International Tables for Crystallography (2016). Vol. A, Section 3.2.1.4, pp. 731–737.

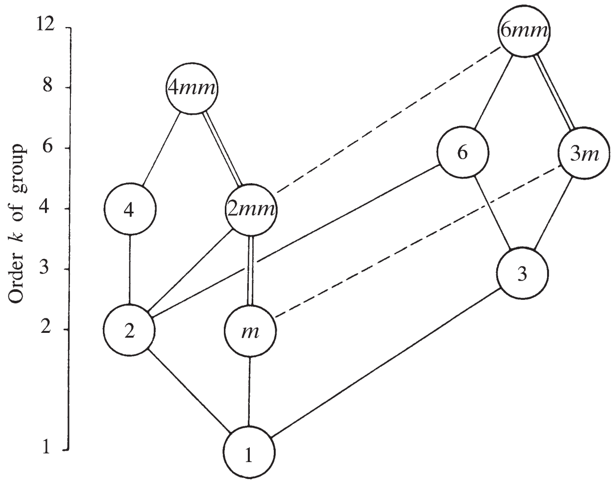


Figure 3.2.1.2
Maximal subgroups and minimal supergroups of the two-dimensional crystallographic point groups. Solid lines indicate maximal normal subgroups; double solid lines mean that there are two maximal normal subgroups with the same symbol. Dashed lines refer to sets of maximal conjugate subgroups.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

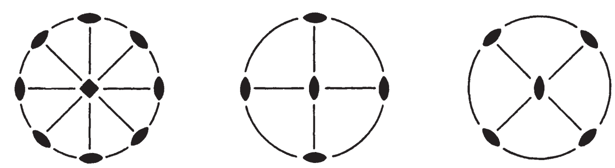
(1) Point group 3*m* has three different mirror planes which are equivalent due to the threefold axis. In each of the three maximal subgroups of type *m*, one of these mirror planes is retained. Hence, the three subgroups *m* are conjugate in 3*m*. This set of conjugate subgroups is represented by *one*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

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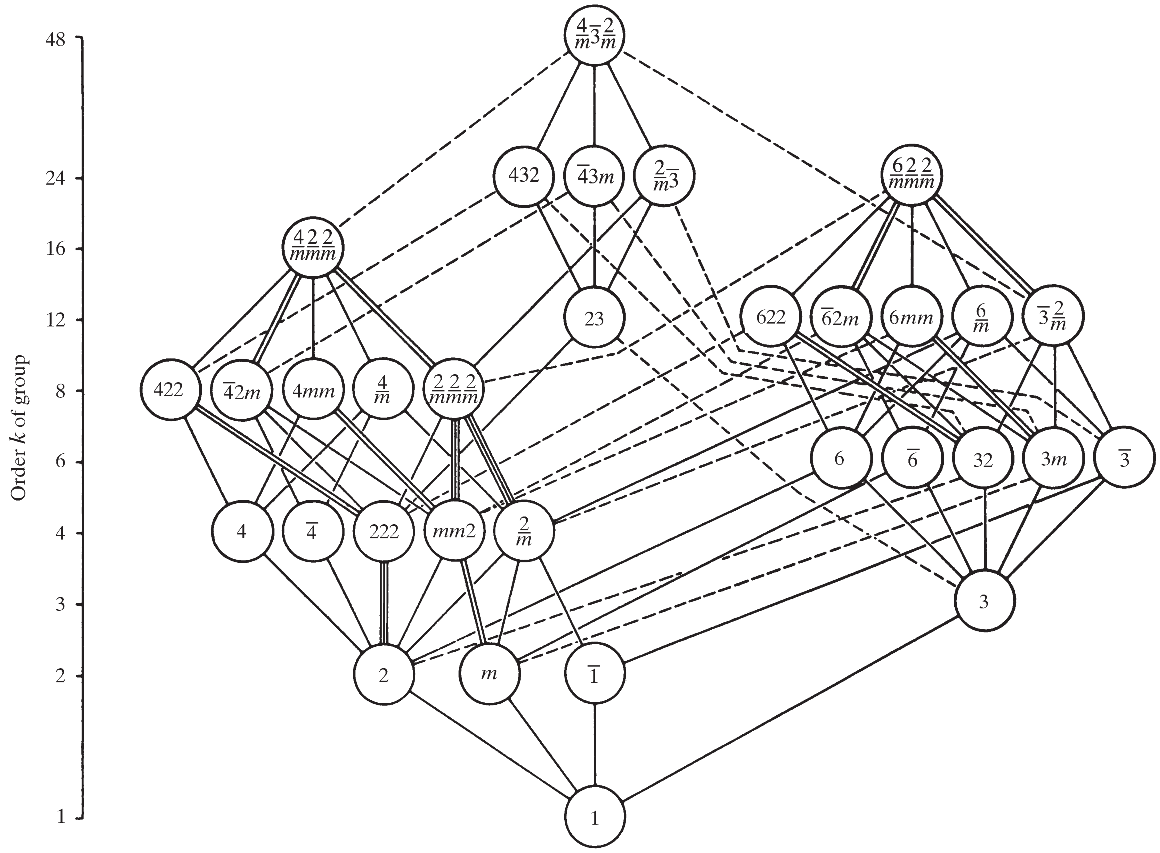

