*International Tables for Crystallography* (2016). Vol. A, Section 1.3.3.1, pp. 28–29.



*Examples*

(i) The lattice **L** spanned by the vectors

$$\mathbf{a} = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}, \quad \mathbf{b} = \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}, \quad \mathbf{c} = \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}$$

has metric tensor

$$\boldsymbol{G} = \begin{pmatrix} 3 & 2 & 0 \\ 2 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix}.$$

The inverse of the metric tensor is

$$\boldsymbol{G}^* = \boldsymbol{G}^{-1} = \frac{1}{2}\begin{pmatrix} 2 & -2 & 0 \\ -2 & 3 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Interpreting the columns of $\boldsymbol{G}^{-1}$ as coordinate vectors with respect to the original basis, one concludes that the reciprocal basis is given by

$$\mathbf{a}^* = \mathbf{a} - \mathbf{b}, \quad \mathbf{b}^* = \tfrac{1}{2}(-2\mathbf{a} + 3\mathbf{b}), \quad \mathbf{c}^* = \tfrac{1}{2}\mathbf{c}.$$

Inserting the columns for **a**, **b**, **c**, one obtains

$$\mathbf{a}^* = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \quad \mathbf{b}^* = \frac{1}{2}\begin{pmatrix} 1 \\ 1 \\ -2 \end{pmatrix}, \quad \mathbf{c}^* = \frac{1}{2}\begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}.$$

For the direct computation, the matrix $\boldsymbol{B}$ with the basis vectors **a**, **b**, **c** as columns is

$$\boldsymbol{B} = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & -1 \\ 1 & 0 & 0 \end{pmatrix}$$

and has as its inverse the matrix

$$\boldsymbol{B}^{-1} = \frac{1}{2}\begin{pmatrix} 0 & 0 & 2 \\ 1 & 1 & -2 \\ 1 & -1 & 0 \end{pmatrix}.$$

The rows of this matrix are indeed the vectors $\mathbf{a}^*$, $\mathbf{b}^*$, $\mathbf{c}^*$ as computed above.

(ii) The body-centred cubic lattice **L** has the vectors

$$\mathbf{a} = \frac{1}{2}\begin{pmatrix} -1 \\ 1 \\ 1 \end{pmatrix}, \quad \mathbf{b} = \frac{1}{2}\begin{pmatrix} 1 \\ -1 \\ 1 \end{pmatrix}, \quad \mathbf{c} = \frac{1}{2}\begin{pmatrix} 1 \\ 1 \\ -1 \end{pmatrix}$$

as primitive basis.
The matrix

$$\boldsymbol{B} = \frac{1}{2}\begin{pmatrix} -1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{pmatrix}$$

with the basis vectors **a**, **b**, **c** as columns has as its inverse the matrix

$$\boldsymbol{B}^{-1} = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}.$$

The rows of $\boldsymbol{B}^{-1}$ are the vectors

$$\mathbf{a}^* = \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}, \quad \mathbf{b}^* = \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}, \quad \mathbf{c}^* = \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix},$$

showing that the reciprocal lattice of a body-centred cubic lattice is a face-centred cubic lattice.

## 1.3.3. The structure of space groups

### 1.3.3.1. Point groups of space groups

The multiplication rule for symmetry operations

$$(\boldsymbol{W}_2,\ \boldsymbol{w}_2)(\boldsymbol{W}_1,\ \boldsymbol{w}_1) = (\boldsymbol{W}_2\boldsymbol{W}_1,\ \boldsymbol{W}_2\boldsymbol{w}_1 + \boldsymbol{w}_2)$$

shows that the mapping $\Pi : (\boldsymbol{W}, \boldsymbol{w}) \mapsto \boldsymbol{W}$ which assigns a space-group operation to its linear part is actually a group homomorphism, because the first component of the combined operation is simply the product of the linear parts of the two operations. As a consequence, the linear parts of a space group form a group themselves, which is called the point group of $\mathcal{G}$. The kernel of the homomorphism $\Pi$ consists precisely of the translations $(\boldsymbol{I}, \boldsymbol{t}) \in \mathcal{T}$, and since kernels of homomorphisms are always normal subgroups (*cf.* Section 1.1.6), the translation subgroup $\mathcal{T}$ forms a normal subgroup of $\mathcal{G}$. According to the *homomorphism theorem* (see Section 1.1.6), the point group is isomorphic to the factor group $\mathcal{G}/\mathcal{T}$.

