International Tables for Crystallography (2006). Vol. A, Section 4.3.6, pp. 75–76.

(*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, $6mm$, $\bar{6}2m$, $6/mmm$ 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 $P321$ and $P31c$; $P6_122$ (178) has subgroups $P3_121$ and $P3_112$, all of index [2].
(3) $P6_3/mcm$ (193) contains the operation $\bar{3}$ [$= (6_3)^2 \times \bar{1}$] and thus has maximal *t* subgroups $P\bar{3}c1$ 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, $6mm$, $\bar{6}2m$ 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 $\bar{4}3m$, 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 [$1\bar{1}0$] (*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, $\bar{4}3m$ 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 [$1\bar{1}0$], one has to choose the somewhat awkward primary and secondary symmetry directions [010] and [$\bar{1}1\bar{1}$].

Examples

(1) In $P\bar{4}3n$ (218), with the choice of the 3 axis along [$\bar{1}1\bar{1}$] and of the $\bar{4}$ axis parallel to [010], one finds $\bar{4} \times 3 = n$, 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.

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 $I\bar{4}3d$ (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* $I\bar{4}3d$.

(*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 $P\bar{4}3m$ (215) and $P\bar{4}3n$ (218) have maximal subgroups $P\bar{4}2m$ and $P\bar{4}2c$.†

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 $P4_2/n\,2/n\,2/m$ and $I4_1/a\,2/c\,2/d$, respectively, $F4_1/d\,\bar{3}\,2/c$ (228) gives rise to $F4_1/d\,2/d\,2/c$, which is equivalent to $I4_1/a\,2/c\,2/d$, 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 $R3c$ 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).

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4.1

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