Figure 3.2.1.3
Maximal subgroups and minimal supergroups of the three-dimensional crystallographic point groups. Solid lines indicate maximal normal subgroups; double or triple solid lines mean that there are two or three maximal normal subgroups with the same symbol. Dashed lines refer to sets of maximal 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 $4mm$ (tetragonal), $8mm$ (octagonal), $12mm$ (dodecagonal), $16mm$ *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*).

Table 3.2.1.6

Classes of general point groups in three dimensions (N = integer ≥ 0)

Short general Hermann–Mauguin symbol, followed by full symbol where different	Schoenflies symbol	Order of group	General face form	General point form	Crystallographic groups
$4N$-gonal system (single n-fold symmetry axis with $n = 4N$)					
n	C_n	n	n-gonal pyramid	Regular n-gon	4
$\bar{n}$	S_n	n	$\frac{1}{2}n$-gonal streptohedron	$\frac{1}{2}n$-gonal antiprism	$\bar{4}$
n/m	C_{nh}	$2n$	n-gonal dipyramid	n-gonal prism	$4/m$
$n22$	D_n	$2n$	n-gonal trapezohedron	Twisted n-gonal antiprism	422
nmm	C_{nv}	$2n$	Di-n-gonal pyramid	Truncated n-gon	$4mm$
$\bar{n}2m$	$D_{\frac{1}{2}nd}$	$2n$	n-gonal scalenohedron	$\frac{1}{2}n$-gonal antiprism sliced off by pinacoid	$\bar{4}2m$
n/mmm, $\frac{n}{m}\frac{2}{m}\frac{2}{m}$	D_{nh}	$4n$	Di-n-gonal dipyramid	Edge-truncated n-gonal prism	$4/mmm$
$(2N+1)$-gonal system (single n-fold symmetry axis with $n = 2N+1$)					
n	C_n	n	n-gonal pyramid	Regular n-gon	1, 3
$\bar{n} = n \times \bar{1}$	C_{ni}	$2n$	n-gonal streptohedron	n-gonal antiprism	$\bar{1}$, $\bar{3} = 3 \times \bar{1}$
$n2$	D_n	$2n$	n-gonal trapezohedron	Twisted n-gonal antiprism	32
nm	C_{nv}	$2n$	Di-n-gonal pyramid	Truncated n-gon	$3m$
$\bar{n}m$, $\bar{n}\frac{2}{m}$	D_{nd}	$4n$	Di-n-gonal scalenohedron	n-gonal antiprism sliced off by pinacoid	$\bar{3}m$
$(4N+2)$-gonal system (single n-fold symmetry axis with $n = 4N+2$)					
n	C_n	n	n-gonal pyramid	Regular n-gon	2, 6
$\bar{n} = \frac{1}{2}n/m$	$C_{\frac{1}{2}nh}$	n	$\frac{1}{2}n$-gonal dipyramid	$\frac{1}{2}n$-gonal prism	$\bar{2} \equiv m$, $\bar{6} \equiv 3/m$
n/m	C_{nh}	$2n$	n-gonal dipyramid	n-gonal prism	$2/m$, $6/m$
$n22$	D_n	$2n$	n-gonal trapezohedron	Twisted n-gonal antiprism	222, 622
nmm	C_{nv}	$2n$	Di-n-gonal pyramid	Truncated n-gon	$mm2$, $6mm$
$\bar{n}2m = \frac{1}{2}n/m2m$	$D_{\frac{1}{2}nh}$	$2n$	Di-$\frac{1}{2}n$-gonal dipyramid	Truncated $\frac{1}{2}n$-gonal prism	$\bar{6}2m$
n/mmm, $\frac{n}{m}\frac{2}{m}\frac{2}{m}$	D_{nh}	$4n$	Di-n-gonal dipyramid	Edge-truncated n-gonal prism	mmm, $6/mmm$
Cubic system (for details see Table 3.2.3.2)					
23	T	12	Pentagon-tritetrahedron	Snub tetrahedron	23
$m\bar{3}$, $\frac{2}{m}\bar{3}$	T_h	24	Didodecahedron	Cube & octahedron & pentagon-dodecahedron	$m\bar{3}$
432	O	24	Pentagon-trioctahedron	Snub cube	432
$\bar{4}3m$	T_d	24	Hexatetrahedron	Cube truncated by two tetrahedra	$\bar{4}3m$
$m\bar{3}m$, $\frac{4}{m}\bar{3}\frac{2}{m}$	O_h	48	Hexaoctahedron	Cube truncated by octahedron and by rhomb-dodecahedron	$m\bar{3}m$
Icosahedral system† (for details see Table 3.2.3.3)					
235	I	60	Pentagon-hexecontahedron	Snub pentagon-dodecahedron	–
$m\bar{3}\bar{5}$, $\frac{2}{m}\bar{3}\bar{5}$	I_h	120	Hecatonicosahedron	Pentagon-dodecahedron truncated by icosahedron and by rhomb-triacontahedron	–
Cylindrical system‡					
∞	C_∞	∞	Rotating cone	Rotating circle	–
$\infty/m \equiv \bar{\infty}$	$C_{\infty h} \equiv S_\infty \equiv C_{\infty i}$	∞	Rotating double cone	Rotating finite cylinder	–
$\infty 2$	D_∞	∞	‘Anti-rotating’ double cone	‘Anti-rotating’ finite cylinder	–
∞m	$C_{\infty v}$	∞	Stationary cone	Stationary circle	–
$\infty/mm \equiv \bar{\infty}m$, $\frac{\infty}{m}\frac{2}{m} \equiv \bar{\infty}\frac{2}{m}$	$D_{\infty h} \equiv D_{\infty d}$	∞	Stationary double cone	Stationary finite cylinder	–
Spherical system§					
2∞, $\infty\infty$	K	∞	Rotating sphere	Rotating sphere	–
$m\bar{\infty}$, $\frac{2}{m}\bar{\infty}$, $\infty\infty m$	K_h	∞	Stationary sphere	Stationary sphere	–

