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