International Tables for Crystallography (2006). Vol. A1, Section 1.5.7, pp. 39–40.

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 by 8, assertion (*a*) also follows if the index of $\mathcal{U}$ is divisible by 8.

For all three-dimensional space groups $\mathcal{R}$, the module $\mathbf{L}(\mathcal{R})/2\mathbf{L}(\mathcal{R})$ [where $\mathcal{T}(\mathcal{R})$ is identified with the corresponding lattice $\mathbf{L}(\mathcal{R})$ in $\tau(\mathbb{E}_3)$ as in Section 1.5.4] is not simple as a module for the point group $\mathcal{P} = \mathcal{R}/\mathcal{T}(\mathcal{R})$. [It suffices to check this property for the two maximal point groups $\mathcal{C}yc_2 \times \mathcal{S}ym_4$ ($= m\overline{3}m$) and $\mathcal{C}yc_2 \times \mathcal{C}yc_2 \times \mathcal{S}ym_3$ ($= 6/mmm$).] This means that $2\mathbf{L}(\mathcal{R})$ is not a maximal $\mathcal{R}$-invariant sublattice of $\mathbf{L}(\mathcal{R})$. Since the translation subgroup $\mathcal{T}(\mathcal{U})$ of a maximal *k*-subgroup $\mathcal{U}$ of index equal to a power of 2 in $\mathcal{R}$ is a maximal $\mathcal{R}$-invariant subgroup of $\mathcal{T}(\mathcal{R})$ that contains $2\mathcal{T}(\mathcal{R})$, one now finds that $\mathcal{R}$ has no maximal *k*-subgroup of index 8.

Now assume that $[\mathcal{R} : \mathcal{U}] = 9$. By Corollary 1.5.7.2.1, one only needs to deal with groups $\mathcal{R}$ such that the order of the point group $\mathcal{P} := \mathcal{R}/\mathcal{T}(\mathcal{R})$ is divisible by 3. $\mathcal{P}$ is isomorphic to a subgroup of $\mathcal{C}yc_2 \times \mathcal{S}ym_4$ or $\mathcal{C}yc_2 \times \mathcal{C}yc_2 \times \mathcal{S}ym_3$. If $\mathcal{A}lt_4 \leq \mathcal{P}$ is a subgroup of $\mathcal{P}$, then $\mathbf{L}(\mathcal{R})/3\mathbf{L}(\mathcal{R})$ is simple and $\mathcal{U}$ is of index 27 in $\mathcal{R}$ [with $\mathbf{L}(\mathcal{U}) = 3\mathbf{L}(\mathcal{R})$]. It turns out that $\mathcal{U}$ is isomorphic to $\mathcal{R}$ in these cases. If $\mathcal{P}$ does not contain a subgroup isomorphic to $\mathcal{A}lt_4$, then the maximality of $\mathcal{U}$ implies that $\mathcal{T}(\mathcal{U}) \leq \mathcal{T}(\mathcal{R})$ is of index 3 in $\mathcal{T}(\mathcal{R})$. Hence $[\mathcal{R} : \mathcal{U}] = 3$ in this case. QED

Corollary 1.5.7.2.3. Let $\mathcal{M}$ be a maximal subgroup of the three-dimensional space group $\mathcal{R}$.

(*a*) If the index of $\mathcal{M}$ is a power of 2, then $[\mathcal{R} : \mathcal{M}] = 2$ or 4.

(*b*) If 3 is a factor of the order of the point group $[\mathcal{R} : \mathcal{T}(\mathcal{R})]$ and the index of $\mathcal{M}$ is a power of 3, then $[\mathcal{R} : \mathcal{M}] = 3$ or 27. For $[\mathcal{R} : \mathcal{M}] = 27$, $\mathcal{M}$ is necessarily isomorphic to $\mathcal{R}$ (by Theorem 1.5.7.2.2). □

This interesting fact explains why there are no maximal subgroups of index 8 in a three-dimensional space group. If there is a maximal subgroup $\mathcal{M}$ of a three-dimensional space group $\mathcal{R}$ of index 9, then the order of the point group of $\mathcal{R}$ is not divisible by three and the subgroup $\mathcal{M}$ is a *k*-subgroup and isomorphic to $\mathcal{R}$.

In particular, there are no maximal subgroups of index 9 for trigonal, hexagonal or cubic space groups, whereas there are such subgroups of tetragonal space groups.

references