of charge from any computer with a web browser *via* the Internet (Aroyo, Perez-Mato *et al.*, 2006; Aroyo, Kirov *et al.*, 2006). Simple retrieval tools give direct access to the figures and tables for any space group. The wavevector database available on the server forms the background of the description and classification of the space-group irreps calculated and applied by different programs of the server.

This chapter is a modification of Chapter 1.5 of the second edition of *International Tables for Crystallography*, Volume B, published in 2001. As in the previous edition, we consider in more detail the reciprocal-space group approach and show that widely used crystallographic conventions can be adopted for the classification of space-group representations. Some basic concepts are developed in Section 1.5.3. Possible conventions are discussed in Section 1.5.4. In contrast to Chapter 1.5 in the second edition of *IT* B, the consequences and advantages of the reciprocal-space group approach are demonstrated and discussed in Section 1.5.5 using examples from the database of the Bilbao Crystallographic Server (1998).

1.5.3. Basic concepts

The aim of this section is to give a brief overview of some of the basic concepts related to groups and their representations. Its content should be of some help to readers who wish to refresh their knowledge of space groups and representations, and to familiarize themselves with the kind of description in this chapter. However, it can not serve as an introductory text for these subjects. The interested reader is referred to books dealing with space-group theory, representations of space groups and their applications in solid-state physics: see BC or Chapter 1.2 of *International Tables for Crystallography* Volume D by Janssen (2003).

1.5.3.1. Representations of finite groups

Group theory is the proper tool for studying symmetry in science. The elements of the crystallographic groups are rigid motions (isometries) with regard to performing one after another. The set of all isometries that map an object onto itself always fulfils the group postulates and is called the symmetry or the symmetry group of that object; the isometry itself is called a symmetry operation. Symmetry groups of crystals are dealt with in this chapter. In addition, groups of matrices with regard to matrix multiplication (matrix groups) are considered frequently. Such groups will sometimes be called realizations or representations of abstract groups.

Many applications of group theory to physical problems are closely related to representation theory, *cf.* Rosen (1981) and references therein. In this section, matrix representations Γ of finite groups $\mathcal{G}$ are considered. The concepts of *homomorphism* and *matrix groups* are of essential importance.

A group $\mathcal{B}$ is a homomorphic image of a group $\mathcal{A}$ if there exists a mapping of the elements a_i of $\mathcal{A}$ onto the elements b_k of $\mathcal{B}$ that preserves the multiplication relation (in general several elements of $\mathcal{A}$ are mapped onto one element of $\mathcal{B}$): if $\mathsf{a}_i \to \mathsf{b}_i$ and $\mathsf{a}_k \to \mathsf{b}_k$, then $\mathsf{a}_i\mathsf{a}_k \to \mathsf{b}_i\mathsf{b}_k$ holds for all elements of $\mathcal{A}$ and $\mathcal{B}$ (the image of the product is equal to the product of the images). In the special case of a one-to-one mapping, the homomorphism is called an *isomorphism*.

A matrix group is a group whose elements are non-singular square matrices. The law of combination is matrix multiplication and the group inverse is the inverse matrix. In the following we will be concerned with some basic properties of finite matrix groups relevant to representations.

Let $\mathcal{M}_1$ and $\mathcal{M}_2$ be two matrix groups whose matrices are of the same dimension. They are said to be equivalent if there exists a (non-singular) matrix $\boldsymbol{S}$ such that $\mathcal{M}_2 = \boldsymbol{S}^{-1}\mathcal{M}_1\boldsymbol{S}$ holds. Equivalence implies isomorphism but the inverse is not true: two matrix groups may be isomorphic without being equivalent. According to the theorem of Schur-Auerbach, every finite matrix group is equivalent to a unitary matrix group (by a unitary matrix group we understand a matrix group consisting entirely of unitary matrices).

A matrix group $\mathcal{M}$ is *reducible* if it is equivalent to a matrix group in which every matrix $\boldsymbol{M}$ is of the form

$$\boldsymbol{R} = \begin{pmatrix} \boldsymbol{D}_1 & \boldsymbol{X} \\ \boldsymbol{O} & \boldsymbol{D}_2 \end{pmatrix},$$

see *e.g.* Lomont (1959), p. 47. The group $\mathcal{M}$ is *completely reducible* if it is equivalent to a matrix group in which for all matrices $\boldsymbol{R}$ the submatrices $\boldsymbol{X}$ are $\boldsymbol{O}$ matrices (consisting of zeros only). According to the theorem of Maschke, a finite matrix group is completely reducible if it is reducible. A matrix group is *irreducible* if it is not reducible.

A (matrix) representation $\Gamma(\mathcal{G})$ of a group $\mathcal{G}$ is a homomorphic mapping of $\mathcal{G}$ onto a matrix group $\mathcal{M}(\mathcal{G})$. In a representation Γ every element $\mathsf{g} \in \mathcal{G}$ is associated with a matrix $\boldsymbol{M}(\mathsf{g})$. The dimension of the matrices is called the dimension of the representation.

The above-mentioned theorems on finite matrix groups can be applied directly to representations: we can restrict the considerations to unitary representations only. Further, since every finite matrix group is either completely reducible into irreducible constituents or irreducible, it follows that the infinite set of all matrix representations of a group is known in principle once the irreps are known. Naturally, the question of how to construct all nonequivalent irreps of a finite group and how to classify them arises.

Linear representations are especially important for applications. In this chapter only linear representations of space groups will be considered. Realizations and representations are homomorphic images of abstract groups, but not all of them are linear. In particular, the action of space groups on point space is a nonlinear realization of the abstract space groups because isometries and thus symmetry operations of space groups $\mathcal{G}$ are nonlinear operations. The same holds for their description by matrix-column pairs $(\boldsymbol{W}, \boldsymbol{w})$,[1] by the general position, or by augmented (4×4) matrices, see *IT* A, Part 8. Therefore, the isomorphic matrix representation of a space group, mostly used by crystallographers and listed in the space-group tables of *IT* A as the general position, is not linear.

1.5.3.2. Space groups

In crystallography one deals with real crystals. In many cases the treatment of the crystal is much simpler, but nevertheless describes the crystal and its properties very well, if the real crystal is replaced by an 'ideal crystal'. The real crystal is then considered to be a finite piece of an undisturbed, periodic, and thus infinitely extended arrangement of particles or their centres: ideal crystals are periodic objects in three-dimensional point space E^3, also called direct space. Periodicity means that there are translations among the symmetry operations of ideal crystals. The symmetry group of an ideal crystal is called its space group $\mathcal{G}$.

Space groups $\mathcal{G}$ are of special interest for our problem because:

(1) their irreps are the subject of the classification to be discussed;

(2) this classification makes use of the isomorphism of certain groups to the so-called symmorphic space groups $\mathcal{G}_0$.

Therefore, space groups are introduced here in a slightly more detailed manner than the other concepts. In doing this we follow the definitions and symbolism of *IT* A, Part 8.

[1] In physics written as the Seitz symbol $(\boldsymbol{W}|\boldsymbol{w})$.