International Tables for Crystallography (2006). Vol. A1, Section 1.5.6, pp. 38–39.

1.5.5.3. *Maximal subgroups of soluble groups*

Now let $\mathcal{G}$ be a soluble group and $\mathcal{M} \leq \mathcal{G}$ a maximal subgroup of finite index in $\mathcal{G}$. Then the set of left cosets $X := \mathcal{G}/\mathcal{M}$ is a primitive finite $\mathcal{G}$-set. Let $\mathcal{K} = \mathrm{core}(\mathcal{M})$ be the kernel of the action of $\mathcal{G}$ on X. Then the factor group $\mathcal{H} := \mathcal{G}/\mathcal{K}$ acts faithfully on X. In particular, $\mathcal{H}$ is a finite group and X is a primitive, faithful $\mathcal{H}$-set. Since $\mathcal{G}$ is soluble, the factor group $\mathcal{H}$ is also a soluble group. Let $\mathcal{H} \trianglerighteq \mathcal{H}_1 \trianglerighteq \ldots \trianglerighteq \mathcal{H}_{n-1} \trianglerighteq \{e\}$ be the derived series of $\mathcal{H}$ with $\mathcal{N} := \mathcal{H}_{n-1} \neq \{e\}$. Then $\mathcal{N}$ is an Abelian normal subgroup of $\mathcal{H}$. The theorem of Galois (Theorem 1.5.5.1.3) states that $\mathcal{N}$ is an elementary Abelian p-group for some prime p and $|X| = |\mathcal{N}| = p^r$ for some $r \in \mathbb{N}$. Since $X = \mathcal{G}/\mathcal{M}$, the order of X is the index $[\mathcal{G} : \mathcal{M}]$ of $\mathcal{M}$ in $\mathcal{G}$. Therefore one gets the following theorem:

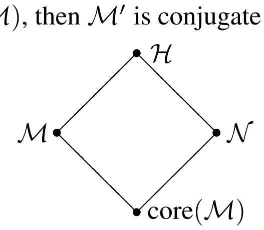
Theorem 1.5.5.3.1. If $\mathcal{M} \leq \mathcal{G}$ is a maximal subgroup of finite index in the soluble group $\mathcal{G}$, then its index $|\mathcal{G}/\mathcal{M}|$ is a prime power. □

In the proof of Theorem 1.5.5.1.3, we have established a bijection between $\mathcal{N}$ and the $\mathcal{H}$-set X, which is now $X := \mathcal{G}/\mathcal{M}$. Taking the full pre-image

$$\mathcal{N}' := \mathcal{N}\mathrm{core}(\mathcal{M})$$

of $\mathcal{N}$ in $\mathcal{G}$, then one has $\mathcal{G} = \mathcal{N}'\mathcal{M}$ and $\mathcal{M} \cap \mathcal{N}' = \mathrm{core}(\mathcal{M})$. Hence we have seen the first part of the following theorem:

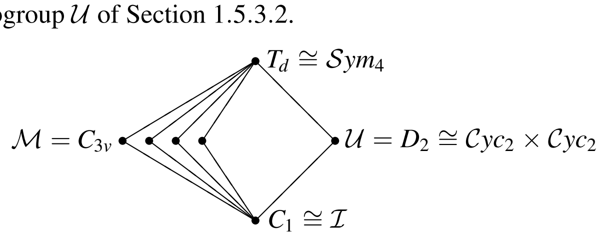
Theorem 1.5.5.3.2. Let $\mathcal{M} \leq \mathcal{G}$ be a maximal subgroup of the soluble group $\mathcal{G}$. Then the factor group $\mathcal{H} := \mathcal{G}/\mathrm{core}(\mathcal{M})$ acts primitively and faithfully on $X := \mathcal{G}/\mathcal{M}$, and there is a normal subgroup $\mathcal{N}' \trianglelefteq \mathcal{G}$ with $\mathcal{M}\mathcal{N}' = \mathcal{G}$ and $\mathcal{M} \cap \mathcal{N}' = \mathrm{core}(\mathcal{M})$. Moreover, if $\mathcal{M}'$ is another subgroup of $\mathcal{G}$, with $\mathcal{M}'\mathcal{N}' = \mathcal{G}$ and $\mathcal{M}' \cap \mathcal{N}' = \mathrm{core}(\mathcal{M})$, then $\mathcal{M}'$ is conjugate to $\mathcal{M}$.



