International Tables for Crystallography (2016). Vol. A, Section 3.2.1.4.1, pp. 731–733.

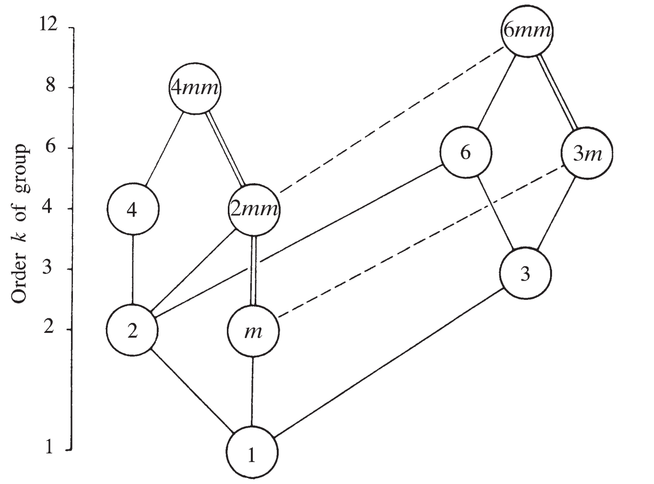


Figure 3.2.1.2
Maximal subgroups and minimal supergroups of the two-dimensional crystallographic point groups. Solid lines indicate maximal normal subgroups; double solid lines mean that there are two maximal normal subgroups with the same symbol. Dashed lines refer to sets of maximal conjugate subgroups. The group orders are given on the left.

or rhombohedral: *e.g.* 'hexagonal ogdohedry' and 'rhombohedral tetartohedry'.

3.2.1.3. Subgroups and supergroups of the crystallographic point groups

In this section, the sub- and supergroup relations between the crystallographic point groups are presented in the form of a 'family tree'.[12] Figs. 3.2.1.2 and 3.2.1.3 apply to two and three dimensions. The sub- and supergroup relations between two groups are represented by solid or dashed lines. For a given point group $\mathcal{P}$ of order k_P the lines to groups of lower order connect $\mathcal{P}$ with all its *maximal subgroups* $\mathcal{H}$ with orders k_H; the index [*i*] of each subgroup is given by the ratio of the orders k_P/k_H. The lines to groups of higher order connect $\mathcal{P}$ with all its *minimal supergroups* $\mathcal{S}$ with orders k_S; the index [*i*] of each supergroup is given by the ratio k_S/k_P. In other words: if the diagram is read downwards, subgroup relations are displayed; if it is read upwards, supergroup relations are revealed. The index is always an integer (theorem of Lagrange) and can be easily obtained from the group orders given on the left of the diagrams. The highest index of a maximal subgroup is [3] for two dimensions and [4] for three dimensions.

Two important kinds of subgroups, namely sets of conjugate subgroups and normal subgroups, are distinguished by dashed and solid lines. They are characterized as follows:

The subgroups $\mathcal{H}_1, \mathcal{H}_2, \ldots, \mathcal{H}_n$ of a group $\mathcal{P}$ are *conjugate* subgroups if $\mathcal{H}_1, \mathcal{H}_2, \ldots, \mathcal{H}_n$ are symmetry-equivalent in $\mathcal{P}$, *i.e.* if for every pair $\mathcal{H}_i, \mathcal{H}_j$ at least one symmetry operation W of $\mathcal{P}$ exists which maps $\mathcal{H}_i$ onto $\mathcal{H}_j$: $W^{-1}\mathcal{H}_i W = \mathcal{H}_j$; *cf.* Sections 1.1.5 and 1.1.8.

Examples

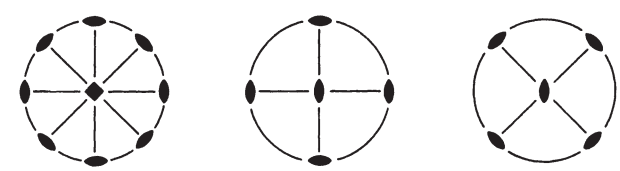
(1) Point group 3*m* has three different mirror planes which are equivalent due to the threefold axis. In each of the three maximal subgroups of type *m*, one of these mirror planes is retained. Hence, the three subgroups *m* are conjugate in 3*m*. This set of conjugate subgroups is represented by *one* dashed line in Figs. 3.2.1.2 and 3.2.1.3.

(2) Similarly, group 432 has three maximal conjugate subgroups of type 422 and four maximal conjugate subgroups of type 32.

