1.4. Space groups and their descriptions

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1.4.1. Symbols of space groups

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1.4.1.1. Introduction

Space groups describe the symmetries of crystal patterns; the point group of the space group is the symmetry of the macroscopic crystal. Both kinds of symmetry are characterized by symbols of which there are different kinds. In this section the space-group numbers as well as the Schoenflies symbols and the Hermann–Mauguin symbols of the space groups and point groups will be dealt with and compared, because these are used throughout this volume. They are rather different in their aims. For the Fedorov symbols, mainly used in Russian crystallographic literature, *cf.* Chapter 3.3. In that chapter the Hermann–Mauguin symbols and their use are also discussed in detail. For computer-adapted symbols of space groups implemented in crystallographic software, such as *Hall symbols* (Hall, 1981*a,b*) or *explicit symbols* (Shmueli, 1984), the reader is referred to Chapter 1.4 of *International Tables for Crystallography*, Volume B (2008).

For the definition of space groups and plane groups, *cf.* Chapter 1.3. The plane groups characterize the symmetries of two-dimensional periodic arrangements, realized in sections and projections of crystal structures or by periodic wallpapers or tilings of planes. They are described individually and in detail in Chapter 2.2. Groups of one- and two-dimensional periodic arrangements embedded in two-dimensional and three-dimensional space are called *subperiodic groups*. They are listed in Vol. E of *International Tables for Crystallography* (2010) (referred to as *IT* E) with symbols similar to the Hermann–Mauguin symbols of plane groups and space groups, and are related to these groups as their subgroups. The space groups *sensu stricto* are the symmetries of periodic arrangements in three-dimensional space, *e.g.* of normal crystals, see also Chapter 1.3. They are described individually and in detail in the space-group tables of Chapter 2.3. In the following, if not specified separately, both space groups and plane groups are covered by the term *space group*.

The description of each space group in the tables of Chapter 2.3 starts with two headlines in which the different symbols of the space group are listed. All these names are explained in this section with the exception of the data for *Patterson symmetry* (*cf.* Chapter 1.6 and Section 2.1.3.5 for explanations of Patterson symmetry).

1.4.1.2. Space-group numbers

The space-group numbers were introduced in *International Tables for X-ray Crystallography* (1952) [referred to as *IT* (1952)] for plane groups (Nos. 1–17) and space groups (Nos. 1–230). They provide a short way of specifying the type of a space group uniquely, albeit without reference to its symmetries. They are particularly convenient for use with computers and have been in use since their introduction.

There are no numbers for the point groups.

1.4.1.3. Schoenflies symbols

The Schoenflies symbols were introduced by Schoenflies (1891, 1923). They describe the point-group type, also known as the geometric crystal class or (for short) crystal class (*cf.* Section 1.3.4.2), of the space group geometrically. The different space-group types within the same crystal class are denoted by a superscript index appended to the point-group symbol.

1.4.1.3.1. Schoenflies symbols of the crystal classes

Schoenflies derived the point groups as groups of crystallographic symmetry operations, but described these crystallographic point groups geometrically by their representation through axes of rotation or rotoreflection and reflection planes (also called mirror planes), *i.e.* by *geometric elements*; for geometric elements of symmetry elements, *cf.* Section 1.2.3, de Wolff *et al.* (1989, 1992) and Flack *et al.* (2000). Rotation axes dominate the description and planes of reflection are added when necessary. Rotoreflection axes are also indicated when necessary. The orientation of a reflection plane, whether *horizontal*, *vertical* or *diagonal*, refers to the plane itself, not to its normal.

A coordinate basis may be chosen by the user: the basis vectors start at the origin which is placed in front of the user. The basis vector **c** points vertically upwards, the basis vectors **a** and **b** lie
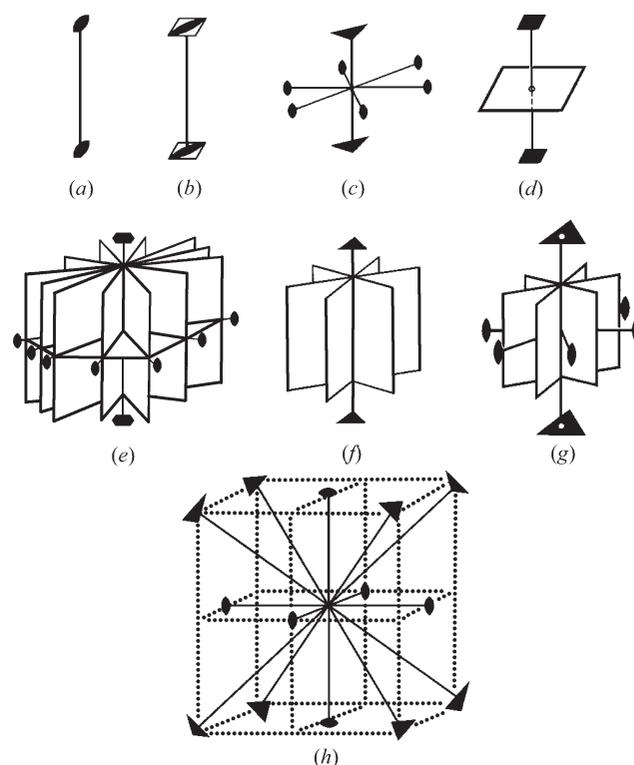

Figure 1.4.1.1
Symmetry-element diagrams of some point groups [adapted from Vainshtein (1994)]. The point groups are specified by their Schoenflies and Hermann–Mauguin symbols. (*a*) $C_2 = 2$, (*b*) $S_4 = \bar{4}$, (*c*) $D_3 = 32$, (*d*) $C_{4h} = 4/m$, (*e*) $D_{6h} = 6/m\,2/m\,2/m$, (*f*) $C_{3v} = 3m$, (*g*) $D_{3d} = \bar{3}\,2/m$, (*h*) $T = 23$. [The cubic frame in part (*h*) has no crystallographic meaning: it has been included to aid visualization of the orientation of the symmetry elements.]