

1.2. GENERAL INTRODUCTION TO THE SUBGROUPS OF SPACE GROUPS

1.2.4. Subgroups

1.2.4.1. Definition

There may be sets of elements  $g_k \in \mathcal{G}$  that do not constitute the full group  $\mathcal{G}$  but nevertheless fulfil the group postulates for themselves.

**Definition 1.2.4.1.1.** A subset  $\mathcal{H}$  of elements of a group  $\mathcal{G}$  is called a *subgroup*  $\mathcal{H}$  of  $\mathcal{G}$  if it fulfils the group postulates with respect to the law of composition of  $\mathcal{G}$ .  $\square$

Remarks:

- (1) The group  $\mathcal{G}$  is considered to be one of its own subgroups. If subgroups  $\mathcal{H}_j$  are discussed where  $\mathcal{G}$  is included among the subgroups, we write  $\mathcal{H}_j \leq \mathcal{G}$  or  $\mathcal{G} \geq \mathcal{H}_j$ . If  $\mathcal{G}$  is excluded from the set  $\{\mathcal{H}_j\}$  of its subgroups, we write  $\mathcal{H}_j < \mathcal{G}$  or  $\mathcal{G} > \mathcal{H}_j$ . A subgroup  $\mathcal{H}_j < \mathcal{G}$  is called a *proper subgroup* of  $\mathcal{G}$ .
- (2) In a relation  $\mathcal{G} \geq \mathcal{H}$  or  $\mathcal{G} > \mathcal{H}$ ,  $\mathcal{G}$  is called a *supergroup* of  $\mathcal{H}$ . The symbols  $\leq$ ,  $\geq$ ,  $<$  and  $>$  are used for supergroups in the same way as they are used for subgroups, cf. Section 2.1.6.
- (3) A subgroup of a finite group is finite. A subgroup of an infinite group may be finite or infinite.
- (4) A subset  $\mathcal{K}$  of elements  $g_k \in \mathcal{G}$  which does not necessarily form a group is designated by the symbol  $\mathcal{K} \subset \mathcal{G}$ .

**Definition 1.2.4.1.2.** A subgroup  $\mathcal{H} < \mathcal{G}$  is a *maximal subgroup* if no group  $\mathcal{Z}$  exists for which  $\mathcal{H} < \mathcal{Z} < \mathcal{G}$  holds. If  $\mathcal{H}$  is a maximal subgroup of  $\mathcal{G}$ , then  $\mathcal{G}$  is a *minimal supergroup* of  $\mathcal{H}$ .  $\square$

This definition is very important for the tables of this volume, as only maximal subgroups of space groups are listed. If all maximal subgroups are known for any given space group, then any general subgroup  $\mathcal{H} < \mathcal{G}$  can be obtained by a (finite) chain of maximal subgroups between  $\mathcal{G}$  and  $\mathcal{H}$ , see Section 1.2.6.2. Moreover, the relations between a space group and its maximal subgroups are particularly transparent, cf. Lemma 1.2.8.1.3.

1.2.4.2. Coset decomposition and normal subgroups

Let  $\mathcal{H} < \mathcal{G}$  be a subgroup of  $\mathcal{G}$  of order  $|\mathcal{H}|$ . Because  $\mathcal{H}$  is a proper subgroup of  $\mathcal{G}$  there must be elements  $g_q \in \mathcal{G}$  that are not elements of  $\mathcal{H}$ . Let  $g_2 \in \mathcal{G}$  be one of them. Then the set of elements  $g_2\mathcal{H} = \{g_2 h_j | h_j \in \mathcal{H}\}^3$  is a subset of elements of  $\mathcal{G}$  with the property that all its elements are different and that the sets  $\mathcal{H}$  and  $g_2\mathcal{H}$  have no element in common. Thus, the set  $g_2\mathcal{H}$  also contains  $|\mathcal{H}|$  elements of  $\mathcal{G}$ . If there is another element  $g_3 \in \mathcal{G}$  which belongs neither to  $\mathcal{H}$  nor to  $g_2\mathcal{H}$ , one can form another set  $g_3\mathcal{H} = \{g_3 h_j | h_j \in \mathcal{H}\}$ . All elements of  $g_3\mathcal{H}$  are different and none occurs already in  $\mathcal{H}$  or in  $g_2\mathcal{H}$ . This procedure can be continued until each element  $g_r \in \mathcal{G}$  belongs to one of these sets. In this way the group  $\mathcal{G}$  can be partitioned, such that each element  $g \in \mathcal{G}$  belongs to exactly one of these sets.

