International Tables for Crystallography (2011). Vol. A1, Section 1.4.4.2, pp. 34–35.

$\mu'(gtg^{-1}) = \overline{g}\mu'(t)$, 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 $\mathcal{M} \ne \mathcal{G}$ 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 $\mathcal{U} \ne \mathcal{R}$ 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.

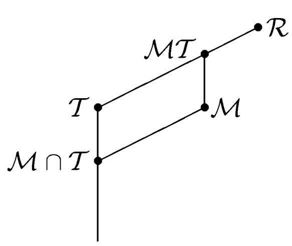
Definition 1.4.4.2.2. Let $\mathcal{U}$ be a subgroup of the space group $\mathcal{R}$ and $\mathcal{T} := \mathcal{T}(\mathcal{R})$.

(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:

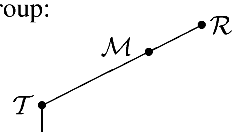


Since $\mathcal{T} \trianglelefteq \mathcal{R}$ and $\mathcal{M} \le \mathcal{R}$, one has by Proposition 1.4.3.2.11 that $\mathcal{M}\mathcal{T} \le \mathcal{R}$. Hence the maximality of $\mathcal{M}$ implies that $\mathcal{M}\mathcal{T} = \mathcal{M}$ or $\mathcal{M}\mathcal{T} = \mathcal{R}$. If $\mathcal{M}\mathcal{T}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

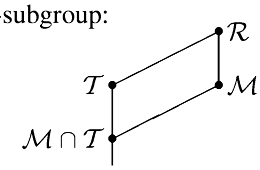
Theorem 1.4.4.2.3. (Hermann) Let $\mathcal{M} \le \mathcal{R}$ be a maximal subgroup of the space group $\mathcal{R}$. Then $\mathcal{M}$ is either a k-subgroup or a t-subgroup. □

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 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 $r \leq n$. □

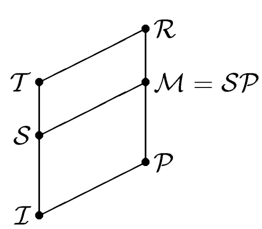
Corollary 1.4.4.2.7. Maximal subgroups of space groups are again space groups and of finite index in the supergroup. □

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

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

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 $g_a\mathcal{M}$ 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.

references