8.1. Basic concepts

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8.1.1. Introduction

The aim of this part is to define and explain some of the concepts and terms frequently used in crystallography, and to present some basic knowledge in order to enable the reader to make best use of the space-group tables.

The reader will be assumed to have some familiarity with analytical geometry and linear algebra, including vector and matrix calculus. Even though one can solve a good number of practical crystallographic problems without this knowledge, some mathematical insight is necessary for a more thorough understanding of crystallography. In particular, the application of symmetry theory to problems in crystal chemistry and crystal physics requires a background of group theory and, sometimes, also of representation theory.

The symmetry of crystals is treated in textbooks by different methods and at different levels of complexity. In this part, a mainly algebraic approach is used, but the geometric viewpoint is presented also. The algebraic approach has two advantages: it facilitates computer applications and it permits statements to be formulated in such a way that they are independent of the dimension of the space. This is frequently done in this part.

A great selection of textbooks and monographs is available for the study of crystallography. Only Giacovazzo (2002) and Vainshtein (1994) will be mentioned here.

Surveys of the history of crystallographic symmetry can be found in Burckhardt (1988) and Lima-de-Faria (1990).

In addition to books, many programs exist by which crystallographic computations can be performed. For example, the programs can be used to derive the classes of point groups, space groups, lattices (Bravais lattices) and crystal families; to calculate the subgroups of point groups and space groups, Wyckoff positions, irreducible representations *etc.* The mathematical program packages *GAP* (Groups, Algorithms and Programming), in particular *CrystGap*, and *Carat* (Crystallographic Algorithms and Tables) are examples of powerful tools for the solution of problems of crystallographic symmetry. For *GAP*, see http://www.gap-system.org/; for *Carat*, see http://wwwb.math.rwth-aachen.de/carat/. Other programs are provided by the crystallographic server in Bilbao: http://www.cryst.ehu.es/cryst/.

Essential for the determination of crystal structures are extremely efficient program systems that implicitly make use of crystallographic (and noncrystallographic) symmetries.

In this part, as well as in the space-group tables of this volume, 'classical' crystallographic groups in three, two and one dimensions are described, *i.e.* space groups, plane groups, line groups and their associated point groups. In addition to three-dimensional crystallography, which is the basis for the treatment of crystal structures, crystallography of two- and one-dimensional space is of practical importance. It is encountered in sections and projections of crystal structures, in mosaics and in frieze ornaments.

There are several expansions of 'classical' crystallographic groups (groups of motions) that are not treated in this volume but will or may be included in future volumes of the *IT* series.

(*a*) Generalization of crystallographic groups to spaces of dimension $n > 3$ is the field of n-dimensional crystallography. Some results are available. The crystallographic symmetry operations for spaces of any dimension n have already been derived by Hermann (1949). The crystallographic groups of four-dimensional space are also completely known and have been tabulated by Brown *et al.* (1978) and Schwarzenberger (1980). The present state of the art and results for higher dimensions are described by Opgenorth *et al.* (1998), Plesken & Schulz (2000) and Souvignier (2003). Some of their results are displayed in Table 8.1.1.1.

(*b*) One can deal with groups of motions whose lattices of translations have lower dimension than the spaces on which the groups act. This expansion yields the *subperiodic groups*. In particular, there are frieze groups (groups in a plane with one-dimensional translations), rod groups (groups in space with one-dimensional translations) and layer groups (groups in space with two-dimensional translations). These subperiodic groups are treated in *IT* E (2002) in a similar way to that in which line groups, plane groups and space groups are treated in this volume. Subperiodic groups are strongly related to 'groups of generalized symmetry'.

(*c*) Incommensurate phases, *e.g.* modulated structures or inclusion compounds, as well as quasicrystals, have led to an extension of crystallography beyond periodicity. Such structures are not really periodic in three-dimensional space but their symmetry may be described as that of an n-dimensional periodic structure, *i.e.* by an n-dimensional space group. In practical cases, $n = 4$, 5 or 6 holds. The crystal structure is then an irrational three-dimensional section through the n-dimensional periodic structure. The description by crystallographic groups of higher-dimensional spaces is thus of practical interest, *cf.* Janssen *et al.* (2004), van Smaalen (1995) or Yamamoto (1996).

(*d*) Generalized symmetry. Other generalizations of crystallographic symmetry combine the geometric symmetry operations with changes of properties: black–white groups, colour groups *etc.* They are treated in the classical book by Shubnikov & Koptsik (1974). Janner (2001) has given an overview of further generalizations.

8.1.2. Spaces and motions

Crystals are objects in the physical three-dimensional space in which we live. A model for the mathematical treatment of this space is the so-called *point space*, which in crystallography is known as *direct* or *crystal space*. In this space, the structures of finite real crystals are idealized as infinite perfect three-dimensional crystal structures (*cf.* Section 8.1.4). This implies that for crystal structures and their symmetries the surfaces of crystals as well as their defects and imperfections are neglected; for most applications, this is an excellent approximation.

The description of crystal structures and their symmetries is not as simple as it appears at first sight. It is useful to consider not only

Table 8.1.1.1. *Number of crystallographic classes for dimensions 1 to 6*

The numbers are those of the *affine* equivalence classes. The numbers for the enantiomorphic pairs are given in parentheses preceded by a + sign (Souvignier, 2003).

Dimension of space	Crystal families	Lattice (Bravais) types	(Geometric) crystal classes	Arithmetic crystal classes	Space-group types
1	1	1	2	2	2
2	4	5	10	13	17
3	6	14	32	73	(+11) 219
4	(+6) 23	(+10) 64	(+44) 227	(+70) 710	(+111) 4783
5	32	189	955	6079	222018
6	91	841	7104	(+30) 85311	(+7052) 28927922

references