1. GENERAL RELATIONSHIPS AND TECHNIQUES

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 $\Gamma$ 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 $a_i \rightarrow b_i$ and $a_k \rightarrow b_k$, then $a_i a_k \rightarrow b_i b_k$ 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 $S$ such that $\mathcal{M}_2 = S^{-1}\mathcal{M}_1 S$ 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 $M$ is of the form

$$R = \begin{pmatrix} D_1 & X \\ O & D_2 \end{pmatrix},$$

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 $R$ the submatrices $X$ are $O$ 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 $\Gamma$ every element $g \in \mathcal{G}$ is associated with a matrix $M(g)$. 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 $(W, w)$,[1] by the general position, or by augmented $(4 \times 4)$ 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.

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

To each space group $\mathcal{G}$ belongs an infinite set $\mathcal{T}$ of translations, the *translation subgroup* of $\mathcal{G}$. The group $\mathcal{T}$ forms an infinite Abelian invariant subgroup of $\mathcal{G}$. For each translation its translation vector is defined. The set of all translation vectors is called the *vector lattice* **L** of $\mathcal{G}$. Because of the finite size of the atoms constituting the real crystal, the lengths of the translation vectors of the ideal crystal cannot be arbitrarily small; rather there is a lower limit $\delta > 0$ for their length in the range of a few Å.

When referred to a coordinate system $(O, \mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3)$, consisting of an origin $O$ and a basis $\mathbf{a}_k$, the symmetry operations, *i.e.* the elements g: $\tilde{\boldsymbol{x}} = \boldsymbol{Wx} + \boldsymbol{w}$ of the space group $\mathcal{G}$, are described by matrix–column pairs $(\boldsymbol{W}, \boldsymbol{w})$ with matrix part $\boldsymbol{W}$ and column part $\boldsymbol{w}$. The translations of $\mathcal{G}$ are represented by pairs $(\boldsymbol{I}, \boldsymbol{t}_i)$, where $\boldsymbol{I}$ is the $(3 \times 3)$ unit matrix and $\boldsymbol{t}_i$ is the column of coefficients of the translation vector $\mathbf{t}_i \in \mathbf{L}$. The basis can always be chosen such that all columns $\boldsymbol{t}_i$ and no other columns of translations consist of integers. Such a basis $\mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_3$ is called a *primitive basis*. For each vector lattice **L** there exists an infinite number of primitive bases.

The space group $\mathcal{G}$ can be decomposed into right cosets relative to $\mathcal{T}$:

$$\mathcal{G} = \mathcal{T} \ \cup \ \mathcal{T}(\boldsymbol{W}_2, \boldsymbol{w}_2) \ \cup \ldots \cup \ \mathcal{T}(\boldsymbol{W}_i, \boldsymbol{w}_i) \ \cup \ldots \cup \ \mathcal{T}(\boldsymbol{W}_n, \boldsymbol{w}_n).$$
$$(1.5.3.1)$$

The coset representatives form the finite set V = $\{(\boldsymbol{W}_\nu, \boldsymbol{w}_\nu)\}$, $\nu = 1, \ldots, n$, with $(\boldsymbol{W}_1, \boldsymbol{w}_1) = (\boldsymbol{I}, \boldsymbol{o})$, where $\boldsymbol{I}$ is the unit matrix and $\boldsymbol{o}$ is the column consisting of zeros only. The factor group $\mathcal{G}/\mathcal{T}$ is isomorphic to the *point group* $\mathcal{P}$ of $\mathcal{G}$ (called $\bar{\mathcal{G}}$ in books on representation theory) describing the symmetry of the external shape of the macroscopic crystal and being represented by the matrices $\boldsymbol{W}_1, \boldsymbol{W}_2, \ldots, \boldsymbol{W}_n$, $\mathcal{P} = \{\boldsymbol{W}_i\}$. If V can be chosen such that all $\boldsymbol{w}_\nu = \boldsymbol{o}$, then $\mathcal{G}$ is called a *symmorphic space group* $\mathcal{G}_0$. A symmorphic space group can be recognized easily from its conventional Hermann–Mauguin symbol which does not contain any screw or glide component. In terms of group theory, a symmorphic space group is the semidirect product of $\mathcal{T}$ and $\mathcal{P}$, *cf.* BC, p. 44. In symmorphic space groups $\mathcal{G}_0$ (and in no others) there are site-symmetry groups which are isomorphic to the point group $\mathcal{P}$ of $\mathcal{G}_0$. (For the term 'site-symmetry group', see Section 1.5.4.2.)

