anomalous dispersion, this function is defined by the formula

$$P(x,y,z) = \frac{1}{V}\sum_h \sum_k \sum_l |F(hkl)|^2 \cos 2\pi(hx + ky + lz).$$

The Patterson function represents the convolution of a structure with its inverse or the pair-correlation function of a structure. A detailed discussion of its use for structure determination is given by Buerger (1959). The space group of the Patterson function is identical to that of the 'vector set' of the structure, and is thus always centrosymmetric and symmorphic.*

The symbol for the Patterson space group of a crystal structure can be deduced from that of its space group in two steps:

(i) Glide planes and screw axes have to be replaced by the corresponding mirror planes and rotation axes, resulting in a symmorphic space group.

(ii) If this symmorphic space group is not centrosymmetric, inversions have to be added.

There are 7 different Patterson symmetries in two dimensions and 24 in three dimensions. They are listed in Table 2.2.5.1. Account is taken of the fact that the Laue class $\bar{3}m$ combines in two ways with the hexagonal translation lattice, namely as $\bar{3}m1$ and as $\bar{3}1m$.

Note: For the four orthorhombic space groups with *A* cells (Nos. 38–41), the standard symbol for their Patterson symmetry, *Cmmm*, is added (between parentheses) after the actual symbol *Ammm* in the space-group tables.

The 'point group part' of the symbol of the Patterson symmetry represents the *Laue class* to which the plane group or space group belongs (*cf.* Table 2.1.2.1). In the absence of anomalous dispersion, the Laue class of a crystal expresses the *point symmetry of its diffraction record, i.e.* the symmetry of the reciprocal lattice weighted with $I(hkl)$.

* A space group is called 'symmorphic' if, apart from the lattice translations, all *generating* symmetry operations leave one common point fixed. Permitted as generators are thus only the point-group operations: rotations, reflections, inversions and rotoinversions (*cf.* Section 8.1.6).