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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

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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

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

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

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

can easily be found as

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

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 $\overrightarrow{PQ}$ 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 gh 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

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

and is called the *subgroup generated by S*. The elements of S are called the *generators* of this group. It is convenient not to list all the elements of a group $\mathcal{G}$ but just to give generators of $\mathcal{G}$ (this also applies to finite groups).

Example 1.4.3.1.3

A well known group is the addition group of integers $\mathbb{Z} = \{0, 1, -1, 2, -2, \ldots\}$ where $\cdot$ is normally denoted by + and the unit element $e \in \mathbb{Z}$ is 0. The group $\mathbb{Z}$ is generated by $\{1\}$. Other generating sets are for example $\{-1\}$ or $\{2, 3\}$. Taking two integers $a, b \in \mathbb{Z}$ which are divisible by some fixed integer $p \in \mathbb{Z}$, then the sum $a + b$ and the negatives $-a$ and $-b$ are again divisible by p. Hence the set $p\mathbb{Z}$ of all integers divisible by p is a subgroup of $\mathbb{Z}$. It is generated by $\{p\}$.

Definition 1.4.3.1.4. The *order* $|\mathcal{G}|$ of a group $\mathcal{G}$ is the number of elements in the set $\mathcal{G}$. □

Most of the groups $\mathcal{G}$ in crystallography, for example $\mathbb{Z}$, $\mathbf{V}_n$, $\mathcal{A}_n$, have infinite order.

Groups that are generated by one element are called *cyclic*. The cyclic group of order n is called $\mathcal{C}yc_n$. (We prefer to use three letters to denote the mathematical names of frequently occurring groups, since the more common symbol $\mathcal{C}_n$ could possibly cause confusion with the Schoenflies symbol C_n.)

The group $\mathbf{V}_n$ is not generated by a finite set.

These two groups $\mathbb{Z}$ and $\mathbf{V}_n$ have the property that for all elements g and h in the group it holds that $g \cdot h = h \cdot g$. Hence these two groups are Abelian in the sense of the following:

Definition 1.4.3.1.5. The group $(\mathcal{G}, \cdot)$ is called *Abelian* if $g \cdot h = h \cdot g$ for all $g, h \in \mathcal{G}$. □

1.4.3.2. Actions of groups on sets

The affine group $\mathcal{A}_n$ is defined *via* its action on the affine space $\mathbb{A}_n$. In general, the greatest significance of groups is that they act on sets.

Definition 1.4.3.2.1. Let $\mathcal{G}$ be a group. A non-empty set M is called a (*left*) $\mathcal{G}$*-set* if there is a mapping $\mathcal{G} \times M \to M$ satisfying the following conditions:

(i) $(gh) \cdot m = g \cdot (h \cdot m)$ for all $g, h \in \mathcal{G}$ and $m \in M$.
(ii) $e \cdot m = m$ for all $m \in M$.

If M is a $\mathcal{G}$-set, one also says that $\mathcal{G}$ acts on M. □

Example 1.4.3.2.2

(*a*) The affine space $\mathbb{A}_n$ is a $\mathcal{G}$-set for the affine group $\mathcal{G} = \mathcal{A}_n$.
(*b*) $\tau(\mathbb{A}_n)$ is an $\mathcal{A}_n$-set, where $\mathcal{A}_n$ acts *via* the linear parts.
(*c*) $\tau(\mathbb{A}_n)$ is also a group and acts on $\mathbb{A}_n$ by translations $\mathbf{v} \cdot P := P + \mathbf{v}$ for $\mathbf{v} \in \tau(\mathbb{A}_n)$, $P \in \mathbb{A}_n$.
(*d*) If $\mathcal{U} \leq \mathcal{G}$ is a subgroup of the group $\mathcal{G}$, then $\mathcal{G}$ is a $\mathcal{U}$-set where $\cdot : \mathcal{U} \times \mathcal{G} \to \mathcal{G}$ is the usual composition law. In particular, each group $\mathcal{G}$ is a $\mathcal{G}$-set and hence every group $\mathcal{G}$ can be viewed as a group of mappings from $\mathcal{G}$ onto $\mathcal{G}$.

Definition 1.4.3.2.3. Let $\mathcal{G}$ be a group and M a $\mathcal{G}$-set. If $m \in M$, then the set $\mathcal{G} \cdot m := \{g \cdot m | g \in \mathcal{G}\}$ is called the *orbit* of m under $\mathcal{G}$.

The $\mathcal{G}$-set M is called *transitive* if $M = \mathcal{G} \cdot m$ for any $m \in M$ consists of a single orbit under $\mathcal{G}$.

If $m \in M$ then the *stabilizer of m in* $\mathcal{G}$ is $\mathrm{Stab}_{\mathcal{G}}(m) := \{g \in \mathcal{G} \mid g \cdot m = m\}$.

For a space group $\mathcal{G}$ and a point P in the point space, the stabilizer $\mathrm{Stab}_{\mathcal{G}}(P)$ is called the *site-symmetry group* of P with respect to $\mathcal{G}$.

The *kernel* $\mathcal{K}$ *of the action* of $\mathcal{G}$ on M is the intersection of the stabilizers of all elements in M,

$$\mathcal{K} := \{g \in \mathcal{G} \mid g \cdot m = m \text{ for all } m \in M\}.$$

M is called a *faithful* $\mathcal{G}$-set and the action of $\mathcal{G}$ on M is also called *faithful* if the kernel of the action is trivial, $\mathcal{K} = \{e\}$. □

Note that any space group $\mathcal{R}$ acts faithfully on the point space.

Remarks

(i) If $m_1, m_2 \in M$, then their orbits are either equal or disjoint. For if there is an element $g_1 \cdot m_1 = g_2 \cdot m_2$, then by the axioms of $\mathcal{G}$-sets $m_1 = em_1 = (g_1^{-1}g_1) \cdot m_1 = g_1^{-1} \cdot (g_1 \cdot m_1) = g_1^{-1} \cdot (g_2 \cdot m_2) = (g_1^{-1}g_2) \cdot m_2$, hence every element $g \cdot m_1$ in the orbit of m_1 is of the form $g \cdot (g_1^{-1}g_2 \cdot m_2) = (gg_1^{-1}g_2) \cdot m_2$ and therefore lies in the orbit of m_2. Hence the set of orbits gives a partition of M into disjoint sets. If M is a finite set, then its order is the sum of the lengths of the different orbits.
(ii) $\mathrm{Stab}_{\mathcal{G}}(m)$ is a subgroup of $\mathcal{G}$, since for $g_1, g_2 \in \mathrm{Stab}_{\mathcal{G}}(m)$, the product $(g_1g_2^{-1}) \cdot m = g_1 \cdot (g_2^{-1} \cdot m) = g_1 \cdot m = m$.
(iii) If $m_1 = g \cdot m_2$, then $\mathrm{Stab}_{\mathcal{G}}(m_1) = g\,\mathrm{Stab}_{\mathcal{G}}(m_2)g^{-1} = \{ghg^{-1} \mid h \in \mathrm{Stab}_{\mathcal{G}}(m_2)\}$.

Example 1.4.3.2.4 (Example 1.4.3.2.2 continued)

(*a*) $\mathbb{A}_n$ is a transitive $\mathcal{A}_n$-set. This is a mathematical expression of the fact that in point space no point is distinguished.
(*b*) The $\mathcal{A}_n$-set $\tau(\mathbb{A}_n)$ decomposes into two orbits $\{\mathbf{o}\}$ and $\{\mathbf{v} \in \tau(\mathbb{A}_n) \mid \mathbf{v} \neq \mathbf{o}\}$. The kernel of the action of $\mathcal{A}_n$ on $\tau(\mathbb{A}_n)$ is the translation subgroup $\mathcal{T}_n$.
(*c*) $\tau(\mathbb{A}_n)$ acts transitively on $\mathbb{A}_n$. The kernel of the action only consists of the zero vector $\mathbf{o}$.

We now introduce some terminology for groups which is nicely formulated using $\mathcal{G}$-sets.

Definition 1.4.3.2.5. The orbit of $g \in \mathcal{G}$ under the action of the subgroup $\mathcal{U} \leq \mathcal{G}$ is the *right coset* $\mathcal{U}g = \{ug \mid u \in \mathcal{U}\}$ (*cf. IT* A, Section 8.1.5). Analogously one defines a *left coset* as

$$g\mathcal{U} = \{gu \mid u \in \mathcal{U}\}$$

and denotes the set of left cosets by $\mathcal{G}/\mathcal{U}$.

If the number of left cosets (which is always equal to the number of right cosets) of $\mathcal{U}$ in $\mathcal{G}$ is finite, then this number is called the *index* $[\mathcal{G} : \mathcal{U}]$ of $\mathcal{U}$ in $\mathcal{G}$. If this number is infinite, one says that the index of $\mathcal{U}$ in $\mathcal{G}$ is infinite. □

Example 1.4.3.2.6

$\mathbb{A}_n$ is a coset of $\mathbf{V}_n$ in $\mathbf{V}_{n+1}$, namely

$$\mathbb{A}_n = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ \hline 1 \end{pmatrix} + \mathbf{V}_n.$$

If one thinks of $\mathbb{A}_2$ as an infinite sheet of paper and puts uncountably many such sheets of paper (one for each real number) one onto the other, one gets the whole 3-space $\mathbf{V}_3$.

Remark. The set of left cosets $\mathcal{G}/\mathcal{U}$ is a left $\mathcal{G}$-set with the operation $g \cdot (m\mathcal{U}) := (gm)\mathcal{U}$ for all $g, m \in \mathcal{G}$. The kernel of the action is the intersection of all subgroups of $\mathcal{G}$ that are conjugate to $\mathcal{U}$ and is called the *core* of $\mathcal{U}$: core $(\mathcal{U}) := \bigcap_{g \in \mathcal{G}} g\mathcal{U}g^{-1}$.

We now assume that $|\mathcal{G}|$ is finite. Let $\mathcal{U} \leq \mathcal{G}$ be a subgroup of $\mathcal{G}$. Then the set $\mathcal{G}$ is partitioned into left cosets of $\mathcal{U}$, $\mathcal{G} = g_1\mathcal{U} \cup \ldots \cup g_i\mathcal{U}$, where $i = [\mathcal{G} : \mathcal{U}]$ is the index of $\mathcal{U}$ in $\mathcal{G}$. Since the orders of the left cosets of $\mathcal{U}$ are all equal to the order of $\mathcal{U}$, one gets

Theorem 1.4.3.2.7. (Theorem of Lagrange.) Let $\mathcal{U}$ be a subgroup of the finite group $\mathcal{G}$. Then

$$|\mathcal{G}| = |\mathcal{U}|[\mathcal{G} : \mathcal{U}].$$

In particular, the order of any subgroup of $\mathcal{G}$ and also the index of any subgroup of $\mathcal{G}$ are divisors of the group order $|\mathcal{G}|$. □

The $\mathcal{G}$-set $\mathcal{G}/\mathcal{U}$ is only a special case of a $\mathcal{G}$-set. It is a transitive $\mathcal{G}$-set. If $M = \mathcal{G} \cdot m$ is a transitive $\mathcal{G}$-set, then the mapping $M \to \mathcal{G}/\mathrm{Stab}_{\mathcal{G}}(m)$, $g \cdot m \mapsto g\,\mathrm{Stab}_{\mathcal{G}}(m)$ is a bijection (in fact an isomorphism of $\mathcal{G}$-sets in the sense of Definition 1.4.3.4.1 below). Therefore, the number of elements of M, which is the length of the orbit of m under $\mathcal{G}$, equals the index of the stabilizer of m in $\mathcal{G}$, whence one gets the following generalization of the theorem of Lagrange:

Theorem 1.4.3.2.8. Let $\mathcal{G}$ be a finite group and M be a $\mathcal{G}$-set. Then

$$|\mathcal{G}| = |\mathcal{G} \cdot m||\mathrm{Stab}_{\mathcal{G}}(m)|$$

for all $m \in M$. □

The point group $\mathcal{G}$ acts on the finite set M of ideal crystal faces. Then the length of the orbit (the number of equivalent crystal faces) times the order of the face-symmetry group is the order of the point group.

Up to now, we have only considered the action of $\mathcal{G}$ upon $\mathcal{G}$ *via* multiplication. There is another natural action of $\mathcal{G}$ on itself *via conjugation*: $\mathcal{G} \times \mathcal{G} \to \mathcal{G}$ defined by $g \cdot m := gmg^{-1}$ for all group elements g and elements m in the $\mathcal{G}$-set $\mathcal{G}$. The stabilizer of m is called the *centralizer* of m in $\mathcal{G}$,

$$\mathrm{Stab}_{\mathcal{G}}(m) = \mathcal{C}_{\mathcal{G}}(m) = \{g \in \mathcal{G} \mid gmg^{-1} = m\}.$$

If $M \subset \mathcal{G}$ is a set of group elements, then the *centralizer of* M is the intersection of the centralizers of the elements in M:

$$\mathcal{C}_{\mathcal{G}}(M) = \{g \in \mathcal{G} \mid gmg^{-1} = m \text{ for all } m \in M\}.$$

Definition 1.4.3.2.9. $\mathcal{G}$ also acts on the set $\mathbf{U}$ of all subgroups of $\mathcal{G}$ by conjugation, $g \cdot \mathcal{U} := g\mathcal{U}g^{-1}$. The stabilizer of an element $\mathcal{U} \in \mathbf{U}$ is called the *normalizer of* $\mathcal{U}$ and denoted by $\mathcal{N}_{\mathcal{G}}(\mathcal{U})$. $\mathcal{U}$ is called a *normal subgroup of* $\mathcal{G}$ (denoted as $\mathcal{U} \trianglelefteq \mathcal{G}$) if $\mathcal{N}_{\mathcal{G}}(\mathcal{U}) = \mathcal{G}$. □

Remarks

(i) Let $\mathcal{U} \leq \mathcal{G}$. Then the index of the normalizer of $\mathcal{U}$ in $\mathcal{G}$ is the number of subgroups of $\mathcal{G}$ that are conjugate to $\mathcal{U}$. Since $\mathcal{U}$ always normalizes itself [hence $\mathcal{U}$ is a subgroup of $\mathcal{N}_{\mathcal{G}}(\mathcal{U})$], the index of the normalizer divides the index of $\mathcal{U}$.

