

1.4. THE MATHEMATICAL BACKGROUND OF THE SUBGROUP TABLES

(c) If  $\mathcal{U} \text{ char } \mathcal{N} \trianglelefteq \mathcal{H}$ , 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  $\mathcal{S} := \text{Stab}_{T_d}(P_1)$  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  $\langle s \rangle \cong \text{Cyc}_2$  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  $\text{Sym}_4$  of degree 4 and the group  $\mathcal{S} \cong \text{Sym}_3$  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  $\{1, \dots, n\}$  onto itself is called the *symmetric group of degree  $n$*  and denoted by

$$\text{Sym}_n := \{f : \{1, \dots, n\} \rightarrow \{1, \dots, n\} \mid f \text{ is bijective}\}.$$

The *alternating group* is the normal subgroup  $\text{Alt}_n$  consisting of all even permutations of  $\{1, \dots, n\}$ .

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,  $\langle r_1 \rangle \cong \mathcal{U}/\langle r_1 \rangle \cong \text{Cyc}_2$ . 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*  $\text{Cyc}_2 \times \text{Cyc}_2$  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  $T_d$ :  $\mathcal{U} = C_{T_d}(\mathcal{U})$ . 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  $T_d/\mathcal{U} \cong \text{Sym}_3$ .

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  $\text{Alt}_4$ , 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  $(\mathbf{b}_1, \dots, \mathbf{b}_n)$  of  $\mathbf{V}_n$  such that

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

- (b) A *crystal structure* is a mapping  $f : \mathbb{E}_n \rightarrow \mathbb{R}$  of the Euclidean point space into the real numbers such that  $\text{Stab}_{\tau(\mathbb{A}_n)}(f) := \{t \in \tau(\mathbb{A}_n) \mid f(P+t) = f(P) \text{ for all } P \in \mathbb{A}_n\}$  is an  $n$ -dimensional lattice in  $\tau(\mathbb{A}_n)$ .
- (c) The Euclidean group  $\mathcal{E}_n$  acts on the set of mappings  $\mathbb{E}_n \rightarrow \mathbb{R}$  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  $f : \mathbb{E}_n \rightarrow \mathbb{R}$ . A *space group*  $\mathcal{R}$  is the stabilizer of a crystal structure  $f : \mathbb{E}_n \rightarrow \mathbb{R}$ ;  $\mathcal{R} = \text{Stab}_{\mathcal{E}_n}(f)$ .
- (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  $\mathcal{T}(\mathcal{R}) := \mathcal{R} \cap T_n$ . □

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  $\mu'$  of the mapping  $\mu$  in Example 1.4.3.4.4 defined by

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

in  $\tau(\mathbb{A}_n)$  is an  $n$ -dimensional lattice  $\mathbf{L}(\mathcal{R})$ . Since  $\mu'$  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  $p$ th 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