International Tables for Crystallography (2011). Vol. A1, Section 1.4.2.4, pp. 28–29.

tuple of n vectors $\mathbf{B} := (\mathbf{a}_1, \ldots, \mathbf{a}_n)$ such that every vector of $\mathbf{V}$ can be written uniquely as a linear combination of the basis vectors: $\mathbf{V} = \{\mathbf{x} = x_1\mathbf{a}_1 + \ldots + x_n\mathbf{a}_n \mid x_1, \ldots, x_n \in \mathbb{R}\}$. Whereas a vector space has many different bases, the number n of vectors of a basis is uniquely determined and is called the *dimension* of $\mathbf{V}$. The isomorphism (see Section 1.4.3.4 for a definition of isomorphism) $\varphi_{\mathbf{B}}$ between $\mathbf{V}$ and $\mathbf{V}_n$ maps the vector $\mathbf{x} = x_1\mathbf{a}_1 + \ldots + x_n\mathbf{a}_n \in \mathbf{V}$ to its coefficient column

$$\boldsymbol{x} = \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix} \in \mathbf{V}_n$$

with respect to the chosen basis $\mathbf{B}$. The mapping $\varphi_{\mathbf{B}}$ respects addition of vectors and multiplication of vectors with real numbers. Moreover, $\varphi_{\mathbf{B}}$ is a bijective mapping, which means that for any coefficient column $\boldsymbol{x} \in \mathbf{V}_n$ there is a unique vector $\mathbf{x} \in \mathbf{V}$ with $\varphi_{\mathbf{B}}(\mathbf{x}) = \boldsymbol{x}$. Therefore one can perform all calculations using the coefficient columns.

An important concept in mathematics is the *automorphism group* of an object. In general, if one has an object (here the vector space $\mathbf{V}$) together with a structure (here the addition of vectors and the multiplication of vectors with real numbers), its automorphism group is the set of all one-to-one mappings of the object onto itself that preserve the structure.

A bijective mapping $\varphi : \mathbf{V} \to \mathbf{V}$ of the vector space $\mathbf{V}$ into itself satisfying $\varphi(\mathbf{v} + \mathbf{w}) = \varphi(\mathbf{v}) + \varphi(\mathbf{w})$ for all $\mathbf{v}, \mathbf{w} \in \mathbf{V}$ and $\varphi(x\mathbf{v}) = x\varphi(\mathbf{v})$ for all real numbers $x \in \mathbb{R}$ and all vectors $\mathbf{v} \in \mathbf{V}$ is called a *linear mapping* and the set of all these linear mappings is the *linear group* of $\mathbf{V}$. To know the image of $\mathbf{x} = x_1\mathbf{a}_1 + \ldots + x_n\mathbf{a}_n$ under a linear mapping φ it suffices to know the images of the basis vectors $\mathbf{a}_1, \ldots, \mathbf{a}_n$ under φ, since $\varphi(\mathbf{x}) = x_1\varphi(\mathbf{a}_1) + \ldots + x_n\varphi(\mathbf{a}_n)$. Writing the coefficient columns of the images of the basis vectors as columns of a matrix $\boldsymbol{A}$ [*i.e.* $\varphi(\mathbf{a}_i) = \sum_{j=1}^{n} \mathbf{a}_j A_{ji}$, $i = 1, \ldots, n$], then the coefficient column of $\varphi(\mathbf{x})$ with respect to the chosen basis $\mathbf{B}$ is just $\boldsymbol{Ax}$. Note that the matrix of a linear mapping depends on the basis $\mathbf{B}$ of $\mathbf{V}$. The matrix that corresponds to the composition of two linear mappings is the product of the two corresponding matrices. We have thus seen that the linear group of a vector space $\mathbf{V}$ of dimension n is isomorphic to the group of all invertible $(n \times n)$ matrices *via* the isomorphism $\varphi_{\mathbf{B}}$ that associates to a linear mapping its corresponding matrix (with respect to the basis $\mathbf{B}$). This means that one can perform all calculations with linear mappings using matrix calculations.

