

4.3. SYMBOLS FOR SPACE GROUPS

(b) Orthorhombic subgroups

No orthorhombic subgroups of trigonal space groups exist, in spite of the existence of an orthohexagonal C cell.

(c) Monoclinic subgroups

All trigonal space groups with secondary or tertiary symmetry elements have monoclinic C -centred maximal t subgroups of index [3].

Example

$P\bar{3}1c$ (163), $P\bar{3}c1$ (165) and $R\bar{3}c$ (167) have subgroups of type $C2/c$.

(d) Triclinic subgroups

All trigonal space groups without secondary or tertiary symmetry elements have triclinic maximal t subgroups of index [3].

Example

$P\bar{3}$ (147) and $R\bar{3}$ (148) have subgroups $P\bar{1}$.

(ii) Hexagonal system

(a) Hexagonal subgroups

Example

$P6_3/m\ 2/c\ 2/m$ (193) has maximal t subgroups $P6_3/m$, $P6_322$, $P6_3cm$, $P\bar{6}2m$ and $P\bar{6}c2$ of index [2].

(b) Trigonal subgroups

The second and fourth powers of sixfold operations are threefold operations; thus, all hexagonal space groups have maximal trigonal t subgroups of index [2]. In space groups of classes 622 , $6mm$, $62m$, $6/mmm$ with secondary and tertiary symmetry elements, trigonal t subgroups always occur in pairs.

Examples

- (1) $P6_1$ (169) contains $P3_1$ of index [2].
- (2) $P\bar{6}2c$ (190) has maximal t subgroups $P3_121$ and $P3_1c$; $P6_122$ (178) has subgroups $P3_121$ and $P3_112$, all of index [2].
- (3) $P6_3/mcm$ (193) contains the operation $\bar{3} [= (6_3)^2 \times 1]$ and thus has maximal t subgroups $P3c1$ and $P\bar{3}1m$ of index [2].

(c) Orthorhombic and monoclinic subgroups

The third power of the sixfold operation is a twofold operation: accordingly, maximal orthorhombic t subgroups of index [3] are derived from the C -cell description of space groups of classes 622 , $6mm$, $62m$ and $6/mmm$. Monoclinic P subgroups of index [3] occur in crystal classes 6 , $\bar{6}$ and $6/m$.

Examples

- (1) $P\bar{6}2c$ (190) becomes $C\bar{6}2c$ in the C cell; with $(\bar{6})^3 = m$, one obtains $C2cm$ (sequence **a**, **b**, **c**) as a maximal t subgroup of index [3]. The standard symbol is $Ama2$.
- (2) $P6_3/mcm$ (193) has maximal orthorhombic t subgroups of type $Cmcm$ of index [3]. With the examples under (a) and (b), this exhausts all maximal t subgroups of $P6_3/mcm$.
- (3) $P6_1$ (169) has a maximal t subgroup $P2_1$; $P6_3/m$ (176) has $P2_1/m$ as a maximal t subgroup.

4.3.6. Cubic system

4.3.6.1. Historical note and arrangement of tables

In the synoptic tables of *IT* (1935) and *IT* (1952), for cubic space groups short and full Hermann–Mauguin symbols were listed. They agree, except that in *IT* (1935) the tertiary symmetry element of the

space groups of class 432 was omitted; it was re-established in *IT* (1952).

In the present edition, the symbols of *IT* (1952) are retained, with one exception. In the space groups of crystal classes $m\bar{3}$ and $m\bar{3}m$, the short symbols contain $\bar{3}$ instead of 3 (cf. Section 2.2.4). In Table 4.3.2.1, short and full symbols for all cubic space groups are given. In addition, for centred groups F and I and for P groups with tertiary symmetry elements, extended space-group symbols are listed. In space groups of classes 432 and $43m$, the product rule (as defined below) is applied in the first line of the extended symbol.

4.3.6.2. Relations between symmetry elements

Conventionally, the representative directions of the primary, secondary and tertiary symmetry elements are chosen as [001], [111], and $[\bar{1}\bar{1}0]$ (cf. Table 2.2.4.1 for the equivalent directions). As in tetragonal and hexagonal space groups, tertiary symmetry elements are not independent. In classes 432, $43m$ and $m\bar{3}m$, there are product rules

$$4 \times 3 = (2); \quad \bar{4} \times 3 = (m) = 4 \times \bar{3},$$

where the tertiary symmetry element is in parentheses; analogous rules hold for the space groups belonging to these classes. When the symmetry directions of the primary and secondary symmetry elements are chosen along [001] and [111], respectively, the tertiary symmetry direction is [011], according to the product rule. In order to have the tertiary symmetry direction along $[\bar{1}\bar{1}0]$, one has to choose the somewhat awkward primary and secondary symmetry directions [010] and $[\bar{1}\bar{1}\bar{1}]$.

Examples

- (1) In $P43n$ (218), with the choice of the 3 axis along $[\bar{1}\bar{1}\bar{1}]$ and of the 4 axis parallel to [010], one finds $4 \times 3 = n$, the n glide plane being in x, x, z , as shown in the space-group diagram.
- (2) In $F\bar{4}3c$ (219), one has the same product rule as above; the centring translation $t(\frac{1}{2}, \frac{1}{2}, 0)$, however, associates with the n glide plane a c glide plane, also located in x, x, z (cf. Table 4.1.2.3). In the space-group diagram and symbol, c was preferred to n .

4.3.6.3. Additional symmetry elements

Owing to periodicity, the tertiary symmetry elements alternate; diagonal axes 2 alternate with parallel screw axes 2_1 ; diagonal planes m alternate with parallel glide planes g ; diagonal n planes, i.e. planes with glide components $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$, alternate with glide planes a, b or c (cf. Chapter 4.1 and Tables 4.1.2.2 and 4.1.2.3). For the meaning of the various glide planes g , see Section 11.1.2 and the entries *Symmetry operations* in Part 7.

4.3.6.4. Group–subgroup relations

4.3.6.4.1. Maximal k subgroups

The extended symbol of $Fm\bar{3}$ (202) shows clearly that $Pm\bar{3}$, $Pn\bar{3}$, $Pb\bar{3}$ ($Pa\bar{3}$) and $Pa\bar{3}$ are maximal subgroups. $Pm\bar{3}m$, $Pn\bar{3}n$, $Pm\bar{3}n$ and $Pn\bar{3}m$ are maximal subgroups of $Im\bar{3}m$ (229). Space groups with d glide planes have no k subgroup of lattice P .

4.3.6.4.2. Maximal t subgroups

(a) Cubic subgroups

The cubic space groups of classes $m\bar{3}$, 432 and $\bar{4}3m$ have maximal cubic subgroups of class 23 which are found by simple inspection of the full symbol.