(ii) If $\mathcal{G}$ is Abelian, then the conjugation action of $\mathcal{G}$ is trivial, hence each subgroup of $\mathcal{G}$ is a normal subgroup.

(iii) The group $\mathcal{G}$ itself and also the trivial subgroup $\{e\} \leq \mathcal{G}$ are always normal subgroups of $\mathcal{G}$.

Normal subgroups play an important role in the investigation of groups. If $\mathcal{N} \trianglelefteq \mathcal{G}$ is a normal subgroup, then the left coset $g\mathcal{N}$ equals the right coset $\mathcal{N}g$ for all $g \in \mathcal{G}$, because $g\mathcal{N} = g(g^{-1}\mathcal{N}g) = \mathcal{N}g$.

The most important property of normal subgroups is that the set of left cosets of $\mathcal{N}$ in $\mathcal{G}$ forms a group, called the *factor group* $\mathcal{G}/\mathcal{N}$, as follows: The set of all products of elements of two left cosets of $\mathcal{N}$ again forms a left coset of $\mathcal{N}$. Let $g, h \in \mathcal{G}$. Then

$$g\mathcal{N}h\mathcal{N} = g(h\mathcal{N}h^{-1})h\mathcal{N} = gh\mathcal{N}\mathcal{N} = gh\mathcal{N}.$$

This defines a natural product on the set of left cosets of $\mathcal{N}$ in $\mathcal{G}$ which turns this set into a group. The unit element is $e\mathcal{N}$.

Hence the philosophy of normal subgroups is that they cut the group into pieces, where the two pieces $\mathcal{G}/\mathcal{N}$ and $\mathcal{N}$ are again groups.

Example 1.4.3.2.10. The group $\mathbb{Z}$ is Abelian. For any number $p \in \mathbb{Z}$, the set $p\mathbb{Z}$ is a subgroup of $\mathbb{Z}$. Hence $p\mathbb{Z}$ is a normal subgroup of $\mathbb{Z}$. The factor group $\mathbb{Z}/p\mathbb{Z}$ inherits the multiplication from the multiplication in $\mathbb{Z}$, since $ap\mathbb{Z} \subset p\mathbb{Z}$ for all $a \in \mathbb{Z}$. If p is a prime number, then all elements $\neq 0 + p\mathbb{Z}$ in $\mathbb{Z}/p\mathbb{Z}$ have a multiplicative inverse, and therefore $\mathbb{Z}/p\mathbb{Z}$ is a field, the *field with p elements*.

Proposition 1.4.3.2.11. Let $\mathcal{N} \trianglelefteq \mathcal{G}$ be a normal subgroup of the group $\mathcal{G}$ and $\mathcal{U} \leq \mathcal{G}$. Then the set

$$\mathcal{N}\mathcal{U} = \mathcal{U}\mathcal{N} := \{un \mid u \in \mathcal{U}, n \in \mathcal{N}\}$$

is a subgroup of $\mathcal{G}$. □

Proof. Let $u_1n_1, u_2n_2 \in \mathcal{U}\mathcal{N}$. Then

$$u_1n_1(u_2n_2)^{-1} = u_1n_1n_2^{-1}u_2^{-1} = u_1u_2^{-1}(u_2n_1n_2^{-1}u_2^{-1}) = un \in \mathcal{U}\mathcal{N},$$

where $u := u_1u_2^{-1} \in \mathcal{U}$, since $\mathcal{U}$ is a subgroup of $\mathcal{G}$, and $n := u_2n_1n_2^{-1}u_2^{-1} \in \mathcal{N}$, since $\mathcal{N}$ is a normal subgroup of $\mathcal{G}$. QED

1.4.3.3. The Sylow theorems

A nice application of the notion of $\mathcal{G}$-sets are the three theorems of Sylow. By Theorem 1.4.3.2.7, the order of any subgroup $\mathcal{U}$ of a group $\mathcal{G}$ divides the order of $\mathcal{G}$. But conversely, given a divisor d of $|\mathcal{G}|$, one cannot predict the existence of a subgroup $\mathcal{U}$ of $\mathcal{G}$ with $|\mathcal{U}| = d$. If $d = p^\beta$ is a prime power that divides $|\mathcal{G}|$, then the following theorem says that such a subgroup exists.

Theorem 1.4.3.3.1. (Sylow) Let $\mathcal{G}$ be a finite group and p be a prime such that p^β divides the order of $\mathcal{G}$. Then $\mathcal{G}$ possesses m subgroups of order p^β, where $m > 0$ satisfies $m \equiv 1 \pmod{p}$. □

In particular this theorem implies that for every prime power that divides the order of the finite group $\mathcal{G}$, the group $\mathcal{G}$ has a subgroup whose order is this prime power. This is not true for composite numbers. For instance, the alternating group $\mathcal{A}lt_4$ of order 12 (Hermann–Mauguin notation 23) has no subgroup of order 6. This group has three subgroups of order 2, a unique subgroup of order 4 = 2^2 and four subgroups of order 3. The group $\mathcal{C}yc_2 \times \mathcal{S}ym_3$ (Hermann–Mauguin notation $\bar{3}m$) also has order 12 but seven subgroups of order 2, three subgroups of order 4 and a unique subgroup of order 3.

Theorem 1.4.3.3.2. (Sylow) If $|\mathcal{G}| = p^\alpha s$ for some prime p not dividing s, then all subgroups of order p^α of $\mathcal{G}$ are conjugate in $\mathcal{G}$. Such a subgroup $\mathcal{U} \leq \mathcal{G}$ of order $|\mathcal{U}| = p^\alpha$ is called a *Sylow p-subgroup*. □

Combining these two theorems with Theorem 1.4.3.2.8, one gets Sylow's third theorem:

Theorem 1.4.3.3.3. (Sylow) The number of Sylow p-subgroups of $\mathcal{G}$ is $\equiv 1 \pmod{p}$ and divides the order of $\mathcal{G}$. □

Proofs of the three theorems above can be found in Ledermann (1976), pp. 158–164, or in Ledermann & Weir (1996), pp. 155–161.

1.4.3.4. Isomorphisms

If one wants to compare objects such as groups or $\mathcal{G}$-sets, to be able to say when they should be considered equal, the concept of isomorphisms should be used:

Definition 1.4.3.4.1. Let $\mathcal{G}$ and $\mathcal{H}$ be groups and M and N be $\mathcal{G}$-sets.

(*a*) A *homomorphism* $\varphi : \mathcal{G} \to \mathcal{H}$ is a mapping of the set $\mathcal{G}$ into the set $\mathcal{H}$ respecting the composition law *i.e.* $\varphi(gh) = \varphi(g)\varphi(h)$ for all $g, h \in \mathcal{G}$.

If φ is bijective, it is called an *isomorphism* and one says $\mathcal{G}$ is *isomorphic* to $\mathcal{H}$ ($\mathcal{G} \cong \mathcal{H}$).

If $e \in \mathcal{H}$ is the unit element of $\mathcal{H}$, then the set of all pre-images of e is called the *kernel* of φ: $\ker(\varphi) := \{g \in \mathcal{G} \mid \varphi(g) = e\}$. An isomorphism $\varphi : \mathcal{G} \to \mathcal{G}$ is called an *automorphism* of $\mathcal{G}$.

(*b*) M and N are called *isomorphic* $\mathcal{G}$-sets if there is a bijection $\varphi : M \to N$ with $g \cdot \varphi(m) = \varphi(g \cdot m)$ for all $g \in \mathcal{G}, m \in M$. □

Example 1.4.3.4.2. In Example 1.4.3.1.3, the group homomorphism $\mathbb{Z} \to p\mathbb{Z}$ defined by $1 \longmapsto p$ is a group isomorphism (from the group $\mathbb{Z}$ onto its subgroup $p\mathbb{Z}$).

Example 1.4.3.4.3. For any group element $g \in \mathcal{G}$, conjugation by g defines an automorphism of $\mathcal{G}$. In particular, if $\mathcal{U}$ is a subgroup of $\mathcal{G}$, then $\mathcal{U}$ and its conjugate subgroup $g\mathcal{U}g^{-1}$ are isomorphic.

Philosophy: If $\mathcal{G}$ and $\mathcal{H}$ are isomorphic groups, then all group-theoretical properties of $\mathcal{G}$ and $\mathcal{H}$ are the same. The calculations in $\mathcal{G}$ can be translated by the isomorphism to calculations in $\mathcal{H}$. Sometimes it is easier to calculate in one group than in the other and translate the result back *via* the inverse of the isomorphism. For example, the isomorphism between $\tau(\mathbb{A}_n)$ and $\mathbf{V}_n$ in Section 1.4.2 is an isomorphism of groups. It even respects scalar multiplication with real numbers, so in fact it is an isomorphism of vector spaces. While the composition of translations is more concrete and easier to imagine, the calculation of the resulting vector is much easier in $\mathbf{V}_n$. The concept of isomorphism says that you can translate to the more convenient group for your calculations and translate back afterwards without losing anything.

Note that a homomorphism is injective, hence an isomorphism onto its image, if and only if its kernel is trivial ($= \{e\}$).

Example 1.4.3.4.4

The mapping μ from the space $\tau(\mathbb{A}_n)$ of translation vectors into the affine group $\mathcal{A}_n$ defined by

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

is a homomorphism of the group $\tau(\mathbb{A}_n)$ into $\mathcal{A}_n$. The kernel of this homomorphism is $\{\boldsymbol{o}\}$ and the image of the mapping is the translation subgroup $\mathcal{T}_n$ of $\mathcal{A}_n$. Hence the groups $\tau(\mathbb{A}_n)$ and $\mathcal{T}_n$ are isomorphic.

The affine group acts (as group of group automorphisms) on the normal subgroup $\mathcal{T}_n \trianglelefteq \mathcal{A}_n$ *via* conjugation: $g \cdot t := gtg^{-1}$. We have seen already in Example 1.4.3.2.4 (*b*) that it also acts (as a group of linear mappings) on $\tau(\mathbb{A}_n)$. The mapping μ is an isomorphism of $\mathcal{A}_n$-sets.

1.4.3.5. Isomorphism theorems

[*cf.* Ledermann (1976), pp. 68–73, or Ledermann & Weir (1996), pp. 85–92.]

Remark. If φ is a homomorphism $\mathcal{G} \to \mathcal{H}$ and $\mathcal{N} \trianglelefteq \mathcal{H}$ is a normal subgroup of $\mathcal{H}$, then the pre-image $\varphi^{-1}(\mathcal{N}) := \{g \in \mathcal{G} \mid \varphi(g) \in \mathcal{N}\}$ is a normal subgroup of $\mathcal{G}$. In particular, it holds that $\ker(\varphi) \trianglelefteq \mathcal{G}$.

Hence the factor group $\mathcal{G}/\ker(\varphi)$ is a well defined group. The following theorem says that this group is isomorphic to the image $\varphi(\mathcal{G}) \leq \mathcal{H}$ of φ:

Theorem 1.4.3.5.1. (First isomorphism theorem.) Let $\varphi : \mathcal{G} \to \mathcal{H}$ be a homomorphism of groups. Then

$$\overline{\varphi} : \mathcal{G}/\ker(\varphi) \to \varphi(\mathcal{G}) \leq \mathcal{H}$$

defined by $\overline{\varphi}(g\ker(\varphi)) = \varphi(g)$ is an isomorphism between the factor group $\mathcal{G}/\ker(\varphi)$ and the image group of φ, which is a subgroup of $\mathcal{H}$. □

For instance, if $\mathcal{R}$ is a space group and φ is mapping any element

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

to its linear part $\boldsymbol{W}$, then the kernel of φ is the translation group $\mathcal{T}(\mathcal{R})$ of $\mathcal{R}$ and the image is the point group $\overline{\mathcal{R}}$ of $\mathcal{R}$. The theorem says that the point group $\overline{\mathcal{R}}$ is isomorphic to the factor group $\mathcal{R}/\mathcal{T}(\mathcal{R})$.

