International Tables for Crystallography (2011). Vol. A1, Section 1.4.4.1, pp. 33–34.

(*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 $\mu'(t_1 t_2) = \mu'(t_1) + \mu'(t_2)$ 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 $\mathcal{M} \le \mathcal{G}$ of a group $\mathcal{G}$ is called *maximal* if $\mathcal{M} \neq \mathcal{G}$ and for all subgroups $\mathcal{U} \le \mathcal{G}$ 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.

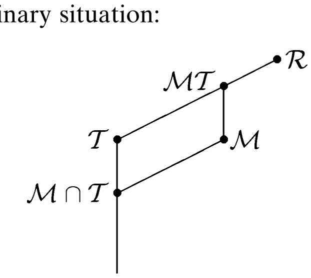
Definition 1.4.4.2.2. Let $\mathcal{U}$ be a subgroup of the space group $\mathcal{R}$ and $\mathcal{T} := \mathcal{T}(\mathcal{R})$.

(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:

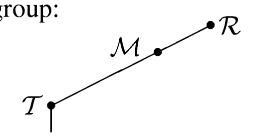


Since $\mathcal{T} \trianglelefteq \mathcal{R}$ and $\mathcal{M} \le \mathcal{R}$, one has by Proposition 1.4.3.2.11 that $\mathcal{M}\mathcal{T} \le \mathcal{R}$. Hence the maximality of $\mathcal{M}$ implies that $\mathcal{M}\mathcal{T} = \mathcal{M}$ or $\mathcal{M}\mathcal{T} = \mathcal{R}$. If $\mathcal{M}\mathcal{T} = \mathcal{M}$ 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:

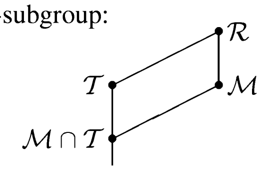
Theorem 1.4.4.2.3. (Hermann) Let $\mathcal{M} \le \mathcal{R}$ be a maximal subgroup of the space group $\mathcal{R}$. Then $\mathcal{M}$ is either a k-subgroup or a t-subgroup. □

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 $\mathcal{T}(\mathcal{R}) \le \mathcal{M}$ 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 $\mathcal{T}(\mathcal{R}) \le \mathcal{M}$ 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 $\mu'(\mathcal{T}(\mathcal{M})) \le \mathbf{L}(\mathcal{R})$ 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 $t_1 \in \mathcal{T} \cap \mathcal{M}$

$$g^{-1}t_1g = m^{-1}t^{-1}t_1tm = m^{-1}t_1m,$$

since $\mathcal{T}$ is Abelian. Since $m \in \mathcal{R}$ and $\mathcal{T}$ is normal in $\mathcal{R}$, one has $m^{-1}t_1m \in \mathcal{T}$. But $m^{-1}t_1m$ is a product of elements in $\mathcal{M}$ and therefore lies in the subgroup $\mathcal{M}$, hence $m^{-1}t_1m \in \mathcal{T} \cap \mathcal{M}$. 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