International Tables for Crystallography (2011). Vol. A1, Section 1.2.8, pp. 23–24.

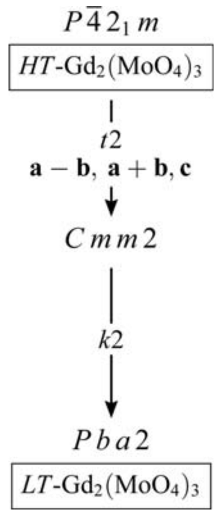

Fig. 1.2.7.1. Group–subgroup relations between the high (HT) and low temperature (LT) forms of gadolinium molybdate (Bärnighausen tree as explained in Section 1.6.3).

To calculate the number of space groups $Pba2$, *i.e.* the number of symmetry states, one determines the normalizer of $Pba2$ in $P\bar{4}2_1m$. From *IT* A, Table 15.2.1.3, one finds $\mathcal{N}_{\mathcal{E}}(Pba2) = P^14/mmm$ for the Euclidean normalizer of $Pba2$ under the PCA, which includes the condition $a' = b'$. P^14/mmm is a supergroup of $P\bar{4}2_1m$. Thus, $\mathcal{N}_{\mathcal{G}}(Pba2) = (\mathcal{N}_{\mathcal{E}}(Pba2) \cap \mathcal{G}) = \mathcal{G}$ and $Pba2$ is a normal subgroup. Therefore, under the PCA all four domain states belong to one space group $Pba2$, *i.e.* there is one symmetry state. Indeed, the tables of Volume A1 list only one subgroup of type $Cmm2$ under $P\bar{4}2_1m$ and only one subgroup $Pba2$ under $Cmm2$ with $[i] = 2$ in both cases. Hermann's group $\mathcal{M}$, $\mathcal{G} > \mathcal{M} > \mathcal{H}$ is of space-group type $Cmm2$ with the point group $mm2$ of $\mathcal{H}$ and with the lattice of $\mathcal{G}$. Because $|\mathcal{G} : \mathcal{M}| = 2$, there are two directional states which belong to the same space group. The directional state of $\mathbf{B}_2$ is obtained from that of $\mathbf{B}_1$ by, for example, the (lost) $\bar{4}$ operation of $P\bar{4}2_1m$: the basis vector $\mathbf{a}$ of $\mathbf{B}_2$ is parallel to $\mathbf{b}$ of $\mathbf{B}_1$, $\mathbf{b}$ of $\mathbf{B}_2$ is parallel to $\mathbf{a}$ of $\mathbf{B}_1$ and $\mathbf{c}$ of $\mathbf{B}_2$ is antiparallel to $\mathbf{c}$ of $\mathbf{B}_1$. The other factor of 2 is caused by the loss of the centring translations of $Cmm2$, $i_T = |\mathcal{M} : \mathcal{H}| = 2$. Therefore, the domain state $\mathbf{B}_3$ is parallel to $\mathbf{B}_1$ but its origin is shifted with respect to that of $\mathbf{B}_1$ by a lost translation, for example, by $t(1, 0, 0)$ of $\mathcal{G}$, which is $t(\frac{1}{2}, \frac{1}{2}, 0)$ in the basis $\mathbf{a}'$, $\mathbf{b}'$ of $Pba2$. The same holds for the domain state $\mathbf{B}_4$ relative to $\mathbf{B}_2$.

1.2.8. Lemmata on subgroups of space groups

There are several lemmata on subgroups $\mathcal{H} < \mathcal{G}$ of space groups $\mathcal{G}$ which may help in getting an insight into the laws governing group–subgroup relations of plane and space groups. They were also used for the derivation and the checking of the tables of Part 2. These lemmata are proved or at least stated and explained in Chapter 1.4. They are repeated here as statements, separated from their mathematical background, and are formulated for the three-dimensional space groups. They are valid by analogy for the (two-dimensional) plane groups.

1.2.8.1. General lemmata

Lemma 1.2.8.1.1. A subgroup $\mathcal{H}$ of a space group $\mathcal{G}$ is a space group again, if and only if the index $i = |\mathcal{G} : \mathcal{H}|$ is finite. □

In this volume, only subgroups of finite index i are listed. However, the index i is not restricted, *i.e.* there is no number I with the property $i < I$ for any i. Subgroups $\mathcal{H} < \mathcal{G}$ with infinite index are considered in *International Tables for Crystallography*, Volume E (2002).

