

10. POINT GROUPS AND CRYSTAL CLASSES

(b) the matrices Y^{-1} , Y^{-2} , Y^{-3} and Y^{-4} for the point coordinates.

This sequence of matrices ensures the same correspondence between the Miller indices and the point coordinates as for the crystallographic point groups in Table 10.1.2.2.

The matrices* are

$$Y = Y^{-4} = \begin{pmatrix} \frac{1}{2} & g & G \\ g & G & -\frac{1}{2} \\ -G & \frac{1}{2} & g \end{pmatrix}, \quad Y^2 = Y^{-3} = \begin{pmatrix} -g & G & \frac{1}{2} \\ G & \frac{1}{2} & -g \\ -\frac{1}{2} & g & -G \end{pmatrix},$$

$$Y^3 = Y^{-2} = \begin{pmatrix} -g & G & -\frac{1}{2} \\ G & \frac{1}{2} & g \\ \frac{1}{2} & -g & -G \end{pmatrix}, \quad Y^4 = Y^{-1} = \begin{pmatrix} \frac{1}{2} & g & -G \\ g & G & \frac{1}{2} \\ G & -\frac{1}{2} & g \end{pmatrix},$$

with†

$$G = \frac{\sqrt{5} + 1}{4} = \frac{\tau}{2} = \cos 36^\circ = 0.80902 \simeq \frac{72}{89}$$

$$g = \frac{\sqrt{5} - 1}{4} = \frac{\tau - 1}{2} = \cos 72^\circ = 0.30902 \simeq \frac{17}{55}.$$

These matrices correspond to counter-clockwise rotations of 72, 144, 216 and 288° around a fivefold axis parallel to $[1\tau 0]$.

The resulting indices h, k, l and coordinates x, y, z are irrational but can be approximated closely by rational (or integral) numbers. This explains the occurrence of almost regular icosahedra or pentagon-dodecahedra as crystal forms (for instance pyrite) or atomic groups (for instance B_{12} icosahedron).

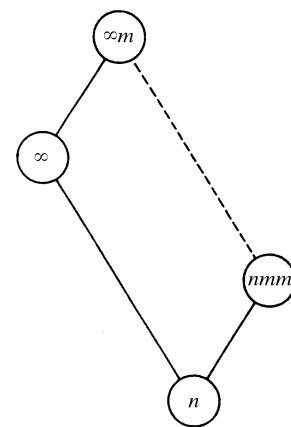
Further descriptions (including diagrams) of noncrystallographic groups are contained in papers by Nowacki (1933) and A. Niggli (1963) and in the textbooks by P. Niggli (1941, pp. 78–80, 96), Shubnikov & Koptsik (1974) and Vainshtein (1994). For the geometry of polyhedra, the well known books by H. S. M. Coxeter (especially Coxeter, 1973) are recommended.

10.1.4.3. Sub- and supergroups of the general point groups

In Figs. 10.1.4.1 to 10.1.4.3, the subgroup and supergroup relations between the two-dimensional and three-dimensional general point groups are illustrated. It should be remembered that the index of a group–subgroup relation between two groups of order infinity may be finite or infinite. For the two spherical groups, for instance, the index is $[2]$; the cylindrical groups, on the other hand, are subgroups of index $[\infty]$ of the spherical groups.

Fig. 10.1.4.1 for two dimensions shows that the two circular groups ∞m and ∞ have subgroups of types nmm and n , respectively, each of index $[\infty]$. The order of the rotation point may be $n = 4N, n = 4N + 2$ or $n = 2N + 1$. In the first case, the subgroups belong to the $4N$ -gonal system, in the latter two cases, they belong to the $(4N + 2)$ -gonal system. [In the diagram of the $(4N + 2)$ -gonal system, the $(2N + 1)$ -gonal groups appear with the symbols $\frac{1}{2}nm$ and $\frac{1}{2}n$.] The subgroups of the circular groups are not maximal because for any given value of N there exists a group with $N' = 2N$ which is both a subgroup of the circular group and a supergroup of the initial group.

