## 3.2. POINT GROUPS AND CRYSTAL CLASSES

above is fulfilled either as $7 \times 1 + 1 = 2 \times 4$ or $7 \times 1 - 1 = 2 \times 3$, *i.e.* $q = 4$ or $q = 3$, and the corresponding Hermann–Mauguin screw operation symbol is either $7_4$ or $7_3$, depending on chirality. The helix is shown in Fig. 3.2.4.1. The $N/r$ symbol cannot be deduced uniquely from the Hermann–Mauguin symbol, because a 7/9 or any other 7/(2 modulo 7) *P*-helix and any 7/(5 modulo 7) *M*-helix also has $\not{p}7_4$ symmetry.

*Layer groups* can have axes of orders of 1, 2, 3, 4 and 6 only. There exist 80 layer-group types. Layer-group symbols refer to a crystallographic coordinate system with **c** (of arbitrary length) perpendicular to the layer defined by the basis vectors **a** and **b**. Layer-group symbols are like space-group symbols, but begin with a lower-case *p* or *c* specifying the centring. Since plane-group symbols also begin by *p* or *c* and can therefore be confused with layer-group symbols, it is advisable to always mention what kind of group is meant.

Rod and layer groups with axis orders of 1, 2, 3, 4 and 6 are the subject of *International Tables for Crystallography* (2010), Volume E, *cf.* Section 1.7.3. Table 3.2.4.1 lists the rod-group types for any axis order.

### 3.2.4.5. Enantiomorphism and chirality

*Definition:* An object is *chiral* if it cannot be superposed by pure rotation and translation on its image formed by inversion through a point.

The symmetry group of a chiral object contains no symmetry operations of the second kind, *i.e.* no inversion, rotoinversion, reflection or glide reflection. As a consequence, a chiral object can occur in two different forms, which are related in the same way as are a right and a left hand. Further terms in this context are (Flack, 2003; Moss, 1996):

| | |
|---|---|
| Absolute configuration | Spatial arrangement of atoms in a chiral molecule and its appropriate designation [*e.g.* by (*R*), (*S*) *etc.*] |
| Absolute (crystal) structure | Spatial arrangement of atoms in a chiral crystal and its description (lattice parameters, space group, atomic coordinates) |
| Enantiomorph | One out of a pair of objects of opposite chirality |
| Enantiomer | One molecule out of a pair of opposite chirality (special designation for enantiomorphic molecules) |
| Racemate | Equimolar mixture of a pair of enantiomers |
| Chirality sense (chirality) | Property which distinguishes enantiomorphs from one another; the two enantiomorphs of a pair have opposite chirality |
| Achiral | Refers to an object that is not chiral |

Possible point groups for chiral molecules correspond to the crystal classes marked in Table 3.2.2.1 with a + sign under the heading 'Enantiomorphism'. In addition, the noncrystallographic point groups $N$, $N2$ ($N$ odd, $N \geq 5$), $N22$ ($N$ even, $N \geq 8$) and $\infty\infty5$ are possible. Chiral crystal structures are compatible only with space groups that have no inversion centres, rotoinversion axes, reflection or glide-reflection planes. For a chiral molecular compound, these symmetry elements would generate the opposite enantiomer and the compound would be a racemate. Chiral

**Table 3.2.4.1**
Classes of rod groups

If $N = 2$, the conventional symbols differ (the symmetry direction with the $N$ must by shifted to the last position of the symbol and $\bar{2}$ is to be replaced by *m*). *n* is an arbitrary positive integer.

| Short symbol | Full symbol | $N$ | $q$ |
|---|---|---|---|
| $\not{p}N$ | | $N = n$ | |
| $\not{p}N_q$ | | $N = n \geq 2$ | $q = 1, \ldots, N-1$ |
| $\not{p}\bar{N}$ | | $N = n$ | |
| $\not{p}N/m$ | | $N = 2n$ | |
| $\not{p}N_q/m$ | | $N = 2n$ | $q = \frac{1}{2}N$ |
| $\not{p}N2$ | | $N = 2n+1$ | |
| $\not{p}N22$ | | $N = 2n$ | |
| $\not{p}N_q2$ | | $N = 2n+1$ | $q = 1, \ldots, N-1$ |
| $\not{p}N_q22$ | | $N = 2n$ | $q = 1, \ldots, N-1$ |
| $\not{p}Nm$ | | $N = 2n+1$ | |
| $\not{p}Nmm$ | | $N = 2n$ | |
| $\not{p}Nc$ | | $N = 2n+1$ | |
| $\not{p}Ncc$ | | $N = 2n$ | |
| $\not{p}N_qmc$ | | $N = 2n$ | $q = \frac{1}{2}N$ |
| $\not{p}\bar{N}m$ | $\not{p}\bar{N}2/m$ | $N = 2n+1$ | |
| $\not{p}\bar{N}2m$ | | $N = 2n$ | |
| $\not{p}\bar{N}c$ | $\not{p}\bar{N}2/c$ | $N = 2n+1$ | |
| $\not{p}\bar{N}2c$ | | $N = 2n$ | |
| $\not{p}N/mmm$ | $\not{p}N/m2/m2/m$ | $N = 2n$ | |
| $\not{p}N/mcc$ | $\not{p}N/m2/c2/c$ | $N = 2n$ | |
| $\not{p}N_q/mmc$ | $\not{p}N_q/m2/m2/c$ | $N = 2n$ | $q = \frac{1}{2}N$ |

crystals belong to one of the 11 crystal classes allowing enantiomorphism (Table 3.2.2.1); they can adopt one out of 65 space-group types. These are called the 65 *Sohncke space-group types* [after L. Sohncke who was the first to derive them; Flack (2003). Julian (2015) calls them 'proper space groups']. The Sohncke space-group types comprise the eleven pairs of enantiomorphic space-group types (*cf.* Section 1.3.4.1) and further 43 non-enantiomorphic space-group types. Whereas an enantiomorphic space group (*e.g.* $P3_1$ or $P4_122$) is chiral in itself, which means that its Euclidean normalizer is noncentrosymmetric, the space groups of the other 43 Sohncke space-group types (*e.g.* $P2_12_12_1$) are not chiral themselves; they have centrosymmetric Euclidean normalizers. Keep in mind that the symmetry of a molecule is specified by its point group; the symmetry of a crystal by its space group; and the symmetry of a space group by its Euclidean normalizer (*cf.* Section 3.5.1.2).[26] However, the arrangement of the atoms in any Sohncke space group is always chiral. In other words, an enantiomorphic space group is a sufficient but not a necessary condition for a chiral crystal structure. Chirality in a non-chiral space group results if the molecules or other building blocks of the crystal consist of only one kind of enantiomers or because the molecules or building blocks, without having to be chiral themselves, are arranged in a chiral manner in the crystal.

*Examples*

Trigonal selenium exhibits two enantiomorphic forms that consist of either right-handed or left-handed helical chain molecules (rod groups $\not{p}3_12$ and $\not{p}3_22$, respectively). The molecules as well as the space groups $P3_121$ and $P3_221$ are enantiomorphic and the helical molecules of right-handed

---

[26] Many structural researchers are not aware of the difference between chiral (enantiomorphic) space groups and Sohncke space groups; frequently, even in textbooks, the term 'chiral space group' is used although an achiral Sohncke space group is meant.

**references**