**Definition 1.2.4.2.1.** The partition just described is called a *decomposition*  $(\mathcal{G} : \mathcal{H})$  into *left cosets* of the group  $\mathcal{G}$  relative to the group  $\mathcal{H}$ . The sets  $g_p\mathcal{H}$ ,  $p = 1, \dots, i$  are called *left cosets*, because the elements  $h_j \in \mathcal{H}$  are multiplied with the new elements from the left-hand side. The procedure is called a *decomposition into right cosets*  $\mathcal{H}g_s$  if the elements  $h_j \in \mathcal{H}$  are multiplied with the new elements  $g_s$  from the right-hand side. The elements  $g_p$  or

$g_s$  are called the *coset representatives*. The number of cosets is called the *index*  $i = |\mathcal{G} : \mathcal{H}|$  of  $\mathcal{H}$  in  $\mathcal{G}$ .  $\square$

Remarks:

- (1) The group  $\mathcal{H} = g_1\mathcal{H}$  with  $g_1 = e$  is the first coset for both kinds of decomposition. It is the only coset which forms a group by itself.
- (2) All cosets have the same *length*, i.e. the same number of elements, which is equal to  $|\mathcal{H}|$ , the order of  $\mathcal{H}$ .
- (3) The index  $i$  is the same for both right and left decompositions. In IT A and in this volume, the index is frequently designated by the symbol  $[i]$ .
- (4) A coset does not depend on its representative element; starting from any of its elements will result in the same coset. The right cosets may be different from the left ones and the representatives of the right and left cosets may also differ.
- (5) If the order  $|\mathcal{G}|$  of  $\mathcal{G}$  is infinite, then either the order  $|\mathcal{H}|$  of  $\mathcal{H}$  or the index  $i = |\mathcal{G} : \mathcal{H}|$  of  $\mathcal{H}$  in  $\mathcal{G}$  or both are infinite.
- (6) The coset decomposition of a space group  $\mathcal{G}$  relative to its translation subgroup  $\mathcal{T}(\mathcal{G})$  is fundamental in crystallography, cf. Section 1.2.5.4.

From its definition and from the properties of the coset decomposition mentioned above, one immediately obtains the fundamental theorem of Lagrange (for another formulation, see Chapter 1.5):

**Lemma 1.2.4.2.2.** *Lagrange's theorem:* Let  $\mathcal{G}$  be a group of finite order  $|\mathcal{G}|$  and  $\mathcal{H} < \mathcal{G}$  a subgroup of  $\mathcal{G}$  of order  $|\mathcal{H}|$ . Then  $|\mathcal{H}|$  is a divisor of  $|\mathcal{G}|$  and the equation  $|\mathcal{H}| \times i = |\mathcal{G}|$  holds where  $i = |\mathcal{G} : \mathcal{H}|$  is the index of  $\mathcal{H}$  in  $\mathcal{G}$ .  $\square$

A special situation exists when the left and right coset decompositions of  $\mathcal{G}$  relative to  $\mathcal{H}$  result in the partition of  $\mathcal{G}$  into the same cosets:

$$g_p\mathcal{H} = \mathcal{H}g_p \text{ for all } 1 \leq p \leq i. \quad (1.2.4.1)$$

Subgroups  $\mathcal{H}$  that fulfil equation (1.2.4.1) are called 'normal subgroups' according to the following definition:

**Definition 1.2.4.2.3.** A subgroup  $\mathcal{H} < \mathcal{G}$  is called a *normal subgroup* or *invariant subgroup* of  $\mathcal{G}$ ,  $\mathcal{H} \triangleleft \mathcal{G}$ , if equation (1.2.4.1) is fulfilled.  $\square$

The relation  $\mathcal{H} \triangleleft \mathcal{G}$  always holds for  $|\mathcal{G} : \mathcal{H}| = 2$ , i.e. subgroups of index 2 are always normal subgroups. The subgroup  $\mathcal{H}$  contains half of the elements of  $\mathcal{G}$ , whereas the other half of the elements forms 'the other' coset. This coset must then be the right as well as the left coset.