*Definition*

The *point group* $\mathcal{P}$ of a space group $\mathcal{G}$ is the group of linear parts of operations occurring in $\mathcal{G}$. It is isomorphic to the factor group $\mathcal{G}/\mathcal{T}$ of $\mathcal{G}$ by the translation subgroup $\mathcal{T}$.

When $\mathcal{G}$ is considered with respect to a coordinate system, the operations of $\mathcal{P}$ are simply $3 \times 3$ matrices.

The point group plays an important role in the analysis of the macroscopic properties of crystals: it describes the symmetry of the set of face normals and can thus be directly observed. It is usually obtained from the *diffraction record* of the crystal, where adding the information about the translation subgroup explains the sharpness of the Bragg peaks in the diffraction pattern.

Although we have already deduced that the translation subgroup $\mathcal{T}$ of a space group $\mathcal{G}$ forms a normal subgroup in $\mathcal{G}$ because it is the kernel of the homomorphism mapping each operation to its linear part, it is worth investigating this fact by an explicit computation. Let $t = (\boldsymbol{I},\ \boldsymbol{t})$ be a translation in $\mathcal{T}$ and $W = (\boldsymbol{W},\ \boldsymbol{w})$ an arbitrary operation in $\mathcal{G}$, then one has

$$\begin{aligned} WtW^{-1} &= (\boldsymbol{W},\ \boldsymbol{w})(\boldsymbol{I},\ \boldsymbol{t})(\boldsymbol{W}^{-1},\ -\boldsymbol{W}^{-1}\boldsymbol{w}) \\ &= (\boldsymbol{W},\ \boldsymbol{W}\boldsymbol{t} + \boldsymbol{w})(\boldsymbol{W}^{-1},\ -\boldsymbol{W}^{-1}\boldsymbol{w}) \\ &= (\boldsymbol{I},\ -\boldsymbol{w} + \boldsymbol{W}\boldsymbol{t} + \boldsymbol{w}) = (\boldsymbol{I},\ \boldsymbol{W}\boldsymbol{t}), \end{aligned}$$

which is again a translation in $\mathcal{G}$, namely by $\boldsymbol{W}\boldsymbol{t}$. This little computation shows an important property of the translation subgroup with respect to the point group, namely that every vector from the translation lattice is mapped again to a lattice vector by each operation of the point group of $\mathcal{G}$.

*Proposition.* Let $\mathcal{G}$ be a space group with point group $\mathcal{P}$ and translation subgroup $\mathcal{T}$ and let $\mathbf{L} = \{\boldsymbol{t} \mid (\boldsymbol{I}, \boldsymbol{t}) \in \mathcal{T}\}$ be the lattice of translations in $\mathcal{T}$. Then $\mathcal{P}$ acts on the lattice $\mathbf{L}$, *i.e.* for every $\boldsymbol{W} \in \mathcal{P}$ and $\boldsymbol{t} \in \mathbf{L}$ one has $\boldsymbol{W}\boldsymbol{t} \in \mathbf{L}$.

A point group that acts on a lattice is a subgroup of the full group of symmetries of the lattice, obtained as the group of orthogonal mappings that map the lattice to itself. With respect to a primitive basis, the group of symmetries of a lattice consists of all integral basis transformations that fix the metric tensor of the lattice.