Theorem 1.4.3.5.2. (Third isomorphism theorem.) Let $\mathcal{N} \trianglelefteq \mathcal{G}$ be a normal subgroup of the group $\mathcal{G}$ and $\mathcal{U} \leq \mathcal{G}$ be an arbitrary subgroup of $\mathcal{G}$. Then $\mathcal{U} \cap \mathcal{N} \trianglelefteq \mathcal{U}$ is a normal subgroup of $\mathcal{U}$ and

$$\mathcal{U}/(\mathcal{U} \cap \mathcal{N}) \cong \mathcal{N}\mathcal{U}/\mathcal{N}.$$

(For the definition of the group $\mathcal{N}\mathcal{U}$ see Proposition 1.4.3.2.11.) □

Definition 1.4.3.5.3. A subgroup $\mathcal{U} \leq \mathcal{H}$ is a *characteristic subgroup* $\mathcal{U} \operatorname{char} \mathcal{H}$ if $\varphi(\mathcal{U}) = \mathcal{U}$ for all automorphisms φ of $\mathcal{H}$. □

Remarks

(*a*) If $\mathcal{H}$ is a finite Abelian group and $\mathcal{P}$ is a Sylow p-subgroup of $\mathcal{H}$, then $\mathcal{P} \operatorname{char} \mathcal{H}$, because $\mathcal{P}$ is the only subgroup of $\mathcal{H}$ of order $|\mathcal{P}|$.

(*b*) If $\mathcal{H}$ is any group and $\mathcal{U} \operatorname{char} \mathcal{H}$, then $\mathcal{U} \trianglelefteq \mathcal{H}$ is also a normal subgroup of $\mathcal{H}$: for $h \in \mathcal{H}$ define the mapping $\kappa_h : \mathcal{H} \to \mathcal{H}$, $x \longmapsto hxh^{-1}$. Then κ_h is an automorphism of $\mathcal{H}$ and $\kappa_h(\mathcal{U}) = h\mathcal{U}h^{-1} = \mathcal{U}$ since $\mathcal{U}$ is characteristic in $\mathcal{H}$.

(*c*) If $\mathcal{U}\,\mathrm{char}\,\mathcal{N} \trianglelefteq \mathcal{H}$, then $\mathcal{U} \trianglelefteq \mathcal{H}$, since the conjugation with any element of $\mathcal{H}$ induces an automorphism of $\mathcal{N}$.

1.4.3.6. An example

Let us consider the tetrahedral group, Schoenflies symbol T_d, which is defined as the symmetry group of a tetrahedron. It permutes the four apices P_1, P_2, P_3, P_4 of the tetrahedron and hence every element of T_d defines a bijection of $V := \{P_1, P_2, P_3, P_4\}$ onto itself. The only element that fixes all the apices is e. Therefore the set V is a faithful T_d-set. Let us calculate the order of $|T_d|$. Since there are elements in T_d that map the first apex P_1 onto each one of the other apices, V is a transitive T_d-set. Let $\mathcal{S} := \mathrm{Stab}_{T_d}(P_1)$ be the stabilizer of P_1. By Theorem 1.4.3.2.8, $|T_d| = |V||\mathcal{S}| = 4|\mathcal{S}|$. The group $\mathcal{S}$ is generated by the threefold rotation r around the 'diagonal' of the tetrahedron through P_1 and the reflection s at the symmetry plane of the tetrahedron which contains the edge (P_1, P_2). In particular, $\mathcal{S}$ acts transitively on the set $\{P_2, P_3, P_4\}$. The stabilizer of P_2 in $\mathcal{S}$ is the cyclic group $\langle s\rangle \cong \mathcal{C}yc_2$ generated by s. (The Schoenflies notation for $\langle s\rangle$ is C_s and the Hermann–Mauguin symbol is m.) Therefore $|\mathcal{S}| = 3|\langle s\rangle| = 6$ and $|T_d| = 24$. In fact, we have seen that T_d is isomorphic to the group of all bijections of V onto itself, which is the symmetric group $\mathcal{S}ym_4$ of degree 4 and the group $\mathcal{S} \cong \mathcal{S}ym_3$ is the symmetric group on $\{P_2, P_3, P_4\}$. The Schoenflies notation for $\mathcal{S}$ is C_{3v} and its Hermann–Mauguin symbol is $3m$.

In general, let $n \in \mathbb{N}$ be a natural number. Then the group of all bijective mappings of the set $\{1, \ldots, n\}$ onto itself is called the *symmetric group of degree n* and denoted by

$$\mathcal{S}ym_n := \{f : \{1, \ldots, n\} \to \{1, \ldots, n\} \mid f \text{ is bijective}\}.$$

The *alternating group* is the normal subgroup $\mathcal{A}lt_n$ consisting of all even permutations of $\{1, \ldots, n\}$.

Let us construct a normal subgroup of T_d. The tetrahedral group contains three twofold rotations r_1, r_2, r_3 around the three axes of the tetrahedron through the midpoints of opposite edges. Since T_d permutes these three axes and hence conjugates the three rotations into each other, the group

$$\mathcal{U} := \langle r_1, r_2, r_3\rangle$$

generated by these three rotations is a normal subgroup of T_d. Since these three rotations commute with each other, the group $\mathcal{U}$ is Abelian. Now $r_1 r_2 = r_3$ and hence $\mathcal{U} = \{e, r_1, r_2, r_3\} \cong D_2$ (in Schoenflies notation) $\cong 222$ (Hermann–Mauguin symbol) is of order 4. There are three normal subgroups of order 2 in $\mathcal{U}$, namely $\langle r_i\rangle$ for $i = 1, 2, 3$. The factor group $\mathcal{U}/\langle r_1\rangle$ is again of order 2. Since all groups of order 2 are cyclic, $\langle r_1\rangle \cong \mathcal{U}/\langle r_1\rangle \cong \mathcal{C}yc_2$. The set $\mathcal{U}$ is the set of all products of elements from the two normal subgroups $\langle r_1\rangle$ and $\langle r_2\rangle$, hence $\mathcal{U}$ is isomorphic to the *direct product* $\mathcal{C}yc_2 \times \mathcal{C}yc_2$ in the sense of the following definition.

Definition 1.4.3.6.1. [*cf.* Ledermann (1976), Section 13, or Ledermann & Weir (1996), Section 2.7.] Let $\mathcal{G}$ and $\mathcal{H}$ be two groups. Then the *direct product* $\mathcal{G} \times \mathcal{H}$ is the group $\mathcal{G} \times \mathcal{H} = \{(g, h) \mid g \in \mathcal{G}, h \in \mathcal{H}\}$ with multiplication $(g, h)(g', h') := (gg', hh')$. □

Let us return to the example above. The centralizer of one of the three rotations, say of r_1, is of index 3 in T_d and hence a Sylow 2-subgroup of T_d with order 8. Following Schoenflies, we will denote this group by D_{2d} (another Schoenflies symbol for this group is S_{4v} and its Hermann–Mauguin symbol is $\bar{4}2m$).

The group $\mathcal{U}$ above is contained in D_{2d}. It is its own centralizer in T_d: $\mathcal{U} = \mathcal{C}_{T_d}(\mathcal{U})$. Therefore, the factor group $T_d/\mathcal{U}$ acts faithfully (and transitively) on the set $\{r_1, r_2, r_3\}$. The stabilizer of r_1 is the subgroup D_{2d} constructed above. Using this, one easily sees that $T_d/\mathcal{U} \cong \mathcal{S}ym_3$.

Another normal subgroup in T_d is the set of all rotations in T_d. This group contains the normal subgroup $\mathcal{U}$ above of index 3 and is of index 2 in T_d (and hence has order 12). It is isomorphic to $\mathcal{A}lt_4$, the alternating group of degree 4, and has Schoenflies symbol T and Hermann–Mauguin symbol 23.

1.4.4. Space groups

1.4.4.1. Definition of space groups

In *IT* A (2005) Section 8.1.6 space groups are introduced as symmetry groups of crystal patterns.

Definition 1.4.4.1.1

(*a*) Let $\mathbf{V}_n$ be the n-dimensional real vector space. A subset $\mathbf{L} \subseteq \mathbf{V}_n$ is called an (n-dimensional) *lattice* if there is a basis $(\mathbf{b}_1, \ldots, \mathbf{b}_n)$ of $\mathbf{V}_n$ such that

$$\mathbf{L} = \mathbb{Z}\mathbf{b}_1 + \ldots + \mathbb{Z}\mathbf{b}_n = \{\sum_{i=1}^{n} a_i \mathbf{b}_i \mid a_i \in \mathbb{Z}\}.$$

(*b*) A *crystal structure* is a mapping $f : \mathbb{E}_n \to \mathbb{R}$ of the Euclidean point space into the real numbers such that $\mathrm{Stab}_{\tau(\mathbb{A}_n)}(f) := \{t \in \tau(\mathbb{A}_n) \mid f(P + t) = f(P) \text{ for all } P \in \mathbb{A}_n\}$ is an n-dimensional lattice in $\tau(\mathbb{A}_n)$.

(*c*) The Euclidean group $\mathcal{E}_n$ acts on the set of mappings $\mathbb{E}_n \to \mathbb{R}$ *via* $(g \cdot f)(P) := f(g^{-1}P)$ for all $P \in \mathbb{E}_n$ and for all $g \in \mathcal{E}_n$ and $f : \mathbb{E}_n \to \mathbb{R}$. A *space group* $\mathcal{R}$ is the stabilizer of a crystal structure $f : \mathbb{E}_n \to \mathbb{R}$; $\mathcal{R} = \mathrm{Stab}_{\mathcal{E}}n(f)$.

(*d*) Let $\mathcal{R} \leq \mathcal{E}_n$ be a space group. The *translation subgroup* $\mathcal{T}(\mathcal{R})$ of $\mathcal{R}$ is defined as $\mathcal{T}(\mathcal{R}) := \mathcal{R} \cap \mathcal{T}_n$. □

The definition introduced space groups in the way they occur in crystallography: The group of symmetries of an ideal crystal stabilizes the crystal structure. This definition is not very helpful in analysing the structure of space groups. If $\mathcal{R}$ is a space group, then the translation subgroup $\mathcal{T} := \mathcal{T}(\mathcal{R})$ is a normal subgroup of $\mathcal{R}$. It is even a characteristic subgroup of $\mathcal{R}$, hence fixed under every automorphism of $\mathcal{R}$. By Definition 1.4.4.1.1, its image under the inverse μ' of the mapping μ in Example 1.4.3.4.4 defined by

$$\mu' : \mathcal{T} \to \tau(\mathbb{E}_n); \begin{pmatrix} \boldsymbol{I} & \boldsymbol{v} \\ \boldsymbol{o}^{\mathrm{T}} & 1 \end{pmatrix} \mapsto \boldsymbol{v}$$

in $\tau(\mathbb{A}_n)$ is an n-dimensional lattice $\mathbf{L}(\mathcal{R})$. Since μ' is an isomorphism from $\mathcal{T}$ onto $\mathbf{L}(\mathcal{R})$, the translation subgroup of $\mathcal{R}$ is isomorphic to the lattice $\mathbf{L}(\mathcal{R})$. In particular, one has $\mu'(t_1 t_2) = \mu'(t_1) + \mu'(t_2)$ and the subgroup $\mathcal{T}^p$, formed by the pth powers of elements in $\mathcal{T}$, is mapped onto $p\mathbf{L}(\mathcal{R})$. Lattices are well understood. Although they are infinite, they have a simple structure, so they can be examined algorithmically. Since they lie in a vector space, one can apply linear algebra to them.

Now we want to look at how this lattice $\mathcal{T}(\mathcal{R})$ fits into the space group $\mathcal{R}$. The affine group $\mathcal{A}_n$ acts on $\mathcal{T}_n$ by conjugation as well as on $\tau(\mathbb{A}_n)$ *via* its linear part. Similarly the space group $\mathcal{R}$ acts on $\mathcal{T}(\mathcal{R})$ by conjugation: For $g \in \mathcal{R}$ and $t \in \mathcal{T}$, one gets

$\mu'(gtg^{-1}) = \overline{g}\mu'(t)$, where $\overline{g}$ is the linear part of g. Therefore, the kernel of this action is on the one hand the centralizer of $\mathcal{T}(\mathcal{R})$ in $\mathcal{R}$, on the other hand, since $\mathbf{L}(\mathcal{R})$ contains a basis of $\tau(\mathbb{E}_n)$, it is equal to the kernel of the mapping $^{-}$, which is $\mathcal{R} \cap \mathcal{T}_n = \mathcal{T}(\mathcal{R})$, hence

$$\mathcal{C}_{\mathcal{R}}(\mathcal{T}(\mathcal{R})) = \mathcal{T}(\mathcal{R}).$$

Hence only the linear part $\overline{\mathcal{R}} \cong \mathcal{R}/\mathcal{T}(\mathcal{R})$ of $\mathcal{R}$ acts faithfully on $\mathcal{T}(\mathcal{R})$ by conjugation and linearly on $\mathbf{L}(\mathcal{R})$. This factor group $\mathcal{R}/\mathcal{T}(\mathcal{R})$ is a finite group. Let us summarize this:

Theorem 1.4.4.1.2. Let $\mathcal{R}$ be a space group. The translation subgroup $\mathcal{T}(\mathcal{R}) = \mathcal{R} \cap \mathcal{T}_n$ is an Abelian normal subgroup of $\mathcal{R}$ which is its own centralizer, $\mathcal{C}_{\mathcal{R}}(\mathcal{T}(\mathcal{R})) = \mathcal{T}(\mathcal{R})$. The finite group $\mathcal{R}/\mathcal{T}(\mathcal{R})$ acts faithfully on $\mathcal{T}(\mathcal{R})$ by conjugation. This action is similar to the action of the linear part $\overline{\mathcal{R}}$ on the lattice $\mu'(\mathcal{T}(\mathcal{R})) = \mathbf{L}(\mathcal{R})$. □

1.4.4.2. Maximal subgroups of space groups

Definition 1.4.4.2.1. A subgroup $\mathcal{M} \leq \mathcal{G}$ of a group $\mathcal{G}$ is called *maximal* if $\mathcal{M} \neq \mathcal{G}$ and for all subgroups $\mathcal{U} \leq \mathcal{G}$ with $\mathcal{M} \subseteq \mathcal{U}$ it holds that either $\mathcal{U} = \mathcal{M}$ or $\mathcal{U} = \mathcal{G}$. □

The translation subgroup $\mathcal{T} := \mathcal{T}(\mathcal{R})$ of the space group $\mathcal{R}$ plays a very important role if one wants to analyse the space group $\mathcal{R}$. Let $\mathcal{U} \neq \mathcal{R}$ be a subgroup of $\mathcal{R}$. Then $\mathcal{U}$ has either fewer translations ($\mathcal{T}(\mathcal{U}) < \mathcal{T}$) or the order of the linear part of $\mathcal{U}$, the index of $\mathcal{T}(\mathcal{U})$ in $\mathcal{U}$, gets smaller ($|\overline{\mathcal{U}}| < |\overline{\mathcal{R}}|$), or both happen.

