International Tables for Crystallography (2011). Vol. A1, Section 1.4.8, pp. 39–40.

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

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

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

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

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

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

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.

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The use of the affine and Euclidean normalizers of a space group $\mathcal{R}$ is described in Part 15 of *IT* A. The *affine normalizer*

$$\mathcal{N} := \mathcal{N}_{\mathcal{A}_n}(\mathcal{R}) = \{g \in \mathcal{A}_n \mid g\mathcal{R}g^{-1} = \mathcal{R}\}$$

of an n-dimensional space group $\mathcal{R} \leq \mathcal{A}_n$ acts on the set of all minimal t-supergroups $\mathcal{S}$ of $\mathcal{R}$ by conjugation.

Theorem 1.4.8.5. $\mathcal{N}$ has finitely many orbits on the set of (minimal) t-supergroups $\mathcal{S}$ of $\mathcal{R}$. □

Proof. Let $\mathcal{S}_1, \ldots, \mathcal{S}_m$ be representatives of the $\mathcal{A}_n$-orbits on the set of n-dimensional space groups, *i.e.* of the types of n-dimensional space groups. For $1 \leq i \leq m$ let

$$\mathcal{M}_i := \{\mathcal{R}_{ij} \mid 1 \leq j \leq a_i\}$$

denote the set of all (maximal) t-subgroups of $\mathcal{S}_i$ that are isomorphic to $\mathcal{R}$.

If $\mathcal{S}$ is a (minimal) t-supergroup of the space group $\mathcal{R}$, then there is some $g \in \mathcal{A}_n$ and $i \in \{1, \ldots, m\}$ such that $g\mathcal{S}g^{-1} = \mathcal{S}_i$ and $g\mathcal{R}g^{-1} = \mathcal{R}_{ij} \in \mathcal{M}_i$, hence the pair of space groups $(\mathcal{R}, \mathcal{S}) = (g^{-1}\mathcal{R}_{ij}g, g^{-1}\mathcal{S}_i g)$ for some $i \in \{1, \ldots, m\}$, $\mathcal{R}_{ij} \in \mathcal{M}_i$ and $g \in \mathcal{A}_n$.

If $\mathcal{S}'$ is a second supergroup of $\mathcal{R}$ and $h \in \mathcal{A}_n$ such that $(\mathcal{R}, \mathcal{S}') = (h^{-1}\mathcal{R}_{ij}h, h^{-1}\mathcal{S}_i h)$ for the same i, j, then $h^{-1}g \in \mathcal{N}$ normalizes $\mathcal{R}$. Hence there are at most $\sum_{i=1}^{m} a_i$ orbits of $\mathcal{N}$ on the set of (minimal) t-supergroups of $\mathcal{R}$. QED

This proof also provides an algorithm to determine representatives of the $\mathcal{N}$-orbits of minimal t-supergroups of a given space group $\mathcal{R}$, provided that one knows representatives of all affine classes of space groups and their maximal t-subgroups. For dimensions 2 and 3 these are given in this volume. Since maximal t-subgroups of three-dimensional space groups have index 2, 3 or 4, this also holds for the minimal t-supergroups of these groups.

Up to dimension $n \leq 4$, the minimal t-supergroups and the minimal k-supergroups of a given space group $\mathcal{R} \leq \mathcal{A}_n$ can be obtained with the commands *TSupergroups* and *KSupergroups* in *CARAT* [see also Heidbüchel (2003)].

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