Space groups can be classified into 219 (*affine*) *space-group types* either by isomorphism or by affine equivalence; the 230 *crystallographic* space-group types are obtained by restricting the transformations available for affine equivalence to those with positive determinant, *cf. IT* A, Section 8.2.1. Many important properties of space groups are shared by all space groups of a type. In such a case one speaks of *properties of the type*. For example, if a space group is symmorphic, then all space groups of its type are symmorphic, so that one normally speaks of a symmorphic space-group type.

With the concept of symmorphic space groups one can also define the arithmetic crystal classes: Let $\mathcal{G}_0$ be a symmorphic space group referred to a primitive basis and V = $\{(\boldsymbol{W}_\nu, \boldsymbol{w}_\nu)\}$ its set of coset representatives with $\boldsymbol{w}_\nu = \boldsymbol{o}$ for all columns. To $\mathcal{G}_0$ all those space groups $\mathcal{G}$ can be assigned for which a primitive basis can be found such that the matrix parts $\boldsymbol{W}_\nu$ of their sets V are the same as those of $\mathcal{G}_0$, only the columns $\boldsymbol{w}_\nu$ may differ. In this way, to a type of symmorphic space groups $\mathcal{G}_0$, other types of space groups are assigned, *i.e.* the space-group types are classified according to the symmorphic space-group types. These classes are called *arithmetic crystal classes* of space groups or of space-group types.

There are 73 arithmetic crystal classes corresponding to the 73 types of symmorphic space groups; between 1 and 16 space-group types belong to an arithmetic crystal class. A matrix-algebraic definition of arithmetic crystal classes and a proposal for their nomenclature can be found in *IT* A, Section 8.2.3; see also Section 8.3.4 and Table 8.3.4.1.

### 1.5.3.3. Representations of the translation group $\mathcal{T}$ and the reciprocal lattice

For representation theory we follow the terminology of BC and CDML.

Let $\mathcal{G}$ be referred to a primitive basis. For the following, the infinite set of translations, based on discrete cyclic groups of infinite order, will be replaced by a (very large) finite set in the usual way, assuming the Born–von Karman boundary conditions

$$(\boldsymbol{I}, \boldsymbol{t}_{bi})^{N_i} = (\boldsymbol{I}, N_i) = (\boldsymbol{I}, \boldsymbol{o}) \qquad (1.5.3.2)$$

to hold, where $\boldsymbol{t}_{bi} = (1, 0, 0), (0, 1, 0)$ or $(0, 0, 1)$ and $N_i$ is a large integer for $i = 1, 2$ or 3, respectively. Then for any lattice translation $(\boldsymbol{I}, \boldsymbol{t})$,

$$(\boldsymbol{I}, \boldsymbol{Nt}) = (\boldsymbol{I}, \boldsymbol{o}) \qquad (1.5.3.3)$$

holds, where $\boldsymbol{Nt}$ is the column $(N_1 t_1, N_2 t_2, N_3 t_3)$. If the (infinitely many) translations mapped in this way onto $(\boldsymbol{I}, \boldsymbol{o})$ form a normal subgroup $\mathcal{T}_1$ of $\mathcal{G}$, then the mapping described by (1.5.3.3) is a homomorphism. There exists a factor group $\mathcal{G}' = \mathcal{G}/\mathcal{T}_1$ of $\mathcal{G}$ relative to $\mathcal{T}_1$ with translation subgroup $\mathcal{T}' = \mathcal{T}/\mathcal{T}_1$ which is finite and is sometimes called the *finite space group*.

