International Tables for Crystallography (2006). Vol. D, Section 3.2.3.2.1, pp. 381–382.

the image of exactly one element of A, then the mapping φ becomes a *one-to-one correspondence between* A *and* B, $\varphi : \mathsf{A} \leftrightarrow \mathsf{B}$. In this case, A and B are of the same order.

One often encounters a situation in which one assigns to each ordered pair $(\mathbf{S}, \mathbf{M})$ an element $\mathbf{N}$, where all three elements $\mathbf{S}, \mathbf{M}, \mathbf{N}$ are elements from the same set A, symbolically $\varphi : (\mathbf{S}, \mathbf{M}) \mapsto \mathbf{N}$; $\mathbf{S}, \mathbf{M}, \mathbf{N} \in \mathsf{A}$ or $\varphi : \mathsf{A} \times \mathsf{A} \rightarrow \mathsf{A}$. Such a mapping is called a *binary operation* or a *composition law* on the set A. A sum of two numbers $a + b = c$ or a product of two numbers $a \cdot b = c$, where a, b, c belong to the set of all real numbers, are elementary examples of binary operations.

3.2.3.1.4. *Equivalence relation on a set, partition of a set*

The notion of the ordered pair allows one to introduce another useful concept, namely the relation on a set. An example will illustrate this notion. Let $\mathbb{Z}$ be a set of integers, $\mathbb{Z} = \{\ldots, -2, -1, 0, 1, 2, \ldots\}$. For each ordered pair (m, n), $m, n \in \mathbb{Z}$, one can decide whether m is smaller than n, $m < n$, or not. All pairs (m, n) that fulfil the condition $m < n$ form a subset R of all possible ordered pairs $\mathbb{Z} \times \mathbb{Z}$. In other words, the relation $m < n$ defines a subset R of the set $\mathbb{Z} \times \mathbb{Z}$, $\mathsf{R} \subset \mathbb{Z} \times \mathbb{Z}$. Similarly, the relation $|m| = |n|$ ($|n|$ denotes absolute value of n) defines another subset of $\mathbb{Z} \times \mathbb{Z}$.

To indicate that an element $\mathbf{S}$ is related to $\mathbf{M}$ by $\overset{\mathsf{R}}{\sim}$, where $\mathbf{S}, \mathbf{M} \in \mathsf{A}$, one writes $\mathbf{S} \overset{\mathsf{R}}{\sim} \mathbf{M}$, where the relation R defines a subset R of all ordered pairs $\mathsf{A} \times \mathsf{A}$, $\mathsf{R} \subset \mathsf{A} \times \mathsf{A}$ (the same letter R is used for the subset and for the relation on A). The opposite also holds: Each subset R of $\mathsf{A} \times \mathsf{A}$ defines a certain relation $\overset{\mathsf{R}}{\sim}$ on A.

A relation $\overset{\mathsf{R}}{\sim}$ is called an *equivalence relation on the set* A if it satisfies three conditions:

$$\mathbf{S} \overset{\mathsf{R}}{\sim} \mathbf{S} \text{ for all } \mathbf{S} \in \mathsf{A} \ (\textit{reflexivity}), \tag{3.2.3.3}$$

$$\text{if } \mathbf{S}, \mathbf{M} \in \mathsf{A} \text{ and } \mathbf{S} \overset{\mathsf{R}}{\sim} \mathbf{M}, \text{ then } \mathbf{M} \overset{\mathsf{R}}{\sim} \mathbf{S} \ (\textit{symmetry}), \tag{3.2.3.4}$$

$$\text{if } \mathbf{S}, \mathbf{M}, \mathbf{N} \in \mathsf{A}, \ \mathbf{S} \overset{\mathsf{R}}{\sim} \mathbf{M} \text{ and } \mathbf{M} \overset{\mathsf{R}}{\sim} \mathbf{N}, \text{ then } \mathbf{S} \overset{\mathsf{R}}{\sim} \mathbf{N} \ (\textit{transitivity}). \tag{3.2.3.5}$$

Thus, for example, it is easy to corroborate that the relation $|m| = |n|$ on the set of integers $\mathbb{Z}$ fulfils all three conditions (3.2.3.3) to (3.2.3.5) and is, therefore, an equivalence relation on the set $\mathbb{Z}$. On the other hand, the relation $m < n$ is not an equivalence relation on $\mathbb{Z}$ since it fulfils neither the reflexivity (3.2.3.3) nor the symmetry condition (3.2.3.4).

