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).

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.* A**32**, 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).]