In crystallography, the translation-vector space has an additional structure: one can measure lengths and angles between vectors. An n-dimensional real vector space with such an additional structure is called a *Euclidean vector space*, $\mathbf{E}_n$. Its automorphism group is the set of all (bijective) linear mappings of $\mathbf{E}_n$ onto itself that preserve lengths and angles and is called the *orthogonal group* $\mathcal{O}_n$ of $\mathbf{E}_n$. If one chooses the basis $\mathbf{B} = (\mathbf{e}_1, \ldots, \mathbf{e}_n)$ to be the unit vectors (which are orthogonal vectors of length 1), then the isomorphism $\varphi_{\mathbf{B}}$ above maps the orthogonal group $\mathcal{O}_n$ onto the set of all $(n \times n)$ matrices $\boldsymbol{A}$ with $\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A} = \boldsymbol{I}$, the $(n \times n)$ unit matrix. $^{\mathrm{T}}$ denotes the transposition operator, which maps columns to rows and rows to columns.

1.4.2.3. *The affine space*

In this section we build up a model for the 'point space'. Let us first assume $n = 2$. Then the affine space $\mathbb{A}_2$ may be imagined as an infinite sheet of paper parallel, let us say, to the $(\mathbf{a}, \mathbf{b})$ plane and cutting the $\mathbf{c}$ axis at $x_3 = 1$ in crystallographic notation. The points of $\mathbb{A}_2$ have coordinates

$$\begin{pmatrix} x_1 \\ x_2 \\ \hline 1 \end{pmatrix},$$

which are the coefficients of the vector from the origin to the point.

This observation is generalized by the following:

Definition 1.4.2.3.1.

$$\mathbb{A}_n := \{ \begin{pmatrix} x_1 \\ \vdots \\ x_n \\ \hline 1 \end{pmatrix} \mid x_i \in \mathbb{R}\}$$

is an n-dimensional *affine space*. □

If

$$P = \begin{pmatrix} x_1 \\ \vdots \\ x_n \\ \hline 1 \end{pmatrix} \text{ and } Q = \begin{pmatrix} y_1 \\ \vdots \\ y_n \\ \hline 1 \end{pmatrix} \in \mathbb{A}_n,$$

then the vector $\overrightarrow{PQ}$ is defined as the difference

$$Q - P = \begin{pmatrix} y_1 - x_1 \\ \vdots \\ y_n - x_n \\ \hline 0 \end{pmatrix}$$

(computed in the vector space $\mathbf{V}_{n+1}$). The set of all $\overrightarrow{PQ}$ with $P, Q \in \mathbb{A}_n$ forms an n-dimensional vector space which is called the *underlying vector space* $\tau(\mathbb{A}_n)$. Omitting the last coefficient, we can identify

$$\tau(\mathbb{A}_n) = \{ \begin{pmatrix} x_1 \\ \vdots \\ x_n \\ \hline 0 \end{pmatrix} \mid x_1, \ldots, x_n \in \mathbb{R}\}$$

with $\mathbf{V}_n$. As the coordinates already indicate, the sets $\mathbb{A}_n$ as well as $\tau(\mathbb{A}_n)$ can be viewed as subsets of $\mathbf{V}_{n+1}$. Computed in $\mathbf{V}_{n+1}$, the sum of two elements in $\tau(\mathbb{A}_n)$ is again in $\tau(\mathbb{A}_n)$, since the last coefficient of the sum is $0 + 0 = 0$ and the sum of a point $P \in \mathbb{A}_n$ and a vector $\mathbf{v} \in \mathbf{V}_n$ is again a point in $\mathbb{A}_n$ (since the last coordinate is $1 + 0 = 1$), but the sum of two points does not make sense.

1.4.2.4. *The affine group*

The affine group of geometry is the set of all mappings of the point space which fulfil the conditions

(1) parallel straight lines are mapped onto parallel straight lines;

(2) collinear points are mapped onto collinear points and the ratio of distances between them remains constant.

In the mathematical model, the affine group is the automorphism group of the affine space and can be viewed as the set of all linear mappings of $\mathbf{V}_{n+1}$ that preserve $\mathbb{A}_n$.