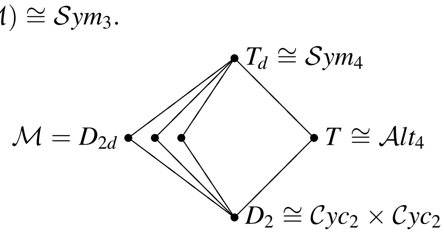
□

Example 1.5.5.3.3.

$\mathcal{G} = \mathcal{S}ym_4 \cong T_d$ is the tetrahedral group from Section 1.5.3.2 and $\mathcal{S}ym_3 \cong \mathcal{M} = C_{3v} \leq \mathcal{G}$ is the stabilizer of one of the four apices in the tetrahedron. Then $\mathrm{core}(\mathcal{M}) = \{e\}$ and $\mathcal{G}/\mathcal{M}$ is a faithful $\mathcal{G}$-set which can be identified with the set of apices of the tetrahedron. The normal subgroup $\mathcal{N} = \mathcal{N}'$ is the normal subgroup $\mathcal{U}$ of Section 1.5.3.2.



Now let $\mathcal{G} = \mathcal{S}ym_4 \cong T_d$ be as above, and take $D_{2d} \cong \mathcal{M} \leq \mathcal{G}$ a Sylow 2-subgroup of $\mathcal{G}$. Then $\mathrm{core}(\mathcal{M}) = D_2 \cong \mathcal{C}yc_2 \times \mathcal{C}yc_2$ is the normal subgroup $\mathcal{U}$ from Section 1.5.3.2 and $\mathcal{H} = \mathcal{G}/\mathrm{core}(\mathcal{M}) \cong \mathcal{S}ym_3$.



These observations result in an algorithm for computing maximal subgroups of soluble groups $\mathcal{G}$:

compute normal subgroups $\mathcal{C}$ [candidates for $\mathrm{core}(\mathcal{M})$];
compute a minimal normal subgroup $\mathcal{N}/\mathcal{C}$ of $\mathcal{G}/\mathcal{C}$;
find $\mathcal{M}/\mathcal{C}$ as a complement of $\mathcal{N}/\mathcal{C}$ in $\mathcal{G}/\mathcal{C}$.

1.5.6. Quantitative results

This section gives estimates for the number of maximal subgroups of a given index in space groups.

1.5.6.1. *General results*

The first very easy but useful remark applies to general groups $\mathcal{G}$:

Remark
Let $\mathcal{M} \leq \mathcal{G}$ be a maximal subgroup of $\mathcal{G}$ of finite index $i := [\mathcal{G} : \mathcal{M}] < \infty$. Then $\mathcal{M} \leq \mathcal{N}_{\mathcal{G}}(\mathcal{M}) \leq \mathcal{G}$. Hence the maximality of $\mathcal{M}$ implies that either $\mathcal{N}_{\mathcal{G}}(\mathcal{M}) = \mathcal{G}$ and $\mathcal{M}$ is a normal subgroup of $\mathcal{G}$ or $\mathcal{N}_{\mathcal{G}}(\mathcal{M}) = \mathcal{M}$ and $\mathcal{G}$ has i maximal subgroups that are conjugate to $\mathcal{M}$.

The smallest possible index of a proper subgroup is 2. It is well known and easy to see that subgroups of index 2 are normal subgroups:

Proposition 1.5.6.1.1. Let $\mathcal{G}$ be a group and $\mathcal{M} \leq \mathcal{G}$ a subgroup of index $2 = |\mathcal{G}/\mathcal{M}|$. Then $\mathcal{M}$ is a normal subgroup of $\mathcal{G}$. □

Proof. Choose an element $g \in \mathcal{G}$, $g \notin \mathcal{M}$. Then $\mathcal{G} = \mathcal{M} \cup g\mathcal{M} = \mathcal{M} \cup \mathcal{M}g$. Hence $g\mathcal{M} = \mathcal{M}g$ and therefore $g\mathcal{M}g^{-1} = \mathcal{M}$. Since this is also true if $g \in \mathcal{M}$, the proposition follows. QED

Let $\mathcal{M}$ be a subgroup of a group $\mathcal{G}$ of index 2. Then $\mathcal{M} \trianglelefteq \mathcal{G}$ is a normal subgroup and the factor group $\mathcal{G}/\mathcal{M}$ is a group of order 2. Since groups of order 2 are Abelian, it follows that the derived subgroup $\mathcal{G}_1$ of $\mathcal{G}$ (*cf.* Definition 1.5.5.2.1) (which is the smallest normal subgroup of $\mathcal{G}$ such that the factor group is Abelian) is contained in $\mathcal{M}$. Hence all maximal subgroups of index 2 in $\mathcal{G}$ contain $\mathcal{G}_1$. If one defines $\mathcal{N} := \cap\{\mathcal{M} \leq \mathcal{G} \mid [\mathcal{G} : \mathcal{M}] = 2\}$, then $\mathcal{G}/\mathcal{N}$ is an elementary Abelian 2-group and hence a vector space over the field with two elements. The maximal subgroups of $\mathcal{G}/\mathcal{N}$ are the maximal subspaces of this vector space, hence their number is $2^a - 1$, where $a := \dim_{\mathbb{Z}/2\mathbb{Z}}(\mathcal{G}/\mathcal{N})$.

