

4.2. Symbols for plane groups (two-dimensional space groups)

BY E. F. BERTAUT

4.2.1. Arrangement of the tables

Comparative tables for the 17 plane groups first appeared in *IT* (1952). The classification of plane groups is discussed in Chapter 2.1. Table 4.2.1.1 lists for each plane group its system, lattice symbol, point group and the plane-group number, followed by the short, full and extended Hermann–Mauguin symbols. Short symbols are included only where different from the full symbols. The next column contains the full symbol for another setting which corresponds to an interchange of the basis vectors **a** and **b**; it is only needed for the rectangular system. Multiple cells *c* and *h* for the square and the hexagonal system are introduced in the last column.

4.2.2. Additional symmetry elements and extended symbols

‘Additional symmetry’ elements are

(i) rotation points 2, 3 and 4, reproduced in the interior of the cell (*cf.* Table 4.1.2.1 and plane-group diagrams in Part 6);

(ii) glide lines *g* which alternate with mirror lines *m*.

In the extended plane-group symbols, only the additional glide lines *g* are listed: they are due either to *c* centring or to ‘inclined’ integral translations, as shown in Table 4.1.2.2.

4.2.3. Multiple cells

The *c* cell in the square system is defined as follows:

$$\mathbf{a}' = \mathbf{a} \mp \mathbf{b}; \quad \mathbf{b}' = \pm \mathbf{a} + \mathbf{b},$$

with ‘centring points’ at $0, 0; \frac{1}{2}, \frac{1}{2}$. It plays the same role as the three-dimensional *C* cell in the tetragonal system (*cf.* Section 4.3.4).

Likewise, the triple cell *h* in the hexagonal system is defined as follows:

$$\mathbf{a}' = \mathbf{a} - \mathbf{b}; \quad \mathbf{b}' = \mathbf{a} + 2\mathbf{b},$$

with ‘centring points’ at $0, 0; \frac{2}{3}, \frac{1}{3}; \frac{1}{3}, \frac{2}{3}$. It is the two-dimensional analogue of the three-dimensional *H* cell (*cf.* Chapter 1.2 and Section 4.3.5).

4.2.4. Group–subgroup relations

The following example illustrates the usefulness of multiple cells.

Example: p3m1 (14)

The symbol of this plane group, described by the triple cell *h*, is *h31m*, where the symmetry elements of the secondary and tertiary positions are interchanged. ‘Decentring’ the *h* cell gives rise to maximal non-isomorphic *k* subgroups *p31m* of index [3], with lattice parameters $a\sqrt{3}, a\sqrt{3}$ (*cf.* Section 4.3.5).

Table 4.2.1.1. *Index of symbols for plane groups*

| System and lattice symbol | Point group | No. of plane group | Hermann–Mauguin symbol | | | Full symbol for other setting | Multiple cell |
|----------------------------|-------------|--------------------|-------------------------------------|--|---------------------------|--|--------------------------------------|
| | | | Short | Full | Extended | | |
| Oblique <i>p</i> | 1 | 1 | | <i>p1</i> | | | |
| | 2 | 2 | | <i>p2</i> | | | |
| Rectangular <i>p, c</i> | <i>m</i> | { 3 4 5 | <i>pm</i> <i>pg</i> <i>cm</i> | <i>p1m1</i> <i>p1g1</i> <i>c1m1</i> | <i>c1m1</i> <i>g</i> | <i>p11m</i> <i>p11g</i> <i>c11m</i> | |
| | <i>2mm</i> | { 6 7 8 9 | | <i>p2mm</i> <i>p2mg</i> <i>p2gg</i> <i>c2mm</i> | <i>c2mm</i> <i>g g</i> | <i>p2mm</i> <i>p2gm</i> <i>p2gg</i> <i>c2mm</i> | |
| Square <i>p</i> | 4 | 10 | | <i>p4</i> <i>p4mm</i> | <i>p4mm</i> <i>g</i> | | <i>c4</i> <i>c4mm</i> <i>g</i> |
| | <i>4mm</i> | { 11 12 | | <i>p4gm</i> | <i>p4gm</i> <i>g</i> | | <i>c4mg</i> <i>g</i> |
| Hexagonal <i>p</i> | 3 | 13 | | <i>p3</i> <i>p3m1</i> | <i>p3m1</i> <i>g</i> | | <i>h3</i> <i>h31m</i> <i>g</i> |
| | <i>3m</i> | { 14 15 | | <i>p31m</i> | <i>p31m</i> <i>g</i> | | <i>h3m1</i> <i>g</i> |
| | 6 | 16 | | <i>p6</i> | | | <i>h6</i> |
| | <i>6mm</i> | 17 | | <i>p6mm</i> | <i>p6mm</i> <i>g g</i> | | <i>h6mm</i> <i>g g</i> |

4. SYNOPTIC TABLES OF SPACE-GROUP SYMBOLS

Examples

$Ia\bar{3}$ (206), full symbol $I2_1/a\bar{3}$, contains $I2_13$. $P2_13$ is a maximal subgroup of $P4_132$ (213) and its enantiomorph $P4_332$ (212). A more difficult example is $I43d$ (220) which contains $I2_13$.*

The cubic space groups of class $m\bar{3}m$ have maximal subgroups which belong to classes 432 and $\bar{4}3m$.

