1.4. The mathematical background of the subgroup tables

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1.4.1. Introduction

This chapter gives a brief introduction to the mathematics involved in the determination of the subgroups of space groups. To achieve this we have to detach ourselves from the geometric point of view in crystallography and introduce more abstract algebraic structures, such as coordinates, which are well known in crystallography and permit the formalization of symmetry operations, and also the abstract notion of a group, which allows us to apply general theorems to the concrete situation of (three-dimensional) space groups.

This algebraic point of view has the following advantages:

(1) Geometric problems can be treated by algebraic calculations. These calculations can be dealt with by well established procedures. In particular, the use of computers and advanced programs enables one to solve even difficult problems in a comparatively short time.
(2) The mappings form groups in the mathematical sense of the word. This means that the very powerful methods of group theory may be applied successfully.
(3) The procedures for the solution may be developed to a great extent independently of the dimension of the space.

In Section 1.4.2, a basis is laid down which gives the reader an understanding of the algebraic point of view of the crystal space (or point space) and special mappings of this space onto itself. The set of these mappings is an example of a group. For a closer connection to crystallography, the reader may consult Section 8.1.1 of *International Tables for Crystallography* Volume A (2005) (abbreviated as *IT* A) or the book by Hahn & Wondratschek (1994).

Section 1.4.3 gives an introduction to abstract groups and states the important theorems of group theory that will be applied in Section 1.4.4 to the most important groups in crystallography, the space groups. In particular, Section 1.4.4 treats maximal subgroups of space groups which have a special structure by the theorem of Hermann. In Section 1.4.5, we come back to abstract group theory stating general facts about maximal subgroups of groups. These general theorems allow us to calculate the possible indices of maximal subgroups of three-dimensional space groups in Section 1.4.6. The next section, Section 1.4.7, deals with the very subtle question of when these maximal subgroups of a space group are isomorphic to this space group. In Section 1.4.8 minimal supergroups of space groups are treated briefly.

1.4.2. The affine space

1.4.2.1. Motivation

The aim of this section is to give a mathematical model for the 'point space' (also known in crystallography as 'direct space' or 'crystal space') which contains the positions of atoms in crystals (the so-called 'points'). This allows us in particular to describe the symmetry groups of crystals and to develop a formalism for calculating with these groups which has the advantage that it works in arbitrary dimensions. Such higher-dimensional spaces up to dimension 6 are used, for example, for the description of quasicrystals and incommensurate phases. For example, the more than 29 000 000 crystallographic groups up to dimension 6 can be parameterized, constructed and identified using the computer package *[CARAT]: Crystallographic AlgoRithms And Tables*, available from http://wwwb.math.rwth-aachen.de/carat/index.html (for a description, see Opgenorth *et al.*, 1998).

As well as the points in point space, there are other objects, called 'vectors'. The vector that connects the point P to the point Q is usually denoted by $\overrightarrow{PQ}$. Vectors are usually visualized by arrows, where parallel arrows of the same length represent the same vector.

Whereas the sum of two points P and Q is not defined, one can add vectors. The sum $\mathbf{v} + \mathbf{w}$ of two vectors $\mathbf{v}$ and $\mathbf{w}$ is simply the sum of the two arrows. Similarly, multiplication of a vector $\mathbf{v}$ by a real number can be defined.

All the points in point space are equally good, but among the vectors one can be distinguished, the null vector $\mathbf{o}$. It is characterized by the property that $\mathbf{v} + \mathbf{o} = \mathbf{v}$ for all vectors $\mathbf{v}$.

Although the notion of a vector seems to be more complicated than that of a point, we introduce vector spaces before giving a mathematical model for the point space, the so-called affine space, which can be viewed as a certain subset of a higher-dimensional vector space, where the addition of a point and a vector makes sense.

1.4.2.2. Vector spaces

We shall now exploit the advantage of being independent of the dimensionality. The following definitions are independent of the dimension by replacing the specific dimensions 2 for the plane and 3 for the space by an unspecified integer number $n > 0$. Although we cannot visualize four- or higher-dimensional objects, we can describe them in such a way that we are able to calculate with such objects and derive their properties.

Algebraically, an n-dimensional (real) vector $\mathbf{v}$ can be represented by a column of n real numbers. The n-dimensional real vector space $\mathbf{V}_n$ is then

$$\mathbf{V}_n = \{\boldsymbol{x} = \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix} \mid x_1, \ldots, x_n \in \mathbb{R}\}.$$

(In crystallography n is normally 3.) The entries $x_1, \ldots, x_n$ are called the *coefficients* of the vector $\mathbf{x}$. On $\mathbf{V}_n$ one can naturally define an addition, where the coefficients of the sum of two vectors are the corresponding sums of the coefficients of the vectors. To multiply a vector by a real number, one just multiplies all its coefficients by this number. The null vector

$$\boldsymbol{o} = \begin{pmatrix} 0 \\ \vdots \\ 0 \end{pmatrix} \in \mathbf{V}_n$$

can be distinguished, since $\mathbf{v} + \mathbf{o} = \mathbf{v}$ for all $\mathbf{v} \in \mathbf{V}_n$.

The identification of a concrete vector space $\mathbf{V}$ with the vector space $\mathbf{V}_n$ can be done by choosing a basis of $\mathbf{V}$. A *basis* of $\mathbf{V}$ is any 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 $\boldsymbol{A}\boldsymbol{x}$. 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

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

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

$$\mathbb{x} = \left(\begin{array}{c} \boldsymbol{x} \\ \hline 1 \end{array}\right) \in \mathbb{A}_n$$

can easily be found as

$$\mathbb{W}\mathbb{x} = \left(\begin{array}{c} \boldsymbol{W}\boldsymbol{x} + \boldsymbol{w} \\ \hline 1 \end{array}\right).$$

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 $\overrightarrow{P\,Q}$ and the angle determined by P, Q and $R \in \mathbb{A}_n$ with vertex Q is obtained from $\cos(P, Q, R) = \cos(\overrightarrow{Q\,P}, \overrightarrow{Q\,R})$. 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 $\mathbf{o}$. 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

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