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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.

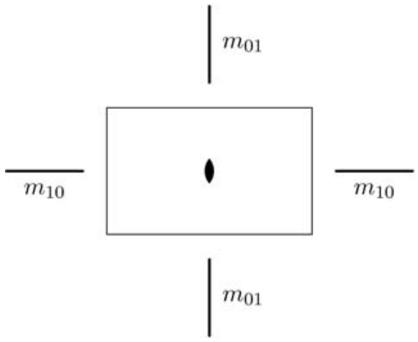

Figure 1.1.2.1
Symmetry group 2*mm* of a rectangle.

Examples

(i) A cyclic group of order 3 consists of the elements $\{g, g^2, g^3 = e\}$. Its multiplication table is

	e	g	g^2
e	e	g	g^2
g	g	g^2	e
g^2	g^2	e	g

(ii) The symmetry group 2*mm* of a rectangle (with unequal sides) consists of a twofold rotation 2, two reflections m_{10}, m_{01} with mirror lines along the coordinate axes and the identity element 1 (see Fig. 1.1.2.1; the small black lenticular symbol in the centre represents the twofold rotation point).

Note that in this and all subsequent examples of crystallographic point groups we will use the Seitz symbols (*cf.* Section 1.4.2.2) for the symmetry operations and the Hermann–Mauguin symbols (*cf.* Section 1.4.1) for the point groups.

The multiplication table of the group 2*mm* is

	1	2	m_{10}	m_{01}
1	1	2	m_{10}	m_{01}
2	2	1	m_{01}	m_{10}
m_{10}	m_{10}	m_{01}	1	2
m_{01}	m_{01}	m_{10}	2	1

The symmetry of the multiplication table (with respect to the main diagonal) shows that this is an abelian group.

(iii) The symmetry group 3*m* of an equilateral triangle consists (apart from the identity element 1) of the threefold rotations 3^+ and 3^- and the reflections m_{10}, m_{01}, m_{11} with mirror lines through a corner of the triangle and the centre of the opposite side (see Fig. 1.1.2.2; the small black triangle in the centre represents the threefold rotation point).

The multiplication table of the group 3*m* is

	1	3^+	3^-	m_{10}	m_{01}	m_{11}
1	1	3^+	3^-	m_{10}	m_{01}	m_{11}
3^+	3^+	3^-	1	m_{11}	m_{10}	m_{01}
3^-	3^-	1	3^+	m_{01}	m_{11}	m_{10}
m_{10}	m_{10}	m_{01}	m_{11}	1	3^+	3^-
m_{01}	m_{01}	m_{11}	m_{10}	3^-	1	3^+
m_{11}	m_{11}	m_{10}	m_{01}	3^+	3^-	1

The fact that $3^+ \cdot m_{10} = m_{11}$, but $m_{10} \cdot 3^+ = m_{01}$ shows that this group is not abelian. It is actually the smallest group (in terms of order) that is not abelian.

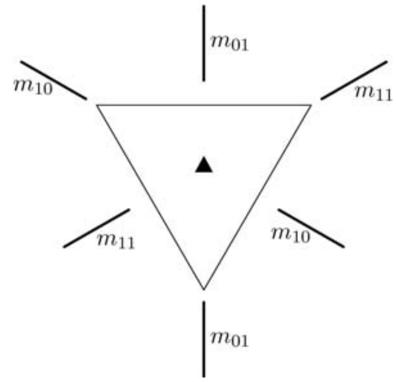

Figure 1.1.2.2
Symmetry group 3*m* of an equilateral triangle.

(iv) The symmetry group 4*mm* of the square consists of the cyclic group generated by the fourfold rotation 4^+ containing the elements $1, 4^+, 2, 4^-$ and the reflections m_{10}, m_{01}, m_{11}, $m_{1\bar{1}}$ with mirror lines along the coordinate axes and the diagonals of the square (see Fig. 1.1.2.3; the small black square in the centre represents the fourfold rotation point).

The multiplication table of the group 4*mm* is

	1	2	4^+	4^-	m_{10}	m_{01}	m_{11}	$m_{1\bar{1}}$
1	1	2	4^+	4^-	m_{10}	m_{01}	m_{11}	$m_{1\bar{1}}$
2	2	1	4^-	4^+	m_{01}	m_{10}	$m_{1\bar{1}}$	m_{11}
4^+	4^+	4^-	2	1	m_{11}	$m_{1\bar{1}}$	m_{01}	m_{10}
4^-	4^-	4^+	1	2	$m_{1\bar{1}}$	m_{11}	m_{10}	m_{01}
m_{10}	m_{10}	m_{01}	$m_{1\bar{1}}$	m_{11}	1	2	4^-	4^+
m_{01}	m_{01}	m_{10}	m_{11}	$m_{1\bar{1}}$	2	1	4^+	4^-
m_{11}	m_{11}	$m_{1\bar{1}}$	m_{10}	m_{01}	4^+	4^-	1	2
$m_{1\bar{1}}$	$m_{1\bar{1}}$	m_{11}	m_{01}	m_{10}	4^-	4^+	2	1

This group is not abelian, because for example $4^+ \cdot m_{10} = m_{11}$, but $m_{10} \cdot 4^+ = m_{1\bar{1}}$.