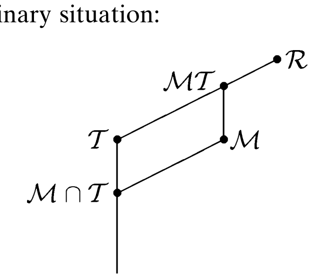
Definition 1.4.4.2.2. Let $\mathcal{U}$ be a subgroup of the space group $\mathcal{R}$ and $\mathcal{T} := \mathcal{T}(\mathcal{R})$.

(t) $\mathcal{U}$ is called a *translationengleiche* or a *t-subgroup* if $\mathcal{U} \cap \mathcal{T} = \mathcal{T}$.

(k) $\mathcal{U}$ is called a *klassengleiche* or a *k-subgroup* if $\mathcal{U}/\mathcal{U} \cap \mathcal{T} \cong \mathcal{R}/\mathcal{T}$. □

Remark. The third isomorphism theorem, Theorem 1.4.3.5.2, implies that if $\mathcal{U}$ is a k-subgroup, then $\mathcal{U}\mathcal{T}/\mathcal{T} \cong \mathcal{U}/\mathcal{U} \cap \mathcal{T} \cong \mathcal{R}/\mathcal{T}$. Hence $\mathcal{U}$ is a k-subgroup if and only if $\mathcal{U}\mathcal{T} = \mathcal{R}$.

Let $\mathcal{M}$ be a maximal subgroup of $\mathcal{R}$. Then we have the following preliminary situation:

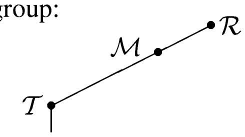


Since $\mathcal{T} \trianglelefteq \mathcal{R}$ and $\mathcal{M} \leq \mathcal{R}$, one has by Proposition 1.4.3.2.11 that $\mathcal{M}\mathcal{T} \leq \mathcal{R}$. Hence the maximality of $\mathcal{M}$ implies that $\mathcal{M}\mathcal{T} = \mathcal{M}$ or $\mathcal{M}\mathcal{T} = \mathcal{R}$. If $\mathcal{M}\mathcal{T} = \mathcal{M}$ then $\mathcal{T} \subseteq \mathcal{M}$, hence $\mathcal{M}$ is a t-subgroup. If $\mathcal{M}\mathcal{T} = \mathcal{R}$, then by the third isomorphism theorem, Theorem 1.4.3.5.2, $\mathcal{R}/\mathcal{T} = \mathcal{M}\mathcal{T}/\mathcal{T} \cong \mathcal{M}/(\mathcal{M} \cap \mathcal{T}) = \mathcal{M}/\mathcal{T}(\mathcal{M})$, hence $\mathcal{M}$ is a k-subgroup. This is given by the following theorem:

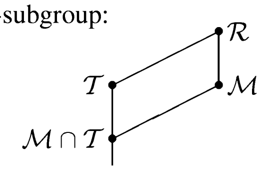
Theorem 1.4.4.2.3. (Hermann) Let $\mathcal{M} \leq \mathcal{R}$ be a maximal subgroup of the space group $\mathcal{R}$. Then $\mathcal{M}$ is either a k-subgroup or a t-subgroup. □

The above picture looks as follows in the two cases:

t-subgroup:



k-subgroup:



Let $\mathcal{M}$ be a t-subgroup of $\mathcal{R}$. Then $\mathcal{T}(\mathcal{R}) \leq \mathcal{M}$ and $\mathcal{M}/\mathcal{T}(\mathcal{R})$ is a subgroup $\mathcal{S}$ of $\mathcal{P} = \mathcal{R}/\mathcal{T}(\mathcal{R})$. On the other hand, any subgroup $\mathcal{S}$ of $\mathcal{P}$ defines a unique t-subgroup $\mathcal{M}$ of $\mathcal{R}$ with $\mathcal{T}(\mathcal{R}) \leq \mathcal{M}$ and $\mathcal{M}/\mathcal{T}(\mathcal{R}) = \mathcal{S}$, namely $\mathcal{M} = \{s \in \mathcal{R} \mid s\mathcal{T}(\mathcal{R}) \in \mathcal{S}\}$. Hence the t-subgroups of $\mathcal{R}$ are in bijection to the subgroups of $\mathcal{P}$, which is a finite group according to the remarks below Definition 1.4.4.1.1. For future reference, we note this in the following corollary:

Corollary 1.4.4.2.4. The t-subgroups of the space group $\mathcal{R}$ are in bijection with the subgroups of the finite group $\mathcal{R}/\mathcal{T}(\mathcal{R})$. □

In the case $n = 3$, which is the most important case in crystallography, the finite groups $\mathcal{R}/\mathcal{T}(\mathcal{R})$ are isomorphic to subgroups of either $\mathcal{C}yc_2 \times \mathcal{S}ym_4$ (Hermann–Mauguin symbol $m\overline{3}m$) or $\mathcal{C}yc_2 \times \mathcal{C}yc_2 \times \mathcal{S}ym_3$ ($= 6/mmm$). Here $\times$ denotes the direct product (*cf.* Definition 1.4.3.6.1), $\mathcal{C}yc_2$ the cyclic group of order 2, and $\mathcal{S}ym_3$ and $\mathcal{S}ym_4$ the symmetric groups of degree 3 or 4, respectively (*cf.* Section 1.4.3.6). Hence the maximal subgroups $\mathcal{M}$ of $\mathcal{R}$ that are t-subgroups can be read off from the subgroups of the two groups above.

An algorithm for calculating the maximal t-subgroups of $\mathcal{R}$ which applies to all three-dimensional space groups is explained in Section 1.4.5.

The more difficult task is the determination of the maximal k-subgroups.

Lemma 1.4.4.2.5. Let $\mathcal{M}$ be a maximal k-subgroup of the space group $\mathcal{R}$. Then $\mathcal{T}(\mathcal{M}) = \mathcal{T} \cap \mathcal{M} \trianglelefteq \mathcal{R}$ is a normal subgroup of $\mathcal{R}$. Hence $\mu'(\mathcal{T}(\mathcal{M})) \leq \mathbf{L}(\mathcal{R})$ is an $\overline{\mathcal{R}}$-invariant lattice. □

Proof. $\mathcal{R} = \mathcal{T}\mathcal{M}$, so every element g in $\mathcal{R}$ can be written as $g = tm$ where $t \in \mathcal{T}$ and $m \in \mathcal{M}$. Therefore one obtains for $t_1 \in \mathcal{T} \cap \mathcal{M}$

$$g^{-1}t_1 g = m^{-1}t^{-1}t_1 tm = m^{-1}t_1 m,$$

since $\mathcal{T}$ is Abelian. Since $m \in \mathcal{R}$ and $\mathcal{T}$ is normal in $\mathcal{R}$, one has $m^{-1}t_1 m \in \mathcal{T}$. But $m^{-1}t_1 m$ is a product of elements in $\mathcal{M}$ and therefore lies in the subgroup $\mathcal{M}$, hence $m^{-1}t_1 m \in \mathcal{T} \cap \mathcal{M}$. QED

The candidates for translation subgroups $\mathcal{T}(\mathcal{M})$ of maximal k-subgroups $\mathcal{M}$ of $\mathcal{R}$ can be found by linear-algebra algorithms using the philosophy explained at the beginning of this section: $\mathcal{R}$ acts on $\mathcal{T}$ by conjugation and this action is isomorphic to the action of the linear part $\overline{\mathcal{R}} \cong \mathcal{R}/\mathcal{T}$ of $\mathcal{R}$ on the lattice $\mathbf{L}(\mathcal{R})$ *via* the isomorphism $\mu' : \mathcal{T} \to \mathbf{L}(\mathcal{R})$. Normal subgroups of $\mathcal{R}$ contained in $\mathcal{T}$ are mapped onto $\overline{\mathcal{R}}$-invariant sublattices of $\mathbf{L}(\mathcal{R})$. An example for such a normal subgroup is the group $\mathcal{T}^p$ formed by the pth powers of elements of $\mathcal{T}$ for any natural number, in particular for prime numbers $p \in \mathbb{N}$. One has $\mu'(\mathcal{T}^p) = p\mathbf{L}(\mathcal{R})$.

If $\mathcal{M}$ is a maximal k-subgroup of $\mathcal{R}$, then $\mathcal{T}(\mathcal{M})$ is a normal subgroup of $\mathcal{R}$ that is maximal in $\mathcal{T}$, which means that $\mu'(\mathcal{T}(\mathcal{M})) = \mathbf{L}(\mathcal{M})$ is a maximal $\overline{\mathcal{R}}$-invariant sublattice of $\mathbf{L}(\mathcal{R})$. Hence it contains $p\mathbf{L}(\mathcal{R})$ for some prime number p. One may view $\mathcal{T}/\mathcal{T}^p \cong \mathbf{L}(\mathcal{R})/p\mathbf{L}(\mathcal{R})$ as a finite $(\mathbb{Z}/p\mathbb{Z})\overline{\mathcal{R}}$-module and find all candidates for such normal subgroups as full pre-images of maximal $(\mathbb{Z}/p\mathbb{Z})\overline{\mathcal{R}}$-submodules of $\mathbf{L}(\mathcal{R})/p\mathbf{L}(\mathcal{R})$. This gives an algorithm for calculating these normal subgroups, which is implemented in the package *[CARAT]*.

The group $\mathcal{G} := \mathcal{T}/\mathcal{T}^p$ is an Abelian group, with the additional property that for all $g \in \mathcal{G}$ one has $g^p = e$. Such a group is called an *elementary Abelian p-group*.

From the reasoning above we find the following lemma.

Lemma 1.4.4.2.6. Let $\mathcal{M}$ be a maximal k-subgroup of the space group $\mathcal{R}$. Then $\mathcal{T}/\mathcal{T}(\mathcal{M})$ is an elementary Abelian p-group for some prime p. The order of $\mathcal{T}/\mathcal{T}(\mathcal{M})$ is p^r with $r \leq n$. □

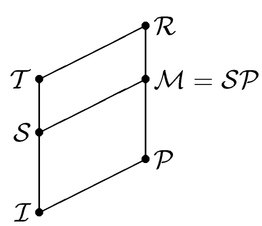
Corollary 1.4.4.2.7. Maximal subgroups of space groups are again space groups and of finite index in the supergroup. □

Hence the first step is the determination of subgroups of $\mathcal{R}$ that are maximal in $\mathcal{T}$ and normal in $\mathcal{R}$, and is solved by linear-algebra algorithms. These subgroups are the candidates for the translation subgroups $\mathcal{T}(\mathcal{M})$ for maximal k-subgroups $\mathcal{M}$. But even if one knows the isomorphism type of $\mathcal{M}/\mathcal{T}(\mathcal{M})$, the group $\mathcal{T}(\mathcal{M})$ does not in general determine $\mathcal{M} \leq \mathcal{R}$. Given such a normal subgroup $\mathcal{S} \trianglelefteq \mathcal{R}$ that is contained in $\mathcal{T}$, one now has to find all maximal k-subgroups $\mathcal{M} \leq \mathcal{R}$ with $\mathcal{S} = \mathcal{T} \cap \mathcal{M}$ and $\mathcal{T}\mathcal{M} = \mathcal{R}$. It might happen that there is no such group $\mathcal{M}$. This case does not occur if $\mathcal{R}$ is a symmorphic space group in the sense of the following definition:

Definition 1.4.4.2.8. A space group $\mathcal{R}$ is called *symmorphic* if there is a subgroup $\mathcal{P} \leq \mathcal{R}$ such that $\mathcal{P} \cap \mathcal{T}(\mathcal{R}) = \mathcal{I}$ and $\mathcal{P}\mathcal{T}(\mathcal{R}) = \mathcal{R}$. The subgroup $\mathcal{P}$ is called a *complement* of the translation subgroup $\mathcal{T}(\mathcal{R})$. □

Note that the group $\mathcal{P}$ in the definition is isomorphic to $\mathcal{R}/\mathcal{T}(\mathcal{R})$ and hence a finite group.

If $\mathcal{R}$ is symmorphic and $\mathcal{P} \leq \mathcal{R}$ is a complement of $\mathcal{T}$, then one may take $\mathcal{M} := \mathcal{S}\mathcal{P}$.