1.2.4.3. Conjugate elements and conjugate subgroups

In a coset decomposition, the set of all elements of the group  $\mathcal{G}$  is partitioned into cosets which form classes in the mathematical sense of the word, i.e. each element of  $\mathcal{G}$  belongs to exactly one coset.

Another equally important partition of the group  $\mathcal{G}$  into classes of elements arises from the following definition:

**Definition 1.2.4.3.1.** Two elements  $g_j, g_k \in \mathcal{G}$  are called *conjugate* if there is an element  $g_q \in \mathcal{G}$  such that  $g_q^{-1}g_jg_q = g_k$ .  $\square$

Remarks:

- (1) Definition 1.2.4.3.1 partitions the elements of  $\mathcal{G}$  into classes of conjugate elements which are called *conjugacy classes of elements*.
- (2) The unit element always forms a conjugacy class by itself.

<sup>3</sup> The formulation  $g_2\mathcal{H} = \{g_2 h_j | h_j \in \mathcal{H}\}$  means: ' $g_2\mathcal{H}$  is the set of the products  $g_2 h_j$  of  $g_2$  with all elements  $h_j \in \mathcal{H}$ '.

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- (3) Each element of an Abelian group forms a conjugacy class by itself.
- (4) Elements of the same conjugacy class have the same order.
- (5) Different conjugacy classes may contain different numbers of elements, *i.e.* have different ‘lengths’.

Not only the individual elements of a group  $\mathcal{G}$  but also the subgroups of  $\mathcal{G}$  can be classified in conjugacy classes.

**Definition 1.2.4.3.2.** Two subgroups  $\mathcal{H}_j, \mathcal{H}_k < \mathcal{G}$  are called *conjugate* if there is an element  $g_q \in \mathcal{G}$  such that  $g_q^{-1} \mathcal{H}_j g_q = \mathcal{H}_k$  holds. This relation is often written  $\mathcal{H}_j^{g_q} = \mathcal{H}_k$ .  $\square$

*Remarks:*

- (1) The ‘trivial subgroup’  $\mathcal{I}$  (consisting only of the unit element of  $\mathcal{G}$ ) and the group  $\mathcal{G}$  itself each form a conjugacy class by themselves.
- (2) Each subgroup of an Abelian group forms a conjugacy class by itself.
- (3) Subgroups in the same conjugacy class are isomorphic and thus have the same order.
- (4) Different conjugacy classes of subgroups may contain different numbers of subgroups, *i.e.* have different lengths.

Equation (1.2.4.1) can be written

$$\mathcal{H} = g_p^{-1} \mathcal{H} g_p \text{ or } \mathcal{H} = \mathcal{H}^{g_p} \text{ for all } p; 1 \leq p \leq i. \quad (1.2.4.2)$$

Using conjugation, Definition 1.2.4.2.3 can be formulated as

**Definition 1.2.4.3.3.** A subgroup  $\mathcal{H}$  of a group  $\mathcal{G}$  is a normal subgroup  $\mathcal{H} \triangleleft \mathcal{G}$  if it is identical with all of its conjugates, *i.e.* if its conjugacy class consists of the one subgroup  $\mathcal{H}$  only.  $\square$

### 1.2.4.4. Factor groups and homomorphism

For the following definition, the ‘product of sets of group elements’ will be used:

**Definition 1.2.4.4.1.** Let  $\mathcal{G}$  be a group and  $\mathcal{K}_j = \{g_{j_1}, \dots, g_{j_n}\}$ ,  $\mathcal{K}_k = \{g_{k_1}, \dots, g_{k_m}\}$  be two arbitrary sets of its elements which are not necessarily groups themselves. Then the product  $\mathcal{K}_j \mathcal{K}_k$  of  $\mathcal{K}_j$  and  $\mathcal{K}_k$  is the set of all products  $\mathcal{K}_j \mathcal{K}_k = \{g_{j_p} g_{k_q} \mid g_{j_p} \in \mathcal{K}_j, g_{k_q} \in \mathcal{K}_k\}$ .<sup>4</sup>  $\square$

The coset decomposition of a group  $\mathcal{G}$  relative to a normal subgroup  $\mathcal{H} \triangleleft \mathcal{G}$  has a property which makes it particularly useful for displaying the structure of a group.