Examples

$F4/m\bar{3}2/c$ (226) contains $F432$ and $F\bar{4}3c$; $I4_1/a\bar{3}2/d$ (230) contains $I4_132$ and $I43d$.

(b) Tetragonal subgroups

In the cubic space groups of classes 432 and $\bar{4}3m$, the primary and tertiary symmetry elements are relevant for deriving maximal tetragonal subgroups.

Examples

The groups $P432$ (207), $P4_232$ (208), $P4_332$ (212) and $P4_132$ (213) have maximal tetragonal t subgroups of index [3]: $P422$, $P4_222$, $P4_32_12$ and $P4_12_12$. $I432$ (211) gives rise to $I422$ with the same cell. $F432$ (209) also gives rise to $I422$, but via $F422$, so that the final unit cell is $a\sqrt{2}/2, a\sqrt{2}/2, a$.

In complete analogy, the groups $P4\bar{3}m$ (215) and $P\bar{4}3n$ (218) have maximal subgroups $P42m$ and $P42c$.†

For the space groups of class $m\bar{3}m$, the full symbols are needed to recognize their tetragonal maximal subgroups of class $4/mmm$. The primary symmetry planes of the cubic space group are conserved in the primary and secondary symmetry elements of the tetragonal

subgroup: m , n and d remain in the tetragonal symbol; a remains a in the primary and becomes c in the secondary symmetry element of the tetragonal symbol.

Example

$P4_2/n\bar{3}2/m$ (224) and $I4_1/a\bar{3}2/d$ (230) have maximal subgroups $P4_2/n2/n2/m$ and $I4_1/a2/c2/d$, respectively, $F4_1/d\bar{3}2/c$ (228) gives rise to $F4_1/d2/d2/c$, which is equivalent to $I4_1/a2/c2/d$, all of index [3].

(c) Rhombohedral subgroups‡

Here the secondary and tertiary symmetry elements of the cubic space-group symbols are relevant. For space groups of classes 23, $m\bar{3}$, 432, the maximal R subgroups are $R3$, $R\bar{3}$ and $R32$, respectively. For space groups of class $\bar{4}3m$, the maximal R subgroup is $R3m$ when the tertiary symmetry element is m and $R\bar{3}c$ otherwise. Finally, for space groups of class $m\bar{3}m$, the maximal R subgroup is $R\bar{3}m$ when the tertiary symmetry element is m and $R\bar{3}c$ otherwise. All subgroups are of index [4].

(d) Orthorhombic subgroups

Maximal orthorhombic space groups of index [3] are easily derived from the cubic space-group symbols of classes 23 and $m\bar{3}$.‡ Thus, $P23$, $F23$, $I23$, $P2_13$, $I2_13$ (195–199) have maximal subgroups $P222$, $F222$, $I222$, $P2_12_12_1$, $I2_12_12_1$, respectively. Likewise, maximal subgroups of $Pm\bar{3}$, $Pn\bar{3}$, $Fm\bar{3}$, $Fd\bar{3}$, $Im\bar{3}$, $Pa\bar{3}$, $Ia\bar{3}$ (200–206) are $Pmmm$, $Pnnn$, $Fmmm$, $Fddd$, $Immm$, $Pbca$, $Ibca$, respectively. The lattice type (P , F , I) is conserved and only the primary symmetry element has to be considered.

* From the product rule it follows that $\bar{4}$ and d have the same translation component so that $(\bar{4})^2 = 2_1$.

† The tertiary cubic symmetry element n becomes c in tetragonal notation.

‡ They have already been given in *IT* (1935).

References

4.1

Internationale Tabellen zur Bestimmung von Kristallstrukturen (1935). 1. Band, edited by C. Hermann. Berlin: Borntraeger. [Revised edition: Ann Arbor: Edwards (1944). Abbreviated as *IT* (1935).]

International Tables for X-ray Crystallography (1952). Vol. I, edited by N. F. M. Henry & K. Lonsdale. Birmingham: Kynoch Press. [Abbreviated as *IT* (1952).]

4.2

International Tables for X-ray Crystallography (1952). Vol. I, edited by N. F. M. Henry & K. Lonsdale. Birmingham: Kynoch Press. [Abbreviated as *IT* (1952).]

4.3

Bertaut, E. F. (1976). *Study of principal subgroups and of their general positions in C and I groups of class mmm-D_{2h}*. *Acta Cryst.* **A32**, 380–387.

Internationale Tabellen zur Bestimmung von Kristallstrukturen (1935). 1. Band, edited by C. Hermann. Berlin: Borntraeger. [Revised edition: Ann Arbor: Edwards (1944). Abbreviated as *IT* (1935).]

International Tables for Crystallography (1995). Vol. A, fourth, revised ed., edited by Th. Hahn. Dordrecht: Kluwer Academic Publishers. [Abbreviated as *IT* (1995).]

International Tables for X-ray Crystallography (1952). Vol. I, edited by N. F. M. Henry & K. Lonsdale. Birmingham: Kynoch Press. [Abbreviated as *IT* (1952).]