The subgroup $\mathcal{H}$ of a group $\mathcal{P}$ is a *normal* (or invariant) subgroup if *no* subgroup $\mathcal{H}'$ of $\mathcal{P}$ exists that is conjugate to $\mathcal{H}$ in $\mathcal{P}$. Note that this does not imply that $\mathcal{H}$ is also a normal subgroup of any supergroup of $\mathcal{P}$. Subgroups of index [2] are always normal and maximal (*cf.* Section 1.1.5). (The role of normal subgroups for the structure of space groups is discussed in Sections 1.3.3 and 1.4.2.3.)

Examples

(1) Fig. 3.2.1.3 shows two solid lines between point groups 422 and 222, indicating that 422 has two maximal normal subgroups 222 of index [2]. The symmetry elements of one subgroup are rotated by 45° around the *c* axis with respect to those of the other subgroup. Thus, in one subgroup the symmetry elements of the two secondary, in the other those of the two tertiary tetragonal symmetry directions (*cf.* Table 2.1.3.1) are retained, whereas the primary twofold axis is the same for both subgroups. There exists no symmetry operation of 422 that maps one subgroup onto the other. This is illustrated by the stereograms below. The two normal subgroups can be indicated by the 'oriented symbols' 222. and 2.22.



422 222. 2.22

(2) Similarly, group 432 has one maximal normal subgroup, 23.

Figs. 3.2.1.2 and 3.2.1.3 show that there exist two 'summits' in both two and three dimensions from which all other point groups can be derived by 'chains' of maximal subgroups. These summits are formed by the square and the hexagonal holohedry in two dimensions and by the cubic and the hexagonal holohedry in three dimensions.

The sub- and supergroups of the point groups are useful both in their own right and as a basis of the *translationengleiche* or *t* subgroups and supergroups of space groups (*cf.* Section 1.7.1). Tables of the sub- and supergroups of the plane groups and space groups are contained in Volume A1 of *International Tables for Crystallography* (2010). A general discussion of sub- and supergroups of crystallographic groups, together with further explanations and examples, is given in Section 1.7.1.

3.2.1.4. Noncrystallographic point groups

3.2.1.4.1. Description of general point groups

In Sections 3.2.1.2 and 3.2.1.3, only the 32 *crystallographic* point groups (crystal classes) are considered. In addition, infinitely many *noncrystallographic* point groups exist that are of interest as possible symmetries of molecules and of quasicrystals and as approximate local site symmetries in crystals. Crystallographic *and* noncrystallographic point groups are collected here under the name *general point groups.* They are reviewed in this section and listed in Tables 3.2.1.5 and 3.2.1.6.

[12] This type of diagram was first used in *International Tables for the Determination of Crystal Structures* (1935): in *International Tables for X-ray Crystallography* (1952) a somewhat different approach was employed.