Consider the coset decomposition with the cosets  $\mathcal{S}_j$  and  $\mathcal{S}_k$  of a group  $\mathcal{G}$  relative to its subgroup  $\mathcal{H} < \mathcal{G}$ . In general the product  $\mathcal{S}_j \mathcal{S}_k$  of two cosets, *cf.* Definition 1.2.4.4.1, will not be a coset again. However, if and only if  $\mathcal{H} \triangleleft \mathcal{G}$  is a normal subgroup of  $\mathcal{G}$ , the product of two cosets is always another coset. This means that for the set of all cosets of a normal subgroup  $\mathcal{H} \triangleleft \mathcal{G}$  there exists a law of composition for which the closure is fulfilled. One can show that the other group postulates are also fulfilled for the cosets and their multiplication if  $\mathcal{H} \triangleleft \mathcal{G}$  holds: there is a neutral element (which is  $\mathcal{H}$ ), for each coset  $g\mathcal{H} = \mathcal{H}g$  the coset  $g^{-1}\mathcal{H} = \mathcal{H}g^{-1}$  forms the inverse element and for the coset multiplication the associative law holds.

**Definition 1.2.4.4.2.** Let  $\mathcal{H} \triangleleft \mathcal{G}$ . The cosets of the decomposition of the group  $\mathcal{G}$  relative to the normal subgroup  $\mathcal{H} \triangleleft \mathcal{G}$  form a group with respect to the composition law of coset multiplication. This

group is called the *factor group*  $\mathcal{G}/\mathcal{H}$ . Its order is  $|\mathcal{G} : \mathcal{H}|$ , *i.e.* the index of  $\mathcal{H}$  in  $\mathcal{G}$ .  $\square$

A factor group  $\mathcal{F} = \mathcal{G}/\mathcal{H}$  is not necessarily isomorphic to a subgroup  $\mathcal{H}_j < \mathcal{G}$ .

Factor groups are indispensable for an understanding of the homomorphism of one group onto the other. The relations between a group  $\mathcal{G}$  and its homomorphic image are very strong and are expressed by the following lemma:

**Lemma 1.2.4.4.3.** Let  $\mathcal{G}'$  be a homomorphic image of the group  $\mathcal{G}$ . Then the set of all elements of  $\mathcal{G}$  that are mapped onto the unit element  $e' \in \mathcal{G}'$  forms a normal subgroup  $\mathcal{X}$  of  $\mathcal{G}$ . The group  $\mathcal{G}'$  is isomorphic to the factor group  $\mathcal{G}/\mathcal{X}$  and the cosets of  $\mathcal{X}$  in  $\mathcal{G}$  are mapped onto the elements of  $\mathcal{G}'$ . The normal subgroup  $\mathcal{X}$  is called the *kernel* of the mapping; it forms the unit element of the factor group  $\mathcal{G}/\mathcal{X}$ . A homomorphic image of  $\mathcal{G}$  exists for any normal subgroup of  $\mathcal{G}$ .  $\square$

The most important homomorphism in crystallography is the relation between a space group  $\mathcal{G}$  and its homomorphic image, the point group  $\mathcal{P}$ , where the kernel is the subgroup  $\mathcal{T}(\mathcal{G})$  of all translations of  $\mathcal{G}$ , *cf.* Section 1.2.5.4.

### 1.2.4.5. Normalizers

The concept of the normalizer  $\mathcal{N}_{\mathcal{G}}(\mathcal{H})$  of a group  $\mathcal{H} < \mathcal{G}$  in a group  $\mathcal{G}$  is very useful for the considerations of the following sections. The size of the conjugacy class of  $\mathcal{H}$  in  $\mathcal{G}$  is determined by this normalizer.

Let  $\mathcal{H} < \mathcal{G}$  and  $h_j \in \mathcal{H}$ . Then  $h_j^{-1} \mathcal{H} h_j = \mathcal{H}$  holds because  $\mathcal{H}$  is a group. If  $\mathcal{H} \triangleleft \mathcal{G}$ , then  $g_k^{-1} \mathcal{H} g_k = \mathcal{H}$  for any  $g_k \in \mathcal{G}$ . If  $\mathcal{H}$  is not a normal subgroup of  $\mathcal{G}$ , there may nevertheless be elements  $g_p \in \mathcal{G}$ ,  $g_p \notin \mathcal{H}$  for which  $g_p^{-1} \mathcal{H} g_p = \mathcal{H}$  holds. We consider the set of all elements  $g_p \in \mathcal{G}$  that have this property.