Definition 1.4.2.4.1. The *affine group* $\mathcal{A}_n$ is the subset of the set of all linear mappings $\varphi: \mathbf{V}_{n+1} \to \mathbf{V}_{n+1}$ with $\varphi(\mathbb{A}_n) = \mathbb{A}_n$. The elements of $\mathcal{A}_n$ are called *affine mappings*. □

Since φ is linear, it holds that

$$\varphi(\overrightarrow{PQ}) = \varphi(Q - P) = \varphi(Q) - \varphi(P) = \overrightarrow{\varphi(P)\varphi(Q)}.$$

Hence an affine mapping also maps $\tau(\mathbb{A}_n)$ into itself.

Since the first n basis vectors of the chosen basis lie in $\tau(\mathbb{A}_n)$ and the last one in $\mathbb{A}_n$, it is clear that with respect to this basis the affine mappings correspond to matrices of the form

$$\mathbb{W} = \left(\begin{array}{c|c} \boldsymbol{W} & \boldsymbol{w} \\ \hline \boldsymbol{o}^{\mathrm{T}} & 1 \end{array}\right).$$

The linear mapping induced by φ on $\tau(\mathbb{A}_n)$ which is represented by the matrix $\boldsymbol{W}$ will be referred to as the *linear part* $\overline{\varphi}$ of φ. The image $\varphi(P)$ of a point P with coordinates

$$\mathbb{x} = \begin{pmatrix} \boldsymbol{x} \\ \hline 1 \end{pmatrix} \in \mathbb{A}_n$$

can easily be found as

$$\mathbb{W}\mathbb{x} = \begin{pmatrix} \boldsymbol{W}\boldsymbol{x} + \boldsymbol{w} \\ \hline 1 \end{pmatrix}.$$

If one has a way to measure lengths and angles (*i.e.* a Euclidean metric) on the underlying vector space $\tau(\mathbb{A}_n)$, one can compute the *distance* between P and $Q \in \mathbb{A}_n$ as the length of the vector $\overrightarrow{PQ}$ and the angle determined by P, Q and $R \in \mathbb{A}_n$ with vertex Q is obtained from $\cos(P, Q, R) = \cos(\overrightarrow{QP}, \overrightarrow{QR})$. In this case, $\mathbb{A}_n$ is the *Euclidean point space*, $\mathbb{E}_n$.

An affine mapping of the Euclidean point space is called an *isometry* if its linear part is an orthogonal mapping of the Euclidean vector space $\tau(\mathbb{A}_n)$. The set of all isometries in $\mathcal{A}_n$ is called the *Euclidean group* and denoted by $\mathcal{E}_n$. Hence $\mathcal{E}_n$ is the set of all distance-preserving mappings of $\mathbb{E}_n$ onto itself. The isometries are the affine mappings with matrices of the form

$$\mathbb{W} = \left(\begin{array}{c|c} \boldsymbol{W} & \boldsymbol{w} \\ \hline \boldsymbol{o}^{\mathrm{T}} & 1 \end{array}\right)$$

where the linear part $\boldsymbol{W}$ belongs to the orthogonal group of $\tau(\mathbb{A}_n)$.

Special isometries are the *translations*, the isometries where the linear part is $\boldsymbol{I}$, with matrix

$$\mathbb{T} = \left(\begin{array}{c|c} \boldsymbol{I} & \boldsymbol{w} \\ \hline \boldsymbol{o}^{\mathrm{T}} & 1 \end{array}\right).$$

The group of all translations in $\mathcal{E}_n$ is the *translation subgroup* of $\mathcal{E}_n$ and is denoted by $\mathcal{T}_n$. Note that composition of two translations means addition of the translation vectors and $\mathcal{T}_n$ is isomorphic to the translation vector space $\tau(\mathbb{E}_n)$.

1.4.3. Groups

1.4.3.1. Groups

The affine group is only one example of the more general concept of a group. The following axiomatic definition sometimes makes it easier to examine general properties of groups.