This shows the following:

Corollary 1.5.6.1.2. The number of subgroups of $\mathcal{G}$ of index 2 is of the form $2^a - 1$ for some $a \geq 0$. □

Dealing with subgroups of index 3, one has the following:

Proposition 1.5.6.1.3. Let $\mathcal{U}$ be a subgroup of the group $\mathcal{G}$ with $[\mathcal{G} : \mathcal{U}] = 3$. Then $\mathcal{U}$ is either a normal subgroup of $\mathcal{G}$ or $\mathcal{G}/\mathrm{core}(\mathcal{U}) \cong \mathcal{S}_3$ and there are three subgroups of $\mathcal{G}$ conjugate to $\mathcal{U}$. □

Proof. $\mathcal{G}/\mathrm{core}(\mathcal{U})$ is isomorphic to a subgroup of $\mathcal{S}ym_3$ that acts primitively on $\{1, 2, 3\}$. Hence either $\mathcal{G}/\mathrm{core}(\mathcal{U}) \cong \mathcal{C}yc_3$ and $\mathcal{U} = \mathrm{core}(\mathcal{U})$ is a normal subgroup of $\mathcal{G}$ or $\mathcal{G}/\mathrm{core}(\mathcal{U}) \cong \mathcal{S}ym_3$, $\mathcal{U}/\mathrm{core}(\mathcal{U}) \cong \mathcal{C}yc_2$ and there are three subgroups of $\mathcal{G}$ conjugate to $\mathcal{U}$. QED

1.5.6.2. *Three-dimensional space groups*

We now come to space groups. By Lemma 1.5.5.2.3, all three-dimensional space groups are soluble. Theorem 1.5.5.3.1 says that the index of a maximal subgroup of a soluble group is a prime power (or infinite). Since the index of a maximal subgroup of a space group is always finite (see Corollary 1.5.4.2.7), we get:

Corollary 1.5.6.2.1. Let $\mathcal{G}$ be a three-dimensional space group and $\mathcal{M} \leq \mathcal{G}$ a maximal subgroup. Then $[\mathcal{G} : \mathcal{M}]$ is a prime power. □

Let $\mathcal{R}$ be a three-dimensional space group and $\mathcal{P} = \mathcal{R}/\mathcal{T}(\mathcal{R})$ its point group. It is well known that the order of $\mathcal{P}$ is of the form $2^a 3^b$ with $a = 0, 1, 2, 3$ or 4 and $b = 0, 1$. By Corollary 1.5.4.2.4, the *t*-subgroups of $\mathcal{R}$ are in one-to-one correspondence with the subgroups of $\mathcal{P}$. Let us look at the *t*-subgroups of $\mathcal{R}$ of index 3. It is clear that $\mathcal{P}$ has no subgroup of index 3 if $b = 0$, since the index of a subgroup divides the order of the finite group $\mathcal{P}$ by the theorem of Lagrange. If $b = 1$, then any subgroup $\mathcal{S}$ of $\mathcal{P}$ of index 3 has order $|\mathcal{P}|/3 = 2^a$ and hence is a Sylow 2-subgroup of $\mathcal{P}$. Therefore there is such a subgroup $\mathcal{S}$ of index 3 in $\mathcal{P}$ by the first theorem of Sylow, Theorem 1.5.3.3.1. By the second theorem of Sylow, Theorem 1.5.3.3.2, all these Sylow 2-subgroups of $\mathcal{P}$ are conjugate in $\mathcal{P}$. Therefore, by Proposition 1.5.6.1.3, the number of these groups is either 1 or 3:

Corollary 1.5.6.2.2. Let $\mathcal{R}$ be a three-dimensional space group.

If the order of the point group of $\mathcal{R}$ is not divisible by 3 then $\mathcal{R}$ has no *t*-subgroups of index 3.

