International Tables for Crystallography (2016). Vol. A, Section 3.2.1.4.2, pp. 733–735.

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, τy 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 $m\bar{3}$ (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 $m\bar{3}\bar{5}$) 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 $\boldsymbol{Y}$, $\boldsymbol{Y}^2$, $\boldsymbol{Y}^3$ 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 [∞] 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,

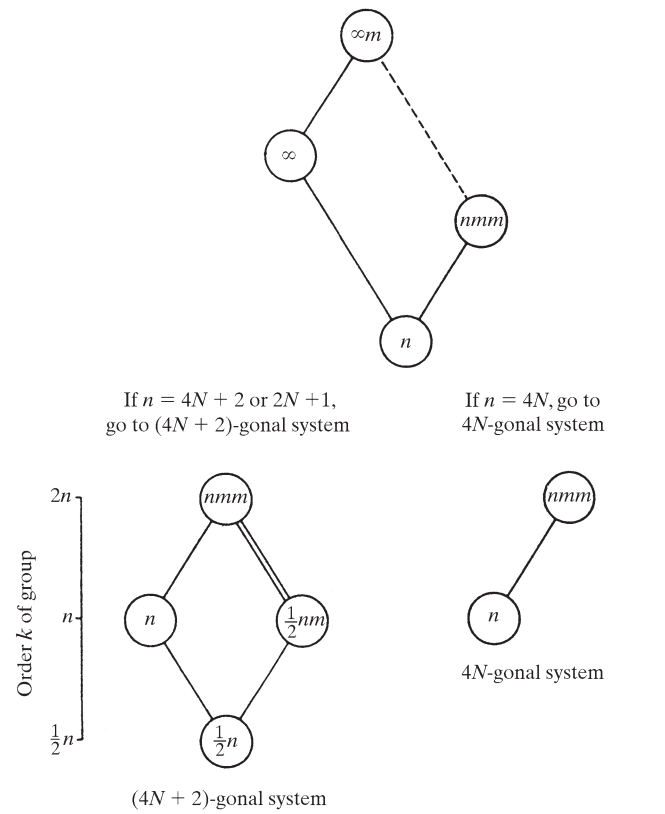

Figure 3.2.1.4
Subgroups and supergroups of the two-dimensional general point groups. Solid lines indicate maximal normal subgroups, double solid lines mean that there are two maximal normal subgroups with the same symbol. Dashed lines refer to sets of maximal conjugate subgroups. For the finite groups,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

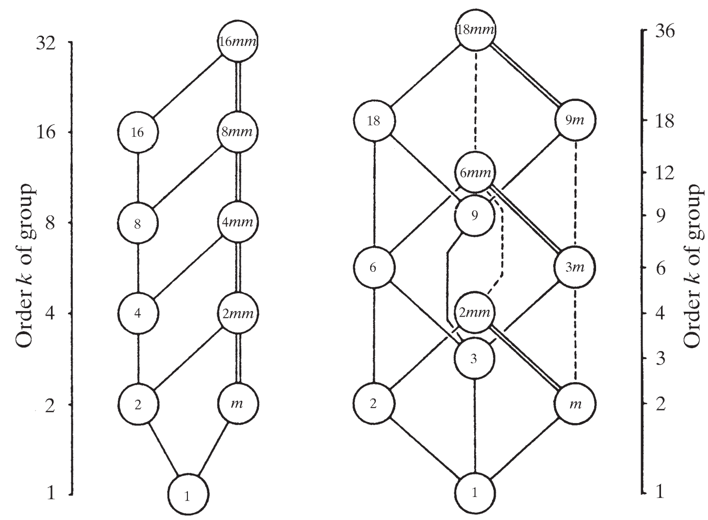

Figure 3.2.1.5
The subgroups of the two-dimensional general point groups 16*mm* (4*N*-gonal system) and 18*mm* [(4*N* + 2)-gonal system, including the (2*N* + 1)-gonal groups]. Compare with Fig. 3.2.1.4 which applies only to one value of *N*.

[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.