

## 3.2. POINT GROUPS AND CRYSTAL CLASSES

Table 3.2.1.5

Classes of general point groups in two dimensions ( $N = \text{integer} \geq 0$ )

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

$$\begin{aligned}
 n = 4N: & \quad \bar{4} = \tilde{4} & \quad \bar{8} = \tilde{8} & \quad \dots & \quad \bar{n} = \tilde{n} \\
 n = 2N + 1: & \quad \bar{1} = \tilde{2} & \quad \bar{3} = \tilde{6} = 3 \times \bar{1} & \quad \dots & \quad \bar{n} = \tilde{2n} = n \times \bar{1} \\
 n = 4N + 2: & \quad \bar{2} = \tilde{1} = m & \quad \bar{6} = \tilde{3} = 3/m & \quad \dots & \quad \bar{n} = \tilde{\frac{1}{2}n} = \frac{1}{2}n/m.
 \end{aligned}$$

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.<sup>17</sup> 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.<sup>18</sup>

## 3.2.1.4.2. The two icosahedral groups

The two point groups 235 and  $m\bar{3}5$  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  $m\bar{3}5$ ) 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  $m\bar{3}5$ ) with index [10]. There occur, furthermore, five maximal conjugate cubic subgroups of types 23 (for 235) and  $m\bar{3}$  (for  $m\bar{3}5$ ) 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  $m\bar{3}5$  instead of the customary symbols 532 and  $\bar{5}3m$ .

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’  $m\bar{3}5$ , the *special* ‘Wyckoff position’ 60*d* 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<sup>19</sup> as follows:

<sup>17</sup> 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 ( $\bar{3}$ ).

<sup>18</sup> 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.

<sup>19</sup> A one-step procedure applies to the icosahedral ‘Wyckoff position’ 12*a*, 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*τ*} and 0, *y*, *z* 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 {0*kl*} 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*).