The groups that are considered in crystallography do not consist of abstract elements but of symmetry operations with a geometric meaning. In the figures illustrating the groups and also in the symbols used for the group elements, this geometric nature is taken into account. For example, the fourfold rotation 4^+ in the group 4*mm* is represented by the small black square placed at the rotation point and the reflection m_{10} by the line fixed by the reflection. To each crystallographic symmetry operation a *geometric element* is assigned which characterizes the type of the

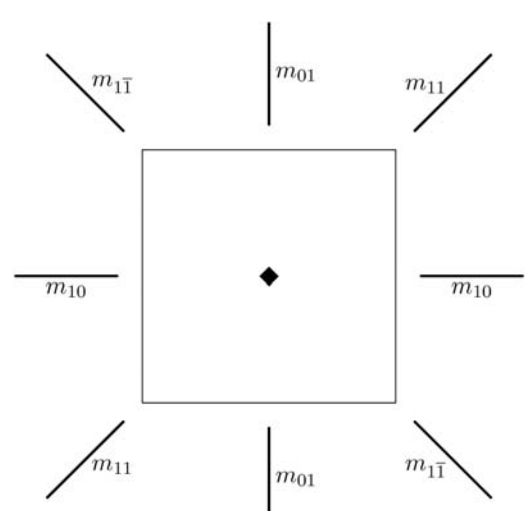

Figure 1.1.2.3
Symmetry group 4*mm* of the square.

symmetry operation. The precise definition of the geometric elements for the different types of operations is given in Section 1.2.3. For a rotation in three-dimensional space the geometric element is the line along the rotation axis and for a reflection it is the plane fixed by the reflection. Different symmetry operations may share the same geometric element, but these operations are then closely related, such as rotations around the same line. One therefore introduces the notion of a *symmetry element*, which is a geometric element together with its associated symmetry operations. In the figures for the crystallographic groups, the symbols like the little black square or the lines actually represent these symmetry elements (and not just a symmetry operation or a geometric element).

It is clear that for larger groups the multiplication table becomes unwieldy to set up and use. Fortunately, for many purposes a full list of all products in the group is actually not required. A very economic alternative of describing a group is to give only a small subset of the group elements from which all other elements can be obtained by forming products.

Definition. A subset $\mathcal{X} \subseteq \mathcal{G}$ is called a set of *generators* for $\mathcal{G}$ if every element of $\mathcal{G}$ can be obtained as a finite product of elements from $\mathcal{X}$ or their inverses. If $\mathcal{X}$ is a set of generators for $\mathcal{G}$, one writes $\mathcal{G} = \langle \mathcal{X} \rangle$.

A group which has a finite generating set is said to be *finitely generated*.

Examples

(i) Every finite group is finitely generated, since $\mathcal{X}$ is allowed to consist of all group elements.

(ii) A cyclic group is generated by a single element. In particular, the infinite cyclic group $(\mathbb{Z}, +)$ is generated by $\mathcal{X} = \{1\}$, but also by $\mathcal{X} = \{-1\}$.

(iii) The symmetry group $4mm$ of the square is generated by a fourfold rotation and any of the reflections, *e.g.* by $\{4^+, m_{10}\}$, but also by two reflections with reflection lines which are not perpendicular, *e.g.* by $\{m_{10}, m_{11}\}$.

(iv) The full symmetry group $m\bar{3}m$ of the cube consists of 48 elements. It can be generated by a fourfold rotation 4^+_{100} around the a axis, a threefold rotation 3^+_{111} around a space diagonal and the inversion $\bar{1}$. It is also possible to generate the group by only two elements, *e.g.* by the fourfold rotation 4^+_{100} and a reflection m_{110} in a plane with normal vector along one of the face diagonals of the cube.

(v) The additive group $(\mathbb{Q}, +)$ of the rational numbers is not finitely generated, because finite sums of finitely many generators $a_1/b_1, a_2/b_2, \ldots, a_n/b_n$ have denominators dividing $b_1 \cdot b_2 \cdot \ldots \cdot b_n$ and thus $1/(1 + b_1 \cdot b_2 \cdot \ldots \cdot b_n)$ is not a finite sum of these generators.

