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The application of Hermann's group $\mathcal{M}$ in group–subgroup relations between space groups

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This paper is devoted to the study of the group–subgroup relations $\mathcal{U} < \mathcal{G}$ between space groups. A procedure has been developed for the derivation of all subgroups $\mathcal{U}_j < \mathcal{G}$ which are obtained from $\mathcal{U}$ by a transformation with a translation ($\mathcal{T}$-equivalent subgroups). All $\mathcal{T}$-equivalent supergroups $\mathcal{G}_k > \mathcal{U}$ can be determined in the same way from one supergroup $\mathcal{G} > \mathcal{U}$. The decisive group in this procedure is the translation part of the (Euclidean) normalizer of Hermann's group $\mathcal{M}$. The group $\mathcal{M}$ is the uniquely determined group $\mathcal{U} \le \mathcal{M} \le \mathcal{G}$ with the translations of $\mathcal{G}$ and the point group of $\mathcal{U}$. The method is particularly useful in the search for supergroups of space groups and is based on several lemmata which are formulated and proven in this paper. The results suggest under special conditions the possibility of a transition with 'region' formation in some analogy to the well known domain formation. This transition could occur from high symmetry to low symmetry or from low symmetry to high symmetry or even both ways.

1. Introduction

1.1. List of symbols

a, **b**, **c**, **t**	Vectors
$\boldsymbol{X}$, $\boldsymbol{I}$	Matrices
$\boldsymbol{x}$, $\boldsymbol{t}$, $\boldsymbol{l}$	Columns
$(\boldsymbol{X}, \boldsymbol{x})$, $(\boldsymbol{I}, \boldsymbol{t})$	Matrix–column pairs
$\mathcal{G}, \mathcal{U}, \mathcal{P}, \mathcal{M}, \mathcal{N}, \ldots$	Groups
$\mathcal{A}, \mathcal{E}, \mathcal{O}, \mathcal{T}$	Particular groups
h, t, x	Group elements

1.2. Aim of the paper

Group–subgroup relations between space groups are a subject of general interest in crystallography. Moreover, they are essential when elucidating the common aspects of different crystal structures in crystal chemistry, when considering continuous phase transitions, when comparing spectra of similar substances *etc.*

The investigation of group–subgroup relations between space groups $\mathcal{G}$ and $\mathcal{U}$, $\mathcal{G} > \mathcal{U}$,[1] was started by Hermann (1929). In his theorem, see lemma 1, he proved that for each pair $\mathcal{G} > \mathcal{U}$ there exists an intermediate group $\mathcal{M}$, $\mathcal{G} \ge \mathcal{M} \ge \mathcal{U}$, later called the *group of Hermann*, which plays a special role in such relations. Its importance has been emphasized by Billiet (1981*a*,*b*). In particular, Billiet pointed out that the subgroups $\mathcal{U}_r < \mathcal{G}$, which can be transformed one into the other by translations (called $\mathcal{T}$-equivalent subgroups), are listed incompletely in the available tables of subgroups $\mathcal{U}$. Such subgroups play a major role in this paper.

Koch (1984) analysed in detail the influence of the Euclidean and affine normalizers of $\mathcal{G}$ and $\mathcal{U}$ on the subgroups $\mathcal{U}_i$ of a space group $\mathcal{G}$. She obtained important results and conjectures on the relations between space groups from a general point of view and from the consideration of many examples. The supergroups $\mathcal{G}$ of a space group $\mathcal{U}$ were treated less completely but interesting laws and rules were also reported for them.

In this paper, the points of view of Billiet (1981*a*,*b*) and Koch (1984) are combined by extending their considerations to the Euclidean normalizer $\mathcal{N}_{\mathcal{E}}(\mathcal{M})$ of Hermann's group $\mathcal{M}$. It turns out that the translation part $\mathcal{T}(\mathcal{N}_{\mathcal{E}}(\mathcal{M}))$ of $\mathcal{N}_{\mathcal{E}}(\mathcal{M})$ determines the $\mathcal{T}$-equivalent subgroups $\mathcal{U}_i$ of a given space group $\mathcal{G}$ as well as the $\mathcal{T}$-equivalent supergroups $\mathcal{G}_k$ of a given space group $\mathcal{U}$. The consequent application of $\mathcal{M}$ and $\mathcal{T}(\mathcal{N}(\mathcal{M}))$ gives a deeper insight into the symmetry relations between space groups. It also makes such relations comprehensible and more transparent and gives an overview of the $\mathcal{T}$-equivalent sub- and supergroups in a group–subgroup relation.

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[1] In this paper, the symbols $<$ and $>$ are used for proper sub- and supergroups; the symbols $\le$ and $\ge$ include $\mathcal{G} = \mathcal{U}$.

Such an investigation does not seem to have been made before. In fact, Koch (1984) has mentioned $\mathcal{N}_{\mathcal{E}}(\mathcal{M})$ in a particular example but our aim is to explore the general properties of that group and its influence on the group–subgroup relations between space groups.

1.3. Nomenclature and definitions

In this paper the following notions are used:

Special groups referred to in this paper are the *affine group* $\mathcal{A}$ of all non-singular affine mappings, the *Euclidean group* $\mathcal{E} < \mathcal{A}$ of all isometries (motions) and the translation group $\mathcal{T} < \mathcal{E}$ of all translations in Euclidean space; in vector space, the group $\mathcal{O}$ of all orthogonal mappings.

The elements of a space group $\mathcal{X}$ are its symmetry operations which are isometries leaving an existing or a possible crystal structure fixed, see *International Tables for Crystallography* (1983), Vol. A (abbreviated as *IT*A), Part 8. Every isometry consists of two parts, called the *linear part* and the *translation part*. Referred to a coordinate system, the linear part of a symmetry operation of $\mathcal{X}$ is described by a matrix $\boldsymbol{X}$, the translation part by a column $\boldsymbol{x}$. Such a description is used in equations (2) and (3).

A subgroup $\mathcal{U} < \mathcal{G}$ is called a *maximal subgroup* of $\mathcal{G}$ if there does not exist a group $\mathcal{X}$ for which $\mathcal{U} < \mathcal{X} < \mathcal{G}$ holds. On the other hand, under the same condition, a supergroup $\mathcal{G} > \mathcal{U}$ of $\mathcal{U}$ is called a *minimal supergroup* of $\mathcal{U}$.

In a group–subgroup or group–supergroup relation between the space groups $\mathcal{G}$ and $\mathcal{U}$, there may be many ways $\mathcal{G} > \mathcal{X} > \mathcal{Y} > \ldots > \mathcal{U}$ from $\mathcal{G}$ to $\mathcal{U}$. Any such way is called a group–subgroup (group–supergroup) *chain* or, for short, *chain*. Only chains of finite index $i = |\mathcal{G} : \mathcal{U}|$ of $\mathcal{U}$ in $\mathcal{G}$ are considered.

Each space group $\mathcal{X}$ has the normal subgroup $\mathcal{T}(\mathcal{X}) < \mathcal{T}$ of all its translations. The coset decomposition $\mathcal{X} : \mathcal{T}(\mathcal{X})$ of a space group $\mathcal{X}$ relative to $\mathcal{T}(\mathcal{X})$ is essential for the discussion of group–subgroup relations between space groups. Because $\mathcal{T}(\mathcal{X})$ is a normal subgroup of $\mathcal{X}$, the cosets of this decomposition form a group, called the *factor group* $\mathcal{X}/\mathcal{T}(\mathcal{X})$. The elements of the same coset have the same linear part and the elements of different cosets have different linear parts such that each coset can be characterized by 'its' linear part. These linear parts form themselves a finite group which is called the *point group* $\mathcal{P}_{\mathcal{X}} < \mathcal{O}$ of the space group $\mathcal{X}$ in crystallography and which is isomorphic to the factor group $\mathcal{X}/\mathcal{T}(\mathcal{X})$. Its order is the number $|\mathcal{X} : \mathcal{T}(\mathcal{X})|$ of cosets. Whereas $\mathcal{X}$ describes the structural symmetry of the crystal, $\mathcal{P}_{\mathcal{X}}$ describes the symmetry of the macroscopic crystal, *i.e.* the symmetry of its ideal shape and of its macroscopic physical properties.

In a relation $\mathcal{U} < \mathcal{G}$ (space group $\mathcal{G}$–subgroup $\mathcal{U}$) or $\mathcal{G} > \mathcal{U}$ (space group $\mathcal{U}$–supergroup $\mathcal{G}$), the corresponding translation groups are $\mathcal{T}(\mathcal{U}) \leq \mathcal{T}(\mathcal{G}) < \mathcal{T}$.

A *general subgroup* $\mathcal{U} < \mathcal{G}$ has less translations than $\mathcal{G}$, $\mathcal{T}(\mathcal{U}) < \mathcal{T}(\mathcal{G})$, as well as less cosets in the decomposition $\mathcal{U} : \mathcal{T}(\mathcal{U})$ than in $\mathcal{G} : \mathcal{T}(\mathcal{G})$, *i.e.* less linear parts in $\mathcal{U}$ than in $\mathcal{G}$. In crystallographic terms, $\mathcal{P}_{\mathcal{U}} < \mathcal{P}_{\mathcal{G}}$. However, there are two important special cases:

A subgroup $\mathcal{U} < \mathcal{G}$ of a space group $\mathcal{G}$ is called *translationengleich*[2] or a *t*-subgroup if $\mathcal{T}(\mathcal{G}) = \mathcal{T}(\mathcal{U})$. Then there are more cosets in $\mathcal{G} : \mathcal{T}(\mathcal{G})$ than in $\mathcal{U} : \mathcal{T}(\mathcal{U})$, *i.e.* more linear parts in $\mathcal{G}$ than in $\mathcal{U}$. In crystallographic terms, $\mathcal{P}_{\mathcal{U}} < \mathcal{P}_{\mathcal{G}}$ is a proper subgroup of $\mathcal{P}_{\mathcal{G}}$.

