International Tables for Crystallography (2011). Vol. A1, Section 1.4.3.5, pp. 32–33.

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 $\mathcal{U} \le \mathcal{G}$ 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 $1 \mapsto p$ 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 $\varphi(\mathcal{G}) \le \mathcal{H}$ of φ:

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

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

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 $\mathcal{U} \le \mathcal{G}$ 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 $\mathcal{U} \le \mathcal{H}$ is a *characteristic subgroup* $\mathcal{U}$ 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 $\mathcal{P}$ 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 $\mathcal{U}$ 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 $\kappa_h : \mathcal{H} \to \mathcal{H}$, $x \mapsto hxh^{-1}$. 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 $\mathcal{R} \le \mathcal{E}_n$ 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

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

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 $\mu'(t_1t_2) = \mu'(t_1) + \mu'(t_2)$ 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

references