† The Hermann–Mauguin symbols of the two icosahedral point groups are often written as 532 and $\bar{5}\bar{3}m$ (see text). ‡ Rotating and ‘anti-rotating’ forms in the cylindrical system have no ‘vertical’ mirror planes, whereas stationary forms have infinitely many vertical mirror planes. In classes ∞ and $\infty 2$, enantiomorphism occurs, *i.e.* forms with opposite senses of rotation. Class $\infty/m \equiv \bar{\infty}$ exhibits no enantiomorphism due to the centre of symmetry, even though the double cone is rotating in one direction. This can be understood as follows: The handedness of a rotating cone depends on the sense of rotation with respect to the axial direction from the base to the tip of the cone. Thus, the rotating double cone consists of two cones with opposite handedness and opposite orientations related by the (single) horizontal mirror plane. In contrast, the ‘anti-rotating’ double cone in class $\infty 2$ consists of two cones of equal handedness and opposite orientations, which are related by the (infinitely many) twofold axes. The term ‘anti-rotating’ means that upper and lower halves of the forms rotate in opposite directions. § The spheres in class 2∞ of the spherical system must rotate around an axis with at least two different orientations, in order to suppress all mirror planes. This class exhibits enantiomorphism, *i.e.* it contains spheres with either right-handed or left-handed senses of rotation around the axes (*cf.* Section 3.2.2.4, *Optical properties*). The stationary spheres in class $m\bar{\infty}$ contain infinitely many mirror planes through the centres of the spheres. Group 2∞ is sometimes symbolized by $\infty\infty$; group $m\bar{\infty}$ by $\bar{\infty}\,\bar{\infty}$ or $\infty\infty m$. The symbols used here indicate the minimal symmetry necessary to generate the groups; they show, furthermore, the relation to the cubic groups. The Schoenflies symbol K is derived from the German name *Kugelgruppe*.