A subgroup $\mathcal{U} < \mathcal{G}$ is called *klassengleich*[2] or a *k*-subgroup if each coset of $\mathcal{G} : \mathcal{T}(\mathcal{G})$ is also represented in $\mathcal{U} : \mathcal{T}(\mathcal{U})$, *i.e.* $\mathcal{G}$ and $\mathcal{U}$ have the same linear parts, or $\mathcal{P}_{\mathcal{G}} = \mathcal{P}_{\mathcal{U}}$. Then $\mathcal{T}(\mathcal{U}) < \mathcal{T}(\mathcal{G})$ is a proper subgroup of $\mathcal{T}(\mathcal{G})$.

The analogous nomenclature *general* supergroup, *t*-supergroup and *k*-supergroup is used for supergroups; the corresponding chains are *general* chains, *t*-chains and *k*-chains.

For the considerations in the next sections, the concept of the normalizer $\mathcal{N}_{\mathcal{H}}(\mathcal{F})$ of a group $\mathcal{F}$ in a group $\mathcal{H}$ is needed in addition.

Definition 1. Let $\mathcal{F} < \mathcal{H}$ be a subgroup of $\mathcal{H}$. The set of all elements $\mathsf{h} \in \mathcal{H}$ that map the group $\mathcal{F}$ onto itself by conjugation, $\mathsf{h}^{-1}\mathcal{F}\,\mathsf{h} = \mathcal{F}$, forms a group $\mathcal{N}_{\mathcal{H}}(\mathcal{F})$, $\mathcal{F} \leq \mathcal{N}_{\mathcal{H}}(\mathcal{F}) \leq \mathcal{H}$, which is called the *normalizer* of $\mathcal{F}$ in $\mathcal{H}$.

In particular, the normalizer of a group $\mathcal{F}$ in the group $\mathcal{E}$ of all isometries is called the *Euclidean normalizer* $\mathcal{N}_{\mathcal{E}}(\mathcal{F})$, that in the group $\mathcal{A}$ of all affine mappings is the *affine normalizer* $\mathcal{N}_{\mathcal{A}}(\mathcal{F})$.

Let $\mathcal{F} < \mathcal{H}$ be a subgroup of $\mathcal{H}$ and $\mathsf{h} \in \mathcal{H}$. Then, $\mathcal{F}' = \mathsf{h}^{-1}\mathcal{F}\mathsf{h} < \mathcal{H}$ is a subgroup of $\mathcal{H}$, which is isomorphic to $\mathcal{F}$. The groups $\mathcal{F}$ and $\mathcal{F}'$ are said to be *conjugate under* $\mathcal{H}$ or $\mathcal{H}$ *conjugate*. Frequently, the group $\mathcal{F}$ will be transformed by an element $\mathsf{x} \in \mathcal{X}$, where $\mathcal{F}$ is not a subgroup of $\mathcal{X}$. Then also the group $\mathsf{x}^{-1}\mathcal{F}\mathsf{x} = \mathcal{F}'$ is not a subgroup of $\mathcal{X}$ but the groups $\mathcal{F}$ and $\mathcal{F}'$ are isomorphic and are called *equivalent under* $\mathcal{X}$ or $\mathcal{X}$*-equivalent*. In particular, groups are called $\mathcal{T}$*-equivalent* if they are equivalent under a translation $\mathsf{t} \in \mathcal{T}$.

The Hermann–Mauguin symbols for the space groups are modified in this paper in comparison with their conventional form in *IT*A. In order to indicate the lattice relations of correlated space groups in a group–subgroup chain, the conventional Hermann–Mauguin symbols have been extended. The coefficients of the basis vectors are put into parentheses (...) and are inserted between the lattice part *P*, *F*, *I etc.* and the rotational part of the Hermann–Mauguin symbol. The following convention is used: the basis vectors of one of the correlated space groups are chosen as the basis to which the lattices of the other space groups are referred. For example, $P(111)m\bar{3}m$ in Fig. 2 means that the basis vectors of the lattice of this space group are 1**a**, 1**b** and 1**c**. The expression $C(11\tfrac{1}{2})4/mmm$ then means that the basis of this space group is $\mathbf{a}' = \mathbf{a}$, $\mathbf{b}' = \mathbf{b}$ and $\mathbf{c}' = \tfrac{1}{2}\mathbf{c}$ with additional translations $\mathsf{t}(\tfrac{1}{2}\tfrac{1}{2}0)$, $\mathsf{t}(00\tfrac{1}{2})$ and $\mathsf{t}(\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2})$ relative to $P(111)m\bar{3}m$; $F(222)4/mmc$ means $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{b}' = 2\mathbf{b}$ and $\mathbf{c}' = 2\mathbf{c}$ with centring translations $\mathsf{t}(110)$, $\mathsf{t}(101)$ and $\mathsf{t}(011)$. Note that the last two symbols are unconventional; their conventional symbols are $P(1'1'\tfrac{1}{2})4/mmm$ and

[2] There do not seem to exist adequate English expressions for the German terms *translationengleich* and *klassengleich*. They were introduced by Hermann (1929) with *zellengleich* instead of *translationengleich*. However, the term *zellengleich* was ambiguous because it could refer to the conventional unit cells and not to the groups $\mathcal{T}(\mathcal{G})$ and $\mathcal{T}(\mathcal{U})$.

$I(2'2'2)4/mcm$ with $1'1'$ meaning $\mathbf{a}' = \frac{1}{2}(\mathbf{a} - \mathbf{b})$, $\mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$ and $2'2'$ meaning $\mathbf{a}' = \mathbf{a} - \mathbf{b}$, $\mathbf{b}' = \mathbf{a} + \mathbf{b}$. In addition, the lattice constants of the tetragonal groups may deviate from the cubic ones within the usual limits because $\mathbf{c}' = \mathbf{a}'$ is no longer strictly necessary in practice for the tetragonal symmetry.

2. Laws for sub- and supergroups

In this section, the laws will be derived and discussed which relate to the group $\mathcal{M}$ in a space-group relation $\mathcal{G} > \mathcal{U}$ and to the translation part $\mathcal{T}(\mathcal{N}_{\mathcal{E}}(\mathcal{M}))$ of its Euclidean normalizer. In any case, $\mathcal{T}(\mathcal{N}_{\mathcal{E}}(\mathcal{M})) = \mathcal{T}(\mathcal{N}_{\mathcal{A}}(\mathcal{M}))$ holds because any translation is an isometry. The laws valid for subgroups and supergroups are dealt with in §2.1. Lemmata for subgroups and for supergroups are treated separately in the next sections. These lemmata are similar but their proofs differ in one important step.

2.1. General laws

The theorem of Hermann and its group $\mathcal{M}$ are important tools for the investigation of relations between space groups (Billiet, 1981*a*,*b*). They are central in this paper.

Lemma 1. *Theorem of Hermann*. For each pair of space groups $\mathcal{U} < \mathcal{G}$, a uniquely defined space group $\mathcal{M}$ exists such that

$$\mathcal{U} \leq \mathcal{M} \leq \mathcal{G} \text{ holds, where} \tag{1}$$

(i) $\mathcal{M}$ is a *t*-subgroup of $\mathcal{G}$, *i.e.* $\mathcal{T}(\mathcal{M}) = \mathcal{T}(\mathcal{G})$, and $\mathcal{M}$ has the same or less linear parts than $\mathcal{G}$, $\mathcal{P}_{\mathcal{M}} \leq \mathcal{P}_{\mathcal{G}}$;

(ii) $\mathcal{U}$ is a *k*-subgroup of $\mathcal{M}$, *i.e.* $\mathcal{G}$ and $\mathcal{M}$ have the same linear parts, $\mathcal{P}_{\mathcal{U}} = \mathcal{P}_{\mathcal{M}}$ and $\mathcal{T}(\mathcal{U}) \leq \mathcal{T}(\mathcal{M})$.

For the proof, see Hermann (1929).

Remark. Lemma 1 has been formulated using subgroups. When looking for supergroups, the formulation: '..., where $\mathcal{G}$ is a *t*-supergroup of $\mathcal{M}$, and $\mathcal{M}$ is a *k*-supergroup of $\mathcal{U}$' is more appropriate.

Corollary. For a *maximal* subgroup $\mathcal{U} < \mathcal{G}$, either $\mathcal{U} = \mathcal{M}$ holds and $\mathcal{U}$ is a *t*-subgroup of $\mathcal{G}$ or $\mathcal{G} = \mathcal{M}$ holds and $\mathcal{U}$ is a *k*-subgroup of $\mathcal{G}$. Therefore, a maximal subgroup $\mathcal{U} < \mathcal{G}$ is either a *t*-subgroup or a *k*-subgroup of $\mathcal{G}$.

For a *minimal* supergroup $\mathcal{G} > \mathcal{U}$, either $\mathcal{M} = \mathcal{U}$ holds and $\mathcal{G}$ is a *t*-supergroup of $\mathcal{U}$ or $\mathcal{M} = \mathcal{G}$ holds and $\mathcal{G}$ is a *k*-supergroup of $\mathcal{U}$. Therefore, a minimal supergroup $\mathcal{G} > \mathcal{U}$ is either a *t*-supergroup or a *k*-supergroup of $\mathcal{U}$.

From the characterization of the group $\mathcal{M}$ in the theorem of Hermann, lemma 2 follows:

Lemma 2. The group $\mathcal{M}$ of Hermann's theorem in the chain $\mathcal{U} \leq \mathcal{M} \leq \mathcal{G}$ is completely determined already by the group $\mathcal{U}$ and the translations of $\mathcal{G}$ as well as by the group $\mathcal{G}$ and the point group $\mathcal{P}_{\mathcal{U}}$.

Indeed, in the first case, the group $\mathcal{M}$ is the group generated by the group $\mathcal{U}$ and the translation group $\mathcal{T}(\mathcal{G})$, *i.e.* it is the smallest group that contains the elements of $\mathcal{U}$ and of $\mathcal{T}(\mathcal{G})$. In the second case, one takes from the cosets of the decomposition $\mathcal{G} : \mathcal{T}(\mathcal{G})$ all those whose linear parts occur in the elements of $\mathcal{U}$, *i.e.* which belong to the point group $\mathcal{P}_{\mathcal{U}}$.