Let $\overset{\mathsf{R}}{\sim}$ be an equivalence relation on A and $\mathbf{S} \in \mathsf{A}$; all elements $\mathbf{M} \in \mathsf{A}$ such that $\mathbf{M} \overset{\mathsf{R}}{\sim} \mathbf{S}$ constitute a subset of A denoted $[\mathbf{S}]_{\mathsf{R}}$ and called the *equivalence class of* $\mathbf{S}$ *with respect to* $\overset{\mathsf{R}}{\sim}$ (or the R-*equivalence class of* $\mathbf{S}$). The element $\mathbf{S}$ is called the *representative* of the class $[\mathbf{S}]_{\mathsf{R}}$. Any other member of the class can be chosen as its representative. Any two elements of the equivalence class $[\mathbf{S}]_{\mathsf{R}}$ are R-*equivalent elements of* A.

From the definition of the equivalence class, it follows that any two elements $\mathbf{M}, \mathbf{N} \in \mathsf{A}$ are either R-equivalent elements of A, $\mathbf{M} \overset{\mathsf{R}}{\sim} \mathbf{N}$, and thus belong to the same class, $[\mathbf{M}]_{\mathsf{R}} = [\mathbf{N}]_{\mathsf{R}}$, or are not R-equivalent, and thus belong to two different classes that are disjoint, $[\mathbf{M}]_{\mathsf{R}} \cap [\mathbf{N}]_{\mathsf{R}} = \emptyset$. In this way, the equivalence relation $\overset{\mathsf{R}}{\sim}$ divides the set A into disjoint subsets (equivalence classes), the union of which is equal to the set itself. Such a decomposition is called a *partition of the set* A *associated with the equivalence relation* $\overset{\mathsf{R}}{\sim}$. For a finite set A this decomposition can be expressed as a union of equivalence classes,

$$\mathsf{A} = [\mathbf{S}]_{\mathsf{R}} \cup [\mathbf{M}]_{\mathsf{R}} \cup \ldots \cup [\mathbf{Q}]_{\mathsf{R}}, \tag{3.2.3.6}$$

where $\mathbf{S}, \mathbf{M}, \ldots, \mathbf{Q}$ are representatives of the equivalence classes.

Generally, any decomposition of a set into a system of disjoint non-empty subsets such that every element of the set is a member of just one subset is called a *partition of the set*. To any partition of a set A there corresponds an equivalence relation $\overset{\mathsf{R}}{\sim}$ such that the R-equivalence classes of A form that partition. This equivalence relation defines two elements as equivalent if and only if they belong to the same subset.

The term 'equivalent' is often used when it is clear from the context what the relevant equivalence relation is. Similarly, the term 'class' is used instead of 'equivalence class'. Sometimes equivalence classes have names that do not explicitly indicate that they are equivalence classes. For example, in group theory, conjugate subgroups, left, right and double cosets form equivalence classes (see Section 3.2.3.2). Often instead of the expression 'partition of a set A' an equivalent expression 'classification of the elements of a set A' is used. The most important equivalence classes in the symmetry analysis of domain structures are called orbits and will be discussed in Section 3.2.3.3.

More details on set theory can be found in Kuratowski & Mostowski (1968), Lipschutz (1981), and Opechowski (1986).

3.2.3.2. *Groups and subgroups*

3.2.3.2.1. *Groups*

Operations (isometries) that act on a body without changing its form and internal state combine in the same way as do elements of a group. Group theory is, therefore, the main mathematical tool for examining transformation properties – symmetry properties in particular – of crystalline objects. The basic concept of group theory is that of a group.

Definition 3.2.3.2. A *group G* is a set that satisfies four postulates:

(1) To each ordered pair (g_i, g_j) of two elements of G, there corresponds a unique element g_k of G, *i.e.* a binary operation (composition law) is defined on the set G. Usually, one writes the ordered pair simply as a 'product' $g_i g_j$ and the composition law as an equation,

$$g_i g_j = g_k, \quad g_i, g_j, g_k \in G. \tag{3.2.3.7}$$

This condition is referred to as *closure of G under multiplication.*

(2) The *multiplication is associative*, *i.e.* for any three elements g_i, g_j, g_k of G it holds that if $g_i g_j = g_l$ and $g_j g_k = g_m$ then $g_l g_k = g_i g_m$. This condition is usually written as one equation,

$$(g_i g_j) g_k = g_i (g_j g_k), \tag{3.2.3.8}$$

which expresses the requirement that the product of any three elements of G is the same, no matter which two of the three one multiplies first, as long as the order in which they stand is not changed. From postulate (2) it follows that the product of any finite sequence of group elements is determined uniquely if the order in which the elements are placed is preserved.