(i) For the face forms the cubic point groups 23 and $m\overline{3}$ (Table 3.2.3.2), and for the point forms the cubic space groups $P23$ (195) and $Pm\overline{3}$ (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 $m\overline{3}$ (for $m\overline{3}\overline{5}$) 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 $Pm\overline{3}$ 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 $\boldsymbol{Y}$, $\boldsymbol{Y}^2$, $\boldsymbol{Y}^3$ and $\boldsymbol{Y}^4$ for the Miller indices;
 (*b*) the matrices $\boldsymbol{Y}^{-1}$, $\boldsymbol{Y}^{-2}$, $\boldsymbol{Y}^{-3}$ and $\boldsymbol{Y}^{-4}$ 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 matrices[20] are

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

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

with[21]

$$G = \frac{\sqrt{5}+1}{4} = \frac{\tau}{2} = \cos 36^\circ = 0.80902 \simeq \frac{72}{89}$$
$$g = \frac{\sqrt{5}-1}{4} = \frac{\tau - 1}{2} = \cos 72^\circ = 0.30902 \simeq \frac{17}{55}.$$

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.

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 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,

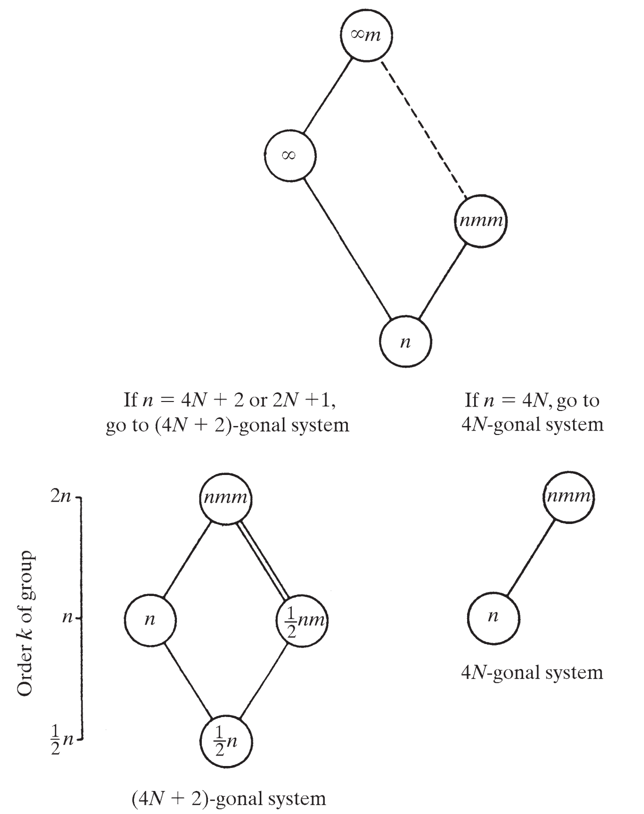

Figure 3.2.1.4
Subgroups and supergroups of the two-dimensional general point groups. Solid lines indicate maximal normal subgroups, double solid lines mean that there are two maximal normal subgroups with the same symbol. Dashed lines refer to sets of maximal conjugate subgroups. For the finite groups,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

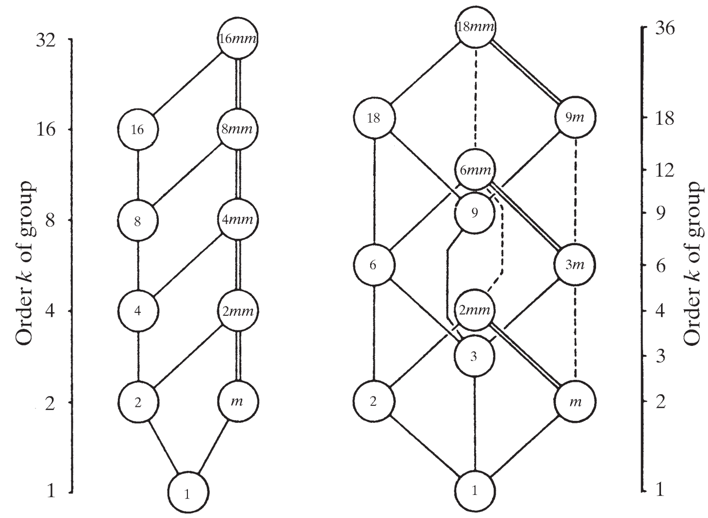

Figure 3.2.1.5
The subgroups of the two-dimensional general point groups 16*mm* (4*N*-gonal system) and 18*mm* [$(4N+2)$-gonal system, including the $(2N+1)$-gonal groups]. Compare with Fig. 3.2.1.4 which applies only to one value of *N*.