Each subgroup $\mathcal{U}$ of a fixed group $\mathcal{G}$ determines 'its' group $\mathcal{M}$. To a set of conjugate subgroups $\mathcal{U}$ there may belong different groups $\mathcal{M}$. For example, if $\mathcal{U}$ is a tetragonal subgroup of a cubic space group $\mathcal{G}$, then there are three conjugate groups $\mathcal{U}$ with the tetragonal axes along [100], [010] and [001]. Thus, there are three conjugate groups $\mathcal{M} \leq \mathcal{G}$, each with the tetragonal axis of 'its' group $\mathcal{U}$.

Definition 2. The group $\mathcal{M}$ is called the *group of Hermann*.

For a given space group $\mathcal{X}$, the normalizers $\mathcal{N}_{\mathcal{E}}(\mathcal{X})$ and $\mathcal{N}_{\mathcal{A}}(\mathcal{X})$ may have more translations than the group $\mathcal{X}$ has. Again, $\mathcal{T}(\mathcal{N}_{\mathcal{E}}(\mathcal{X})) = \mathcal{T}(\mathcal{N}_{\mathcal{A}}(\mathcal{X}))$ holds because any translation is an isometry. Using the matrix-column description of the isometries, the additional translations t of these normalizers $\mathcal{N}(\mathcal{X})$ of $\mathcal{X}$ can be calculated from the equation

$$(\boldsymbol{I},\ \boldsymbol{t})^{-1}\{(\boldsymbol{X}_i,\ \boldsymbol{x}_i + \boldsymbol{l}_j)\}(\boldsymbol{I},\ \boldsymbol{t}) = \{(\boldsymbol{X}_p,\ \boldsymbol{x}_p + \boldsymbol{l}_q)\}, \tag{2}$$

where $(\boldsymbol{I},\ \boldsymbol{t})$ is the matrix–column pair of a translation of $\mathcal{T}(\mathcal{N}(\mathcal{X}))$, $\{(\boldsymbol{X}_i,\ \boldsymbol{x}_i)\}$ and $\{(\boldsymbol{X}_p,\ \boldsymbol{x}_p)\}$ are sets of matrix–column pairs representing the space group $\mathcal{X}$, listed *e.g.* as the general position of $\mathcal{X}$, and $\boldsymbol{l}_j$ and $\boldsymbol{l}_q$ are the columns of coefficients of translations of $\mathcal{X}$. The indices i and p are running over all representatives and the indices j and q are running over all translations of $\mathcal{T}(\mathcal{X})$.

From equation (2) follow the equations

$$(\boldsymbol{X}_i - \boldsymbol{I})\,\boldsymbol{t}_{\mathcal{N}} \in \boldsymbol{T}(\mathcal{X}), \tag{3}$$

where $\boldsymbol{X}_i$ are the matrices of a set of generators of $\mathcal{P}_{\mathcal{X}}$, $\boldsymbol{I}$ is the unit matrix, $\boldsymbol{t}_{\mathcal{N}}$ is the column of a translation of $\mathcal{T}(\mathcal{N}(\mathcal{X}))$ and $\boldsymbol{T}(\mathcal{X})$ is the set of columns of all translations of $\mathcal{X}$, see *e.g.* Boisen *et al.* (1990).

Let $\mathcal{U} < \mathcal{G}$. When calculating $\mathcal{T}(\mathcal{N}(\mathcal{U}))$ using equations (3), attention has to be paid to the following fact. Suppose the subgroup $\mathcal{U}$ has more free lattice parameters than the space group $\mathcal{G}$ has, *i.e.* $\mathcal{G}$ and $\mathcal{U}$ do not belong to the same crystal family. Then the lattice parameters of $\mathcal{U}$ cannot be general but have to obey special relations. For example, if $\mathcal{G}$ is cubic and $\mathcal{U}$ is tetragonal as in example 3.2.1, the relation c/a of the lattice parameters of $\mathcal{U}$ is not arbitrary as it is normally for a tetragonal space group but is fixed, *e.g.* 1. Thus, the actual symmetry of the translation lattice of $\mathcal{U}$ may be cubic with a threefold rotation as an additional generator. This generator is not imposed by the tetragonal symmetry of $\mathcal{U}$. Generators of such additional (from the view point of $\mathcal{U}$ accidental) symmetries do not enter equations (3). The generators in (3) refer to the point group $\mathcal{P}_{\mathcal{X}}$ of the space group $\mathcal{X}$, not to the point group of its lattice.

Euclidean normalizers of space groups with 'accidental' lattice symmetries are listed by Koch & Müller (1990) and in the forthcoming edition of *International Tables for Crystallography* (2001), Part 15.

It is obvious from (3) that $\mathcal{T}(\mathcal{N}(\mathcal{X}))$ cannot decrease with increasing $\mathcal{T}(\mathcal{X})$ because more elements in $\mathcal{T}(\mathcal{X})$ provide more possibilities for translations $\mathsf{t}_{\mathcal{N}}$ to fulfil equations (3). On the other hand, $\mathcal{T}(\mathcal{N}(\mathcal{X}))$ cannot increase with an increase in the number of independent generators of $\mathcal{P}_{\mathcal{X}}$ because each equation of the system of equations (3) restricts the translations of $\mathcal{T}(\mathcal{N}(\mathcal{X}))$, and to have more independent generators means to have more restrictive relations to be fulfilled for the translations $\mathsf{t} \in \mathcal{T}(\mathcal{N}(\mathcal{X}))$.

Consider the chain $\mathcal{G} \geq \mathcal{M} \geq \mathcal{U}$. According to lemma 1, $\mathcal{M}$ is a *t*-subgroup of $\mathcal{G}$. Therefore, $\mathcal{T}(\mathcal{M}) = \mathcal{T}(\mathcal{G})$ and $\mathcal{P}_{\mathcal{M}} \leq \mathcal{P}_{\mathcal{G}}$ and thus $\mathcal{T}(\mathcal{N}(\mathcal{M})) \geq \mathcal{T}(\mathcal{N}(\mathcal{G}))$. On the other hand, $\mathcal{U}$ is a *k*-subgroup of $\mathcal{M}$. Therefore, $\mathcal{P}_{\mathcal{M}} = \mathcal{P}_{\mathcal{U}}$ and $\mathcal{T}(\mathcal{U}) \leq \mathcal{T}(\mathcal{M})$ and thus $\mathcal{T}(\mathcal{N}(\mathcal{M})) \geq \mathcal{T}(\mathcal{N}(\mathcal{U}))$. From these formulae, one obtains the following lemma:

Lemma 3. For the chain of space groups $\mathcal{G} \geq \mathcal{M} \geq \mathcal{U}$, where $\mathcal{M}$ is the group of Hermann in lemma 1, the inequality $\mathcal{T}(\mathcal{N}(\mathcal{U})) \leq \mathcal{T}(\mathcal{N}(\mathcal{M})) \geq \mathcal{T}(\mathcal{N}(\mathcal{G}))$ holds.

From lemma 3, the lemmata 4 and 5 follow immediately by specialization.

Lemma 4. If $\mathcal{U}$ is a *t*-subgroup of $\mathcal{G}$ (or $\mathcal{G}$ a *t*-supergroup of $\mathcal{U}$), then $\mathcal{U} = \mathcal{M}$ and $\mathcal{T}(\mathcal{N}(\mathcal{U})) \geq \mathcal{T}(\mathcal{N}(\mathcal{G}))$.

Do there exist *t*-subgroups $\mathcal{U}$ of $\mathcal{G}$ for which $\mathcal{N}(\mathcal{G}) > \mathcal{N}(\mathcal{U})$ holds? Koch (1984) states: 'Group–subgroup relations of type (2) [*i.e.* $\mathcal{N}(\mathcal{G}) > \mathcal{N}(\mathcal{U})$] seem to be confined to class-equivalent subgroups [*i.e.* *k*-subgroups], if only maximal subgroups are considered'. It is clear that because of lemma 4 such relations will be scarce; they require $\mathcal{T}(\mathcal{N}(\mathcal{U})) = \mathcal{T}(\mathcal{N}(\mathcal{G}))$ and $\mathcal{P}_{\mathcal{N}(\mathcal{G})} > \mathcal{P}_{\mathcal{N}(\mathcal{U})}$. However, the example $F(111)m\bar{3}m$–$F(111)4/mmm \sim I(1'1'1)4/mmm$ of index 3 with the same lattice parameters for $Fm\bar{3}m$ and $F4/mmm$ shows that such a relation is possible. The normalizers are $P(\frac{1}{2}\frac{1}{2}\frac{1}{2})m\bar{3}m$ with $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ and $P(\frac{1}{2}\frac{1}{2}\frac{1}{2})4/mmm$ with $\mathbf{a}' = \mathbf{c}' = \frac{1}{2}\mathbf{a}$, so that $\mathcal{T}(\mathcal{N}(\mathcal{U})) = \mathcal{T}(\mathcal{N}(\mathcal{G}))$ is fulfilled, and $\mathcal{P}_{\mathcal{N}(\mathcal{G})} > \mathcal{P}_{\mathcal{N}(\mathcal{U})}$ of index $|\mathcal{N}(\mathcal{G}) : \mathcal{N}(\mathcal{U})| = 3$. Another example is the similar pair $Pm\bar{3}m$–$R\bar{3}m$ of index 4.

Lemma 5. If $\mathcal{U}$ is a *k*-subgroup of $\mathcal{G}$ (or $\mathcal{G}$ a *k*-supergroup of $\mathcal{U}$), then $\mathcal{G} = \mathcal{M}$ and $\mathcal{T}(\mathcal{N}(\mathcal{U})) \leq \mathcal{T}(\mathcal{N}(\mathcal{G}))$.

This lemma has been formulated and proved in another way by Koch (1984).

Lemma 3 can be extended to any intermediate group $\mathcal{X}$ of any group–subgroup or group–supergroup chain between $\mathcal{U}$ and $\mathcal{G}$, independent of the number of intermediate members of the chain and of $\mathcal{M}$ being a member of the selected chain or not. This is expressed by the following lemma:

Lemma 6. Let $\mathcal{U} \leq \ldots \leq \mathcal{X} \leq \ldots \leq \mathcal{G}$ be an arbitrary chain between $\mathcal{G}$ and $\mathcal{U}$, and $\mathcal{X}$ be an arbitrary intermediate group including $\mathcal{X} = \mathcal{U}$ or $\mathcal{X} = \mathcal{G}$. Then $\mathcal{T}(\mathcal{N}(\mathcal{M})) \geq \mathcal{T}(\mathcal{N}(\mathcal{X}))$ holds.