(3) The set G contains an *identity* or *unit element e* such that

$$eg = ge = g \text{ for any element } g \in G. \tag{3.2.3.9}$$

(4) For any element $g \in G$ there exists an *inverse element* g^{-1} such that

$$gg^{-1} = g^{-1}g = e. \tag{3.2.3.10}$$

The number of elements of a group G is called the *order of the group*. If the order of the group is finite, it is denoted by $|G|$.

The multiplication of group elements is, in general, not commutative, *i.e.* $g_i g_j \neq g_j g_i$ may hold for some $g_i, g_j \in G$. If the multiplication is commutative, *i.e.* if $g_i g_j = g_j g_i$ for all $g_i, g_j \in G$, then the group G is called a *commutative* or *Abelian group*. All groups of orders 1 to 5 are Abelian. In Abelian groups, an *additive notation* is sometimes used instead of the *multiplicative notation*, *i.e.* if g_i and g_k are elements of an Abelian group G then one writes $g_i + g_k$ instead of $g_i g_k$. Additive notation is usually used in groups of translations.

The *nth power* g^n of an element $g \in G$, where n is a positive integer, is defined recursively in the following manner:

(i) $g^0 = e$, $g^1 = g$, where e is a unit element of G;
(ii) $g^{n+1} = g^n g$;
(iii) $g^{-n} = (g^n)^{-1}$.

If G is written additively, one writes ng instead of g^n and speaks of a *multiple of g*.

If m and n are integers and g is an element of G then the following *laws of exponents* hold:

$$g^m g^n = g^{m+n} = g^n g^m, \qquad (3.2.3.11)$$

$$(g^m)^n = g^{mn} = (g^n)^m. \qquad (3.2.3.12)$$

A set of elements $\{g_1, g_2, \ldots\}$ of a group G is called a *set of generators of G* if any element of the group G can be written as a product of powers of these generators. In general, a group may have several sets of generators.

The *order of an element g* is the smallest positive integer m such that $g^m = e$. An element g and the inverse element g^{-1} have the same order. The order m of any element g of a finite group G is a factor of the order $|G|$.

Two groups G and G' with elements $g_1, g_2, \ldots, g_i, \ldots$ and $g'_1, g'_2, \ldots, g'_i, \ldots$, respectively, are *isomorphic* if there is an one-to-one correspondence φ between G and G',

$$\varphi : g_i \leftrightarrow g'_i \text{ for each } g_i \in G, \qquad (3.2.3.13)$$

such that

$$\text{whenever } \varphi : g_i \leftrightarrow g'_i \text{ and } \varphi : g_j \leftrightarrow g'_j, \text{ then } \varphi : g_i g_j \leftrightarrow g'_i g'_j. \qquad (3.2.3.14)$$

In other words, the *isomorphism of two groups G and G′* is a one-to-one mapping of G onto G' [(3.2.3.13)] which preserves the products of the elements of the two groups [(3.2.3.14)]. Two isomorphic groups G and G' are denoted as $G \cong G'$.

Isomorphism is an equivalence relation that divides the set of all groups into classes of isomorphic groups. Between two groups G and G' there may exist several isomorphisms.

Groups that appear in Chapters 3.3 and 3.4 are mostly *crystallographic groups* [for their definition and properties see Bradley & Cracknell (1972), Hahn & Wondratschek (1994), *IT* A (2002), *IT* A1 (2003), Janssen (1973), Opechowski (1986), and Vainshtein (1994)]. Elements of these groups are distance-preserving transformations (mappings) called *isometries*, *Euclidean transformations*, *motions* or *crystallographic operations*. Whenever we encounter crystallographic groups we shall use the term 'crystallographic operation' or just 'operation' or 'isometry' instead of 'element'.

In what follows, the group G may be a crystallographic point group or a crystallographic space group. Since we shall be mainly concerned with a continuum approach, we shall have in mind point groups. When we consider space groups, we shall mention this explicitly and, if possible, use calligraphic letters, *e.g.* $\mathcal{G}$, $\mathcal{F}$ *etc.* for space groups.