[20] Note that for orthogonal matrices $\boldsymbol{Y}^{-1} = \boldsymbol{Y}^t$ (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.

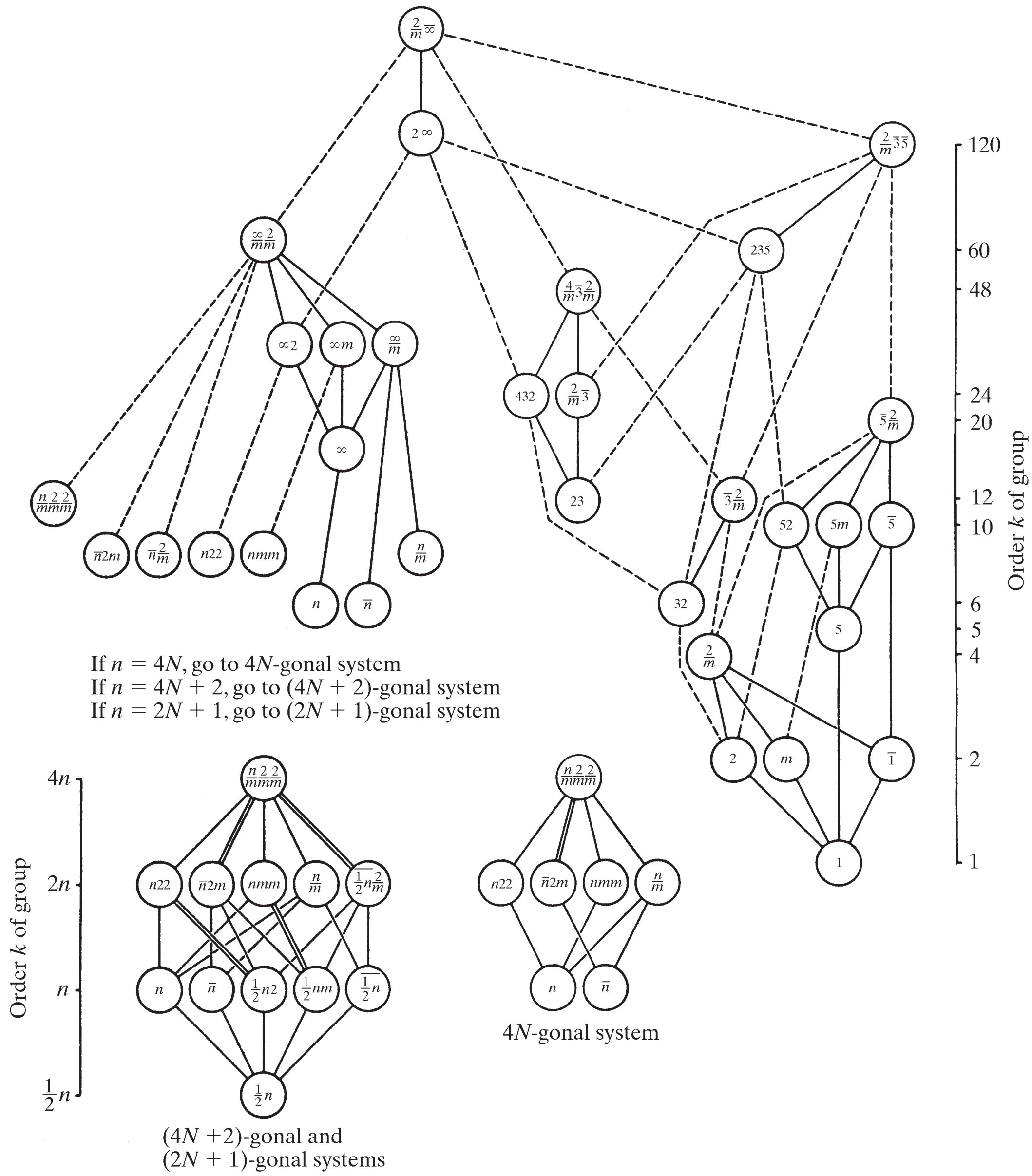

Figure 3.2.1.6

Subgroups and supergroups of the three-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 and on the right. Note that the subgroups of the five cylindrical groups are not maximal and that the diagram applies only to a specified value of N (see text). Only those crystallographic point groups are included that are maximal subgroups of noncrystallographic point groups, *cf.* Fig. 3.2.1.3. Full Hermann–Mauguin symbols are used.