This shows the following:

Lemma 1.4.4.2.9. Let $\mathcal{R}$ be a symmorphic space group with translation subgroup $\mathcal{T}$ and $\mathcal{T}_1 \leq \mathcal{T}$ an $\mathcal{R}$-invariant subgroup of $\mathcal{T}$ (*i.e.* $\mathcal{T}_1 \trianglelefteq \mathcal{R}$). Then there is at least one k-subgroup $\mathcal{U} \leq \mathcal{R}$ with translation subgroup $\mathcal{T}_1$. □

In any case, the maximal k-subgroups, $\mathcal{M}$, of $\mathcal{R}$ satisfy

$\mathcal{M}\mathcal{T} = \mathcal{R}$ and
$\mathcal{M} \cap \mathcal{T} = \mathcal{S}$ is a maximal $\mathcal{R}$-invariant subgroup of $\mathcal{T}$.

To find these maximal subgroups, $\mathcal{M}$, one first chooses such a subgroup $\mathcal{S}$. It then suffices to compute in the finite group $\mathcal{R}/\mathcal{S} =: \overline{\mathcal{R}}$. If there is a complement $\overline{\mathcal{M}}$ of $\overline{\mathcal{T}} = \mathcal{T}/\mathcal{S}$ in $\overline{\mathcal{R}}$, then every element $x \in \overline{\mathcal{R}}$ may be written uniquely as $x = mt$ with $m \in \overline{\mathcal{M}}$, $t \in \overline{\mathcal{T}}$. In particular, any other complement $\overline{\mathcal{M}'}$ of $\overline{\mathcal{T}}$ in $\overline{\mathcal{R}}$ is of the form $\overline{\mathcal{M}'} = \{mt_m \mid m \in \overline{\mathcal{M}}, t_m \in \overline{\mathcal{T}}\}$. One computes $m_1 t_{m_1} m_2 t_{m_2} = m_1 m_2 (m_2^{-1} t_{m_1} m_2) t_{m_2}$. Since $\overline{\mathcal{M}'}$ is a subgroup of $\overline{\mathcal{R}}$, it holds that $t_{m_1 m_2} = (m_2^{-1} t_{m_1} m_2) t_{m_2}$. Moreover, every mapping $\overline{\mathcal{M}} \to \overline{\mathcal{T}};\ m \mapsto t_m$ with this property defines some maximal subgroup $\mathcal{M}'$ as above. Since $\overline{\mathcal{M}}$ and $\overline{\mathcal{T}}$ are finite, it is a finite problem to find all such mappings.

If there is no such complement $\overline{\mathcal{M}}$, this means that there is no (maximal) k-subgroup $\mathcal{M}$ of $\mathcal{R}$ with $\mathcal{M} \cap \mathcal{T} = \mathcal{S}$.

1.4.5. Maximal subgroups

1.4.5.1. Maximal subgroups and primitive $\mathcal{G}$-sets

To determine the maximal t-subgroups of a space group $\mathcal{R}$, essentially one has to calculate the maximal subgroups of the finite group $\mathcal{R}/\mathcal{T}(\mathcal{R})$. There are fast algorithms to calculate these maximal subgroups if this finite group is soluble (see Definition 1.4.5.2.1), which is the case for three-dimensional space groups. To explain this method and obtain theoretical consequences for the index of maximal subgroups in soluble space groups, we consider abstract groups again in this section.

For an arbitrary group $\mathcal{G}$, one has a fast method of checking whether a given subgroup $\mathcal{U} \leq \mathcal{G}$ of finite index $[\mathcal{G} : \mathcal{U}]$ is maximal by inspection of the $\mathcal{G}$-set $\mathcal{G}/\mathcal{U}$ of left cosets of $\mathcal{U}$ in $\mathcal{G}$. Assume that $\mathcal{U} \leq \mathcal{M} \leq \mathcal{G}$ and let $\mathcal{M}/\mathcal{U} := \{m_1\mathcal{U}, \ldots, m_k\mathcal{U}\}$ with $m_i \in \mathcal{M}$, $m_1 = e$ and $\mathcal{G}/\mathcal{M} := \{g_1\mathcal{M}, \ldots, g_l\mathcal{M}\}$ with $g_i \in \mathcal{G}$, $g_1 = e$. Then the set $\mathcal{G}/\mathcal{U}$ may be written as

$$\mathcal{G}/\mathcal{U} = \begin{array}{lll} \{g_1 m_1 \mathcal{U}, & \ldots, & g_1 m_k \mathcal{U}, \\ g_2 m_1 \mathcal{U}, & \ldots, & g_2 m_k \mathcal{U}, \\ \vdots, & \ldots, & \vdots, \\ g_l m_1 \mathcal{U}, & \ldots, & g_l m_k \mathcal{U}\} \end{array}.$$

Then $\mathcal{G}$ permutes the lines of the rectangle above: For all $g \in \mathcal{G}$ and all $j \in \{1, \ldots, l\}$, the left coset $gg_j\mathcal{M}$ is equal to some $g_a\mathcal{M}$ for an $a \in \{1, \ldots, l\}$. Hence the jth line is mapped onto the set

$$\{gg_j m_1 \mathcal{U}, \ldots, gg_j m_k \mathcal{U}\} = \{g_a m_1 \mathcal{U}, \ldots, g_a m_k \mathcal{U}\}.$$

Definition 1.4.5.1.1. Let $\mathcal{G}$ be a group and X a $\mathcal{G}$-set.

(i) A *congruence* $\{S_1, \ldots, S_l\}$ on X is a partition of X into non-empty subsets $X = \dot\bigcup_{i=1}^{l} S_i$ such that for all $x_1, x_2 \in S_i$, $g \in \mathcal{G}$, $gx_1 \in S_j$ implies $gx_2 \in S_j$.

(ii) The congruences $\{X\}$ and $\{\{x\} \mid x \in X\}$ are called the *trivial congruences*.

(iii) X is called a *primitive* $\mathcal{G}$-set if $\mathcal{G}$ is transitive on X, $|X| > 1$ and X has only the trivial congruences. □

Hence the considerations above have proven the following lemma.

Lemma 1.4.5.1.2. Let $\mathcal{M} \leq \mathcal{G}$ be a subgroup of the group $\mathcal{G}$. Then $\mathcal{M}$ is a maximal subgroup if and only if the $\mathcal{G}$-set $\mathcal{G}/\mathcal{M}$ is primitive. □

The advantage of this point of view is that the groups $\mathcal{G}$ having a faithful, primitive, finite $\mathcal{G}$-set have a special structure. It will turn out that this structure is very similar to the structure of space groups.

If X is a $\mathcal{G}$-set and $\mathcal{N} \trianglelefteq \mathcal{G}$ is a normal subgroup of $\mathcal{G}$, then $\mathcal{G}$ acts on the set of $\mathcal{N}$-orbits on X, hence $\{\mathcal{N}x \mid x \in X\}$ is a congruence on X. If X is a primitive $\mathcal{G}$-set, then this congruence is trivial, hence $\mathcal{N}x = \{x\}$ or $\mathcal{N}x = X$ for all $x \in X$. This means that $\mathcal{N}$ either acts trivially or transitively on X.

One obtains the following:

Theorem 1.4.5.1.3. [Theorem of Galois (*ca* 1830).] Let $\mathcal{H}$ be a finite group and let X be a faithful, primitive $\mathcal{H}$-set. Assume that $\{e\} \neq \mathcal{N} \trianglelefteq \mathcal{H}$ is an Abelian normal subgroup. Then

(*a*) $\mathcal{N}$ is a minimal normal subgroup of $\mathcal{H}$ (*i.e.* for all $\mathcal{N}_1 \trianglelefteq \mathcal{H}$, $\mathcal{N}_1 \subseteq \mathcal{N} \Leftrightarrow \mathcal{N}_1 = \mathcal{N}$ or $\mathcal{N}_1 = \{e\}$).

(*b*) $\mathcal{N}$ is an elementary Abelian p-group for some prime p and $|X| = |\mathcal{N}|$ is a prime power.

(*c*) $\mathcal{C}_{\mathcal{H}}(\mathcal{N}) = \mathcal{N}$ and $\mathcal{N}$ is the unique minimal normal subgroup of $\mathcal{H}$. □

Proof. Let $\{e\} \neq \mathcal{N} \trianglelefteq \mathcal{H}$ be an Abelian normal subgroup. Then $\mathcal{N}$ acts faithfully and transitively on X. To establish a bijection between the sets $\mathcal{N}$ and X, choose $x \in X$ and define $\varphi: \mathcal{N} \to X; n \mapsto n \cdot x$. Since $\mathcal{N}$ is transitive, φ is surjective. To show the injectivity of φ, let $n_1, n_2 \in \mathcal{N}$ with $\varphi(n_1) = \varphi(n_2)$. Then $n_1 \cdot x = n_2 \cdot x$, hence $n_1^{-1} n_2 x = x$. But then $n_1^{-1} n_2$ acts trivially on X, because if $y \in X$ then the transitivity of $\mathcal{N}$ implies that there is an $n \in \mathcal{N}$ with $n \cdot x = y$. Then $n_1^{-1} n_2 \cdot y = n_1^{-1} n_2 n \cdot x = n n_1^{-1} n_2 \cdot x = n \cdot x = y$, since $\mathcal{N}$ is Abelian. Since X is a faithful $\mathcal{H}$-set, this implies $n_1^{-1} n_2 = e$ and therefore $n_1 = n_2$. This proves $|\mathcal{N}| = |X|$. Since this equality holds for all nontrivial Abelian normal subgroups of $\mathcal{H}$, statement (*a*) follows. If p is some prime dividing $|\mathcal{N}|$, then the Sylow p-subgroup of $\mathcal{N}$ is normal in $\mathcal{N}$, since $\mathcal{N}$ is Abelian. Therefore, it is also a characteristic subgroup of $\mathcal{N}$ and hence a normal subgroup in $\mathcal{H}$ (see the remarks below Definition 1.4.3.5.3). Since $\mathcal{N}$ is a minimal normal subgroup of $\mathcal{H}$, this implies that $\mathcal{N}$ is equal to its Sylow p-subgroup. Therefore, the order of $\mathcal{N}$ is a prime power $|\mathcal{N}| = p^r$ for some prime p and $r \in \mathbb{N}$. Similarly, the set $\mathcal{N}^p := \{n^p \mid n \in \mathcal{N}\}$ is a normal subgroup of $\mathcal{H}$ properly contained in $\mathcal{N}$. Therefore, $\mathcal{N}^p = \{e\}$ and $\mathcal{N}$ is elementary Abelian. This establishes (*b*).

To see that (*c*) holds, let $g \in \mathcal{C}_{\mathcal{H}}(\mathcal{N})$. Choose $x \in X$. Then $g \cdot x = y \in X$. Since $\mathcal{N}$ acts transitively, there is an $n \in \mathcal{N}$ such that $n \cdot x = y$. Hence $n^{-1} g \cdot x = x$. As above, let $z \in X$ be any element of X. Then there is an element $n_1 \in \mathcal{N}$ with $z = n_1 \cdot x$. Hence $n^{-1} g \cdot z = n^{-1} g n_1 \cdot x = n_1 n^{-1} g \cdot x = n_1 \cdot x = z$. Since z was arbitrary and X is faithful, this implies that $g = n \in \mathcal{N}$. Therefore, $\mathcal{C}_{\mathcal{H}}(\mathcal{N}) \subseteq \mathcal{N}$. Since $\mathcal{N}$ is Abelian, one has $\mathcal{N} \subseteq \mathcal{C}_{\mathcal{H}}(\mathcal{N})$, hence $\mathcal{N} = \mathcal{C}_{\mathcal{H}}(\mathcal{N})$. To see that $\mathcal{N}$ is unique, let $\mathcal{P} \neq \mathcal{N}$ be another normal subgroup of $\mathcal{H}$. Since $\mathcal{N}$ is a minimal normal subgroup, one has $\mathcal{N} \cap \mathcal{P} = \{e\}$, and, therefore, for $p \in \mathcal{P}, n \in \mathcal{N}$: $n^{-1} p^{-1} n p \in \mathcal{N} \cap \mathcal{P} = \{e\}$. Hence $\mathcal{P}$ centralizes $\mathcal{N}$, $\mathcal{P} \subseteq \mathcal{C}_{\mathcal{H}}(\mathcal{N}) = \mathcal{N}$, which is a contradiction. QED

Hence the groups $\mathcal{H}$ that satisfy the hypotheses of the theorem of Galois are certain subgroups of an affine group $\mathcal{A}_n(\mathbb{Z}/p\mathbb{Z})$ over a finite field $\mathbb{Z}/p\mathbb{Z}$. This affine group is defined in a way similar to the affine group $\mathcal{A}_n$ over the real numbers where one has to replace the real numbers by this finite field. Then $\mathcal{N}$ is the translation subgroup of $\mathcal{A}_n(\mathbb{Z}/p\mathbb{Z})$ isomorphic to the n-dimensional vector space

$$(\mathbb{Z}/p\mathbb{Z})^n = \{\boldsymbol{x} = \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix} \mid x_1, \ldots, x_n \in \mathbb{Z}/p\mathbb{Z}\}$$

over $\mathbb{Z}/p\mathbb{Z}$. The set X is the corresponding affine space $\mathbb{A}_n(\mathbb{Z}/p\mathbb{Z})$. The factor group $\overline{\mathcal{H}} = \mathcal{H}/\mathcal{N}$ is isomorphic to a subgroup of the linear group of $(\mathbb{Z}/p\mathbb{Z})^n$ that does not leave invariant any nontrivial subspace of $(\mathbb{Z}/p\mathbb{Z})^n$.