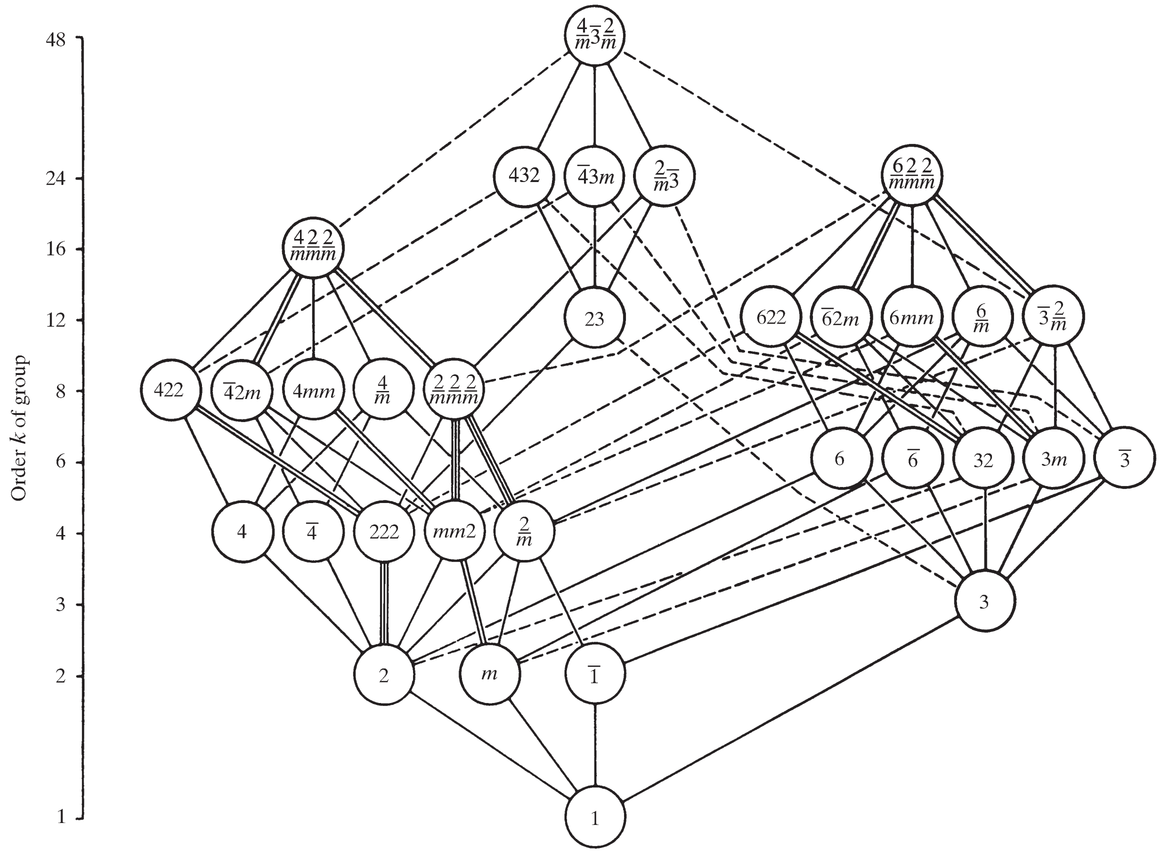


Figure 3.2.1.3

Maximal subgroups and minimal supergroups of the three-dimensional crystallographic point groups. Solid lines indicate maximal normal subgroups; double or triple solid lines mean that there are two or three maximal normal subgroups with the same symbol. Dashed lines refer to sets of maximal conjugate subgroups. The group orders are given on the left. Full Hermann–Mauguin symbols are used.

Because of the infinite number of these groups only *classes of general point groups* (*general classes*)[13] can be listed. They are grouped into *general systems*, which are similar to the crystal systems. The 'general classes' are of two kinds: in the cubic, icosahedral, circular, cylindrical and spherical system, each general class contains *one* point group only, whereas in the $4N$-gonal, $(2N+1)$-gonal and $(4N+2)$-gonal system, each general class contains *infinitely* many point groups, which differ in their principal n-fold symmetry axis, with $n = 4, 8, 12, \ldots$ for the $4N$-gonal system, $n = 1, 3, 5, \ldots$ for the $(2N+1)$-gonal system and $n = 2, 6, 10, \ldots$ for the $(4N+2)$-gonal system.

Furthermore, some general point groups are of order infinity because they contain symmetry axes (rotation or rotoinversion axes) of order infinity[14] (∞-fold axes). These point groups occur in the circular system (two dimensions) and in the cylindrical and spherical systems (three dimensions).

The Hermann–Mauguin and Schoenflies symbols for the general point groups follow the rules of the crystallographic point groups (*cf.* Sections 1.4.1, 2.1.3.4 and 3.3.1). This extends also to the infinite groups where symbols like ∞m or $C_{\infty v}$ are immediately obvious.

In *two dimensions* (Table 3.2.1.5), the eight general classes are collected into three systems. Two of these, the $4N$-gonal and the $(4N+2)$-gonal systems, contain only point groups of finite order with one n-fold rotation point each. These systems are generalizations of the square and hexagonal crystal systems. The circular system consists of two infinite point groups, with one ∞-fold rotation point each.

In *three dimensions* (Table 3.2.1.6), the 33 general classes are collected into seven systems. Three of these, the $4N$-gonal, the $(2N+1)$-gonal and the $(4N+2)$-gonal systems,[15] contain only point groups of finite order with one principal n-fold symmetry axis each. These systems are generalizations of the tetragonal, trigonal and hexagonal crystal systems (*cf.* Table 3.2.3.2). The five cubic groups are well known as crystallographic groups. The two icosahedral groups of orders 60 and 120, characterized by special combinations of twofold, threefold and fivefold symmetry axes, are discussed in more detail below. The groups of the cylindrical and the spherical systems are all of order infinity; they describe the symmetries of cylinders, cones, rotation ellipsoids, spheres *etc.*[16]