Lemma 1.2.8.1.2. Hermann's theorem. For any group–subgroup chain $\mathcal{G} > \mathcal{H}$ between space groups there exists a uniquely defined space group $\mathcal{M}$ with $\mathcal{G} \geq \mathcal{M} \geq \mathcal{H}$, where $\mathcal{M}$ is a *translationengleiche* subgroup of $\mathcal{G}$ and $\mathcal{H}$ is a *klassengleiche* subgroup of $\mathcal{M}$. □

The decisive point is that any group–subgroup chain between space groups can be split into a *translationengleiche* subgroup chain between the space groups $\mathcal{G}$ and $\mathcal{M}$ and a *klassengleiche* subgroup chain between the space groups $\mathcal{M}$ and $\mathcal{H}$.

It may happen that either $\mathcal{G} = \mathcal{M}$ or $\mathcal{H} = \mathcal{M}$ holds. In particular, one of these equations must hold if $\mathcal{H} < \mathcal{G}$ is a maximal subgroup of $\mathcal{G}$.

Lemma 1.2.8.1.3. (Corollary to Hermann's theorem.) A maximal subgroup of a space group is either a *translationengleiche* subgroup or a *klassengleiche* subgroup, never a general subgroup. □

The following lemma holds for space groups but not for arbitrary groups of infinite order.

Lemma 1.2.8.1.4. For any space group, the number of subgroups with a given finite index i is *finite*. □

This number of subgroups can be further specified, see Chapter 1.4. Although for each index i the number of subgroups is finite, the number of all subgroups with finite index is infinite because there is no upper limit for the number i.

1.2.8.2. Lemmata on maximal subgroups

Even the set of all *maximal* subgroups of finite index is not finite, as can be seen from the following lemma.

Lemma 1.2.8.2.1. The index i of a maximal subgroup of a space group is always of the form p^n, where p is a prime number and n = 1 or 2 for plane groups and n = 1, 2 or 3 for space groups. □

This lemma means that a subgroup of, say, index 6 cannot be maximal. Moreover, because of the infinite number of primes, the set of all maximal subgroups of a given space group cannot be finite.

An index of p^2, $p > 2$, occurs for isomorphic subgroups of tetragonal space groups when the basis vectors are enlarged to $p\mathbf{a}$, $p\mathbf{b}$; for trigonal and hexagonal space groups, the enlargement $p\mathbf{a}$, $p\mathbf{b}$ is allowed for $p = 2$ and for all or part of the primes $p > 3$. An index of p^3 occurs for and only for isomorphic subgroups of cubic space groups with cell enlargements of $p\mathbf{a}$, $p\mathbf{b}$, $p\mathbf{c}$ ($p > 2$).

There are even stronger restrictions for *maximal non-isomorphic* subgroups.

Lemma 1.2.8.2.2. The index of a maximal non-isomorphic subgroup of a plane group is 2 or 3; for a space group the index is 2, 3 or 4. □

This lemma can be specified further:

Lemma 1.2.8.2.3. The index of a maximal non-isomorphic subgroup $\mathcal{H}$ is always 2 for oblique, rectangular and square plane groups and for triclinic, monoclinic, orthorhombic and tetragonal space groups $\mathcal{G}$. The index is 2 or 3 for hexagonal plane groups and for trigonal and hexagonal space groups $\mathcal{G}$. The index is 2, 3 or 4 for cubic space groups $\mathcal{G}$. □

There are also lemmata for the number of subgroups of a certain index. The most important are:

Lemma 1.2.8.2.4. The number of subgroups of index 2 is $2^N - 1$ with $0 \leq N \leq 6$ for space groups and $0 \leq N \leq 4$ for plane groups. The number of *translationengleiche* subgroups of index 2 is $2^M - 1$ with $0 \leq M \leq 3$ for space groups and $0 \leq M \leq 2$ for plane groups. □

Examples are:

$N = 0: \ 2^0 - 1 = 0$ subgroups of index 2 for *p*3, No. 13, and *F*23, No. 196;

$N = 1: \ 2^1 - 1 = 1$ subgroup of index 2 for *p*3*m*1, No. 14, and *P*3, No. 143; ...;

$N = 4: \ 2^4 - 1 = 15$ subgroups of index 2 for *p*2*mm*, No. 6, and $P\overline{1}$, No. 2;

$N = 6: \ 2^6 - 1 = 63$ subgroups of index 2 for *Pmmm*, No. 47.

Lemma 1.2.8.2.5. The number of isomorphic subgroups of each space group is infinite and this applies even to the number of maximal isomorphic subgroups. □

Nevertheless, their listing is possible in the form of infinite series. The series are specified by parameters.

Lemma 1.2.8.2.6. For each space group, each maximal isomorphic subgroup $\mathcal{H}$ can be listed as a member of one of at most four series of maximal isomorphic subgroups. Each member is specified by a set of parameters. □

The series of maximal isomorphic subgroups are discussed in Section 2.1.5.

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