If 3 is a factor of the order of the point group of $\mathcal{R}$, then $\mathcal{R}$ has either one *t*-subgroup of index 3 (which is then normal in $\mathcal{R}$) or three conjugate *t*-subgroups of index 3. □

1.5.7. Qualitative results

1.5.7.1. *General theory*

In this section, we want to comment on the very subtle question of deciding whether two space groups $\mathcal{R}_1$ and $\mathcal{R}_2$ are isomorphic.

This problem can be treated in several stages:

Let $\mathcal{R}_1$ and $\mathcal{R}_2$ be space groups. Since the translation subgroups $\mathcal{T}(\mathcal{R}_i)$ are characteristic subgroups of $\mathcal{R}_i$ (the maximal Abelian normal subgroup of finite index), each isomorphism $\varphi : \mathcal{R}_1 \to \mathcal{R}_2$ induces isomorphisms of the corresponding translation subgroups

$$\varphi' : \mathcal{T}(\mathcal{R}_1) \to \mathcal{T}(\mathcal{R}_2)$$

(by restriction) as well as of the point groups

$$\overline{\varphi} : \mathcal{P}_1 := \mathcal{R}_1/\mathcal{T}(\mathcal{R}_1) \to \mathcal{R}_2/\mathcal{T}(\mathcal{R}_2) =: \mathcal{P}_2.$$

It is convenient to view $\mathcal{T}(\mathcal{R}_i)$ as a lattice on which the point group $\mathcal{P}_i$ acts as group of linear mappings (*cf.* the start of Section 1.5.4). Then the isomorphism φ' is an isomorphism of $\mathcal{P}_1$-sets, where $\mathcal{P}_1$ acts on $\mathcal{T}(\mathcal{R}_1)$ *via* conjugation and on $\mathcal{T}(\mathcal{R}_2)$ *via*

$$g\mathcal{T}(\mathcal{R}_1) \cdot t := \varphi(g)t\varphi(g)^{-1} \text{ for all } g\mathcal{T}(\mathcal{R}_1) \in \mathcal{P}_1, t \in \mathcal{T}(\mathcal{R}_2).$$

Since $\varphi(\mathcal{T}(\mathcal{R}_1)) = \mathcal{T}(\mathcal{R}_2)$ and $\mathcal{T}(\mathcal{R}_2)$ centralizes itself, this action is well defined, *i.e.* independent of the choice of the coset representative g.

The following theorem will show that the isomorphism of sufficiently large factor groups of $\mathcal{R}_1$ and $\mathcal{R}_2$ implies a 'near' isomorphism of the space groups themselves. To give a precise formulation we need one further definition.

Definition 1.5.7.1.1. For $d \in \mathbb{N}$ define

$$O_d := \{\frac{a}{b} \mid a, b \in \mathbb{Z}, b \neq 0, \gcd(b, d) = 1\} \leq \mathbb{Q},$$

which is the set of all rational numbers for which the denominator is prime to d. For the space group $\mathcal{R} \leq \mathcal{E}_n$ let $\mathcal{R} \leq \mathcal{R}_{(d)} \leq \mathcal{E}_n$ be the group $\mathcal{R}_{(d)} := \langle \mathcal{T}(\mathcal{R})_{(d)}, \mathcal{R} \rangle$, where

$$\mathcal{T}(\mathcal{R})_{(d)} = \{at \mid a \in O_{(d)}, t \in \mathcal{T}(\mathcal{R})\} \leq \mathcal{T}_n,$$

i.e. one allows denominators that are prime to d in the translation subgroup. □

One has the following:

Theorem 1.5.7.1.2. Let $\mathcal{R}_1$ and $\mathcal{R}_2$ be two space groups with point groups of order $d_i := |\mathcal{R}_i/\mathcal{T}(\mathcal{R}_i)|$. Let $\mathbf{N}(\mathcal{R}_i)$ denote the set of normal subgroups of $\mathcal{R}_i$ having finite index in $\mathcal{R}_i$. Then the following three conditions are equivalent:

(i) There are normal subgroups $\mathcal{S}_i \trianglelefteq \mathcal{R}_i$ with $\mathcal{R}_1/\mathcal{S}_1 \cong \mathcal{R}_2/\mathcal{S}_2$ and with $\mathcal{S}_i \subseteq d_i^2\mathcal{T}(\mathcal{R}_i)$ if $d_i \neq 2$ and $\mathcal{S}_i \subseteq 16\mathcal{T}(\mathcal{R}_i)$ if $d_i = 2$ $(i = 1, 2)$.

(ii) $(\mathcal{R}_1)_{(d_1)} \cong (\mathcal{R}_2)_{(d_2)}$.

