International Tables for Crystallography (2006). Vol. A1, Section 1.5.4, pp. 34–36.

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 1.5.3.2.4 (*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.

1.5.3.5. *Isomorphism theorems*

[*cf.* Ledermann (1976), pp. 68–73.]

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

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

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

Theorem 1.5.3.5.2. (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 1.5.3.2.11.) □

Definition 1.5.3.5.3. A subgroup $\mathcal{U} \leq \mathcal{H}$ 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 $\mathcal{U}$ 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 $\mathcal{N}$.

1.5.3.6. *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 1.5.3.2.8, $|T_d| = |V||\mathcal{S}| = 4|\mathcal{S}|$. 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 1.5.3.6.1. [*cf.* Ledermann (1976), Section 13.] 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.

1.5.4. Space groups

1.5.4.1. *Definition of space groups*

In *IT* A (2002), Section 8.1.6, space groups are introduced as symmetry groups of crystal patterns.

Definition 1.5.4.1.1.
(*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 affine *n*-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 1.5.4.1.1, its image under the inverse μ' of the mapping μ in Example 1.5.3.4.4 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 a full 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 *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 $\mu'(gtg^{-1}) = \overline{g}\mu'(t)$, 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 $\bar{}$, 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 1.5.4.1.2. 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 $\mu'(\mathcal{T}(\mathcal{R})) = \mathbf{L}(\mathcal{R})$. □

1.5.4.2. *Maximal subgroups of space groups*

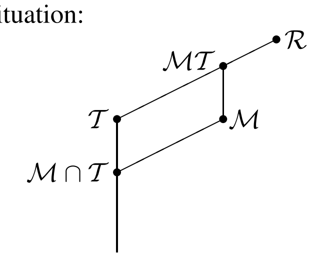
Definition 1.5.4.2.1. A subgroup $\mathcal{M} \leq \mathcal{G}$ of a group $\mathcal{G}$ is called *maximal* if $\mathcal{M} \neq \mathcal{G}$ and for all subgroups $\mathcal{U} \leq \mathcal{G}$ with $\mathcal{M} \subseteq \mathcal{U}$ it holds that either $\mathcal{U} = \mathcal{M}$ or $\mathcal{U} = \mathcal{G}$. □

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 1.5.4.2.2. 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-subgroups* if $\mathcal{U}/\mathcal{U} \cap \mathcal{T} \cong \mathcal{R}/\mathcal{T}$. □

Remark
The third isomorphism theorem, Theorem 1.5.3.5.2, 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:

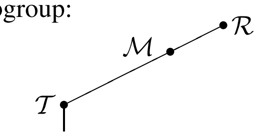


Since $\mathcal{T} \trianglelefteq \mathcal{R}$ and $\mathcal{M} \leq \mathcal{R}$, one has by Proposition 1.5.3.2.11 that $\mathcal{M}\mathcal{T} \leq \mathcal{R}$. Hence the maximality of $\mathcal{M}$ implies that $\mathcal{M}\mathcal{T} = \mathcal{M}$ or $\mathcal{M}\mathcal{T} = \mathcal{R}$. If $\mathcal{M}\mathcal{T} = \mathcal{M}$ 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 1.5.3.5.2, $\mathcal{R}/\mathcal{T} = \mathcal{M}\mathcal{T}/\mathcal{T} \cong \mathcal{M}/(\mathcal{M} \cap \mathcal{T}) = \mathcal{M}/\mathcal{T}(\mathcal{M})$, hence $\mathcal{M}$ is a *k*-subgroup. This is given by the following theorem:

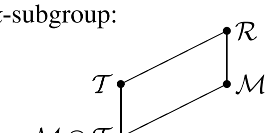
Theorem 1.5.4.2.3. (Hermann) Let $\mathcal{M} \leq \mathcal{R}$ be a maximal subgroup of the space group $\mathcal{R}$. Then $\mathcal{M}$ is either a *k*-subgroup or a *t*-subgroup. □

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 1.5.4.1.1. For future reference, we note this in the following corollary:

Corollary 1.5.4.2.4. 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 1.5.3.6.1), $\mathcal{C}yc_2$ 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 1.5.3.6). 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 1.5.5.

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

Lemma 1.5.4.2.5. 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 $t_1 \in \mathcal{T} \cap \mathcal{M}$

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

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 *p*th powers of elements of $\mathcal{T}$ for any natural number $p \in \mathbb{N}$. 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 1.5.4.2.6. 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 $r \leq n$. □

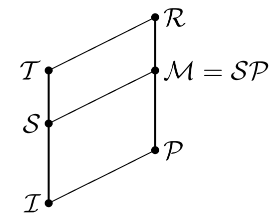
Corollary 1.5.4.2.7. Maximal subgroups of space groups are again space groups and of finite index in the supergroup. □

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 1.5.4.2.8. 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 1.5.4.2.9. 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 $\mathcal{M} \cap \mathcal{T} = \mathcal{S}$.

1.5.5. Maximal subgroups

1.5.5.1. *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 1.5.5.2.1), 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

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

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 $g_a\mathcal{M}$