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conjugate in $\mathcal{P}$. Therefore, by Proposition 1.4.6.1.3, the number of these groups is either 1 or 3:

Corollary 1.4.6.2.2. 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. □

1.4.7. Qualitative results

1.4.7.1. 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 1.4.4). 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 1.4.7.1.1. 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 1.4.7.1.2. 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.

1.4.7.2. Three-dimensional space groups

Corollary 1.4.7.2.1. 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 1.4.4.2.2, $\mathcal{U}$ 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 1.4.3.5.2, 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 1.4.7.1.2 (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 1.4.7.2.2. 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 1.4.5.3.1). If p is not a factor of $|\mathcal{R}/\mathcal{T}(\mathcal{R})|$, the statement follows from Corollary 1.4.7.2.1. 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 1.4.4] 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 1.4.7.2.1, 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 1.4.7.2.3. 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 1.4.7.2.2). □

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.

1.4.8. Minimal supergroups

For several problems, for example for the prediction of a phase transition or in the search for overlooked symmetry in crystal-structure determinations *etc.*, it is helpful to know all space groups $\mathcal{S}$ containing a given space group $\mathcal{R}$, which means that $\mathcal{R} \leq \mathcal{S}$. Then $\mathcal{S}$ is called a *supergroup* of $\mathcal{R}$. Note that – in contrast to subgroups – the supergroups $\mathcal{G} \geq \mathcal{R}$ containing a space group $\mathcal{R}$ of finite index need not be space groups. For instance, the one-dimensional translation group

$$\mathcal{R} = \langle \left(\begin{array}{c|c} 1 & 1 \\ \hline 0 & 1 \end{array}\right) \rangle \cong \mathbb{Z}$$

has a supergroup $\mathcal{G}$ of index 2 isomorphic to $\mathcal{C}yc_2 \times \mathbb{Z}$ which is not a subgroup of the one-dimensional affine group. $\mathcal{G}$ is Abelian but has an element of finite order, so $\mathcal{G}$ cannot be a space group. For the applications in crystallography, we are restricted to those supergroups $\mathcal{S}$ of $\mathcal{R}$ that are again space groups.

Definition 1.4.8.1. Let $\mathcal{S}$ be a space group that is a supergroup of the space group $\mathcal{R}$ and $\mathcal{T} := \mathcal{T}(\mathcal{S})$.

(i) $\mathcal{S}$ is called a *translationengleiche* or a *t*-supergroup if $\mathcal{R} \cap \mathcal{T} = \mathcal{T}$.

(ii) $\mathcal{S}$ is called a *klassengleiche* or a *k*-supergroup if $\mathcal{R}/\mathcal{R} \cap \mathcal{T} \cong \mathcal{S}/\mathcal{T}$. □

Clearly $\mathcal{S}$ is a *t*-supergroup (or *k*-supergroup, respectively) of $\mathcal{R}$ if and only if $\mathcal{R}$ is a *t*-subgroup (or *k*-subgroup) of $\mathcal{S}$ and the theorem of Hermann implies the following:

Theorem 1.4.8.2. (Theorem of Hermann.) Let $\mathcal{S}$ and $\mathcal{R}$ be space groups such that $\mathcal{S} \geq \mathcal{R}$ is a minimal supergroup of $\mathcal{R}$. Then $\mathcal{S}$ is either a *k*-supergroup or a *t*-supergroup. □

The determination of the *k*-supergroups of a given space group $\mathcal{R}$ is the easier task. For instance, if $\mathcal{R}$ is a symmorphic space group then all its *k*-supergroups are also symmorphic. This is not true for *k*-subgroups of $\mathcal{R}$.

