***International Tables for Crystallography* (2011). Vol. A1, Section 1.2.4, pp. 12–14.**

different space groups allows one to classify the infinite number of space groups into a finite number of *isomorphism types of space groups*, which is one of the bases of crystallography, see Section 1.2.5.

Isomorphism provides a very strong relation between groups: the groups are identical in their group-theoretical properties. One can weaken this relation by omitting the condition of reversibility of the mapping. One then admits that more than one element of the group $\mathcal{G}$ is mapped onto the same element of $\mathcal{G}'$. This concept leads to the definition of homomorphism.

Definition 1.2.3.2.3. A mapping of a group $\mathcal{G}$ onto a group $\mathcal{G}'$ is called *homomorphic*, and $\mathcal{G}'$ is called a *homomorphic image* of the group $\mathcal{G}$, if for any pair of elements of $\mathcal{G}$ the image of the product is equal to the product of the images and if any element of $\mathcal{G}'$ is the image of at least one element of $\mathcal{G}$. The relation of $\mathcal{G}$ and $\mathcal{G}'$ is called a *homomorphism*. More formally: For the mapping $\mathcal{G}$ onto $\mathcal{G}'$, $(g_j\, g_k)' = g_j'\, g_k'$ holds. □

The formulation 'mapping onto' implies that each element $g' \in \mathcal{G}'$ occurs among the images of the elements $g \in \mathcal{G}$ at least once.[3]

The very important concept of homomorphism is discussed further in Lemma 1.2.4.4.3. The crystallographic point groups are homomorphic images of the space groups, see Section 1.2.5.4.

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 $\mathcal{G}$. □

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 $\mathcal{H}$. □

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 $g_2\,\mathcal{H} = \{g_2\, h_j \mid h_j \in \mathcal{H}\}$[4] 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 $g_3\mathcal{H} = \{g_3 h_j \mid h_j \in \mathcal{H}\}$. 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 $g_p\,\mathcal{H}$, $p = 1, \ldots, i$ 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 $\mathcal{G}$. □

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 1.4):

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 $\mathcal{G}$. □

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:

[3] In mathematics, the term 'homomorphism' includes mappings of a group $\mathcal{G}$ *into* a group $\mathcal{G}'$, *i.e.* mappings in which not every $g' \in \mathcal{G}'$ is the image of some element of $g \in \mathcal{G}$. The term 'homomorphism onto' defined above is also known as an *epimorphism, e.g.* in Ledermann (1976) and Ledermann & Weir (1996). In the older literature the term 'multiple isomorphism' can also be found.

[4] The formulation $g_2\,\mathcal{H} = \{g_2\, h_j \mid h_j \in \mathcal{H}\}$ means: '$g_2\,\mathcal{H}$ is the set of the products $g_2\, h_j$ of g_2 with all elements $h_j \in \mathcal{H}$.'

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

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 $\mathcal{G}$, $\mathcal{H} \lhd \mathcal{G}$, if equation (1.2.4.1) is fulfilled. □

The relation $\mathcal{H} \lhd \mathcal{G}$ 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 $g_q^{-1} g_j\, g_q = g_k$. □

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.
(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 $\mathcal{H}_j^{g_q} = \mathcal{H}_k$. □

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

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

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 $\mathcal{H} \lhd \mathcal{G}$ if it is identical with all of its conjugates, *i.e.* if its conjugacy class consists of the one subgroup $\mathcal{H}$ only. □

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 $\mathcal{K}_j = \{g_{j_1}, \ldots, g_{j_n}\}$, $\mathcal{K}_k = \{g_{k_1}, \ldots, g_{k_m}\}$ 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 $\mathcal{K}_j\,\mathcal{K}_k = \{g_{j_p}\, g_{k_q} \mid g_{j_p} \in \mathcal{K}_j,\ g_{k_q} \in \mathcal{K}_k\}$.[5] □

The coset decomposition of a group $\mathcal{G}$ relative to a normal subgroup $\mathcal{H} \lhd \mathcal{G}$ 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 $\mathcal{H} \lhd \mathcal{G}$ 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 $\mathcal{H} \lhd \mathcal{G}$ 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 $\mathcal{H} \lhd \mathcal{G}$ 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 $\mathcal{H} \lhd \mathcal{G}$. The cosets of the decomposition of the group $\mathcal{G}$ relative to the normal subgroup $\mathcal{H} \lhd \mathcal{G}$ 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 $\mathcal{G}$. □

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 $\mathcal{G}$. □

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 length 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 $\mathcal{H} \lhd \mathcal{G}$, then $g_k^{-1}\mathcal{H}g_k = \mathcal{H}$ for any $g_k \in \mathcal{G}$. If $\mathcal{H}$ is not a

[5] 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.

