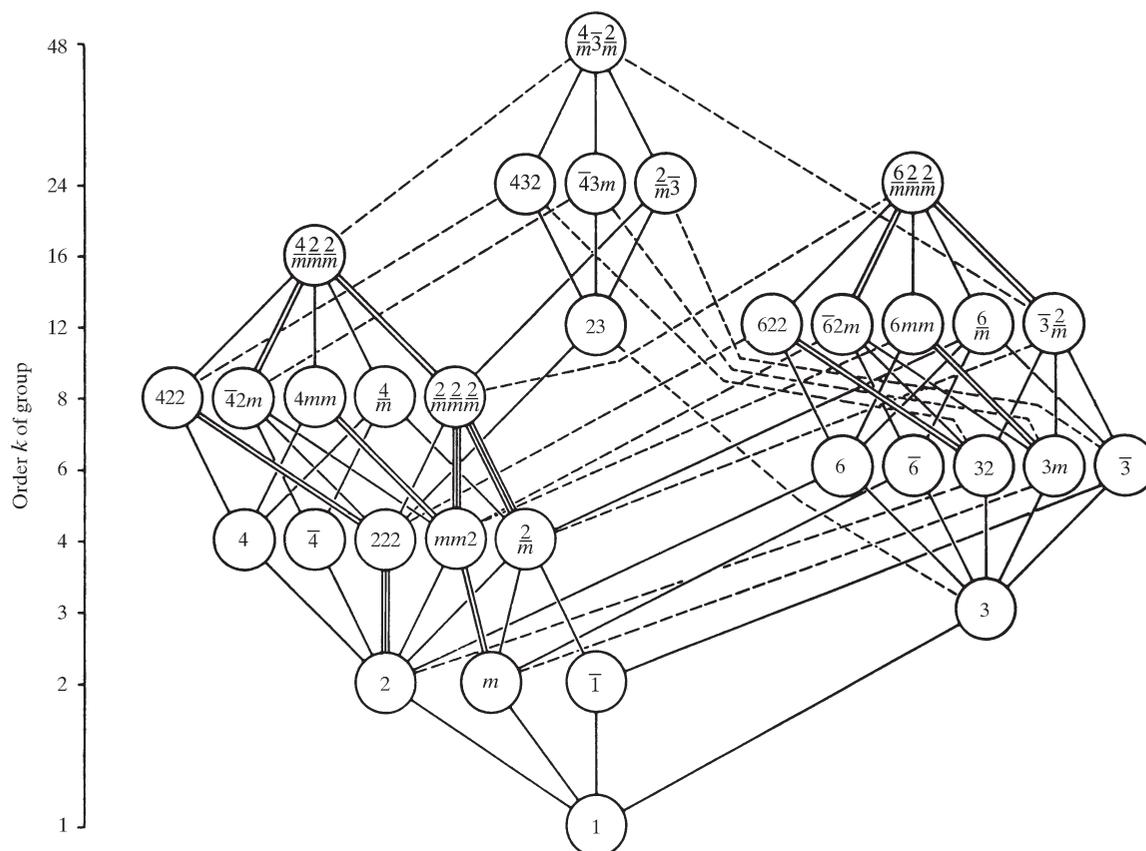


## 3. ADVANCED TOPICS ON SPACE-GROUP SYMMETRY

**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)*<sup>13</sup> 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  $n = 4, 8, 12, \dots$  for the  $4N$ -gonal system,  $n = 1, 3, 5, \dots$  for the  $(2N + 1)$ -gonal system and  $n = 2, 6, 10, \dots$  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<sup>14</sup> ( $\infty$ -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  $\infty m$  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  $\infty$ -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,<sup>15</sup> 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.*<sup>16</sup>

<sup>15</sup> 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).

<sup>16</sup> 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  $\infty$ ) or presence ( $\infty m$ ,  $\infty \bar{m}$ ) of ‘vertical’ mirror planes in these groups or order  $\infty$ .

<sup>13</sup> 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.*

<sup>14</sup> 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  $\infty$  or  $C_{\infty}$ ; note that the Hermann–Mauguin symbols  $\infty/m$  and  $\infty \bar{m}$  are equivalent, and so are the Schoenflies symbols  $C_{\infty h}$ ,  $S_{\infty}$  and  $C_{\infty v}$ . (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.)