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 values of N, until the crystallographic groups (Fig. 3.2.1.2) are reached. This is illustrated for both systems in Fig. 3.2.1.5.

Fig. 3.2.1.6 for *three dimensions* illustrates that the two spherical groups $2/m\overline{\infty}$ and 2∞ each have one infinite set of cylindrical maximal conjugate subgroups, as well as one infinite set of cubic and one infinite set of icosahedral maximal finite conjugate subgroups, all of index $[\infty]$.

Each of the two icosahedral groups 235 and $2/m\,\bar{3}\,\bar{5}$ has one set of five cubic, one set of six pentagonal and one set of ten trigonal maximal conjugate subgroups of indices [5], [6] and [10], respectively (*cf.* Section 3.2.1.4.2, *The two icosahedral groups*); they are listed on the right of Fig. 3.2.1.6. For the crystallographic groups, Fig. 3.2.1.3 applies. The subgroup types of the five cylindrical point groups are shown on the upper left part of Fig. 3.2.1.6. As explained above for two dimensions, these subgroups are *not maximal* and of index $[\infty]$. Depending upon whether the main symmetry axis has the multiplicity 4N, $4N + 2$ or $2N + 1$, the subgroups belong to the 4N-gonal, $(4N + 2)$-gonal or $(2N + 1)$-gonal system.

The subgroup and supergroup relations within these three systems are displayed in the lower left part of Fig. 3.2.1.6. They are analogous to the crystallographic groups. To facilitate the use of the diagrams, the $(4N+2)$-gonal and the $(2N+1)$-gonal systems are combined, with the consequence that the five classes of the $(2N+1)$-gonal system now appear with the symbols $\overline{\frac{1}{2}n}\frac{2}{m}$, $\frac{1}{2}n2$, $\frac{1}{2}nm$, $\overline{\frac{1}{2}n}$ and $\frac{1}{2}n$. Again, the diagrams apply to a specified value of *N*. A finite number of further maximal subgroups is obtained for lower values of *N*, until the crystallographic groups (Fig. 3.2.1.3) are reached (*cf.* the two-dimensional examples in Fig. 3.2.1.5).

3.2.2. Point-group symmetry and physical properties of crystals

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In the previous section (Section 3.2.1), the crystallographic and noncrystallographic point groups are treated under geometrical aspects only. In the present section the point-group symmetries of the physical properties are considered. Among the physical properties, those represented by tensors are accessible to a mathematical treatment of their symmetries, which are apparent by the invariance of tensor components under symmetry operations. For more details the reader is referred to Nye (1957, 1985), Paufler (1986), Schwarzenbach & Chapuis (2006) and Shuvalov (1988). A similar comprehensive treatment of non-tensorial properties, such as cleavage, plasticity, hardness or crystal growth does not exist, but these properties are, of course, also governed by the crystallographic point-group symmetry.

3.2.2.1. General restrictions on physical properties imposed by symmetry

3.2.2.1.1. Neumann's principle

Neumann's principle (Neumann, 1885) describes the relation between the symmetry $\mathcal{Q}$ of a physical property and the crystallographic point group $\mathcal{P}$ of a crystal. It states that the symmetry of any physical property of a crystal is higher than, or at least equal to, its crystallographic point-group symmetry, or in the language of groups, the symmetry $\mathcal{Q}$ of any physical property of a crystal is a proper or improper supergroup of its crystallographic symmetry $\mathcal{P}$: $\mathcal{Q} \subseteq \mathcal{P}$. This is easily illustrated for polar second-rank tensors, which are represented by ellipsoids and hyperboloids. The representation surfaces of triclinic, monoclinic and orthorhombic crystals are general ellipsoids or hyperboloids of symmetry $\mathcal{Q} = 2/m\,2/m\,2/m$, which is a proper supergroup of all triclinic, monoclinic and orthorhombic point groups with the only exception of the orthorhombic holohedry $\mathcal{P} = 2/m\,2/m\,2/m$, for which the two symmetries are the same. For the uniaxial crystals of the trigonal, tetragonal and hexagonal systems the representation ellipsoids and hyperboloids have rotation symmetries with the cylindrical point group $\mathcal{Q} = \infty/m\,2/m$ (see Table 3.2.1.6), which is a proper supergroup of all uniaxial crystallographic point groups. For cubic crystals, second-rank tensors are isotropic and represented by a sphere with point-group symmetry $\mathcal{Q} = 2/m\,\overline{\infty}$ ($\infty\infty m$), a proper supergroup of all cubic crystallographic point groups. For more details the reader is referred to Paufler (1986) and Authier (2014). A short resume is given by Klapper & Hahn (2005).