The proof follows from equations (3) and the relations $\mathcal{T}(\mathcal{X}) \leq \mathcal{T}(\mathcal{G}) = \mathcal{T}(\mathcal{M})$ and $\mathcal{P}_{\mathcal{X}} \geq \mathcal{P}_{\mathcal{U}} = \mathcal{P}_{\mathcal{M}}$.

Remark. Because of $\mathcal{T}(\mathcal{N}(\mathcal{X})) \geq \mathcal{T}(\mathcal{X})$, one can decompose $\mathcal{T}(\mathcal{N}(\mathcal{X}))$ into cosets relative to $\mathcal{T}(\mathcal{X})$. The representatives of these cosets are known in X-ray crystallography as the *permissible origins* (Giacovazzo, 1992). According to lemma 6, the group $\mathcal{M}$ is the group with the highest number of permissible origins among all the groups of any chain between $\mathcal{G}$ and $\mathcal{U}$.

Remark. Both the groups $\mathcal{T}(\mathcal{N}(\mathcal{G}))$ and $\mathcal{T}(\mathcal{N}(\mathcal{U}))$ are subgroups of $\mathcal{T}(\mathcal{N}(\mathcal{M}))$ but they need not be in a group–subgroup relation themselves. The possible relations between $\mathcal{T}(\mathcal{N}(\mathcal{G}))$ and $\mathcal{T}(\mathcal{N}(\mathcal{U}))$ are discussed in §3.1.

All these relations as well as those for subgroups and supergroups in the next two sections are valid independently of the dimension of the Euclidean space.

2.2. A law for subgroups

Additional conclusions from lemma 3 refer to those subgroups $\mathcal{U}_i < \mathcal{G}$ which are $\mathcal{T}$-equivalent to a subgroup $\mathcal{U} < \mathcal{G}$. Their number is stated for many examples in Billiet (1981*a*,*b*) and Koch (1984) without an indication of how it is obtained. It results directly from the following lemma.

Lemma 7. *Subgroup theorem*. The number of subgroups $\mathcal{U}_i < \mathcal{G}$ which are $\mathcal{T}$-equivalent to a subgroup $\mathcal{U} < \mathcal{G}$ is equal to the index $|\mathcal{T}(\mathcal{N}(\mathcal{M})) : \mathcal{T}(\mathcal{N}(\mathcal{U}))|$ of $\mathcal{T}(\mathcal{N}(\mathcal{U}))$ in $\mathcal{T}(\mathcal{N}(\mathcal{M}))$.

Proof. The proof is performed by coset decomposition of $\mathcal{T}(\mathcal{N}(\mathcal{M}))$ relative to $\mathcal{T}(\mathcal{N}(\mathcal{U}))$ and the choice of appropriate representatives of the cosets. The representatives themselves are then the translations by which the subgroups $\mathcal{U}_i$ are $\mathcal{T}$-equivalent to the subgroup $\mathcal{U} < \mathcal{G}$; the number of representatives is the number of the $\mathcal{T}$-equivalent subgroups $\mathcal{U}_i$.

Each of these $\mathcal{T}$-equivalent groups $\mathcal{U}_i$ is a subgroup of $\mathcal{G}$. Although $\mathcal{G}$ may be shifted to another group $\mathcal{G}'$ when shifting $\mathcal{U}$ to $\mathcal{U}'$ by a translation $\mathsf{t} \in \mathcal{T}(\mathcal{N}(\mathcal{M}))$, $\mathcal{M}$ will be mapped onto itself. Thus, $\mathcal{U}' \leq \mathcal{M} \leq \mathcal{G}$ holds.

There are no $\mathcal{T}$-equivalent subgroups $\mathcal{U}_i < \mathcal{G}$ other than those of lemma 7. This second part of lemma 7 will be proven using lemma 2. Suppose a subgroup $\mathcal{U}' < \mathcal{G}$ exists which is obtained from the subgroup $\mathcal{U} < \mathcal{G}$ by a translation $\mathsf{t}' \notin \mathcal{T}(\mathcal{N}(\mathcal{M}))$, where $\mathcal{U}' = \mathsf{t}'^{-1}\mathcal{U}\mathsf{t}'$, $\mathcal{M}' = \mathsf{t}'^{-1}\mathcal{M}\mathsf{t}'$ and $\mathcal{G}' = \mathsf{t}'^{-1}\mathcal{G}\mathsf{t}'$. The group $\mathcal{P}_{\mathcal{U}}$ is invariant under the transformation with a translation. According to lemma 2, Hermann's group of the pair $\mathcal{U}' < \mathcal{G}$ is the group $\mathcal{M}$, not $\mathcal{M}'$. Therefore, in addition to $\mathcal{U}' \leq \mathcal{M}'$, also $\mathcal{U}' \leq \mathcal{M}$ would be fulfilled. Then, $\mathcal{U}'$ would also be a subgroup of the intersection $\mathcal{V}$ of the groups $\mathcal{M}$ and $\mathcal{M}'$. However, $\mathcal{M} \neq \mathcal{M}'$, otherwise $\mathsf{t}' \in \mathcal{T}(\mathcal{N}(\mathcal{M}))$. As cosets are either equal or have no element in common, there must be cosets of $\mathcal{M}$ which are not cosets of $\mathcal{M}'$ and thus $\mathcal{P}_{\mathcal{V}} < \mathcal{P}_{\mathcal{M}} = \mathcal{P}_{\mathcal{U}'}$. This contradicts the assumption that $\mathcal{U}' \leq \mathcal{V}$. But if $\mathcal{U}' \not\leq \mathcal{V}$, then because of $\mathcal{U}' \leq \mathcal{M}'$ also $\mathcal{U}' \not\leq \mathcal{M}$ and thus $\mathcal{U}' \not\leq \mathcal{G}$. ■

$\mathcal{T}$-equivalent subgroups $\mathcal{U}_i < \mathcal{G}$ may also be $\mathcal{T}(\mathcal{N}(\mathcal{G}))$-equivalent. If $\mathcal{T}(\mathcal{N}(\mathcal{G})) \geq \mathcal{T}(\mathcal{N}(\mathcal{U}))$, the number u of these groups may be calculated by the formula $u = |\mathcal{T}(\mathcal{N}(\mathcal{G})) : \mathcal{T}(\mathcal{N}(\mathcal{U}))|$ directly. Otherwise one has to decompose $\mathcal{T}(\mathcal{N}(\mathcal{G}))$ relative to $\mathcal{T}(\mathcal{D})$, where $\mathcal{D}$ is the intersection $\mathcal{N}(\mathcal{G}) \cap \mathcal{N}(\mathcal{U})$ of the groups $\mathcal{N}(\mathcal{G})$ and $\mathcal{N}(\mathcal{U})$, see Koch (1984). The representatives of this decomposition yield the $\mathcal{T}(\mathcal{N}(\mathcal{G}))$-equivalent subgroups $\mathcal{U}_i$, their number is given by $u = |\mathcal{T}(\mathcal{N}(\mathcal{G})) : \mathcal{T}(\mathcal{D})|$. The classification of the group–subgroup pairs according to the relations between $\mathcal{T}(\mathcal{N}(\mathcal{G}))$ and $\mathcal{T}(\mathcal{N}(\mathcal{U}))$ is considered in §3.1.

In Koch's (1984) paper, the $\mathcal{N}(\mathcal{G})$-equivalent subgroups $\mathcal{U}$ play a distinguished role. However, general criteria on the implication of such a relationship for crystal structures do not seem to be known. Only the $\mathcal{G}$ conjugacy is primarily relevant for the crystal structures with subgroups $\mathcal{U} < \mathcal{G}$, as has been emphasized by Billiet (1981*a*). Other relations, *e.g.* conjugacy or equivalence under normalizers, are relevant for the symmetries but not directly for the crystal structures. This has been demonstrated at derived structures of the perovskite type by Billiet (1981*a*). One probably has to analyse and compare the pertinent crystal structures in order to judge the consequences of $\mathcal{N}(\mathcal{G})$ or $\mathcal{T}(\mathcal{N}(\mathcal{G}))$ conjugacy and similar relations on structural relationships, see example 3.2.3.

2.3. A law for supergroups

It is trivial that in a phase transition both directions may occur, *viz* to lower and to higher symmetry. Nevertheless, the supergroups $\mathcal{G}_k$ of a space group $\mathcal{U}$ are treated much less frequently in the literature than the subgroups $\mathcal{U}_i$ of a space group $\mathcal{G}$. The main reason is probably the lack of a phenomenon for supergroups of a group $\mathcal{U}$ which compares with the conjugacy of subgroups of a group $\mathcal{G}$ with its formation of twin and antiphase domains. Another reason may be the restriction of the search for subgroups to the elements of the supergroup $\mathcal{G}$ only. The search for supergroups has to take into consideration the Euclidean group $\mathcal{E}$ of all isometries which is a continuous group. Therefore, searching for supergroups is more involved than searching for subgroups and cannot be performed simply by an inversion of the subgroup data. In addition, for every proper subgroup $\mathcal{U}$ the inequality $\mathcal{U} < \mathcal{G} \leq \mathcal{N}(\mathcal{G})$ holds, whereas the relation $\mathcal{G} \leq \mathcal{N}(\mathcal{U})$ holds only if $\mathcal{U}$ is a normal subgroup of $\mathcal{G}, \mathcal{U} \triangleleft \mathcal{G}$.

The search for supergroups should be a necessary companion of the search for subgroups as soon as relationships are considered which are less direct than $\mathcal{G}$ conjugacy. If one does not take into consideration $\mathcal{T}$-equivalent supergroups when dealing with $\mathcal{T}$-equivalent subgroups, distorted views are possible. When looking only for the subgroups of a space group $\mathcal{G}$, one may find differences in $\mathcal{T}$-equivalent subgroups $\mathcal{U}_r$, which can be misleading. It is then necessary to ask also for the $\mathcal{T}$-equivalent supergroups $\mathcal{G}_s$ of these subgroups. Only the simultaneous treatment of subgroups *and* supergroups displays the real relations for such sets of supergroup–subgroup chains. This is shown by the example 3.2.1 which deals with the chains between $P(111)m\bar{3}m$ and $F(222)4/mmc \sim I(2'2'2)4/mcm$.