[13] The 'classes of general point groups' are not the same as the commonly used 'crystal classes' because some of them contain point groups of *different orders*. All these orders, however, follow a common scheme. In this sense, the 'general classes' are an extension of the concept of (geometric) crystal classes. For example, the general class *nmm* of the $4N$-gonal system contains the point groups 4*mm* (tetragonal), 8*mm* (octagonal), 12*mm* (dodecagonal), 16*mm etc.*

[14] The axes of order infinity, as considered here, do not correspond to cyclic groups (as do the axes of finite order) because there is no smallest rotation from which all other rotations can be derived as higher powers, *i.e.* by successive application. Instead, rotations of all possible angles exist. Nevertheless, it is customary to symbolize these axes as ∞ or C_∞; note that the Hermann–Mauguin symbols ∞/m and $\overline{\infty}$ are equivalent, and so are the Schoenflies symbols $C_{\infty h}$, S_∞ and $C_{\infty i}$. (There exist also axes of order infinity that do correspond to cyclic groups, namely axes based upon smallest rotations with irrational values of the rotation angle.)

[15] Here, the $(2N+1)$-gonal and the $(4N+2)$-gonal systems are distinguished in order to bring out the analogy with the trigonal and the hexagonal crystal systems. They could equally well be combined into one, in correspondence with the hexagonal 'crystal family' (*cf.* Sections 1.3.4.4 and 2.1.1).

[16] The terms 'rotating' and 'stationary' in the circular, cylindrical and spherical systems do not imply any relation to dynamical properties (motions) of crystals or molecules. They only serve to illustrate the absence (group ∞) or presence (∞m, $\overline{\infty}m$) of 'vertical' mirror planes in these groups or order ∞.

Table 3.2.1.5
Classes of general point groups in two dimensions (N = integer ≥ 0)

General Hermann–Mauguin symbol	Order of group	General edge form	General point form	Crystallographic groups
$4N$-gonal system (n-fold rotation point with $n = 4N$)				
n	n	Regular n-gon	Regular n-gon	4
nmm	$2n$	Semiregular di-n-gon	Truncated n-gon	$4mm$
$(4N+2)$-gonal system (n-fold or $\frac{1}{2}n$-fold rotation point with $n = 4N+2$)				
$\frac{1}{2}n$	$\frac{1}{2}n$	Regular $\frac{1}{2}n$-gon	Regular $\frac{1}{2}n$-gon	1, 3
$\frac{1}{2}nm$	n	Semiregular di-$\frac{1}{2}n$-gon	Truncated $\frac{1}{2}n$-gon	m, $3m$
n	n	Regular n-gon	Regular n-gon	2, 6
nmm	$2n$	Semiregular di-n-gon	Truncated n-gon	$2mm$, $6mm$
Circular system†				
∞	∞	Rotating circle	Rotating circle	–
∞m	∞	Stationary circle	Stationary circle	–

† A rotating circle has no mirror lines; there exist two enantiomorphic circles with opposite senses of rotation. A stationary circle has infinitely many mirror lines through its centre.

It is possible to define the three-dimensional point groups on the basis of either rotoinversion axes $\bar{n}$ or rotoreflection axes $\tilde{n}$. The equivalence between these two descriptions is apparent from the following examples:

$$\begin{array}{llll} n = 4N: & \bar{4} = \tilde{4} & \bar{8} = \tilde{8} & \ldots\ \bar{n} = \tilde{n} \\ n = 2N+1: & \bar{1} = \tilde{2} & \bar{3} = \tilde{6} = 3 \times \bar{1} & \ldots\ \bar{n} = \widetilde{2n} = n \times \bar{1} \\ n = 4N+2: & \bar{2} = \tilde{1} = m & \bar{6} = \tilde{3} = 3/m & \ldots\ \bar{n} = \widetilde{\tfrac{1}{2}n} = \tfrac{1}{2}n/m. \end{array}$$

In the present tables, the standard convention of using rotoinversion axes is followed.

Tables 3.2.1.5 and 3.2.1.6 contain for each class its general Hermann–Mauguin and Schoenflies symbols, the group order and the names of the general face form and its dual, the general point form.[17] Special and limiting forms are not given, nor are 'Miller indices' (hkl) and point coordinates x, y, z. They can be derived easily from Tables 3.2.3.1 and 3.2.3.2 for the crystallographic groups.[18]

3.2.1.4.2. The two icosahedral groups

The two point groups 235 and $m\bar{3}\bar{5}$ of the icosahedral system (orders 60 and 120) are of particular interest among the noncrystallographic groups because of the occurrence of fivefold axes and their increasing importance as symmetries of molecules (viruses), of quasicrystals, and as approximate local site symmetries in crystals (alloys, B_{12} icosahedron). Furthermore, they contain as special forms the two noncrystallographic *platonic solids*, the regular icosahedron (20 faces, 12 vertices) and its dual, the regular pentagon-dodecahedron (12 faces, 20 vertices).