*Definition*

Let **L** be a three-dimensional lattice with metric tensor $\boldsymbol{G}$ with respect to a primitive basis **a**, **b**, **c**.

(i) An *automorphism* of **L** is an isometry mapping **L** to itself. Written with respect to the basis **a**, **b**, **c**, an automorphism of **L** is an integral basis transformation fixing the metric tensor of **L**, *i.e.* it is an integral matrix $\boldsymbol{W} \in \mathrm{GL}_3(\mathbb{Z})$ with $\boldsymbol{W}^{\mathrm{T}} \cdot \boldsymbol{G} \cdot \boldsymbol{W} = \boldsymbol{G}$.

(ii) The group

$$\mathcal{B} := Aut(\mathbf{L}) = \{\boldsymbol{W} \in \mathrm{GL}_3(\mathbb{Z}) \mid \boldsymbol{W}^{\mathrm{T}} \cdot \boldsymbol{G} \cdot \boldsymbol{W} = \boldsymbol{G}\}$$

of all automorphisms of **L** is called the *automorphism group* or *Bravais group* of **L**. Note that $Aut(\mathbf{L})$ acts on the coordinate columns of **L**, which are simply columns with integral coordinates.

Since the isometries in the Bravais group of a lattice preserve distances, the possible images of the vectors in a basis are vectors of the same lengths as the basis vectors. But due to its discreteness, a lattice contains only finitely many lattice vectors up to a given length. This means that a lattice automorphism can only permute the finitely many vectors up to the maximum length of a basis vector. Thus, there can only be finitely many automorphisms of a lattice. This argument proves the following important fact:

*Theorem.* The Bravais group of a lattice is finite. As a consequence, point groups of space groups are finite groups.

As subgroups of the Bravais group of a lattice, point groups can be realized as integral matrix groups when written with respect to a primitive basis. For a centred lattice, it is possible that the Bravais group of a lattice contains non-integral matrices, because the centring vector is a column with non-integral entries. However, in dimensions two and three the conventional bases are chosen such that the Bravais groups of all lattices are integral when written with respect to a conventional basis.

Information on the Bravais groups of the primitive lattices in two- and three-dimensional space is displayed in Tables 1.3.3.1 and 1.3.3.2. The columns of the tables contain the names of the lattices, the metric tensor with respect to the conventional basis (with only the upper half given, the lower half following by the symmetry of the metric tensor), the Hermann–Mauguin symbol for the type of the Bravais group and generators of the Bravais group (given in the shorthand notation introduced in Section 1.2.2.1 and the corresponding Seitz symbols discussed in Section 1.4.2.2).

The finiteness and integrality of the point groups has important consequences. For example, it implies the *crystallographic restriction* that rotations in space groups of two- and three-dimensional space can only have orders 1, 2, 3, 4 or 6. On the one hand, an integral matrix clearly has an integral trace.[1] But a matrix $\boldsymbol{W}$ with the property that $\boldsymbol{W}^k = \boldsymbol{I}$ can be diagonalized over the complex numbers and the diagonal entries have to be $k$th roots of unity, *i.e.* powers of $\zeta_k = \exp(2\pi i/k)$. Since diagonalization does not change the trace, the sum of these $k$th roots of unity still has to be an integer and in particular these roots of unity have to occur in complex conjugate pairs. In dimension 2 this means that the two diagonal entries are complex conjugate and the only possible ways to obtain an integral trace are $\zeta_1 + \zeta_1^{-1} = 2$, $\zeta_2 + \zeta_2^{-1} = -2$, $\zeta_3 + \zeta_3^{-1} = -1$, $\zeta_4 + \zeta_4^{-1} = 0$ and $\zeta_6 + \zeta_6^{-1} = 1$. In dimension 3 the third diagonal entry does not have a complex conjugate partner, and therefore has to be $\pm 1$.

[1] The trace of a matrix is the sum of its diagonal entries.