Additional conclusions from lemma 3 refer to supergroups $\mathcal{G}_k > \mathcal{U}$ which are $\mathcal{T}$-equivalent to a supergroup $\mathcal{G} > \mathcal{U}$. Their number results directly from the following lemma.

Lemma 8. *Supergroup theorem*. The number of supergroups $\mathcal{G}_k > \mathcal{U}$ which are $\mathcal{T}$-equivalent to a supergroup $\mathcal{G} > \mathcal{U}$ is equal to the index $|\mathcal{T}(\mathcal{N}(\mathcal{M})) : \mathcal{T}(\mathcal{N}(\mathcal{G}))|$ of $\mathcal{T}(\mathcal{N}(\mathcal{G}))$ in $\mathcal{T}(\mathcal{N}(\mathcal{M}))$.

Proof. The proof is performed by coset decomposition of $\mathcal{T}(\mathcal{N}(\mathcal{M}))$ relative to $\mathcal{T}(\mathcal{N}(\mathcal{G}))$ and the choice of appropriate representatives of the cosets. The representatives themselves are the translations by which the supergroups $\mathcal{G}_k$ are $\mathcal{T}$-equivalent; their number is the number of $\mathcal{T}$-equivalent supergroups $\mathcal{G}_k$. All groups obtained in this way are really supergroups of $\mathcal{U}$. Although $\mathcal{U}$ may be shifted to another group $\mathcal{U}'$ when shifting $\mathcal{G}$ to $\mathcal{G}'$ by a translation $\mathsf{t} \in \mathcal{T}(\mathcal{N}(\mathcal{M}))$, $\mathcal{M}$ will be mapped onto itself. Thus, $\mathcal{G}' \geq \mathcal{M} \geq \mathcal{U}$ holds.

There are no $\mathcal{T}$-equivalent supergroups $\mathcal{G}' > \mathcal{U}$ other than those of lemma 8. Suppose a supergroup $\mathcal{G}' > \mathcal{U}$ exists which is obtained from the supergroup $\mathcal{G} > \mathcal{U}$ by a translation $\mathsf{t}' \notin \mathcal{T}(\mathcal{N}(\mathcal{M}))$, where $\mathcal{G}' = \mathsf{t}'^{-1}\mathcal{G}\mathsf{t}'$, $\mathcal{M}' = \mathsf{t}'^{-1}\mathcal{M}\mathsf{t}'$ and $\mathcal{U}' = \mathsf{t}'^{-1}\mathcal{U}\mathsf{t}'$. The group $\mathcal{T}(\mathcal{G})$ is invariant under the transformation with a translation. According to lemma 2, Hermann's group of the chain $\mathcal{U} < \mathcal{G}'$ is the group $\mathcal{M}$, *i.e.* the group $\mathcal{U}$ with its cosets expanded by the translations of $\mathcal{G}'$, it is not the group $\mathcal{M}'$. Thus, in addition to $\mathcal{G}' \geq \mathcal{M}'$ also $\mathcal{G}' \geq \mathcal{M}$ would be fulfilled. Then also $\mathcal{G}' \geq \mathcal{W}$ would hold, where $\mathcal{W}$ is the group generated from the groups $\mathcal{M}$ and $\mathcal{M}'$, *i.e.* the smallest group which contains all elements of $\mathcal{M}$ and $\mathcal{M}'$. However, because $\mathcal{M}$ and $\mathcal{M}'$ are different, $\mathcal{W}$ must have cosets of the coset decomposition $\mathcal{W} : \mathcal{T}(\mathcal{W})$ which have more elements than the corresponding cosets of $\mathcal{M}$ have. Therefore, $\mathcal{G}' \geq \mathcal{W}$ cannot be true. From this follows that also $\mathcal{G}' \geq \mathcal{M}$ and $\mathcal{G}' \geq \mathcal{U}$ cannot be fulfilled. ∎

$\mathcal{T}$-equivalent supergroups of $\mathcal{U}$ may also be $\mathcal{T}(\mathcal{N}(\mathcal{U}))$-equivalent. If $\mathcal{T}(\mathcal{N}(\mathcal{U})) \geq \mathcal{T}(\mathcal{N}(\mathcal{G}))$ holds, their number g can be calculated by the formula $g = |\mathcal{T}(\mathcal{N}(\mathcal{U})) : \mathcal{T}(\mathcal{N}(\mathcal{G}))|$ directly. Otherwise, if $\mathcal{T}(\mathcal{N}(\mathcal{U}))$ and $\mathcal{T}(\mathcal{N}(\mathcal{G}))$ are not in a group–supergroup relation, one has to decompose $\mathcal{T}(\mathcal{N}(\mathcal{U}))$ relative to $\mathcal{T}(\mathcal{D})$, where $\mathcal{D}$ is the intersection $\mathcal{N}(\mathcal{G}) \cap \mathcal{N}(\mathcal{U})$ of the groups $\mathcal{N}(\mathcal{G})$ and $\mathcal{N}(\mathcal{U})$, see Koch (1984). The representatives of this decomposition yield the $\mathcal{T}(\mathcal{N}(\mathcal{U}))$-equivalent supergroups $\mathcal{G}$. Their number is given by $g = |\mathcal{T}(\mathcal{N}(\mathcal{U})) : \mathcal{T}(\mathcal{D})|$. The classification of the group–supergroup pairs according to the relations between $\mathcal{T}(\mathcal{N}(\mathcal{U}))$ and $\mathcal{T}(\mathcal{N}(\mathcal{G}))$ will be considered in the next section.

Also for the $\mathcal{T}(\mathcal{N}(\mathcal{U}))$-equivalent supergroups general criteria on the implication of such a relationship for crystal structures do not seem to be known, *cf.* the last paragraph of §2.2.

3. Applications

3.1. Peculiarities of $\mathcal{T}$-equivalent sub- and supergroups

Koch (1984) has distributed the group $\mathcal{G}$–subgroup $\mathcal{U}$ and group $\mathcal{U}$–supergroup $\mathcal{G}$ chains into four cases with respect to the relations between the normalizers $\mathcal{N}(\mathcal{G})$ and $\mathcal{N}(\mathcal{U})$:

1. $\mathcal{N}(\mathcal{G}) = \mathcal{N}(\mathcal{U})$
2. $\mathcal{N}(\mathcal{G}) > \mathcal{N}(\mathcal{U})$
3. $\mathcal{N}(\mathcal{G}) < \mathcal{N}(\mathcal{U})$
4. $\mathcal{N}(\mathcal{G}) \not\leq \mathcal{N}(\mathcal{U})$ and $\mathcal{N}(\mathcal{G}) \not\geq \mathcal{N}(\mathcal{U})$.

These four cases are elucidated by many examples, mostly taken from *t*- and *k*-chains, in particular from those with maximal subgroups and minimal supergroups. Here the considerations are restricted primarily to the relations between $\mathcal{T}(\mathcal{N}(\mathcal{G}))$ and $\mathcal{T}(\mathcal{N}(\mathcal{U}))$ because with respect to $\mathcal{T}$-equivalence there are clear rules for these translation subgroups of the normalizers. They are part of the $\mathcal{N}(\mathcal{G})$–$\mathcal{N}(\mathcal{U})$ relations which, however, may belong to other types, see the following examples. In analogy to Koch (1984), four cases will be distinguished, their relations are listed with examples:

(1) $\mathcal{T}(\mathcal{N}(\mathcal{G})) = \mathcal{T}(\mathcal{N}(\mathcal{U}))$. The *t*-chain $P(111)m\bar{3}m$–$P(111)23$, the *k*-chain $I(111)23$–$P(111)23$, both with the normalizer $I(111)m\bar{3}m$; many other *t*- and *k*-chains; the general chains of the example 3.2.3.

The corresponding normalizers $\mathcal{N}(\mathcal{G})$ and $\mathcal{N}(\mathcal{U})$ may be equal too, as in the specified examples but also all other cases may occur:

(*a*) $\mathcal{N}(\mathcal{G}) > \mathcal{N}(\mathcal{U})$: $I(111)a\bar{3}$–$P(111)a\bar{3}$ with the normalizers $I(111)a\bar{3}d$ and $I(111)a\bar{3}$;

(*b*) $\mathcal{N}(\mathcal{G}) < \mathcal{N}(\mathcal{U})$: $P(111)a\bar{3}$–$P(111)2_13$ with the normalizers $I(111)a\bar{3}$ and $I(111)a\bar{3}d$;

(*c*) $\mathcal{N}(\mathcal{G}) \not\leq \mathcal{N}(\mathcal{U})$ and $\mathcal{N}(\mathcal{G}) \not\geq \mathcal{N}(\mathcal{U})$: see example 3.2.2.

(2) $\mathcal{T}(\mathcal{N}(\mathcal{G})) > \mathcal{T}(\mathcal{N}(\mathcal{U}))$. The *k*-pair $F(111)23$–$P(111)23$ with the normalizers $I(\frac{1}{2}\frac{1}{2}\frac{1}{2})m\bar{3}m$ and $I(111)m\bar{3}m$; many other *k*-chains; the general chains of the example 3.2.1.

For the corresponding normalizers, $\mathcal{N}(\mathcal{G}) > \mathcal{N}(\mathcal{U})$ may hold, as in the first example, otherwise $\mathcal{N}(\mathcal{G}) \not\leq \mathcal{N}(\mathcal{U})$ and $\mathcal{N}(\mathcal{G}) \not\geq \mathcal{N}(\mathcal{U})$, as in the $\mathcal{G}$–$\mathcal{U}$ pair (referred to a hexagonal basis) $R(111)\bar{3}$–$P(111)\bar{3}$ with the normalizers $\mathcal{N}(\mathcal{G}) = R_{\rm rev}(11\frac{1}{2})\bar{3}m$ and $\mathcal{N}(\mathcal{U}) = P(11\frac{1}{2})6/mmm$.