(iii) There is a bijection $\mu : \mathbf{N}(\mathcal{R}_1) \to \mathbf{N}(\mathcal{R}_2)$ such that $\mathcal{R}_1/\mathcal{N} \cong \mathcal{R}_2/\mu(\mathcal{N})$ for all $\mathcal{N} \in \mathbf{N}(\mathcal{R}_1)$. □

For a proof of this theorem, see Finken *et al.* (1980).

Remark

If $\mathcal{R}_i$ are three- or four-dimensional space groups, the isomorphism in (ii) already implies the isomorphism of $\mathcal{R}_1$ and $\mathcal{R}_2$, but there are counterexamples for dimension 5.

1.5.7.2. *Three-dimensional space groups*

Corollary 1.5.7.2.1. Let $\mathcal{R}$ be a three-dimensional space group with translation subgroup $\mathcal{T}$ and p be a prime not dividing the order of the point group $\mathcal{R}/\mathcal{T}$. Let $\mathcal{U}$ be a subgroup of $\mathcal{R}$ of index p^α for some $\alpha \in \mathbb{Z}_{>0}$. Then

(*a*) $\mathcal{U}$ is a *k*-subgroup.

(*b*) $\mathcal{U}$ is isomorphic to $\mathcal{R}$. □

Proof:

(*a*) $\mathcal{U} \leq \mathcal{U}\mathcal{T} \leq \mathcal{R}$ implies that $[\mathcal{R} : \mathcal{U}\mathcal{T}]$ divides $[\mathcal{R} : \mathcal{U}] = p^\alpha$. Since $\mathcal{T} \leq \mathcal{U}\mathcal{T} \leq \mathcal{R}$, one obtains $[\mathcal{R} : \mathcal{U}\mathcal{T}]$ as a factor of $[\mathcal{R} : \mathcal{T}]$. But p is not a factor of $[\mathcal{R} : \mathcal{T}]$, hence $[\mathcal{R} : \mathcal{U}\mathcal{T}] = 1$ and $\mathcal{R} = \mathcal{U}\mathcal{T}$. According to the remark following Definition 1.5.4.2.2, $\mathcal{U}$ is a *k*-subgroup.

(*b*) Let $d_1 := |\mathcal{R}/\mathcal{T}| = |\mathcal{U}/\mathcal{T}(\mathcal{U})|$. Let $d := d_1^2$ if $d_1 \neq 2$ and $d := 16$ otherwise, and let $\mathcal{T}' := d\mathcal{T}$. Since $\gcd([\mathcal{R} : \mathcal{U}], d) = 1$, one has $\mathcal{U}\mathcal{T}' = \mathcal{R}$ and $\mathcal{T}' \cap \mathcal{U} = d\mathcal{T}(\mathcal{U})$. By the third isomorphism theorem, Theorem 1.5.3.5.2, it follows that

$$\mathcal{R}/\mathcal{T}' = \mathcal{U}\mathcal{T}'/\mathcal{T}' \cong \mathcal{U}/\mathcal{T}' \cap \mathcal{U} = \mathcal{U}/d\mathcal{T}(\mathcal{U}).$$

By Theorem 1.5.7.1.2 (i) ⇒ (ii), one has $\mathcal{R}_{(d_1)} \cong \mathcal{U}_{(d_1)}$. By the remark above, this already implies that $\mathcal{R}$ and $\mathcal{U}$ are isomorphic. QED

Theorem 1.5.7.2.2. Let $\mathcal{R}$ be a three-dimensional space group and $\mathcal{U}$ be a maximal subgroup of $\mathcal{R}$ of index > 4. Then

(*a*) $\mathcal{U}$ is a *k*-subgroup.

(*b*) $\mathcal{U}$ is isomorphic to $\mathcal{R}$. □

Proof. Since $\mathcal{R}$ is soluble, the index $[\mathcal{R} : \mathcal{U}] = p^\alpha$ is a prime power (see Theorem 1.5.5.3.1). If p is not a factor of $|\mathcal{R}/\mathcal{T}(\mathcal{R})|$, the statement follows from Corollary 1.5.7.2.1. Hence we only have to consider the cases $p = 2$, $\alpha > 2$ and $p = 3$, $\alpha > 1$. Since 9 is not a factor of the order of any crystallographic point group in dimension 3, assertion (*a*) follows if the index of $\mathcal{U}$ is divisible by 9. If $\mathcal{U}$ is a maximal *t*-subgroup, then $\mathcal{R}/\mathcal{U}$ is a primitive $\mathcal{P}$-set for the point group $\mathcal{P}$ of $\mathcal{R}$. Since the point groups $\mathcal{P}$ of dimension 3 have no primitive $\mathcal{P}$-sets of order divisible

references