The icosahedral groups (*cf.* diagrams in Table 3.2.3.3) are characterized by six fivefold axes that include angles of 63.43°. Each fivefold axis is surrounded by five threefold and five twofold axes, with angular distances of 37.38° between a fivefold and a threefold axis and of 31.72° between a fivefold and a twofold axis. The angles between neighbouring threefold axes are 41.81°, between neighbouring twofold axes 36°. The smallest angle between a threefold and a twofold axis is 20.90°.

Each of the six fivefold axes is perpendicular to five twofold axes; there are thus six maximal conjugate pentagonal subgroups of types 52 (for 235) and $\bar{5}m$ (for $m\bar{3}\bar{5}$) with index [6]. Each of the ten threefold axes is perpendicular to three twofold axes, leading to ten maximal conjugate trigonal subgroups of types 32 (for 235) and $\bar{3}m$ (for $m\bar{3}\bar{5}$) with index [10]. There occur, furthermore, five maximal conjugate cubic subgroups of types 23 (for 235) and $m\bar{3}$ (for $m\bar{3}\bar{5}$) with index [5].

The two icosahedral groups are listed in Table 3.2.3.3, in a form similar to the cubic point groups in Table 3.2.3.2. Each group is illustrated by stereographic projections of the symmetry elements and the general face poles (general points); the complete sets of symmetry elements are listed below the stereograms. Both groups are referred to a cubic coordinate system, with the coordinate axes along three twofold rotation axes and with four threefold axes along the body diagonals. This relation is well brought out by symbolizing these groups as 235 and $m\bar{3}\bar{5}$ instead of the customary symbols 532 and $\bar{5}\bar{3}m$.

The table contains also the multiplicities, the Wyckoff letters and the names of the general and special face forms and their duals, the point forms, as well as the oriented face- and site-symmetry symbols. In the icosahedral 'holohedry' $m\bar{3}\bar{5}$, the *special* 'Wyckoff position' $60d$ occurs in three realizations, *i.e.* with three types of polyhedra. In 235, however, these three types of polyhedra are different realizations of the limiting *general* forms, which depend on the location of the poles with respect to the axes 2, 3 and 5. For this reason, the three entries are connected by braces; *cf.* Section 3.2.1.2.4, *Notes on crystal and point forms*, item (viii).

Not included are the sets of equivalent Miller indices and point coordinates. Instead, only the 'initial' triplets (hkl) and x, y, z for each type of form are listed. The complete sets of indices and coordinates can be obtained in two steps[19] as follows:

[17] The noncrystallographic face and point forms are extensions of the corresponding crystallographic forms: *cf.* Section 3.2.1.2.4, *Notes on crystal and point forms*. The name *streptohedron* applies to the general face forms of point groups $\bar{n}$ with $n = 4N$ and $n = 2N+1$; it is thus a generalization of the tetragonal disphenoid or tetragonal tetrahedron ($\bar{4}$) and the rhombohedron ($\bar{3}$).

[18] The term 'Miller indices' is used here also for the noncrystallographic point groups. Note that these indices do not have to be integers or rational numbers, as for the crystallographic point groups. Irrational indices, however, can always be closely approximated by integers, quite often even by small integers.

[19] A one-step procedure applies to the icosahedral 'Wyckoff position' $12a$, the face poles and points of which are located on the fivefold axes. Here, step (ii) is redundant and can be omitted. The forms $\{01\tau\}$ and $0, y, \tau y$ are contained in the cubic point groups 23 and $m\bar{3}$ and in the cubic space groups $P23$ and $Pm\bar{3}$ as limiting cases of Wyckoff positions$\{0kl\}$ and $0, y, z$ with specialized (irrational) values of the indices and coordinates. In geometric terms, the regular pentagon-dodecahedron is a noncrystallographic 'limiting polyhedron' of the 'crystallographic' pentagon-dodecahedron and the regular icosahedron is a 'limiting polyhedron' of the 'irregular' icosahedron (*cf.* Section 3.2.1.2.2, *Crystal and point forms*).