Although one usually chooses generating sets with as few elements as possible, it is sometimes convenient to actually include some redundancy. For example, it may be useful to generate the symmetry group $4mm$ of the square by $\{2, m_{10}, m_{11}\}$. The element 2 is redundant, since $2 = (m_{10}m_{11})^2$, but this generating set explicitly shows the different types of elements of order 2 in the group.

1.1.3. Subgroups

The group of symmetry operations of a crystal pattern may alter if the crystal undergoes a phase transition. Often, some symmetries are preserved, while others are lost, *i.e.* symmetry breaking takes place. The symmetry operations that are preserved form a subset of the original symmetry group which is itself a group. This gives rise to the concept of a subgroup.

Definition. A subset $\mathcal{H} \subseteq \mathcal{G}$ is called a *subgroup* of $\mathcal{G}$ if its elements form a group by themselves. This is denoted by $\mathcal{H} \leq \mathcal{G}$. If $\mathcal{H}$ is a subgroup of $\mathcal{G}$, then $\mathcal{G}$ is called a *supergroup* of $\mathcal{H}$. In order to be a subgroup, $\mathcal{H}$ is required to contain the identity element e of $\mathcal{G}$, to contain inverse elements and to be closed with respect to composition of elements. Thus, technically, every group is a subgroup of itself.

The subgroups of $\mathcal{G}$ that are not equal to $\mathcal{G}$ are called *proper subgroups* of $\mathcal{G}$. A proper subgroup $\mathcal{H}$ of $\mathcal{G}$ is called a *maximal subgroup* if it is not a proper subgroup of any proper subgroup $\mathcal{H}'$ of $\mathcal{G}$.

It is often convenient to specify a subgroup $\mathcal{H}$ of $\mathcal{G}$ by a set $\{h_1, \ldots, h_s\}$ of generators. This is denoted by $\mathcal{H} = \langle h_1, \ldots, h_s \rangle$. The order of $\mathcal{H}$ is not *a priori* obvious from the set of generators. For example, in the symmetry group $4mm$ of the square the pairs $\{m_{10}, m_{01}\}$ and $\{m_{11}, m_{1\bar{1}}\}$ both generate subgroups of order 4, whereas the pair $\{m_{10}, m_{11}\}$ generates the full group of order 8.

The subgroups of a group can be visualized in a *subgroup diagram*. In such a diagram the subgroups are arranged with subgroups of higher order above subgroups of lower order. Two subgroups are connected by a line if one is a maximal subgroup of the other. By following downward paths in this diagram, all group–subgroup relations in a group can be derived. Additional information is provided by connecting subgroups of the same order by a horizontal line if they are *conjugate* (see Section 1.1.7).

Examples

(i) The set $\{e\}$ consisting only of the identity element of $\mathcal{G}$ is a subgroup, called the *trivial subgroup* of $\mathcal{G}$.

(ii) For the group $\mathbb{Z}$ of the integers, all subgroups are cyclic and generated by some integer n, *i.e.* they are of the form $n\mathbb{Z} := \{na \mid a \in \mathbb{Z}\}$ for an integer n. Such a subgroup is maximal if n is a prime number.

(iii) For every element g of a group $\mathcal{G}$, the powers of g form a subgroup of $\mathcal{G}$ which is a cyclic group.

(iv) In $\mathrm{GL}_n(\mathbb{R})$ the matrices of determinant 1 form a subgroup, since the determinant of the matrix product $\boldsymbol{A} \cdot \boldsymbol{B}$ is equal to the product of the determinants of $\boldsymbol{A}$ and $\boldsymbol{B}$.

(v) In the symmetry group $3m$ of an equilateral triangle the rotations form a subgroup of order 3 (see Fig. 1.1.3.1).

(vi) The symmetry group $2mm$ of a rectangle has three subgroups of order 2, generated by the reflection m_{10}, the twofold rotation 2 and the reflection m_{01}, respectively (see Fig. 1.1.3.2).

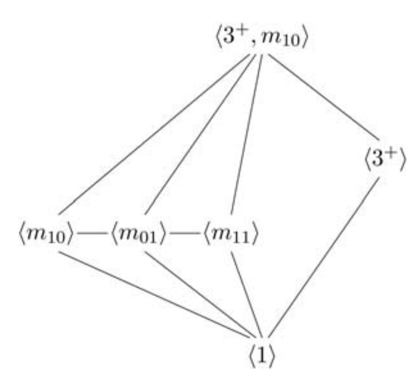

Figure 1.1.3.1
Subgroup diagram for the symmetry group $3m$ of an equilateral triangle.