Theorem 1.4.8.3. Let $\mathcal{S}$ be a *k*-supergroup of the space group $\mathcal{R}$. Then $\mathcal{S} = \mathcal{R}\mathcal{T}(\mathcal{S})$. If $\mathcal{S}$ is a minimal *k*-supergroup of $\mathcal{R}$ then the translation lattice $\mathbf{L}(\mathcal{S})$ of $\mathcal{S}$ is an $\overline{\mathcal{R}}$-invariant lattice that contains $\mathbf{L}(\mathcal{R})$ as a maximal sublattice. □

Proof. Let $\mathcal{T} := \mathcal{T}(\mathcal{S})$ be the translation subgroup of $\mathcal{S}$. Then $\mathcal{T} \cap \mathcal{R} = \mathcal{T}(\mathcal{R})$ and $\mathcal{R}/(\mathcal{T} \cap \mathcal{R})$ is isomorphic to the point group $\overline{\mathcal{R}}$, which is a finite group. By the isomorphism theorem

$$\mathcal{R}/(\mathcal{T} \cap \mathcal{R}) \cong \mathcal{R}\mathcal{T}/\mathcal{T}.$$

Therefore, group $\mathcal{R}\mathcal{T}$ generated by $\mathcal{T}$ and $\mathcal{R}$ is a subgroup of $\mathcal{S}$ containing $\mathcal{T}$ with the same index and, therefore, $\mathcal{R}\mathcal{T} = \mathcal{S}$. Moreover, $\mathcal{T}$ contains $\mathcal{T}(\mathcal{R})$ and hence $\mathbf{L}(\mathcal{S})$ contains $\mathbf{L}(\mathcal{R})$. Since $\mathcal{T}$ is a normal subgroup of $\mathcal{S}$, the space group $\mathcal{R}$ acts on $\mathcal{T}$ by conjugation and therefore $\mathbf{L}(\mathcal{S})$ is $\overline{\mathcal{R}}$ invariant. If there is an $\overline{\mathcal{R}}$ invariant lattice $\mathbf{L}$ such that $\mathbf{L}(\mathcal{R}) \subset \mathbf{L} \subset \mathbf{L}(\mathcal{S})$, then, applying the isomorphism μ from Example 1.4.3.4.4, the group $\mathcal{G} := \mathcal{R}\mu^{-1}(\mathbf{L})$ is a space group with $\mathcal{R} \leq \mathcal{G} \leq \mathcal{S}$. Hence the minimality of the supergroup $\mathcal{S}$ implies that $\mathbf{L}(\mathcal{S})$ is an $\overline{\mathcal{R}}$-invariant lattice that contains $\mathbf{L}(\mathcal{R})$ as a maximal sublattice. QED

As for maximal *k*-subgroups, the index $[\mathcal{S} : \mathcal{R}]$ of a minimal *k*-supergroup $\mathcal{S}$ of $\mathcal{R}$ is a prime power and for each prime p there is some $a \in \mathbb{N}$ such that $\mathcal{R}$ has a minimal *k*-supergroup $\mathcal{S}$ of index $[\mathcal{S} : \mathcal{R}] = p^a$. Because of the infinite number of prime numbers, a space group $\mathcal{R}$ has infinitely many minimal *k*-supergroups, but there are only finitely many minimal *k*-supergroups containing a given space group $\mathcal{R}$ of given index.

This is different for *t*-supergroups, as the following example shows.

Example 1.4.8.4

Let

$$\mathcal{R} = \langle \left(\begin{array}{cc|c} 1 & 0 & 1 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & 1 & 1 \\ \hline 0 & 0 & 1 \end{array}\right) \rangle \cong \mathbb{Z}^2$$

be the two-dimensional translation group $p1$. Then for all $x \in \mathbb{R}$ the group

$$\mathcal{S}_x := \langle \mathcal{R}, \left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & -1 & x \\ \hline 0 & 0 & 1 \end{array}\right) \rangle$$

is a minimal *t*-supergroup of $\mathcal{R}$ containing $\mathcal{R}$ of index 2. These groups are conjugate under the normalizer of $\mathcal{R}$ in the affine group $\mathcal{A}_2$ [see Example 3.47 in Heidbüchel (2003)],

$$\left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & 1 & -x/2 \\ \hline 0 & 0 & 1 \end{array}\right) \mathcal{S}_x \left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & 1 & x/2 \\ \hline 0 & 0 & 1 \end{array}\right) = \mathcal{S}_0.$$

Visually this means that the discrete sets of symmetry lines of the different plane groups may be shifted by any real distance against each other or relative to an arbitrarily chosen origin. This yields uncountably many different *t*-supergroups of $p1$ which are all of the same type.