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 $2mm$.

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

No. 2: Change from $p211$ to $p2$.

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*	*p2mm*
7	*pmg*	*p2mg*
8	*pgg*	*p2gg*
9	*cmm*	*c2mm*
11	*p4m*	*p4mm*
12	*p4g*	*p4gm*
17	*p6m*	*p6mm*

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).

references