(3) $\mathcal{T}(\mathcal{N}(\mathcal{G})) < \mathcal{T}(\mathcal{N}(\mathcal{U}))$. The *t*-chain $P(111)m\bar{3}$–$P(111)\bar{1}$ with the normalizers $I(111)m\bar{3}m$ and $P(\frac{1}{2}\frac{1}{2}\frac{1}{2})m\bar{3}m$; many other *t*-chains; the general chain $I(111)23$–$P(111)222$ with the normalizers $I(111)m\bar{3}m$ and $P(\frac{1}{2}\frac{1}{2}\frac{1}{2})m\bar{3}m$.

For the corresponding normalizers, $\mathcal{N}(\mathcal{G}) < \mathcal{N}(\mathcal{U})$ may hold, as in the specified examples, otherwise $\mathcal{N}(\mathcal{G}) \not\leq \mathcal{N}(\mathcal{U})$ and $\mathcal{N}(\mathcal{G}) \not\geq \mathcal{N}(\mathcal{U})$, as in the pair $P(111)432$–$P(111)422$, tetragonal axis along *z*, with $\mathcal{N}(\mathcal{G}) = I(111)m\bar{3}m$, $\mathcal{N}(\mathcal{U}) = C(11\frac{1}{2})4/mmm$.

Example 3.2.1 Extended diagram of the pair $P(111)m\bar{3}m - F(222)4/mmc \sim I(2'2'2)4/mcm$

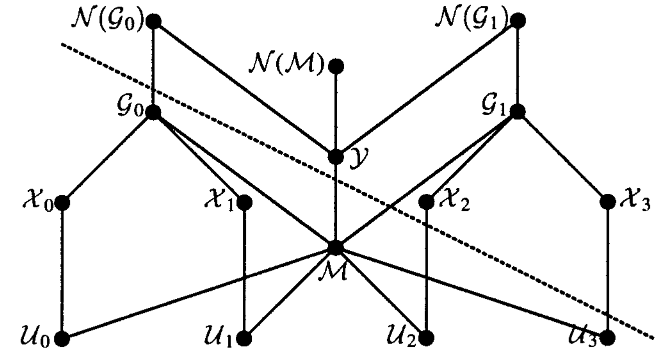

Figure 1

This example has been treated by Billiet (1981*a*) and Koch (1984). The lower part of the diagram to the left of the dotted line is contained in Fig. 2 of Billiet (1981*a*). On the way from $\mathcal{G}_0$ to the subgroups $\mathcal{U}_r$, the groups $\mathcal{X}_0$, $\mathcal{X}_1$ and $\mathcal{M}$ are passed. The upper right part has been added in order to show the positions of the group $\mathcal{G}_1$, both groups $\mathcal{N}(\mathcal{G}_0)$, $\mathcal{N}(\mathcal{G}_1)$, the group $\mathcal{Y} = \mathcal{N}(\mathcal{G}_0) \cap \mathcal{N}(\mathcal{M}) = \mathcal{N}(\mathcal{G}_0) \cap \mathcal{N}(\mathcal{G}_1) = \mathcal{N}(\mathcal{M}) \cap \mathcal{N}(\mathcal{G}_1)$, the groups $\mathcal{X}_2$ and $\mathcal{X}_3$ and the group $\mathcal{N}(\mathcal{M})$. The full view upwards from the subgroups $\mathcal{U}_r$ results from the complete diagram. All normalizers are the Euclidean normalizers; the lattices of the tetragonal groups have cubic symmetry.

The basic space group is $\mathcal{G}_0 = P(111)m\bar{3}m$ with $a = b = c$ and the conventional origin in the point $\langle 000\rangle$. The group $\mathcal{G}_1$ is $\mathcal{T}$-equivalent to $\mathcal{G}_0$ with the conventional origin in $\langle 00\frac{1}{2}\rangle$. The normalizers $\mathcal{N}(\mathcal{G}_s)$ are $\mathcal{N}(\mathcal{G}_0) = I(111)m\bar{3}m$ $\langle 000\rangle$ and $\mathcal{N}(\mathcal{G}_1) = I(111)m\bar{3}m$ $\langle 00\frac{1}{2}\rangle$. The $\mathcal{T}$-equivalent groups $\mathcal{U}_r$ with the tetragonal axis along *z* are $\mathcal{U}_0 = F(222)4/mmc$ $\langle \frac{1}{2}\frac{1}{2}0\rangle$; $\mathcal{U}_1 = F(222)4/mmc$ $\langle 00\frac{1}{2}\rangle$; $\mathcal{U}_2 = F(222)4/mmc$ $\langle \frac{1}{2}\frac{1}{2}\frac{1}{2}\rangle$; $\mathcal{U}_3 = F(222)4/mmc$ $\langle 000\rangle$. Hermann's group $\mathcal{M}$, which is accidentally equal to the normalizers $\mathcal{N}(\mathcal{U}_r)$, its normalizer $\mathcal{N}(\mathcal{M})$ and the group $\mathcal{Y}$ are $\mathcal{M} = \mathcal{N}(\mathcal{U}_r) = P(111)4/mmm$; $\mathcal{N}(\mathcal{M}) = C(11\frac{1}{2})4/mmm$; $\mathcal{Y} = I(111)4/mmm$, all with the origin in $\langle 000\rangle$. The groups $\mathcal{X}_q$ are members of other chains between $\mathcal{U}_r$ and $\mathcal{G}_s$ (the shift coefficients $\langle\ldots\rangle$ of the groups $\mathcal{X}_r$ are different from those of the groups $\mathcal{U}_r$ because the standard origins in *ITA* are different), $\mathcal{X}_0 = F(222)m\bar{3}c$ $\langle 000\rangle$; $\mathcal{X}_1 = F(222)m\bar{3}c$ $\langle \frac{1}{2}\frac{1}{2}\frac{1}{2}\rangle$; $\mathcal{X}_2 = F(222)m\bar{3}c$ $\langle 00\frac{1}{2}\rangle$; $\mathcal{X}_3 = F(222)m\bar{3}c$ $\langle \frac{1}{2}\frac{1}{2}0\rangle$.

From the diagram, one takes that each group $\mathcal{G}_s$ has as subgroups $\mathcal{M}$, two groups of type $\mathcal{X}$ and the four groups $\mathcal{U}_r$. Each group $\mathcal{U}_r$ has the supergroups $\mathcal{M}$, $\mathcal{X}_r$ and the two groups $\mathcal{G}_s$. If only the group $\mathcal{G}_0$ is taken into consideration, the four subgroups $\mathcal{U}_r < \mathcal{G}_0$ split into two kinds of two subgroups each. The subgroups $\mathcal{U}_0$ and $\mathcal{U}_1$ have 'its' supergroup $\mathcal{X}_q$ each, $q = 0, 1$; the subgroups $\mathcal{U}_2$ and $\mathcal{U}_3$ have none. However, the complete diagram is nicely symmetric; the simultaneous view to sub- and supergroups and the influence of the group $\mathcal{N}(\mathcal{M})$ unveil the real relationship between the involved $\mathcal{T}$-equivalent groups.

This figure displays the subgroups $\mathcal{U}$ with the tetragonal axis along one of the coordinate directions, say the *z* axis. The same diagram holds for the conjugate subgroups with their tetragonal axis along the *x* or the *y* axis. Altogether, there are 12 subgroups of type $\mathcal{U}$, forming four conjugate classes with three subgroups each (Billiet, 1981*a*).

Example 3.2.1, cont. The chain $\mathcal{G}_0 - \mathcal{U}_0$ of the relation $P(111)\,m\bar{3}m - F(222)\,4/mmc \sim I(2'2'2)\,4/mcm$

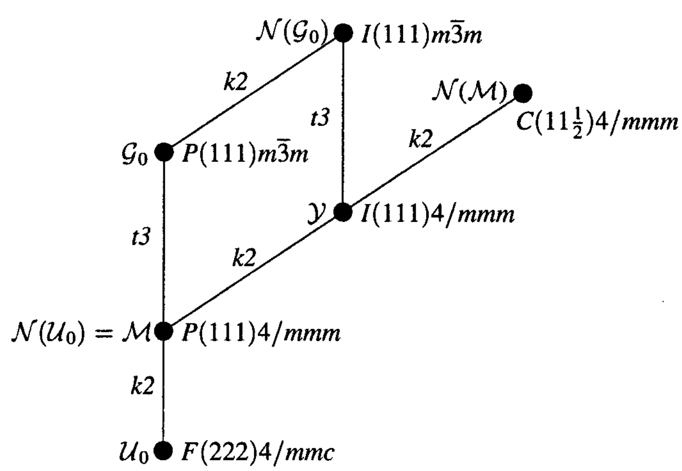

Figure 2

The group–subgroup chain $\mathcal{G}_0$–$\mathcal{U}_0$ of Fig. 1 as seen from another point of view. Displayed is the chain $\mathcal{G}_0$–$\mathcal{M}$–$\mathcal{U}_0$ with the normalizers of these groups. The number of four $\mathcal{T}$-equivalent subgroups $\mathcal{U}_r$ of $\mathcal{G}_0$ and that of two $\mathcal{T}$-equivalent supergroups $\mathcal{G}_s$ of $\mathcal{U}_r$ is not displayed but can be determined conveniently also from this diagram $|\mathcal{T}(\mathcal{N}(\mathcal{M})) : \mathcal{T}(\mathcal{N}(\mathcal{U}_0))| = 4$; $|\mathcal{T}(\mathcal{N}(\mathcal{M})) : \mathcal{T}(\mathcal{Y})| = 2$, where $\mathcal{Y} = \mathcal{N}(\mathcal{G}_0) \cap \mathcal{N}(\mathcal{M}) = I(111)4/mmm$. The action of $\mathcal{G}_0$ on $\mathcal{M}$ triples the number of subgroups, changing the tetragonal axis from *z* to *x* and *y*. The conventional symbols of $C(11\frac{1}{2})4/mmm$ and $F(222)4/mmc$ are $P(1'1'\frac{1}{2})4/mmm$ with $1'1'$ meaning $\mathbf{a}' = \frac{1}{2}(\mathbf{a} - \mathbf{b})$ and $\mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$ and $I(2'2'2)4/mcm$ with $2'2'$ meaning $\mathbf{a}' = \mathbf{a} - \mathbf{b}$ and $\mathbf{b}' = \mathbf{a} + \mathbf{b}$. The symbols *k*2 and *t*3 attached to the lines mean *k*- or *t*-subgroup of index 2 or 3.