Crystallographic operations of crystallographic point groups and products of these operations can be found by means of the multiplication calculator in the software *GI⋆KoBo*-1 under the menu item *Group Elements* (see the manual for *GI⋆KoBo*-1).

3.2.3.2.2. *Subgroups*

Definition 3.2.3.3. Let G be a group. A subset F of G is a *subgroup of G* if it forms a group under the product rule of G, *i.e.* if it fulfils the group postulates (1) to (4).

For finite groups these requirements can be replaced by a single condition [see *e.g.* Opechowski (1986)]: The product of any two elements f_i, f_j of F belongs to F,

$$f_i f_j = f_k, \quad f_k \in F \text{ for any } f_i, f_j \in F. \qquad (3.2.3.15)$$

The groups G and F are denoted the *high-symmetry group* and the *low-symmetry group*, respectively. The pair '*group G – subgroup F*' is called the *symmetry descent* $G \supset F$, *dissymmetrization* $G \supset F$ or *symmetry reduction* $G \supset F$. A symmetry descent is a basic specification of a phase transition and corresponding domain structure (see Chapters 3.1 and 3.4).

Each group G always has at least two subgroups: the group G itself (sometimes called the *improper subgroup*) and the *trivial subgroup* consisting of the unit element only. The symbol $F \subseteq G$ signifies that F is a subgroup of G including the improper subgroup G, whereas $F \subset G$ means that F is a *proper subgroup* of G which differs from G. By this definition, the trivial subgroup is a proper subgroup. This definition of a proper subgroup [used *e.g.* in Volume A of the present series (*IT* A, 2002) and by Opechowski (1986)] is convenient for our purposes, although often by the term 'proper subgroup' one understands a subgroup different from G and from the trivial subgroup.

A proper subgroup F of G is a *maximal subgroup of G* if it is not a proper subgroup of some other proper subgroup H, *i.e.* if there exists no group H such that $F \subset H \subset G$. A group can have more than one maximal subgroup.

A group P for which G is subgroup is called a *supergroup of G*, $G \subseteq P$. If G is a proper subgroup of Q, $G \subset Q$, then Q is a *proper supergroup of G*. If G is a maximal subgroup of P, then P is called a *minimal supergroup of G*.

Let a group L be a proper supergroup of a group F, $F \subset L$, and simultaneously a proper subgroup of a group G, $L \subset G$. Then the sequence of subgroups

$$F \subset L \subset G \qquad (3.2.3.16)$$

will be called a *group–subgroup chain* and the group L an *intermediate group* of the chain (3.2.3.16).

Subgroups of crystallographic point groups are listed in Table 3.4.2.7 and are displayed in Figs. 3.1.3.1 and 3.1.3.2 (see also the software *GI⋆KoBo*-1, menu item *Subgroups*).

3.2.3.2.3. *Left and right cosets*

If F_1 is a proper subgroup of G and g_i is a fixed element of G, then the set of all products $g_i f$, where f runs over all elements of the subgroup F_1, is denoted $g_i F_1$ and is called the *left coset of F_1 in G*,

$$g_i F_1 = \{g_i f \,|\, \forall f \in F_1\}, \quad g_i \in G, \quad F_1 \subset G, \qquad (3.2.3.17)$$

where the sign $\forall$ means 'for all'. Similarly, one defines a *right coset of F_1 in G*:

$$F_1 g_i = \{f g_i \,|\, \forall f \in F_1\}, \quad g_i \in G, \quad F_1 \subset G. \qquad (3.2.3.18)$$

[Some authors, *e.g.* Hall (1959), call the set $g_i F_1$ a right coset of F_1 in G and the set $F_1 g_i$ a left coset of F_1 in G.] Since in the application of cosets in the symmetry analysis of domain structures left cosets are used almost exclusively, all statements that follow are formulated for left cosets. Each statement about left cosets has a complementary statement about right cosets which can in most cases be obtained by replacing 'left' with 'right'.

The element g_i which appears explicitly in the symbol $g_i F_1$ of the left coset of F_1 is called a *representative of the left coset* $g_i F_1$. Any element of a left coset can be chosen as its representative.

Left coset criterion: Two elements g_i and g_j belong to the same left coset, $g_i F_1 = g_j F_1$, if and only if $g_i^{-1} g_j$ belongs to the subgroup F_1, $g_i^{-1} g_j \in F_1$.