Only the irreps of these finite space groups will be considered. The definitions of space-group type, symmorphic space group *etc.* can be transferred to these groups. Because $\mathcal{T}$ is Abelian, $\mathcal{T}'$ is also Abelian. Replacing the space group $\mathcal{G}$ by $\mathcal{G}'$ means that the especially well developed theory of representations of finite groups can be applied, *cf.* Lomont (1959), Jansen & Boon (1967). For convenience, the prime $'$ will be omitted and the symbol $\mathcal{G}$ will be used instead of $\mathcal{G}'$; $\mathcal{T}'$ will be denoted by $\mathcal{T}$ in the following.

Because $\mathcal{T}$ (formerly $\mathcal{T}'$) is Abelian, its irreps $\Gamma(\mathcal{T})$ are one-dimensional and consist of (complex) roots of unity. Owing to equations (1.5.3.2) and (1.5.3.3), the irreps $\Gamma^{q_1 q_2 q_3}[(\boldsymbol{I}, \boldsymbol{t})]$ of $\mathcal{T}$ have the form

$$\Gamma^{q_1 q_2 q_3}[(\boldsymbol{I}, \boldsymbol{t})] = \exp\left[-2\pi i\left(q_1 \frac{t_1}{N_1} + q_2 \frac{t_2}{N_2} + q_3 \frac{t_3}{N_3}\right)\right], \quad (1.5.3.4)$$

where $\boldsymbol{t}$ is the column $(t_1, t_2, t_3)$, $q_j = 0, 1, 2, \ldots, N_j - 1$, $j = 1, 2, 3$, and $t_k$ and $q_j$ are integers.

Given a primitive basis $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ of **L**, mathematicians and crystallographers define the *basis of the dual or reciprocal lattice* $\mathbf{L}^*$ by

$$\mathbf{a}_i \cdot \mathbf{a}_j^* = \delta_{ij}, \qquad (1.5.3.5)$$

where $\mathbf{a} \cdot \mathbf{a}^*$ is the scalar product between the vectors and $\delta_{ij}$ is the unit matrix (see *e.g.* Chapter 1.1, Section 1.1.3). Texts on the physics of solids redefine the basis $\mathbf{a}_1^*, \mathbf{a}_2^*, \mathbf{a}_3^*$ of the *reciprocal lattice* $\mathbf{L}^*$, lengthening each of the basis vectors $\mathbf{a}_j^*$ by the factor $2\pi$. Therefore, in the physicist's convention the relation between the bases of direct and reciprocal lattice reads (*cf.* BC, p. 86):

$$\mathbf{a}_i \cdot \mathbf{a}_j^* = 2\pi \delta_{ij}. \qquad (1.5.3.6)$$

In the present chapter only the physicist's basis of the reciprocal lattice is employed, and hence the use of $\mathbf{a}_j^*$ should not lead to misunderstandings. The set of all vectors $\mathbf{K}$,[2]

$$\mathbf{K} = k_1 \mathbf{a}_1^* + k_2 \mathbf{a}_2^* + k_3 \mathbf{a}_3^*, \qquad (1.5.3.7)$$

$k_i$ integer, is called the lattice reciprocal to **L** or the *reciprocal lattice* $\mathbf{L}^*$.[3]

If one adopts the notation of *IT* A, Part 5, the basis of direct space is denoted by a row $(\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3)^T$, where $(\ )^T$ means trans-

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[2] See Note (1) in Section 1.5.1.
[3] The lattice **L** is often called the *direct lattice*. These names are historically introduced and cannot be changed, although equations (1.5.3.5) and (1.5.3.6) show that essentially neither of the lattices is preferred: they form a pair of *mutually reciprocal* lattices.