**Definition 1.2.4.5.1.** The set of all elements  $g_p \in \mathcal{G}$  that map the subgroup  $\mathcal{H} < \mathcal{G}$  onto itself by conjugation,  $\mathcal{H} = g_p^{-1} \mathcal{H} g_p = \mathcal{H}^{g_p}$ , forms a group  $\mathcal{N}_{\mathcal{G}}(\mathcal{H})$ , called the *normalizer of  $\mathcal{H}$  in  $\mathcal{G}$* , where  $\mathcal{H} \triangleleft \mathcal{N}_{\mathcal{G}}(\mathcal{H}) \leq \mathcal{G}$ .  $\square$

*Remarks:*

- (1) The group  $\mathcal{H} < \mathcal{G}$  is a normal subgroup of  $\mathcal{G}$ ,  $\mathcal{H} \triangleleft \mathcal{G}$ , if and only if  $\mathcal{N}_{\mathcal{G}}(\mathcal{H}) = \mathcal{G}$ .
- (2) Let  $\mathcal{N}_{\mathcal{G}}(\mathcal{H}) = \{g_p\}$ . One can decompose  $\mathcal{G}$  into right cosets relative to  $\mathcal{N}_{\mathcal{G}}(\mathcal{H})$ . All elements  $g_p g_r$  of a right coset  $\mathcal{N}_{\mathcal{G}}(\mathcal{H}) g_r$  of this decomposition ( $\mathcal{G} : \mathcal{N}_{\mathcal{G}}(\mathcal{H})$ ) transform  $\mathcal{H}$  into the same subgroup  $g_r^{-1} g_p^{-1} \mathcal{H} g_p g_r = g_r^{-1} \mathcal{H} g_r < \mathcal{G}$ , which is thus conjugate to  $\mathcal{H}$  in  $\mathcal{G}$  by  $g_r$ .
- (3) The elements of different cosets of ( $\mathcal{G} : \mathcal{N}_{\mathcal{G}}(\mathcal{H})$ ) transform  $\mathcal{H}$  into different conjugates of  $\mathcal{H}$ . The number of cosets of  $\mathcal{N}_{\mathcal{G}}(\mathcal{H})$  is equal to the index  $i_N = |\mathcal{G} : \mathcal{N}_{\mathcal{G}}(\mathcal{H})|$  of  $\mathcal{N}_{\mathcal{G}}(\mathcal{H})$  in  $\mathcal{G}$ . Therefore, the number  $N_{\mathcal{H}}$  of conjugates in the conjugacy class of  $\mathcal{H}$  is equal to the index  $i_N$  and is thus determined by the order of  $\mathcal{N}_{\mathcal{G}}(\mathcal{H})$ . From  $\mathcal{N}_{\mathcal{G}}(\mathcal{H}) \geq \mathcal{H}$ ,  $i_N = |\mathcal{G} : \mathcal{N}_{\mathcal{G}}(\mathcal{H})| \leq |\mathcal{G} : \mathcal{H}| = i$  follows. This means that the number of conjugates of a subgroup  $\mathcal{H} < \mathcal{G}$  cannot exceed the index  $i = |\mathcal{G} : \mathcal{H}|$ .
- (4) If  $\mathcal{H} < \mathcal{G}$  is a maximal subgroup of  $\mathcal{G}$ , then either  $\mathcal{N}_{\mathcal{G}}(\mathcal{H}) = \mathcal{G}$  and  $\mathcal{H} \triangleleft \mathcal{G}$  is a normal subgroup of  $\mathcal{G}$  or  $\mathcal{N}_{\mathcal{G}}(\mathcal{H}) = \mathcal{H}$  and the number of conjugates is equal to the index  $i = |\mathcal{G} : \mathcal{H}|$ .
- (5) For the normalizers of the space groups, see the corresponding part of Section 1.2.6.3.

<sup>4</sup> The right-hand side of this equation is the set of all products  $g_r = g_{j_p} g_{k_q}$ , where  $g_{j_p}$  runs through all elements of  $\mathcal{K}_j$  and  $g_{k_q}$  through all elements of  $\mathcal{K}_k$ . Each element  $g_r$  is taken only once in the set.