1.4.5.2. Soluble groups

Definition 1.4.5.2.1. Let $\mathcal{G}$ be a group. The *derived series* of $\mathcal{G}$ is the series $(\mathcal{G}_0, \mathcal{G}_1, \ldots)$ defined *via* $\mathcal{G}_0 := \mathcal{G}$, $\mathcal{G}_i := \langle g^{-1} h^{-1} g h \mid g, h \in \mathcal{G}_{i-1} \rangle$. The group $\mathcal{G}_1$ is called the *derived subgroup* of $\mathcal{G}$. The group $\mathcal{G}$ is called *soluble* if $\mathcal{G}_n = \{e\}$ for some $n \in \mathbb{N}$. □

Remarks

(i) The $\mathcal{G}_i$ are characteristic subgroups of $\mathcal{G}$.

(ii) $\mathcal{G}$ is Abelian if and only if $\mathcal{G}_1 = \{e\}$.

(iii) $\mathcal{G}_1$ is characterized as the smallest normal subgroup of $\mathcal{G}$, such that $\mathcal{G}/\mathcal{G}_1$ is Abelian, in the sense that every normal subgroup of $\mathcal{G}$ with an Abelian factor group contains $\mathcal{G}_1$.

(iv) Subgroups and factor groups of soluble groups are soluble.

(v) If $\mathcal{N} \trianglelefteq \mathcal{G}$ is a normal subgroup, then $\mathcal{G}$ is soluble if and only if $\mathcal{G}/\mathcal{N}$ and $\mathcal{N}$ are both soluble.

Example 1.4.5.2.2

The derived series of $\mathcal{C}yc_2 \times \mathcal{S}ym_4$ is

$$\mathcal{C}yc_2 \times \mathcal{S}ym_4 \trianglerighteq \mathcal{A}lt_4 \trianglerighteq \mathcal{C}yc_2 \times \mathcal{C}yc_2 \trianglerighteq \mathcal{I}$$

(or in Hermann–Mauguin notation $m\bar{3}m \trianglerighteq 23 \trianglerighteq 222 \trianglerighteq 1$) and that of $\mathcal{C}yc_2 \times \mathcal{C}yc_2 \times \mathcal{S}ym_3$ is

$$\mathcal{C}yc_2 \times \mathcal{C}yc_2 \times \mathcal{S}ym_3 \trianglerighteq \mathcal{C}yc_3 \trianglerighteq \mathcal{I}$$

(Hermann–Mauguin notation: $6/mmm \trianglerighteq 3 \trianglerighteq 1$).

Hence these two groups are soluble. (For an explanation of the groups that occur here and later, see Section 1.4.3.6.)

Now let $\mathcal{R} \leq \mathcal{E}_3$ be a three-dimensional space group. Then $\mathcal{T}(\mathcal{R})$ is an Abelian normal subgroup, hence $\mathcal{T}(\mathcal{R})$ is soluble. The factor group $\mathcal{R}/\mathcal{T}(\mathcal{R})$ is isomorphic to a subgroup of either $\mathcal{C}yc_2 \times \mathcal{S}ym_4$ or $\mathcal{C}yc_2 \times \mathcal{C}yc_2 \times \mathcal{S}ym_3$ and therefore also soluble. Using the remark above, one deduces that all three-dimensional space groups are soluble.

Lemma 1.4.5.2.3. Let $\mathcal{R}$ be a three-dimensional space group. Then $\mathcal{R}$ is soluble. □

1.4.5.3. Maximal subgroups of soluble groups

Now let $\mathcal{G}$ be a soluble group and $\mathcal{M} \leq \mathcal{G}$ a maximal subgroup of finite index in $\mathcal{G}$. Then the set of left cosets $X := \mathcal{G}/\mathcal{M}$ is a primitive finite $\mathcal{G}$-set. Let $\mathcal{K} = \mathrm{core}(\mathcal{M})$ be the kernel of the action of $\mathcal{G}$ on X. Then the factor group $\mathcal{H} := \mathcal{G}/\mathcal{K}$ acts faithfully on X. In particular, $\mathcal{H}$ is a finite group and X is a primitive, faithful $\mathcal{H}$-set. Since $\mathcal{G}$ is soluble, the factor group $\mathcal{H}$ is also a soluble group. Let $\mathcal{H} \trianglerighteq \mathcal{H}_1 \trianglerighteq \ldots \trianglerighteq \mathcal{H}_{n-1} \trianglerighteq \{e\}$ be the derived series of $\mathcal{H}$ with $\mathcal{N} := \mathcal{H}_{n-1} \neq \{e\}$. Then $\mathcal{N}$ is an Abelian normal subgroup of $\mathcal{H}$. The theorem of Galois (Theorem 1.4.5.1.3) states that $\mathcal{N}$ is an elementary Abelian p-group for some prime p and $|X| = |\mathcal{N}| = p^r$ for some $r \in \mathbb{N}$. Since $X = \mathcal{G}/\mathcal{M}$, the order of X is the index $[\mathcal{G} : \mathcal{M}]$ of $\mathcal{M}$ in $\mathcal{G}$. Therefore one gets the following theorem:

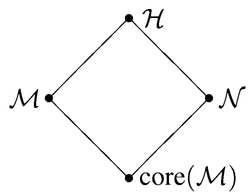
Theorem 1.4.5.3.1. If $\mathcal{M} \leq \mathcal{G}$ is a maximal subgroup of finite index in the soluble group $\mathcal{G}$, then its index $|\mathcal{G}/\mathcal{M}|$ is a prime power. □

In the proof of Theorem 1.4.5.1.3, we have established a bijection between $\mathcal{N}$ and the $\mathcal{H}$-set X, which is now $X := \mathcal{G}/\mathcal{M}$. Taking the full pre-image

$$\mathcal{N}' := \mathcal{N}\,\mathrm{core}\,(\mathcal{M})$$

of $\mathcal{N}$ in $\mathcal{G}$, then one has $\mathcal{G} = \mathcal{N}'\mathcal{M}$ and $\mathcal{M} \cap \mathcal{N}' = \mathrm{core}\,(\mathcal{M})$. Hence we have seen the first part of the following theorem:

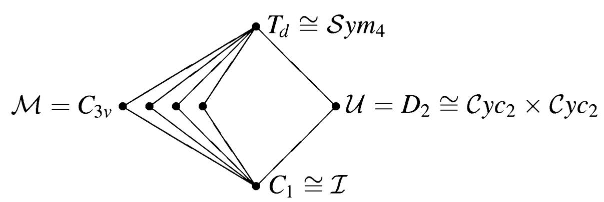
Theorem 1.4.5.3.2. Let $\mathcal{M} \leq \mathcal{G}$ be a maximal subgroup of the soluble group $\mathcal{G}$. Then the factor group $\mathcal{H} := \mathcal{G}/\mathrm{core}(\mathcal{M})$ acts primitively and faithfully on $X := \mathcal{G}/\mathcal{M}$, and there is a normal subgroup $\mathcal{N}' \trianglelefteq \mathcal{G}$ with $\mathcal{M}\mathcal{N}' = \mathcal{G}$ and $\mathcal{M} \cap \mathcal{N}' = \mathrm{core}(\mathcal{M})$. Moreover, if $\mathcal{M}'$ is another subgroup of $\mathcal{G}$, with $\mathcal{M}'\mathcal{N}' = \mathcal{G}$ and $\mathcal{M}' \cap \mathcal{N}' = \mathrm{core}(\mathcal{M})$, then $\mathcal{M}'$ is conjugate to $\mathcal{M}$.



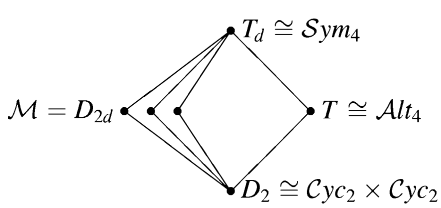
□

Example 1.4.5.3.3

$\mathcal{G} = \mathcal{S}ym_4 \cong T_d$ is the tetrahedral group from Section 1.4.3.2 and $\mathcal{S}ym_3 \cong \mathcal{M} = C_{3v} \leq \mathcal{G}$ is the stabilizer of one of the four apices in the tetrahedron. Then $\mathrm{core}(\mathcal{M}) = \{e\}$ and $\mathcal{G}/\mathcal{M}$ is a faithful $\mathcal{G}$-set which can be identified with the set of apices of the tetrahedron. The normal subgroup $\mathcal{N} = \mathcal{N}'$ is the normal subgroup $\mathcal{U}$ of Section 1.4.3.2.



Now let $\mathcal{G} = \mathcal{S}ym_4 \cong T_d$ be as above, and take $D_{2d} \cong \mathcal{M} \leq \mathcal{G}$ a Sylow 2-subgroup of $\mathcal{G}$. Then $\mathrm{core}(\mathcal{M}) = D_2 \cong \mathcal{C}yc_2 \times \mathcal{C}yc_2$ is the normal subgroup $\mathcal{U}$ from Section 1.4.3.2 and $\mathcal{H} = \mathcal{G}/\mathrm{core}(\mathcal{M}) \cong \mathcal{S}ym_3$.



These observations result in an algorithm for computing maximal subgroups of soluble groups $\mathcal{G}$:

(1) compute normal subgroups $\mathcal{C}$ [candidates for core($\mathcal{M}$)];
(2) compute a minimal normal subgroup $\mathcal{N}/\mathcal{C}$ of $\mathcal{G}/\mathcal{C}$;
(3) find $\mathcal{M}/\mathcal{C}$ as a complement of $\mathcal{N}/\mathcal{C}$ in $\mathcal{G}/\mathcal{C}$.

1.4.6. Quantitative results

This section gives estimates for the number of maximal subgroups of a given index in space groups.

1.4.6.1. General results

The first very easy but useful remark applies to general groups $\mathcal{G}$:

Remark. Let $\mathcal{M} \leq \mathcal{G}$ be a maximal subgroup of $\mathcal{G}$ of finite index $i := [\mathcal{G} : \mathcal{M}] < \infty$. Then $\mathcal{M} \leq \mathcal{N}_{\mathcal{G}}(\mathcal{M}) \leq \mathcal{G}$. Hence the maximality of $\mathcal{M}$ implies that either $\mathcal{N}_{\mathcal{G}}(\mathcal{M}) = \mathcal{G}$ and $\mathcal{M}$ is a normal subgroup of $\mathcal{G}$ or $\mathcal{N}_{\mathcal{G}}(\mathcal{M}) = \mathcal{M}$ and $\mathcal{G}$ has i maximal subgroups that are conjugate to $\mathcal{M}$.

The smallest possible index of a proper subgroup is 2. It is well known and easy to see that subgroups of index 2 are normal subgroups:

Proposition 1.4.6.1.1. Let $\mathcal{G}$ be a group and $\mathcal{M} \leq \mathcal{G}$ a subgroup of index $2 = |\mathcal{G}/\mathcal{M}|$. Then $\mathcal{M}$ is a normal subgroup of $\mathcal{G}$. □

Proof. Choose an element $g \in \mathcal{G}, g \notin \mathcal{M}$. Then $\mathcal{G} = \mathcal{M} \cup g\mathcal{M} = \mathcal{M} \cup \mathcal{M}g$. Hence $g\mathcal{M} = \mathcal{M}g$ and therefore $g\mathcal{M}g^{-1} = \mathcal{M}$. Since this is also true if $g \in \mathcal{M}$, the proposition follows. QED

Let $\mathcal{M}$ be a subgroup of a group $\mathcal{G}$ of index 2. Then $\mathcal{M} \trianglelefteq \mathcal{G}$ is a normal subgroup and the factor group $\mathcal{G}/\mathcal{M}$ is a group of order 2. Since groups of order 2 are Abelian, it follows that the derived subgroup $\mathcal{G}_1$ of $\mathcal{G}$ (*cf.* Definition 1.4.5.2.1) (which is the smallest normal subgroup of $\mathcal{G}$ such that the factor group is Abelian) is contained in $\mathcal{M}$. Hence all maximal subgroups of index 2 in $\mathcal{G}$ contain $\mathcal{G}_1$. If one defines $\mathcal{N} := \cap\{\mathcal{M} \leq \mathcal{G} \mid [\mathcal{G} : \mathcal{M}] = 2\}$, then $\mathcal{G}/\mathcal{N}$ is an elementary Abelian 2-group and hence a vector space over the field with two elements. The maximal subgroups of $\mathcal{G}/\mathcal{N}$ are the maximal subspaces of this vector space, hence their number is $2^a - 1$, where $a := \dim_{\mathbb{Z}/2\mathbb{Z}}(\mathcal{G}/\mathcal{N})$.

