

3.2. POINT GROUPS AND CRYSTAL CLASSES

- (i) For the face forms the cubic point groups 23 and $m\bar{3}$ (Table 3.2.3.2), and for the point forms the cubic space groups $P23$ (195) and $Pm\bar{3}$ (200) have to be considered. For each 'initial' triplet (hkl) , the set of Miller indices of the (general or special) crystal form with the same face symmetry in 23 (for group 235) or $m\bar{3}$ (for $m\bar{3}5$) is taken. For each 'initial' triplet x, y, z , the coordinate triplets of the (general or special) position with the same site symmetry in $P23$ or $Pm\bar{3}$ are taken.
- (ii) To obtain the complete set of icosahedral Miller indices and point coordinates, the 'cubic' (hkl) triplets (as rows) and x, y, z triplets (as columns) have to be multiplied with the identity matrix and with
 - (a) the matrices Y, Y^2, Y^3 and Y^4 for the Miller indices;
 - (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 3.2.3.2.

The matrices²⁰ are

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

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

with²¹

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

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

These matrices correspond to counter-clockwise rotations of $72^\circ, 144^\circ, 216^\circ$ 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.

3.2.1.4.3. Sub- and supergroups of the general point groups

In Figs. 3.2.1.4 to 3.2.1.6, 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

²⁰ Note that for orthogonal matrices $Y^{-1} = Y^t$ (t = transposed).
²¹ The number $\tau = 2G = 2g + 1 = (\sqrt{5} + 1)/2 = 1.618034$ (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.

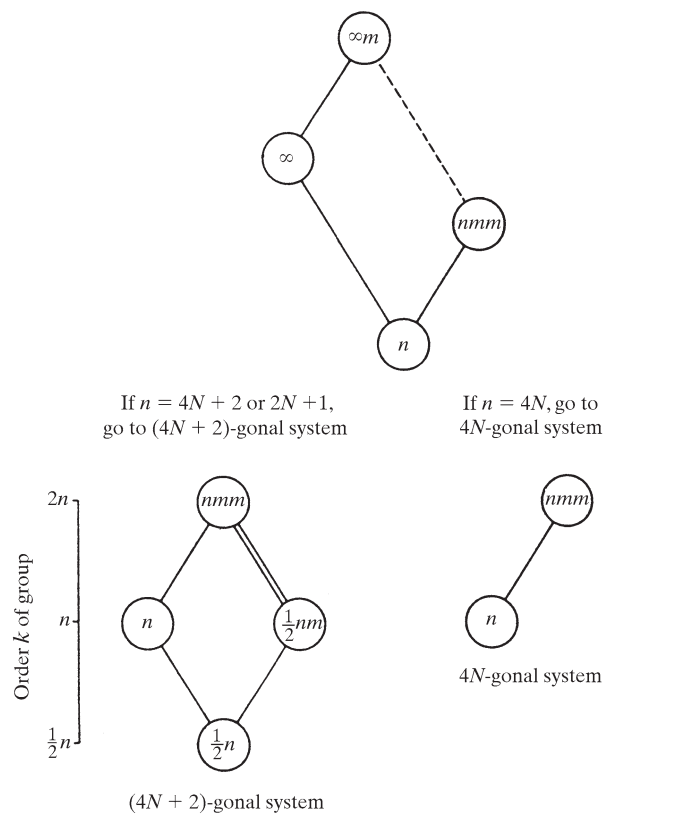


Figure 3.2.1.4 Subgroups and supergroups of the two-dimensional general point groups. Solid lines indicate maximal normal subgroups, double solid lines mean that there are two maximal normal subgroups with the same symbol. Dashed lines refer to sets of maximal conjugate subgroups. For the finite groups, 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. 3.2.1.5.

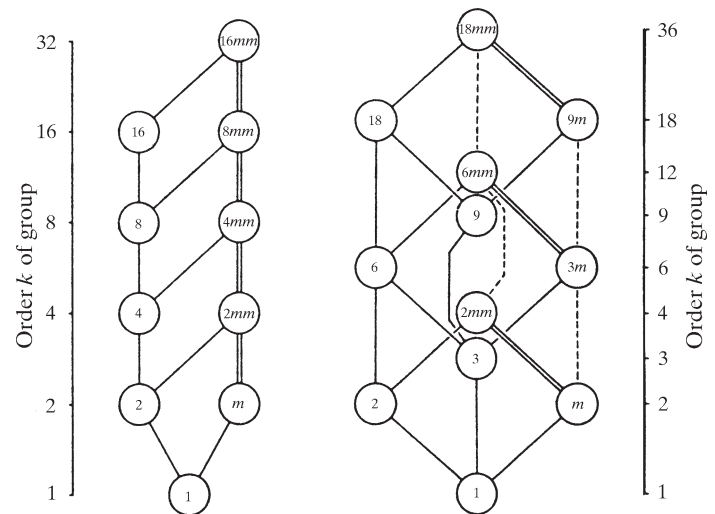


Figure 3.2.1.5 The subgroups of the two-dimensional general point groups $16mm$ ($4N$ -gonal system) and $18mm$ [$(4N + 2)$ -gonal system, including the $(2N + 1)$ -gonal groups]. Compare with Fig. 3.2.1.4 which applies only to one value of N .

groups, for instance, the index is $[2]$; the cylindrical groups, on the other hand, are subgroups of index $[\infty]$ of the spherical groups.

Fig. 3.2.1.4 for two dimensions shows that the two circular groups ∞m and ∞ have subgroups of types nmm and n ,