Definition 1.4.3.1.1. A *group* $(\mathcal{G}, \cdot)$ is a set $\mathcal{G}$ with a mapping $\mathcal{G} \times \mathcal{G} \to \mathcal{G}; (g, h) \mapsto g \cdot h$, called the *composition law* or *multiplication* of $\mathcal{G}$, satisfying the following three axioms:

(i) $(g \cdot h) \cdot k = g \cdot (h \cdot k)$ for all $g, h, k \in \mathcal{G}$ (associative law).
(ii) There is an element $e \in \mathcal{G}$ called the *unit element* of $\mathcal{G}$ with $e \cdot g = g \cdot e = g$ for all $g \in \mathcal{G}$.
(iii) For all $g \in \mathcal{G}$, there is an element $g^{-1} \in \mathcal{G}$, called the *inverse* of g, with $g \cdot g^{-1} = g^{-1} \cdot g = e$. □

Normally the symbol $\cdot$ is omitted, hence the product $g \cdot h$ is just written as $g\,h$ and the set $\mathcal{G}$ is called a group.

One should note that in particular property (i), the associative law, of a group is something very natural if one thinks of group elements as mappings. Clearly the composition of mappings is associative. In general, one can think of groups as groups of mappings as explained in Section 1.4.3.2.

A subset of elements of a group $\mathcal{G}$ which themselves form a group is called a subgroup:

Definition 1.4.3.1.2. A non-empty subset $\emptyset \neq \mathcal{U} \subseteq \mathcal{G}$ is called a *subgroup* of $\mathcal{G}$ (abbreviated as $\mathcal{U} \leq \mathcal{G}$) if $g \cdot h^{-1} \in \mathcal{U}$ for all $g, h \in \mathcal{U}$. □

The affine group is an example of a group where $\cdot$ is given by the composition of mappings. The unit element $e \in \mathcal{A}_n$ is the identity mapping given by the matrix

$$\mathbb{I} = \left(\begin{array}{c|c} \boldsymbol{I} & \boldsymbol{o} \\ \hline \boldsymbol{o}^{\mathrm{T}} & 1 \end{array}\right),$$

which also represents the translation by the vector **o**. The composition of two affine mappings is again an affine mapping and the inverse of an affine mapping $\mathbb{W}$ has matrix

$$\mathbb{W}^{-1} = \left(\begin{array}{c|c} \boldsymbol{W}^{-1} & -\boldsymbol{W}^{-1}\boldsymbol{w} \\ \hline \boldsymbol{o}^{\mathrm{T}} & 1 \end{array}\right).$$

Since the inverse of an isometry and the composition of two isometries are again isometries, the set of isometries $\mathcal{E}_n$ is a subgroup of the affine group $\mathcal{A}_n$. The translation subgroup $\mathcal{T}_n$ is a subgroup of $\mathcal{E}_n$.

Any vector space $\mathbf{V}_n$ is a group with the usual vector addition as composition law. Therefore $\tau(\mathbb{A}_n)$ is also a group.

Remarks

(i) For every group $\mathcal{G}$, the set $\{e\}$ consisting only of the unit element of $\mathcal{G}$ is a subgroup of $\mathcal{G}$ called the *trivial subgroup* $\mathcal{I} = \{e\}$.
(ii) If $\mathcal{U}$ is a subgroup of $\mathcal{V}$ and $\mathcal{V}$ is a subgroup of the group $\mathcal{G}$, then $\mathcal{U}$ is a subgroup of $\mathcal{G}$.
(iii) If $\mathcal{U}$ and $\mathcal{V}$ are subgroups of the group $\mathcal{G}$, then the intersection $\mathcal{U} \cap \mathcal{V}$ is also a subgroup of $\mathcal{G}$.
(iv) If $S \subseteq \mathcal{G}$ is a subset of the group $\mathcal{G}$, then the smallest subgroup of $\mathcal{G}$ containing S is denoted by

$$\langle S \rangle := \bigcap \{\mathcal{U} \leq \mathcal{G} \mid S \subseteq \mathcal{U}\}$$

references