This shows the following:

Corollary 1.4.6.1.2. The number of subgroups of $\mathcal{G}$ of index 2 is of the form $2^a - 1$ for some $a \geq 0$. □

Dealing with subgroups of index 3, one has the following:

Proposition 1.4.6.1.3. Let $\mathcal{U}$ be a subgroup of the group $\mathcal{G}$ with $[\mathcal{G} : \mathcal{U}] = 3$. Then $\mathcal{U}$ is either a normal subgroup of $\mathcal{G}$ or $\mathcal{G}/\mathrm{core}(\mathcal{U}) \cong \mathcal{S}_3$ and there are three subgroups of $\mathcal{G}$ conjugate to $\mathcal{U}$. □

Proof. $\mathcal{G}/\mathrm{core}\,(\mathcal{U})$ is isomorphic to a subgroup of $\mathcal{S}ym_3$ that acts primitively on $\{1, 2, 3\}$. Hence either $\mathcal{G}/\mathrm{core}\,(\mathcal{U}) \cong \mathcal{C}yc_3$ and $\mathcal{U} = \mathrm{core}\,(\mathcal{U})$ is a normal subgroup of $\mathcal{G}$ or $\mathcal{G}/\mathrm{core}\,(\mathcal{U}) \cong \mathcal{S}ym_3$, $\mathcal{U}/\mathrm{core}\,(\mathcal{U}) \cong \mathcal{C}yc_2$ and there are three subgroups of $\mathcal{G}$ conjugate to $\mathcal{U}$. QED

1.4.6.2. Three-dimensional space groups

We now come to space groups. By Lemma 1.4.5.2.3, all three-dimensional space groups are soluble. Theorem 1.4.5.3.1 says that the index of a maximal subgroup of a soluble group is a prime power (or infinite). Since the index of a maximal subgroup of a space group is always finite (see Corollary 1.4.4.2.7), we get:

Corollary 1.4.6.2.1. Let $\mathcal{G}$ be a three-dimensional space group and $\mathcal{M} \leq \mathcal{G}$ a maximal subgroup. Then $[\mathcal{G} : \mathcal{M}]$ is a prime power. □

Let $\mathcal{R}$ be a three-dimensional space group and $\mathcal{P} = \mathcal{R}/\mathcal{T}(\mathcal{R})$ its point group. It is well known that the order of $\mathcal{P}$ is of the form 2^a3^b with $a = 0, 1, 2, 3$ or 4 and $b = 0, 1$. By Corollary 1.4.4.2.4, the *t*-subgroups of $\mathcal{R}$ are in one-to-one correspondence with the subgroups of $\mathcal{P}$. Let us look at the *t*-subgroups of $\mathcal{R}$ of index 3. It is clear that $\mathcal{P}$ has no subgroup of index 3 if $b = 0$, since the index of a subgroup divides the order of the finite group $\mathcal{P}$ by the theorem of Lagrange. If $b = 1$, then any subgroup $\mathcal{S}$ of $\mathcal{P}$ of index 3 has order $|\mathcal{P}|/3 = 2^a$ and hence is a Sylow 2-subgroup of $\mathcal{P}$. Therefore there is such a subgroup $\mathcal{S}$ of index 3 in $\mathcal{P}$ by the first theorem of Sylow, Theorem 1.4.3.3.1. By the second theorem of Sylow, Theorem 1.4.3.3.2, all these Sylow 2-subgroups of $\mathcal{P}$ are conjugate in $\mathcal{P}$. Therefore, by Proposition 1.4.6.1.3, the number of these groups is either 1 or 3:

Corollary 1.4.6.2.2. Let $\mathcal{R}$ be a three-dimensional space group.

If the order of the point group of $\mathcal{R}$ is not divisible by 3 then $\mathcal{R}$ has no *t*-subgroups of index 3.

If 3 is a factor of the order of the point group of $\mathcal{R}$, then $\mathcal{R}$ has either one *t*-subgroup of index 3 (which is then normal in $\mathcal{R}$) or three conjugate *t*-subgroups of index 3. □

1.4.7. Qualitative results

1.4.7.1. General theory

In this section, we want to comment on the very subtle question of deciding whether two space groups $\mathcal{R}_1$ and $\mathcal{R}_2$ are isomorphic.

This problem can be treated in several stages:

Let $\mathcal{R}_1$ and $\mathcal{R}_2$ be space groups. Since the translation subgroups $\mathcal{T}(\mathcal{R}_i)$ are characteristic subgroups of $\mathcal{R}_i$ (the maximal Abelian normal subgroup of finite index), each isomorphism $\varphi : \mathcal{R}_1 \to \mathcal{R}_2$ induces isomorphisms of the corresponding translation subgroups

$$\varphi' : \mathcal{T}(\mathcal{R}_1) \to \mathcal{T}(\mathcal{R}_2)$$

(by restriction) as well as of the point groups

$$\overline{\varphi} : \mathcal{P}_1 := \mathcal{R}_1/\mathcal{T}(\mathcal{R}_1) \to \mathcal{R}_2/\mathcal{T}(\mathcal{R}_2) =: \mathcal{P}_2.$$

It is convenient to view $\mathcal{T}(\mathcal{R}_i)$ as a lattice on which the point group $\mathcal{P}_i$ acts as group of linear mappings (*cf.* the start of Section 1.4.4). Then the isomorphism φ' is an isomorphism of $\mathcal{P}_1$-sets, where $\mathcal{P}_1$ acts on $\mathcal{T}(\mathcal{R}_1)$ *via* conjugation and on $\mathcal{T}(\mathcal{R}_2)$ *via*

$$g\mathcal{T}(\mathcal{R}_1) \cdot t := \varphi(g)t\varphi(g)^{-1} \text{ for all } g\mathcal{T}(\mathcal{R}_1) \in \mathcal{P}_1, t \in \mathcal{T}(\mathcal{R}_2).$$

Since $\varphi(\mathcal{T}(\mathcal{R}_1)) = \mathcal{T}(\mathcal{R}_2)$ and $\mathcal{T}(\mathcal{R}_2)$ centralizes itself, this action is well defined, *i.e.* independent of the choice of the coset representative g.

The following theorem will show that the isomorphism of sufficiently large factor groups of $\mathcal{R}_1$ and $\mathcal{R}_2$ implies a 'near' isomorphism of the space groups themselves. To give a precise formulation we need one further definition.

Definition 1.4.7.1.1. For $d \in \mathbb{N}$ define

$$O_d := \{\frac{a}{b} \mid a, b \in \mathbb{Z}, b \neq 0, \gcd(b, d) = 1\} \leq \mathbb{Q},$$

which is the set of all rational numbers for which the denominator is prime to d. For the space group $\mathcal{R} \leq \mathcal{E}_n$ let $\mathcal{R} \leq \mathcal{R}_{(d)} \leq \mathcal{E}_n$ be the group $\mathcal{R}_{(d)} := \langle \mathcal{T}(\mathcal{R})_{(d)}, \mathcal{R} \rangle$, where

$$\mathcal{T}(\mathcal{R})_{(d)} = \{at \mid a \in O_{(d)}, t \in \mathcal{T}(\mathcal{R})\} \leq \mathcal{T}_n,$$

i.e. one allows denominators that are prime to d in the translation subgroup. □

One has the following:

Theorem 1.4.7.1.2. Let $\mathcal{R}_1$ and $\mathcal{R}_2$ be two space groups with point groups of order $d_i := |\mathcal{R}_i/\mathcal{T}(\mathcal{R}_i)|$. Let $\mathbf{N}(\mathcal{R}_i)$ denote the set of normal subgroups of $\mathcal{R}_i$ having finite index in $\mathcal{R}_i$. Then the following three conditions are equivalent:

(i) There are normal subgroups $\mathcal{S}_i \trianglelefteq \mathcal{R}_i$ with $\mathcal{R}_1/\mathcal{S}_1 \cong \mathcal{R}_2/\mathcal{S}_2$ and with $\mathcal{S}_i \subseteq d_i^2\mathcal{T}(\mathcal{R}_i)$ if $d_i \neq 2$ and $\mathcal{S}_i \subseteq 16\mathcal{T}(\mathcal{R}_i)$ if $d_i = 2$ $(i = 1, 2)$.

(ii) $(\mathcal{R}_1)_{(d_1)} \cong (\mathcal{R}_2)_{(d_2)}$.

(iii) There is a bijection $\mu : \mathbf{N}(\mathcal{R}_1) \to \mathbf{N}(\mathcal{R}_2)$ such that $\mathcal{R}_1/\mathcal{N} \cong \mathcal{R}_2/\mu(\mathcal{N})$ for all $\mathcal{N} \in \mathbf{N}(\mathcal{R}_1)$. □

For a proof of this theorem, see Finken *et al.* (1980).

Remark. If $\mathcal{R}_i$ are three- or four-dimensional space groups, the isomorphism in (ii) already implies the isomorphism of $\mathcal{R}_1$ and $\mathcal{R}_2$, but there are counterexamples for dimension 5.

1.4.7.2. Three-dimensional space groups

Corollary 1.4.7.2.1. Let $\mathcal{R}$ be a three-dimensional space group with translation subgroup $\mathcal{T}$ and p be a prime not dividing the order of the point group $\mathcal{R}/\mathcal{T}$. Let $\mathcal{U}$ be a subgroup of $\mathcal{R}$ of index p^α for some $\alpha \in \mathbb{Z}_{>0}$. Then

(*a*) $\mathcal{U}$ is a *k*-subgroup.

(*b*) $\mathcal{U}$ is isomorphic to $\mathcal{R}$. □

Proof:

(*a*) $\mathcal{U} \leq \mathcal{U}\mathcal{T} \leq \mathcal{R}$ implies that $[\mathcal{R} : \mathcal{U}\mathcal{T}]$ divides $[\mathcal{R} : \mathcal{U}] = p^\alpha$. Since $\mathcal{T} \leq \mathcal{U}\mathcal{T} \leq \mathcal{R}$, one obtains $[\mathcal{R} : \mathcal{U}\mathcal{T}]$ as a factor of $[\mathcal{R} : \mathcal{T}]$. But p is not a factor of $[\mathcal{R} : \mathcal{T}]$, hence $[\mathcal{R} : \mathcal{U}\mathcal{T}] = 1$ and $\mathcal{R} = \mathcal{U}\mathcal{T}$. According to the remark following Definition 1.4.4.2.2, $\mathcal{U}$ is a *k*-subgroup.

(*b*) Let $d_1 := |\mathcal{R}/\mathcal{T}| = |\mathcal{U}/\mathcal{T}(\mathcal{U})|$. Let $d := d_1^2$ if $d_1 \neq 2$ and $d := 16$ otherwise, and let $\mathcal{T}' := d\mathcal{T}$. Since $\gcd([\mathcal{R} : \mathcal{U}], d) = 1$, one has $\mathcal{U}\mathcal{T}' = \mathcal{R}$ and $\mathcal{T}' \cap \mathcal{U} = d\mathcal{T}(\mathcal{U})$. By the third isomorphism theorem, Theorem 1.4.3.5.2, it follows that

$$\mathcal{R}/\mathcal{T}' = \mathcal{U}\mathcal{T}'/\mathcal{T}' \cong \mathcal{U}/\mathcal{T}' \cap \mathcal{U} = \mathcal{U}/d\mathcal{T}(\mathcal{U}).$$

By Theorem 1.4.7.1.2 (i) ⇒ (ii), one has $\mathcal{R}_{(d_1)} \cong \mathcal{U}_{(d_1)}$. By the remark above, this already implies that $\mathcal{R}$ and $\mathcal{U}$ are isomorphic. QED

Theorem 1.4.7.2.2. Let $\mathcal{R}$ be a three-dimensional space group and $\mathcal{U}$ be a maximal subgroup of $\mathcal{R}$ of index > 4. Then

(*a*) $\mathcal{U}$ is a *k*-subgroup.

(*b*) $\mathcal{U}$ is isomorphic to $\mathcal{R}$. □

Proof. Since $\mathcal{R}$ is soluble, the index $[\mathcal{R} : \mathcal{U}] = p^\alpha$ is a prime power (see Theorem 1.4.5.3.1). If p is not a factor of $|\mathcal{R}/\mathcal{T}(\mathcal{R})|$, the statement follows from Corollary 1.4.7.2.1. Hence we only have to consider the cases $p = 2, \alpha > 2$ and $p = 3, \alpha > 1$. Since 9 is not a factor of the order of any crystallographic point group in dimension 3, assertion (*a*) follows if the index of $\mathcal{U}$ is divisible by 9. If $\mathcal{U}$ is a maximal *t*-subgroup, then $\mathcal{R}/\mathcal{U}$ is a primitive $\mathcal{P}$-set for the point group $\mathcal{P}$ of $\mathcal{R}$. Since the point groups $\mathcal{P}$ of dimension 3 have no primitive $\mathcal{P}$-sets of order divisible by 8, assertion (*a*) also follows if the index of $\mathcal{U}$ is divisible by 8.

For all three-dimensional space groups $\mathcal{R}$, the module $\mathbf{L}(\mathcal{R})/2\mathbf{L}(\mathcal{R})$ [where $\mathcal{T}(\mathcal{R})$ is identified with the corresponding lattice $\mathbf{L}(\mathcal{R})$ in $\tau(\mathbb{E}_3)$ as in Section 1.4.4] is not simple as a module for the point group $\mathcal{P} = \mathcal{R}/\mathcal{T}(\mathcal{R})$. [It suffices to check this property for the two maximal point groups $\mathcal{C}yc_2 \times \mathcal{S}ym_4$ ($= m\overline{3}m$) and $\mathcal{C}yc_2 \times \mathcal{C}yc_2 \times \mathcal{S}ym_3$ ($= 6/mmm$).] This means that $2\mathbf{L}(\mathcal{R})$ is not a maximal $\mathcal{R}$-invariant sublattice of $\mathbf{L}(\mathcal{R})$. Since the translation subgroup $\mathcal{T}(\mathcal{U})$ of a maximal *k*-subgroup $\mathcal{U}$ of index equal to a power of 2 in $\mathcal{R}$ is a maximal $\mathcal{R}$-invariant subgroup of $\mathcal{T}(\mathcal{R})$ that contains $2\mathcal{T}(\mathcal{R})$, one now finds that $\mathcal{R}$ has no maximal *k*-subgroup of index 8.