(4) $\mathcal{T}(\mathcal{N}(\mathcal{G})) \not\leq \mathcal{T}(\mathcal{N}(\mathcal{U}))$ and $\mathcal{T}(\mathcal{N}(\mathcal{G})) \not\geq \mathcal{T}(\mathcal{N}(\mathcal{U}))$. The general chains $P(111)m\bar{3}m$–$P(112)4/mmm$, tetragonal axis along z, with the normalizers $I(111)m\bar{3}m$ and $C(111)4/mmm$; other general chains.

If the translation parts of the normalizers are not in a group–subgroup relation, then also the normalizers $\mathcal{N}(\mathcal{G})$ and $\mathcal{N}(\mathcal{U})$ themselves are not.

Special relations hold for *t*-chains and *k*-chains. They are described in the next two paragraphs.

If the chain $\mathcal{G}_0$–$\mathcal{U}_0$ is a *t*-chain, then $\mathcal{U}_0 = \mathcal{M}$. According to lemma 4, $\mathcal{T}(\mathcal{N}(\mathcal{M})) = \mathcal{T}(\mathcal{N}(\mathcal{U}_0)) \geq \mathcal{T}(\mathcal{N}(\mathcal{G}_0))$. There are no other subgroups of $\mathcal{G}_0$ which are $\mathcal{T}$-equivalent to $\mathcal{U}_0$. If $\mathcal{T}(\mathcal{N}(\mathcal{U}_0)) = \mathcal{T}(\mathcal{N}(\mathcal{G}_0))$ then there are also no other supergroups of $\mathcal{U}_0$ which are $\mathcal{T}$-equivalent to $\mathcal{G}_0$. If $\mathcal{T}(\mathcal{N}(\mathcal{U}_0)) > \mathcal{T}(\mathcal{N}(\mathcal{G}_0))$, then $\mathcal{T}(\mathcal{N}(\mathcal{U}_0))$ is decomposed relative to $\mathcal{T}(\mathcal{N}(\mathcal{G}_0))$ into $|\mathcal{T}(\mathcal{N}(\mathcal{U}_0)) : \mathcal{T}(\mathcal{N}(\mathcal{G}_0))| = g$ cosets, whose representatives generate g different $\mathcal{T}$-equivalent *t*-supergroups $\mathcal{G}_s$ from $\mathcal{G}_0$.

If the chain $\mathcal{G}_0$–$\mathcal{U}_0$ is a *k*-chain, then $\mathcal{G}_0 = \mathcal{M}$. According to lemma 5, $\mathcal{T}(\mathcal{N}(\mathcal{M})) = \mathcal{T}(\mathcal{N}(\mathcal{G}_0)) \geq \mathcal{T}(\mathcal{N}(\mathcal{U}_0))$. There are no other supergroups of $\mathcal{U}_0$ which are $\mathcal{T}$-equivalent to $\mathcal{G}_0$. If $\mathcal{T}(\mathcal{N}(\mathcal{U}_0)) = \mathcal{T}(\mathcal{N}(\mathcal{G}_0))$, then there are no other subgroups of $\mathcal{G}_0$ which are $\mathcal{T}$-equivalent to $\mathcal{U}_0$. If $\mathcal{T}(\mathcal{N}(\mathcal{G}_0)) > \mathcal{T}(\mathcal{N}(\mathcal{U}_0))$, then $\mathcal{T}(\mathcal{N}(\mathcal{G}_0))$ is decomposed into cosets relative to $\mathcal{T}(\mathcal{N}(\mathcal{U}_0))$ with $|\mathcal{T}(\mathcal{N}(\mathcal{G}_0)) : \mathcal{T}(\mathcal{N}(\mathcal{U}_0))| = u$ cosets, whose

Example 3.2.2 The chains $P(111)23 - F(222)222$

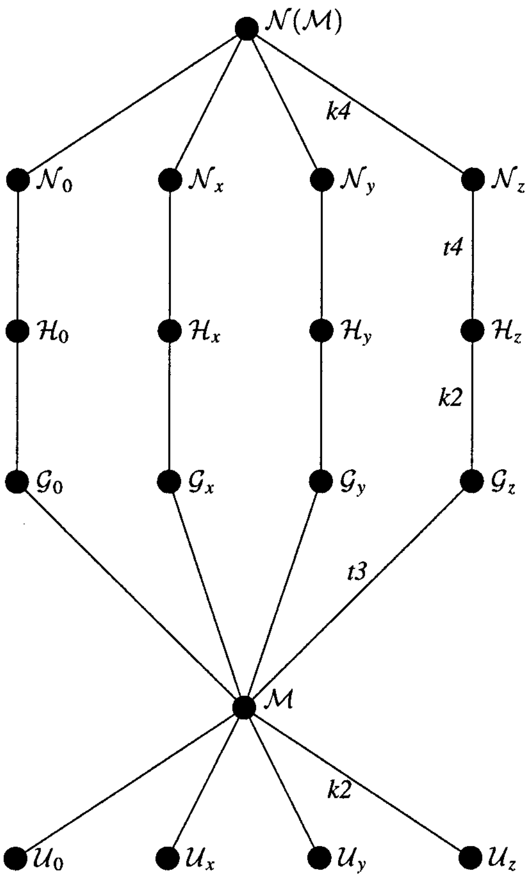

Figure 3
Starting from the supergroup $\mathcal{G}_0 = P(111)23$ with the conventional origin in the point $\langle 000 \rangle$ and its general subgroup $\mathcal{U}_0 = F(222)222$ of index 6 with the same conventional origin, one finds for this chain the Euclidean normalizers $\mathcal{N}(\mathcal{G}_0) = \mathcal{N}(\mathcal{U}_0) = I(111)m\bar{3}m$, called $\mathcal{N}_0$ in the figure, with the same conventional origin. Then $\mathcal{M} = P(111)222$ and $\mathcal{N}(\mathcal{M}) = P(\frac{1}{2}\frac{1}{2}\frac{1}{2})m\bar{3}m$, also with the origin in $\langle 000 \rangle$. The group $\mathcal{N}_0$ is a subgroup of $\mathcal{N}(\mathcal{M})$ of index 4, its normalizer in $\mathcal{N}(\mathcal{M})$ is $\mathcal{N}_0$ itself. Therefore, there are four $\mathcal{T}$-equivalent subgroups of $\mathcal{N}(\mathcal{M})$, of the type $I(111)m\bar{3}m$, designated $\mathcal{N}_0, \mathcal{N}_x, \mathcal{N}_y$ and $\mathcal{N}_z$ in the diagram, because their origins are in $\langle 000 \rangle$, $\langle \frac{1}{2}00 \rangle$, $\langle 0\frac{1}{2}0 \rangle$ and $\langle 00\frac{1}{2} \rangle$, referred to the coordinate system introduced above. Analogously, there are four $\mathcal{T}$-equivalent supergroups $\mathcal{G}_0, \ldots, \mathcal{G}_z$ and four $\mathcal{T}$-equivalent subgroups $\mathcal{U}_0, \ldots, \mathcal{U}_z$ with the corresponding origins in $\langle 000 \rangle, \ldots, \langle 00\frac{1}{2} \rangle$. The groups $\mathcal{H}_s$ of the type $I(111)23$ are inserted in the chains; they have the corresponding origins and separate the enhancement of the lattice from that of the point group on the way from $\mathcal{G}_s$ to $\mathcal{N}(\mathcal{G}_s)$. The symbols $k2$, $k4$, $t3$ and $t4$ attached to the lines mean *k*- or *t*-subgroup of index 2, 3 or 4. For the relations between $\mathcal{N}(\mathcal{G}_s)$ and $\mathcal{N}(\mathcal{U}_r)$, see the end of §3.1.

Example 3.2.3 The chains $c(11)2mm - p(11)2$

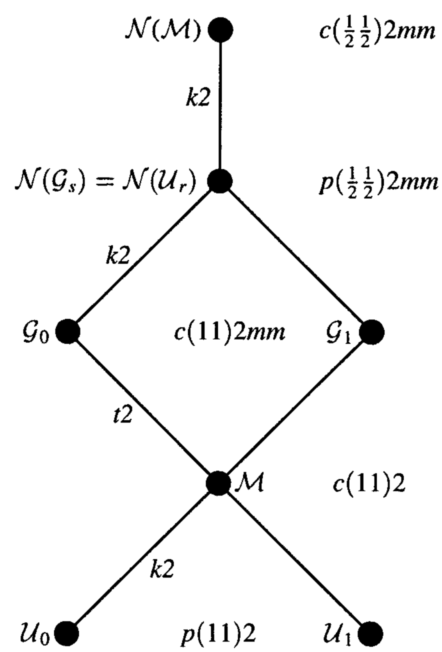

Figure 4
Structural implications can be recognized in the example of the general chains $c(11)2mm$–$p(11)2$, $\mathcal{M} = c(11)2$. Here $\mathcal{U}_0$ is a subgroup of index 4 of $\mathcal{G}_0$ with the conventional unit cell of $\mathcal{G}_0$, *i.e.* $\gamma = 90^\circ$, conventional origin in $\langle 00 \rangle$. The normalizers are $\mathcal{N}(\mathcal{G}_0) = \mathcal{N}(\mathcal{U})_0 = p(\frac{1}{2}\frac{1}{2})2mm$ and $\mathcal{N}(\mathcal{M}) = c(\frac{1}{2}\frac{1}{2})2mm$, both with origin in $\langle 00 \rangle$. The $\mathcal{T}$-equivalent groups are $\mathcal{U}_1$ and $\mathcal{G}_1$ with their origins in $\langle \frac{1}{4}\frac{1}{4} \rangle$ and the same normalizers as $\mathcal{U}_0$ and $\mathcal{G}_0$. The symbols $k2$ and $t2$ attached to the lines mean *k*- or *t*-subgroup of index 2.