As a consequence of the invariance of tensor components under a symmetry operation (or alternatively: under a transformation of the coordinate system to a symmetry-equivalent one), some of the tensor components are equal or even zero. The number of independent components decreases when the symmetry of the crystal increases. Thus, an increase of the point-group symmetry from 1 (triclinic) to $4/m\,\bar{3}\,2/m$ (cubic) or to the sphere group $\infty\infty m$ (*i.e.* isotropy) reduces the number of tensor components for symmetrical second-rank tensors from 6 to 1. Even more drastic is this reduction for all tensors of odd rank (such as pyroelectricity and piezoelectricity) or axial tensors of second rank (*e.g.* optical activity): all components are zero if an inversion centre is present, *i.e.* properties described by these tensors do not exist in centrosymmetric crystals (see the textbooks of tensor physics mentioned above). These properties, which exist only in noncentrosymmetric crystals are, as a rule, the most important ones, not only for physical applications but also for structure determination, because they allow a proof of the absence of a symmetry centre.

For the description of noncentrosymmetric crystals and their specific properties, certain notions are of importance and these are explained in the following two sections.

3.2.2.1.2. Curie's principle

Curie's principle (Curie, 1894) describes the crystallographic symmetry $\mathcal{P}_F$ of a macroscopic crystal which is subject to an external influence *F*, for example to an electric field **E**, to uniaxial stress σ_{ii}, to a temperature change ΔT *etc*. For this treatment, the point-group symmetries $\mathcal{R}$ of the external influences (Curie groups) are defined as follows (see Authier, 2014, p. 11; Paufler, 1986, p. 29):

Homogeneous electric field **E**: $\mathcal{R} = \infty m$ (polar continuous rotation axis with 'parallel' mirror planes, *i.e.* symmetry of a stationary cone) [Note that a rotating cone (left- or right-handed) represents geometrically the polar enantiomorphous group ∞; a stationary cone represents the polar group ∞m with 'vertical' mirror planes, *cf.* Section 3.2.1.4.1.];

Homogeneous magnetic field **H**: $\mathcal{R} = \infty/m$ (symmetry of a rotating cylinder);

Uniaxial stress σ_{ii}: $\mathcal{R} = \infty/m\,2/m$ (symmetry of a stationary centrosymmetric cylinder);

Temperature change ΔT or hydrostatic pressure *p* (scalars): $\mathcal{R} = 2/m\,\overline{\infty}$ ($\infty\infty m$) (symmetry of a stationary centrosymmetric sphere);

Shear stress σ_{ij}: $\mathcal{R} = 2/m\,2/m\,2/m$ (orthorhombic).

According to Curie's principle, the point-group symmetry $\mathcal{P}_F$ of the crystal under the external field *F* is the intersection symmetry of the two point groups: $\mathcal{P}$ of the crystal without field and $\mathcal{R}$ of the field without crystal: $\mathcal{P}_F = \mathcal{R} \cap \mathcal{P}$; *i.e.* $\mathcal{P}_F$ is a (proper or improper) subgroup of both groups $\mathcal{R}$ and $\mathcal{P}$.

As examples we consider the effect of an electric field ($\mathcal{R} = \infty m$) and of a uniaxial stress ($\mathcal{R} = \infty/m\,2/m$) along one of the (four) threefold rotoinversion axes $\bar{3}$ of cubic crystals with point groups $\mathcal{P} = 2/m\,\bar{3}$ and $\mathcal{P} = 4/m\,\bar{3}\,2/m$.

Electric field parallel to [111]:

$2/m\,\bar{3} \cap \infty m$:	$\mathcal{P}_F = 3$	along [111] (polar, pyroelectric, optically active; *cf*. Sections 3.2.2.5 and 3.2.2.4.2)
$4/m\,\bar{3}\,2/m \cap \infty m$:	$\mathcal{P}_F = 3m$	along [111] (polar, pyroelectric, not optically active)

references