1.2. General introduction to the subgroups of space groups

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1.2.1. General remarks

The performance of simple vector and matrix calculations, as well as elementary operations with groups, are nowadays common practice in crystallography, especially since computers and suitable programs have become widely available. The authors of this volume therefore assume that the reader has at least some practical experience with matrices and groups and their crystallographic applications. The explanations and definitions of the basic terms of linear algebra and group theory in these first sections of this introduction are accordingly short. Rather than replace an elementary textbook, these first sections aim to acquaint the reader with the method of presentation and the terminology that the authors have chosen for the tables and graphs of this volume. The concepts of groups, their subgroups, isomorphism, coset decomposition and conjugacy are considered to be essential for the use of the tables and for their practical application to crystal structures; for a deeper understanding the concept of normalizers is also necessary. Frequently, however, an 'intuitive feeling' obtained by practical experience may replace a full comprehension of the mathematical meaning. From Section 1.2.6 onwards, the presentation will be more detailed because the subjects are more specialized (but mostly not more difficult) and are seldom found in textbooks.

1.2.2. Mappings and matrices

1.2.2.1. *Crystallographic symmetry operations*

A crystal is a finite block of an infinite periodic array of atoms in physical space. The infinite periodic array is called the *crystal pattern*. The finite block is called the *macroscopic crystal*.

Periodicity implies that there are *translations* which map the crystal pattern onto itself. Geometric mappings have the property that for each point P of the space, and thus of the object, there is a uniquely determined point $\tilde{P}$, the *image point*. The mapping is *reversible* if each image point $\tilde{P}$ is the image of one point P only.

Translations belong to a special category of mappings which leave all distances in the space invariant (and thus within an object and between objects in the space). Furthermore, a mapping of an object onto itself (German: *Deckoperation*) is the basis of the concept of geometric symmetry. This is expressed by the following two definitions.

Definition 1.2.2.1.1. A mapping is called a *motion*, a *rigid motion* or an *isometry* if it leaves all distances invariant (and thus all angles, as well as the size and shape of an object). In this volume the term 'isometry' is used. □

An isometry is a special kind of affine mapping. In an *affine mapping*, parallel lines are mapped onto parallel lines; lengths and angles may be distorted but quotients of lengths on the same line are preserved. In Section 1.2.2.3, the description of affine mappings is discussed, because this type of description also applies to isometries. Affine mappings are important for the classification of crystallographic symmetries, *cf.* Section 1.2.5.2.

Definition 1.2.2.1.2. A mapping is called a *symmetry operation* of an object if

(1) it is an isometry,
(2) it maps the object onto itself. □

Instead of 'maps the object onto itself', one frequently says 'leaves the object invariant (as a whole)'. This does not mean that each point of the object is mapped onto itself; rather, the object is mapped in such a way that an observer cannot distinguish the states of the object before and after the mapping.

Definition 1.2.2.1.3. A symmetry operation of a crystal pattern is called a *crystallographic symmetry operation*. □

The symmetry operations of a macroscopic crystal are also crystallographic symmetry operations, but they belong to another kind of mapping which will be discussed in Section 1.2.5.4.

There are different types of isometries which may be crystallographic symmetry operations. These types are described and discussed in many textbooks of crystallography and in mathematical, physical and chemical textbooks. They are listed here without further treatment. Fixed points are very important for the characterization of isometries.

Definition 1.2.2.1.4. A point P is a *fixed point* of a mapping if it is mapped onto itself, *i.e.* the *image point* $\tilde{P}$ is the same as the original point P: $\tilde{P} = P$. □

The set of all fixed points of an isometry may be the whole space, a plane in the space, a straight line, a point, or the set may be empty (no fixed point).

The following kinds of isometries exist:

(1) The *identity operation*, which maps each point of the space onto itself. It is a symmetry operation of every object and, although trivial, is indispensable for the group properties which are discussed in Section 1.2.3.
(2) A *translation* t which shifts every object. A translation is characterized by its translation vector $\mathbf{t}$ and has no fixed point: if $\boldsymbol{x}$ is the column of coordinates of a point P, then the coordinates $\tilde{x}$ of the image point $\tilde{P}$ are $\tilde{\boldsymbol{x}} = \boldsymbol{x} + \boldsymbol{t}$. If a translation is a symmetry operation of an object, the object extends infinitely in the directions of $\mathbf{t}$ and $-\mathbf{t}$. A translation preserves the 'handedness' of an object, *e.g.* it maps any right-hand glove onto a right-hand one and any left-hand glove onto a left-hand one.
(3) A *rotation* is an isometry that leaves one line fixed pointwise. This line is called the *rotation axis*. The degree of rotation about this axis is described by its rotation angle φ. In particular, a rotation is called an *N-fold rotation* if the rotation angle is $\varphi = k \times 360°/N$, where k and N are relatively prime integers. A rotation preserves the 'handedness' of any object.
(4) A *screw rotation* is a rotation coupled with a translation parallel to the rotation axis. The rotation axis is now called the *screw axis*. The translation vector is called the *screw vector*. A screw rotation has no fixed points. The screw axis is invariant as a whole under the screw rotation but not pointwise.
(5) An N-fold *rotoinversion* is an N-fold rotation coupled with inversion through a point on the rotation axis. This point is called the *centre of the rotoinversion*. For $N \neq 2$ it is the only fixed point. The axis of the rotation is invariant as a whole

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