The subgroup relations, for a specified value of N , within the $4N$ -gonal and the $(4N + 2)$ -gonal system, are shown in the lower part of the figure. They correspond to those of the crystallographic groups. A finite number of further maximal subgroups is obtained for lower



If $n = 4N$, go to $4N$ -gonal system
If $n = 4N + 2$ or $2N + 1$, go to $(4N + 2)$ -gonal system

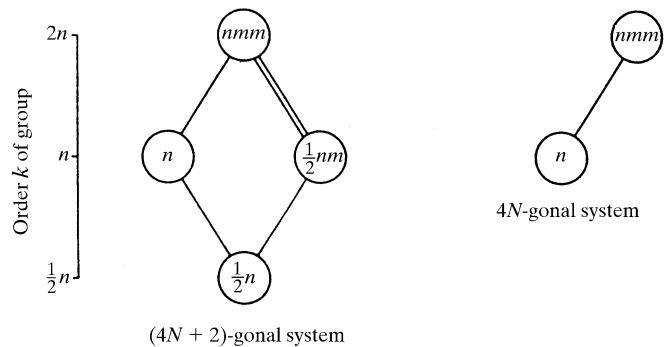


Fig. 10.1.4.1. Subgroups and supergroups of the two-dimensional general point groups. Solid lines indicate maximal normal subgroups, double solid lines mean that there are two maximal normal subgroups with the same symbol. Dashed lines refer to sets of maximal conjugate subgroups. For the finite groups, the orders are given on the left. Note that the subgroups of the two circular groups are not maximal and the diagram applies only to a specified value of N (see text). For complete examples see Fig. 10.1.4.2.

values of N , until the crystallographic groups (Fig. 10.1.3.1) are reached. This is illustrated for the case $N = 4$ in Fig. 10.1.4.2.

Fig. 10.1.4.3 for three dimensions illustrates that the two spherical groups $2/m\infty$ and 2∞ each have one infinite set of cylindrical maximal conjugate subgroups, as well as one infinite set

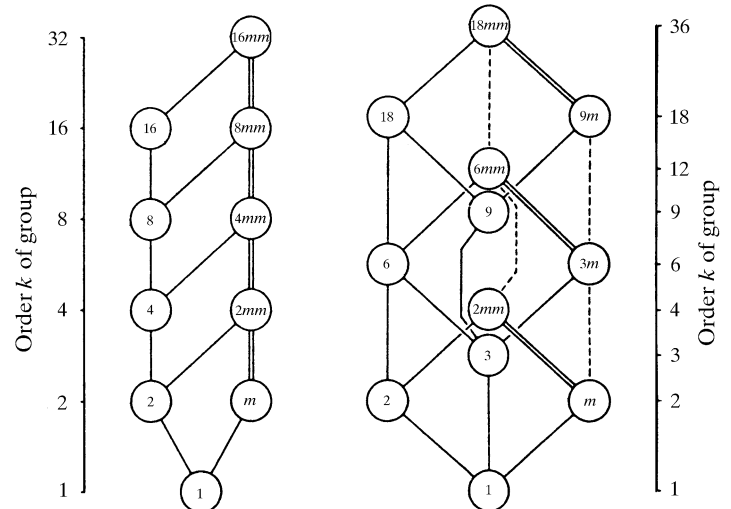


Fig. 10.1.4.2. The subgroups of the two-dimensional general point groups $16mm$ ($4N$ -gonal system) and $18mm$ [$(4N + 2)$ -gonal system including the $(2N + 1)$ -gonal groups]. Compare with Fig. 10.1.4.1 which applies only to one value of N .

* Note that for orthogonal matrices $Y^{-1} = Y^t$ (t = transposed).
† The number $\tau = 2G = 2g + 1 = 1.618034$ (Fibonacci number) is the characteristic value of the golden section $(\tau + 1) : \tau = \tau : 1$, i.e. $\tau(\tau - 1) = 1$. Furthermore, τ is the distance between alternating vertices of a regular pentagon of unit edge length and the distance from centre to vertex of a regular decagon of unit edge length.