**Table 1.3.3.1**
Automorphism groups of two-dimensional primitive lattices

| Lattice | Metric tensor | Bravais group: Hermann–Mauguin symbol | Bravais group: Generators |
|---|---|---|---|
| Oblique | $\begin{pmatrix} g_{11} & g_{12} \\ & g_{22} \end{pmatrix}$ | 2 | $2\colon \bar{x}, \bar{y}$ |
| Rectangular | $\begin{pmatrix} g_{11} & 0 \\ & g_{22} \end{pmatrix}$ | $2mm$ | $2\colon \bar{x}, \bar{y}$<br>$m_{10}\colon \bar{x}, y$ |
| Square | $\begin{pmatrix} g_{11} & 0 \\ & g_{11} \end{pmatrix}$ | $4mm$ | $4^+\colon \bar{y}, x$<br>$m_{10}\colon \bar{x}, y$ |
| Hexagonal | $\begin{pmatrix} g_{11} & -\frac{1}{2}g_{11} \\ & g_{11} \end{pmatrix}$ | $6mm$ | $6^+\colon x-y, x$<br>$m_{21}\colon \bar{x}, \bar{x}+y$ |

Thus the possible orders in dimension 3 are the same as in dimension 2.

A much stronger result was obtained by H. Minkowski (1887). He gave an explicit bound for the maximal power $p^m$ of a prime $p$ which can divide the order of an $n$-dimensional finite integral matrix group. In dimension 2 this theorem implies that the orders of the point groups divide 24 and in dimension 3 the orders of the point groups divide 48. The Bravais groups $4mm$ (of order 8) and $6mm$ (of order 12) of the square and hexagonal lattices in dimension 2 and the Bravais group $m\bar{3}m$ (of order 48) of the cubic lattice in dimension 3 show that Minkowski's result is the best possible in these dimensions.

#### 1.3.3.2. Coset decomposition with respect to the translation subgroup

The translation subgroup $\mathcal{T}$ of a space group $\mathcal{G}$ can be used to distribute the operations of $\mathcal{G}$ into different classes by grouping together all operations that differ only by a translation. This results in the decomposition of $\mathcal{G}$ into cosets with respect to $\mathcal{T}$ (see Section 1.1.4 for details of cosets).

*Definition*

Let $\mathcal{G}$ be a space group with translation subgroup $\mathcal{T}$.

(i) The *right coset* $\mathcal{T}W$ of an operation $W \in \mathcal{G}$ with respect to $\mathcal{T}$ is the set $\{tW \mid t \in \mathcal{T}\}$.
Analogously, the set $W\mathcal{T} = \{Wt \mid t \in \mathcal{T}\}$ is called the *left coset* of $W$ with respect to $\mathcal{T}$.

(ii) A set $\{W_1, \ldots, W_m\}$ of operations in $\mathcal{G}$ is called a system of *coset representatives* relative to $\mathcal{T}$ if every operation $W$ in $\mathcal{G}$ is contained in exactly one coset $\mathcal{T}W_i$.

(iii) Writing $\mathcal{G}$ as the disjoint union

$$\mathcal{G} = \mathcal{T}W_1 \cup \ldots \cup \mathcal{T}W_m$$

is called the *coset decomposition of* $\mathcal{G}$ *relative to* $\mathcal{T}$.

If the translation subgroup $\mathcal{T}$ is a subgroup of index $[i]$ in $\mathcal{G}$, a set of coset representatives for $\mathcal{G}$ relative to $\mathcal{T}$ consists of $[i]$ operations $W_1, W_2, \ldots, W_{[i]}$, where $W_1$ is assumed to be the identity element $e$ of $\mathcal{G}$. The cosets of $\mathcal{G}$ relative to $\mathcal{T}$ can be imagined as columns of an infinite array with $[i]$ columns, labelled by the coset representatives, as displayed in Table 1.3.3.3.