Now assume that $[\mathcal{R} : \mathcal{U}] = 9$. By Corollary 1.4.7.2.1, one only needs to deal with groups $\mathcal{R}$ such that the order of the point group $\mathcal{P} := \mathcal{R}/\mathcal{T}(\mathcal{R})$ is divisible by 3. $\mathcal{P}$ is isomorphic to a subgroup of $\mathcal{C}yc_2 \times \mathcal{S}ym_4$ or $\mathcal{C}yc_2 \times \mathcal{C}yc_2 \times \mathcal{S}ym_3$. If $\mathcal{A}lt_4 \leq \mathcal{P}$ is a subgroup of $\mathcal{P}$, then $\mathbf{L}(\mathcal{R})/3\mathbf{L}(\mathcal{R})$ is simple and $\mathcal{U}$ is of index 27 in $\mathcal{R}$ [with $\mathbf{L}(\mathcal{U}) = 3\mathbf{L}(\mathcal{R})$]. It turns out that $\mathcal{U}$ is isomorphic to $\mathcal{R}$ in these cases. If $\mathcal{P}$ does not contain a subgroup isomorphic to $\mathcal{A}lt_4$, then the maximality of $\mathcal{U}$ implies that $\mathcal{T}(\mathcal{U}) \leq \mathcal{T}(\mathcal{R})$ is of index 3 in $\mathcal{T}(\mathcal{R})$. Hence $[\mathcal{R} : \mathcal{U}] = 3$ in this case. QED

Corollary 1.4.7.2.3. Let $\mathcal{M}$ be a maximal subgroup of the three-dimensional space group $\mathcal{R}$.

(*a*) If the index of $\mathcal{M}$ is a power of 2, then $[\mathcal{R} : \mathcal{M}] = 2$ or 4.

(*b*) If 3 is a factor of the order of the point group $[\mathcal{R} : \mathcal{T}(\mathcal{R})]$ and the index of $\mathcal{M}$ is a power of 3, then $[\mathcal{R} : \mathcal{M}] = 3$ or 27. For $[\mathcal{R} : \mathcal{M}] = 27$, $\mathcal{M}$ is necessarily isomorphic to $\mathcal{R}$ (by Theorem 1.4.7.2.2). □

This interesting fact explains why there are no maximal subgroups of index 8 in a three-dimensional space group. If there is a maximal subgroup $\mathcal{M}$ of a three-dimensional space group $\mathcal{R}$ of index 9, then the order of the point group of $\mathcal{R}$ is not divisible by three and the subgroup $\mathcal{M}$ is a *k*-subgroup and isomorphic to $\mathcal{R}$.

In particular, there are no maximal subgroups of index 9 for trigonal, hexagonal or cubic space groups, whereas there are such subgroups of tetragonal space groups.

1.4.8. Minimal supergroups

For several problems, for example for the prediction of a phase transition or in the search for overlooked symmetry in crystal-structure determinations *etc.*, it is helpful to know all space groups $\mathcal{S}$ containing a given space group $\mathcal{R}$, which means that $\mathcal{R} \leq \mathcal{S}$. Then $\mathcal{S}$ is called a *supergroup* of $\mathcal{R}$. Note that – in contrast to subgroups – the supergroups $\mathcal{G} \geq \mathcal{R}$ containing a space group $\mathcal{R}$ of finite index need not be space groups. For instance, the one-dimensional translation group

$$\mathcal{R} = \langle \left(\begin{array}{c|c} 1 & 1 \\ \hline 0 & 1 \end{array}\right) \rangle \cong \mathbb{Z}$$

has a supergroup $\mathcal{G}$ of index 2 isomorphic to $\mathcal{C}yc_2 \times \mathbb{Z}$ which is not a subgroup of the one-dimensional affine group. $\mathcal{G}$ is Abelian but has an element of finite order, so $\mathcal{G}$ cannot be a space group. For the applications in crystallography, we are restricted to those supergroups $\mathcal{S}$ of $\mathcal{R}$ that are again space groups.

Definition 1.4.8.1. Let $\mathcal{S}$ be a space group that is a supergroup of the space group $\mathcal{R}$ and $\mathcal{T} := \mathcal{T}(\mathcal{S})$.

(i) $\mathcal{S}$ is called a *translationengleiche* or a *t*-supergroup if $\mathcal{R} \cap \mathcal{T} = \mathcal{T}$.

(ii) $\mathcal{S}$ is called a *klassengleiche* or a *k*-supergroup if $\mathcal{R}/\mathcal{R} \cap \mathcal{T} \cong \mathcal{S}/\mathcal{T}$. □

Clearly $\mathcal{S}$ is a *t*-supergroup (or *k*-supergroup, respectively) of $\mathcal{R}$ if and only if $\mathcal{R}$ is a *t*-subgroup (or *k*-subgroup) of $\mathcal{S}$ and the theorem of Hermann implies the following:

Theorem 1.4.8.2. (Theorem of Hermann.) Let $\mathcal{S}$ and $\mathcal{R}$ be space groups such that $\mathcal{S} \geq \mathcal{R}$ is a minimal supergroup of $\mathcal{R}$. Then $\mathcal{S}$ is either a *k*-supergroup or a *t*-supergroup. □

The determination of the *k*-supergroups of a given space group $\mathcal{R}$ is the easier task. For instance, if $\mathcal{R}$ is a symmorphic space group then all its *k*-supergroups are also symmorphic. This is not true for *k*-subgroups of $\mathcal{R}$.

Theorem 1.4.8.3. Let $\mathcal{S}$ be a *k*-supergroup of the space group $\mathcal{R}$. Then $\mathcal{S} = \mathcal{R}\mathcal{T}(\mathcal{S})$. If $\mathcal{S}$ is a minimal *k*-supergroup of $\mathcal{R}$ then the translation lattice $\mathbf{L}(\mathcal{S})$ of $\mathcal{S}$ is an $\overline{\mathcal{R}}$-invariant lattice that contains $\mathbf{L}(\mathcal{R})$ as a maximal sublattice. □

Proof. Let $\mathcal{T} := \mathcal{T}(\mathcal{S})$ be the translation subgroup of $\mathcal{S}$. Then $\mathcal{T} \cap \mathcal{R} = \mathcal{T}(\mathcal{R})$ and $\mathcal{R}/(\mathcal{T} \cap \mathcal{R})$ is isomorphic to the point group $\overline{\mathcal{R}}$, which is a finite group. By the isomorphism theorem

$$\mathcal{R}/(\mathcal{T} \cap \mathcal{R}) \cong \mathcal{R}\mathcal{T}/\mathcal{T}.$$

Therefore, group $\mathcal{R}\mathcal{T}$ generated by $\mathcal{T}$ and $\mathcal{R}$ is a subgroup of $\mathcal{S}$ containing $\mathcal{T}$ with the same index and, therefore, $\mathcal{R}\mathcal{T} = \mathcal{S}$. Moreover, $\mathcal{T}$ contains $\mathcal{T}(\mathcal{R})$ and hence $\mathbf{L}(\mathcal{S})$ contains $\mathbf{L}(\mathcal{R})$. Since $\mathcal{T}$ is a normal subgroup of $\mathcal{S}$, the space group $\mathcal{R}$ acts on $\mathcal{T}$ by conjugation and therefore $\mathbf{L}(\mathcal{S})$ is $\overline{\mathcal{R}}$ invariant. If there is an $\overline{\mathcal{R}}$ invariant lattice $\mathbf{L}$ such that $\mathbf{L}(\mathcal{R}) \subset \mathbf{L} \subset \mathbf{L}(\mathcal{S})$, then, applying the isomorphism μ from Example 1.4.3.4.4, the group $\mathcal{G} := \mathcal{R}\mu^{-1}(\mathbf{L})$ is a space group with $\mathcal{R} \leq \mathcal{G} \leq \mathcal{S}$. Hence the minimality of the supergroup $\mathcal{S}$ implies that $\mathbf{L}(\mathcal{S})$ is an $\overline{\mathcal{R}}$-invariant lattice that contains $\mathbf{L}(\mathcal{R})$ as a maximal sublattice. QED

As for maximal *k*-subgroups, the index $[\mathcal{S} : \mathcal{R}]$ of a minimal *k*-supergroup $\mathcal{S}$ of $\mathcal{R}$ is a prime power and for each prime p there is some $a \in \mathbb{N}$ such that $\mathcal{R}$ has a minimal *k*-supergroup $\mathcal{S}$ of index $[\mathcal{S} : \mathcal{R}] = p^a$. Because of the infinite number of prime numbers, a space group $\mathcal{R}$ has infinitely many minimal *k*-supergroups, but there are only finitely many minimal *k*-supergroups containing a given space group $\mathcal{R}$ of given index.

This is different for *t*-supergroups, as the following example shows.

Example 1.4.8.4

Let

$$\mathcal{R} = \langle \left(\begin{array}{cc|c} 1 & 0 & 1 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & 1 & 1 \\ \hline 0 & 0 & 1 \end{array}\right) \rangle \cong \mathbb{Z}^2$$

be the two-dimensional translation group $p1$. Then for all $x \in \mathbb{R}$ the group

$$\mathcal{S}_x := \langle \mathcal{R}, \left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & -1 & x \\ \hline 0 & 0 & 1 \end{array}\right) \rangle$$

is a minimal *t*-supergroup of $\mathcal{R}$ containing $\mathcal{R}$ of index 2. These groups are conjugate under the normalizer of $\mathcal{R}$ in the affine group $\mathcal{A}_2$ [see Example 3.47 in Heidbüchel (2003)],

$$\left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & 1 & -x/2 \\ \hline 0 & 0 & 1 \end{array}\right) \mathcal{S}_x \left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & 1 & x/2 \\ \hline 0 & 0 & 1 \end{array}\right) = \mathcal{S}_0.$$

Visually this means that the discrete sets of symmetry lines of the different plane groups may be shifted by any real distance against each other or relative to an arbitrarily chosen origin. This yields uncountably many different *t*-supergroups of $p1$ which are all of the same type.

The use of the affine and Euclidean normalizers of a space group $\mathcal{R}$ is described in Part 15 of *IT* A. The *affine normalizer*

$$\mathcal{N} := \mathcal{N}_{\mathcal{A}_n}(\mathcal{R}) = \{g \in \mathcal{A}_n \mid g\mathcal{R}g^{-1} = \mathcal{R}\}$$

of an n-dimensional space group $\mathcal{R} \leq \mathcal{A}_n$ acts on the set of all minimal t-supergroups $\mathcal{S}$ of $\mathcal{R}$ by conjugation.

Theorem 1.4.8.5. $\mathcal{N}$ has finitely many orbits on the set of (minimal) t-supergroups $\mathcal{S}$ of $\mathcal{R}$. □

Proof. Let $\mathcal{S}_1, \ldots, \mathcal{S}_m$ be representatives of the $\mathcal{A}_n$-orbits on the set of n-dimensional space groups, *i.e.* of the types of n-dimensional space groups. For $1 \leq i \leq m$ let

$$\mathcal{M}_i := \{\mathcal{R}_{ij} \mid 1 \leq j \leq a_i\}$$

denote the set of all (maximal) t-subgroups of $\mathcal{S}_i$ that are isomorphic to $\mathcal{R}$.

If $\mathcal{S}$ is a (minimal) t-supergroup of the space group $\mathcal{R}$, then there is some $g \in \mathcal{A}_n$ and $i \in \{1, \ldots, m\}$ such that $g\mathcal{S}g^{-1} = \mathcal{S}_i$ and $g\mathcal{R}g^{-1} = \mathcal{R}_{ij} \in \mathcal{M}_i$, hence the pair of space groups $(\mathcal{R}, \mathcal{S}) = (g^{-1}\mathcal{R}_{ij}g, g^{-1}\mathcal{S}_i g)$ for some $i \in \{1, \ldots, m\}$, $\mathcal{R}_{ij} \in \mathcal{M}_i$ and $g \in \mathcal{A}_n$.

If $\mathcal{S}'$ is a second supergroup of $\mathcal{R}$ and $h \in \mathcal{A}_n$ such that $(\mathcal{R}, \mathcal{S}') = (h^{-1}\mathcal{R}_{ij}h, h^{-1}\mathcal{S}_i h)$ for the same i, j, then $h^{-1}g \in \mathcal{N}$ normalizes $\mathcal{R}$. Hence there are at most $\sum_{i=1}^{m} a_i$ orbits of $\mathcal{N}$ on the set of (minimal) t-supergroups of $\mathcal{R}$. QED

This proof also provides an algorithm to determine representatives of the $\mathcal{N}$-orbits of minimal t-supergroups of a given space group $\mathcal{R}$, provided that one knows representatives of all affine classes of space groups and their maximal t-subgroups. For dimensions 2 and 3 these are given in this volume. Since maximal t-subgroups of three-dimensional space groups have index 2, 3 or 4, this also holds for the minimal t-supergroups of these groups.

Up to dimension $n \leq 4$, the minimal t-supergroups and the minimal k-supergroups of a given space group $\mathcal{R} \leq \mathcal{A}_n$ can be obtained with the commands *TSupergroups* and *KSupergroups* in *CARAT* [see also Heidbüchel (2003)].

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