1.1. A general introduction to groups

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In this chapter we give a general introduction to group theory, which provides the mathematical background for considering symmetry properties. Starting from basic principles, we discuss those properties of groups that are of particular interest in crystallography. To readers interested in a more elaborate treatment of the theoretical background, the standard textbooks by Armstrong (2010), Hill (1999) or Sternberg (2008) are recommended; an account from the perspective of crystallography can also be found in Müller (2013).

1.1.1. Introduction

Crystal structures may be investigated and classified according to their symmetry properties. But in a strict sense, crystal structures in nature are never perfectly symmetric, due to impurities, structural imperfections and especially their finite extent. Therefore, symmetry considerations deal with *idealized* crystal structures that are free from impurities and structural imperfections and that extend infinitely in all directions. In the mathematical model of such an idealized crystal structure, the atoms are replaced by points in a three-dimensional point space and this model will be called a *crystal pattern*.

A symmetry operation of a crystal pattern is a transformation of three-dimensional space that preserves distances and angles and that leaves the crystal pattern as a whole unchanged. The symmetry of a crystal pattern is then understood as the collection of all symmetry operations of the pattern.

The following simple statements about the symmetry operations of a crystal pattern are almost self-evident:

(*a*) If two symmetry operations are applied successively, the crystal pattern is still invariant, thus the combination of the two operations (called their *composition*) is again a symmetry operation.

(*b*) Every symmetry operation can be reversed by simply moving every point back to its original position.

These observations (together with the fact that leaving all points in their position is also a symmetry operation) show that the symmetry operations of a crystal pattern form an algebraic structure called a *group*.

1.1.2. Basic properties of groups

Although groups occur in innumerable contexts, their basic properties are very simple and are captured by the following definition.

Definition. Let $\mathcal{G}$ be a set of elements on which a binary operation is defined which assigns to each pair (g, h) of elements the composition $g \circ h \in \mathcal{G}$. Then $\mathcal{G}$, together with the binary operation $\circ$, is called a *group* if the following hold:

(i) the binary operation is associative, *i.e.* $(g \circ h) \circ k = g \circ (h \circ k)$;

(ii) there exists a *unit element* or *identity element* $e \in \mathcal{G}$ such that $g \circ e = g$ and $e \circ g = g$ for all $g \in \mathcal{G}$;

(iii) every $g \in \mathcal{G}$ has an inverse element, denoted by g^{-1}, for which $g \circ g^{-1} = g^{-1} \circ g = e$.

In most cases, the composition of group elements is regarded as a *product* and is written as $g \cdot h$ or even gh instead of $g \circ h$. An exception is groups where the composition is addition, *e.g.* a group of translations. In such a case, the composition $\mathbf{a} \circ \mathbf{b}$ is more conveniently written as $\mathbf{a} + \mathbf{b}$.

Examples

(i) The group consisting only of the identity element e (with $e \circ e = e$) is called the *trivial group*.

(ii) The group $3m$ of all symmetries of an equilateral triangle is a group with the composition of symmetry operations as binary operation. The group contains six elements, namely three reflections, two rotations and the identity element. It is schematically displayed in Fig. 1.1.2.2.

(iii) The set $\mathbb{Z}$ of all integers forms a group with addition as operation. The identity element is 0, the inverse element for $a \in \mathbb{Z}$ is $-a$.

(iv) The set of complex numbers with absolute value 1 forms a circle in the complex plane, the *unit circle* S^1. The unit circle can be described by $S^1 = \{\exp(2\pi i\, t) \mid 0 \le t < 1\}$ and forms a group with (complex) multiplication as operation.

(v) The set of all real $n \times n$ matrices with determinant $\neq 0$ is a group with matrix multiplication as operation. This group is called the *general linear group* and denoted by $\mathrm{GL}_n(\mathbb{R})$.

If a group $\mathcal{G}$ contains finitely many elements, it is called a *finite group* and the number of its elements is called the *order* of the group, denoted by $|\mathcal{G}|$. A group with infinitely many elements is called an *infinite group*.

For a group element g, its *order* is the smallest integer $n > 0$ such that $g^n = e$ is the identity element. If there is no such integer, then g is said to be of *infinite order*.

The group operation is not required to be *commutative*, *i.e.* in general one will have $gh \neq hg$. However, a group $\mathcal{G}$ in which $gh = hg$ for all g, h is said to be a *commutative* or *abelian group*.

The inverse of the product gh of two group elements is the product of the inverses of the two elements in reversed order, *i.e.* $(gh)^{-1} = h^{-1}g^{-1}$.

A particularly simple type of groups is *cyclic groups* in which all elements are powers of a single element g. A finite cyclic group $\mathcal{C}_n$ of order n can be written as $\mathcal{C}_n = \{g, g^2, \ldots, g^{n-1}, g^n = e\}$. For example, the rotations that are symmetry operations of an equilateral triangle constitute a cyclic group of order 3.

The group $\mathbb{Z}$ of integers (with addition as operation) is an example of an infinite cyclic group in which negative powers also have to be considered, *i.e.* where $\mathcal{G} = \{\ldots, g^{-2}, g^{-1}, e = g^0, g^1, g^2, \ldots\}$.

Groups of small order may be displayed by their *multiplication table*, which is a square table with rows and columns indexed by the group elements and where the intersection of the row labelled by g and of the column labelled by h is the product gh. It follows immediately from the invertibility of the group elements that each row and column of the multiplication table contains every group element precisely once.

references