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 $\mathcal{H} \trianglelefteq \mathcal{N}_{\mathcal{G}}(\mathcal{H}) \leq \mathcal{G}$. □

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.

1.2.5. Space groups

1.2.5.1. Space groups and their description

The set of all symmetry operations of a three-dimensional crystal pattern, *i.e.* its symmetry group, is the *space group* of this crystal pattern. In a plane, the symmetry group of a two-dimensional crystal pattern is its *plane group*. In the following, the term 'space group' alone will be used and the plane groups are included because they are the space groups of two-dimensional space.

A crystal pattern is a periodic array. This means that there are translations among its symmetry operations. The translations of crystals are small (up to a few hundred ångströms) but cannot be arbitrarily short because of the finite size of the particles in crystal structures. One thus defines for any finite integer n:

Definition 1.2.5.1.1. A group $\mathcal{G}$ of isometries in n-dimensional space is called an n-dimensional space group if

(1) $\mathcal{G}$ contains n linearly independent translations.

(2) There is a minimum length $\delta > 0$ such that the length r of any translation vector is at least $r = \delta$. □

Condition (2) is justified because crystal structures contain atoms of finite size, and it is necessary to avoid infinitely small translations as elements of space groups. Several fundamental properties would not hold without this condition, such as the existence of a lattice of translation vectors and the restriction to only a few rotation angles.

In this volume, only the dimensions $n = 2$ and $n = 3$ will be dealt with. However, the space groups (more precisely, the space-group types, *cf.* Section 1.2.5.3) and other crystallographic items are also known for dimensions n = 4, 5 and 6. For example, the number of affine space-group types for n = 6 is 28 927 922 (Plesken & Schulz, 2000). 7052 of these affine space-group types split into enantiomorphic pairs of space groups, such that there are 28 934 974 crystallographic space-group types (Souvignier, 2003).

One of the characteristics of a space group is its translation group. Any space group $\mathcal{G}$ is an infinite group because the number of its translations is already infinite. The set of all translations of $\mathcal{G}$ forms the infinite translation subgroup $\mathcal{T}(\mathcal{G}) \triangleleft \mathcal{G}$ with the composition law of performing one translation after the other, represented by the multiplication of matrix–column pairs. The group $\mathcal{T}(\mathcal{G})$ is a normal subgroup of $\mathcal{G}$ of finite index. The vector lattice **L**, *cf.* Section 1.2.2.2, forms a group with the composition law of vector addition. This group is isomorphic to the group $\mathcal{T}(\mathcal{G})$.

The matrix–column pairs of the symmetry operations of a space group $\mathcal{G}$ are mostly referred to the *conventional coordinate system*. Its basis is chosen as a lattice basis and in such a way that the matrices for the linear parts of the symmetry operations of $\mathcal{G}$ are particularly simple. The origin is chosen such that as many coset representatives as possible can be selected with their column coefficients to be zero, or such that the origin is situated on a centre of inversion. This means (for details and examples see Section 8.3.1 of *IT* A):

(1) The basis is always chosen such that all matrix coefficients are 0 or ± 1.

(2) If possible, the basis is chosen such that all matrices have main diagonal form; then six of the nine coefficients are 0 and three are ± 1.

(3) If (2) is not possible, the basis is chosen such that the matrices are orthogonal. Again, six coefficients are 0 and three are ± 1.

(4) If (3) is not possible, the basis is hexagonal. At least five of the nine matrix coefficients are 0 and at most four are ± 1.

(5) The conventional basis chosen according to these rules is not always primitive, *cf.* the first example of Section 8.3.1 of *IT* A. If the conventional basis is primitive, then the lattice is also called *primitive*; if the conventional basis is not primitive, then the lattice referred to this (non-primitive) basis is called a *centred lattice*.

(6) The matrix parts of a translation and of an inversion are

$$\boldsymbol{I} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \text{ and } \bar{\boldsymbol{I}} = \begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix},$$

i.e. the unit matrix and the negative unit matrix. They are independent of the basis.

(7) The basis vectors of a crystallographic basis are lattice vectors. This makes the description of the lattice and of the symmetry operations of a crystal pattern independent of the actual metrics of the lattice, for example independent of temperature and pressure. It also means that the description of the symmetry may be the same for space groups of the same type, *cf.* Section 1.2.5.3.

(8) The origin is chosen at a point of highest site symmetry which is left invariant by as many symmetry operations as possible. The column parts $\boldsymbol{w}_k$ of these symmetry operations are $\boldsymbol{w}_k = \boldsymbol{o}$, *i.e.* the columns consist of zeroes only.

It is obviously impossible to list all elements of an infinite group individually. One can define the space group by a set of generators, because the number of necessary generators for any space group is finite: theoretically, up to six generators might be