The group–subgroup relations are displayed. A phase transition from $\mathcal{G}_0$ may result in two $\mathcal{T}$-equivalent subgroups $\mathcal{U}_0$ and $\mathcal{U}_1$; a phase transition from $\mathcal{U}_0$ may result in two $\mathcal{T}$-equivalent supergroups $\mathcal{G}_0$ and $\mathcal{G}_1$. This is clear from the symmetry diagrams in Figs. 5(*a*) to (*e*) and the two-dimensional structure models in Figs. 6(*a*) to (*e*). The two-dimensional 'crystal structures' of the two $\mathcal{T}$-equivalent subgroups $\mathcal{U}_r$ as well as those of the two $\mathcal{T}$-equivalent supergroups $\mathcal{G}_s$ are different. Therefore, simultaneous phase transitions are unlikely. If they could occur for special compounds, a kind of shift-domain formation should be observed which is called *region formation* in this paper. Shift domains are formed by the same crystal structure differing only in the position. Unlike domains, regions are formed by different crystal structures (modifications) with the same orientation but shifted symmetry frames. This effect could either happen in the transition to the low-symmetry phase or in that to the high-symmetry phase or even in both directions.

representatives generate u different $\mathcal{T}$-equivalent k-subgroups $\mathcal{U}_r$ of $\mathcal{G}_0$.

Definition 3. Two chains $\mathcal{G}_1$–$\mathcal{U}_1$ and $\mathcal{G}_2$–$\mathcal{U}_2$ are called $\mathcal{T}$-equivalent if there exists a translation $\mathsf{t} \in \mathcal{T}$ such that $\mathcal{G}_2 = \mathsf{t}^{-1}\mathcal{G}_1\mathsf{t}$ and $\mathcal{U}_2 = \mathsf{t}^{-1}\mathcal{U}_1\mathsf{t}$.

From the last two paragraphs it follows that for t relations $\mathcal{G} > \mathcal{U}$ all chains are of the type $\mathcal{G}_s$–$\mathcal{U}_0$ and are thus $\mathcal{T}$-equivalent. For k relations $\mathcal{G} > \mathcal{U}$, all chains are of the type $\mathcal{G}_0$–$\mathcal{U}_r$ and are also $\mathcal{T}$-equivalent.

As can be seen from the examples under (1) to (4), general chains may belong to any of the four types of the $\mathcal{T}(\mathcal{N}(\mathcal{G}))$–$\mathcal{T}(\mathcal{N}(\mathcal{U}))$ relations. Moreover, different chains between $\mathcal{T}$-equivalent sets of general subgroups $\mathcal{U}_r$ and general supergroups $\mathcal{G}_s$ may belong to different types of $\mathcal{N}(\mathcal{G})$–$\mathcal{N}(\mathcal{U})$ relations. This phenomenon is demonstrated for $\mathcal{T}(\mathcal{N}(\mathcal{G})) = \mathcal{T}(\mathcal{N}(\mathcal{U}))$ in example 3.2.2. The four chains between $\mathcal{G}_s = P(111)23$ and $\mathcal{U}_r = F(222)222$ with $s = r$ belong to Koch's (1984) case 1, $\mathcal{N}(\mathcal{G}) = \mathcal{N}(\mathcal{U})$. The other 12 chains with $s \neq r$ belong to case 4, $\mathcal{N}(\mathcal{G}) \not\leq \mathcal{N}(\mathcal{U})$ and $\mathcal{N}(\mathcal{G}) \not\geq \mathcal{N}(\mathcal{U})$.

For example, $\mathcal{N}(\mathcal{G}_0) = \mathcal{N}(\mathcal{U}_0) = I(111)m\bar{3}m$ with the origin in $\langle 000 \rangle$. Therefore, the chain $\mathcal{G}_0$–$\mathcal{U}_0$ belongs to case 1 of Koch (1984). On the other hand, $\mathcal{N}(\mathcal{U}_x) = I(111)m\bar{3}m$ with the origin in $\langle \frac{1}{2}00 \rangle$. Therefore, the intersection $\mathcal{N}(\mathcal{G}_0) \cap \mathcal{N}(\mathcal{U}_x) = I(111)4_x/mmm$, *i.e.* the chain $\mathcal{G}_0$–$\mathcal{U}_x$ belongs to case 4 of Koch (1984).

Such a diversity can only happen for general chains because for them the different chains $\mathcal{G}_s$–$\mathcal{U}_r$ are not necessarily all $\mathcal{T}$-equivalent.

An analogous example for $\mathcal{T}(\mathcal{N}(\mathcal{G})) > \mathcal{T}(\mathcal{N}(\mathcal{U}))$ is formed by the general relation $P(111)m\bar{3}$–$F(222)mmm$ with the types of normalizers $\mathcal{N}(\mathcal{G}) = I(111)m\bar{3}m$ and $\mathcal{N}(\mathcal{U}) = P(111)m\bar{3}m$. With $\mathcal{M} = P(111)mmm$ and $\mathcal{N}(\mathcal{M}) = P(\frac{1}{2}\frac{1}{2}\frac{1}{2})m\bar{3}m$, one finds similarly as in example 3.2.2 four normalizers $\mathcal{N}(\mathcal{G})$, eight normalizers $\mathcal{N}(\mathcal{U})$, four groups $\mathcal{G}_s$ and eight groups $\mathcal{U}_r$. Altogether there are 32 chains $\mathcal{G}_s$–$\mathcal{U}_r$. For eight of them $\mathcal{N}(\mathcal{G}) > \mathcal{N}(\mathcal{U})$ holds; the other 24 belong again to case 4, $\mathcal{N}(\mathcal{G}) \not\leq \mathcal{N}(\mathcal{U})$ and $\mathcal{N}(\mathcal{G}) \not\geq \mathcal{N}(\mathcal{U})$.

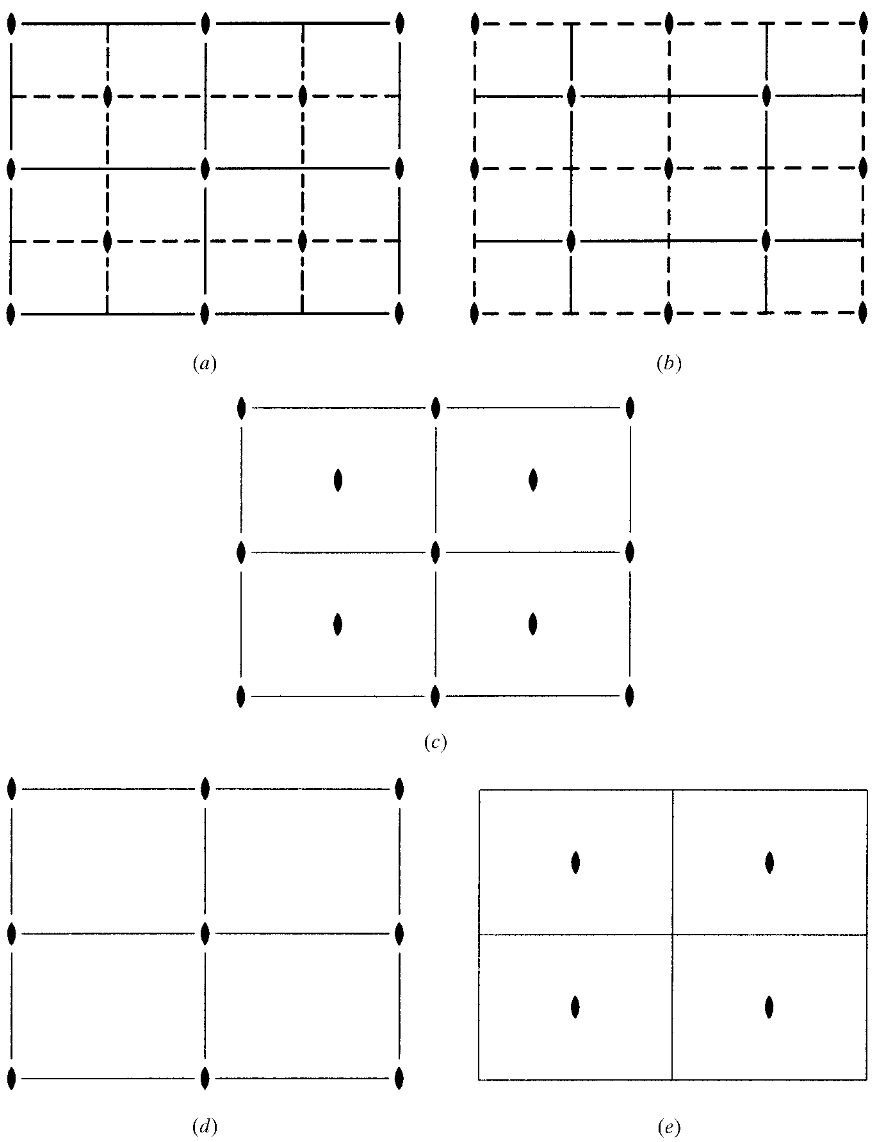

Figure 5
(*a*) Supergroup $\mathcal{G}_0$; one unit cell of $c(11)2mm$; origin in $\langle 00 \rangle$. (*b*) $\mathcal{T}$-equivalent supergroup $\mathcal{G}_1$; one unit cell of $c(11)2mm$; origin in $\langle \frac{1}{4}\frac{1}{4} \rangle$. (*c*) Hermann's group $\mathcal{M}$; one unit cell of $c(11)2$; unconventional setting; origin in $\langle 00 \rangle$. (*d*) Subgroup $\mathcal{U}_0$; one unit cell of $p(11)2$; origin in $\langle 00 \rangle$. (*e*) $\mathcal{T}$-equivalent subgroup $\mathcal{U}_1$; one unit cell of $p(11)2$; origin in $\langle \frac{1}{4}\frac{1}{4} \rangle$.

3.2. Examples

In this section, examples are displayed in order to demonstrate the application and the consequences of the derived formulae. The Hermann–Mauguin space-group symbols which are attached to the diagrams of the group–subgroup trees are slightly modified, see §1.3.

In example 3.2.1, Figs. 1 and 2 show the subgroups of the space group $Pm\bar{3}m$ of perovskite. They have been extensively discussed by Billiet (1981*a*) and Koch (1984) without the group $\mathcal{T}(\mathcal{N}(\mathcal{M}))$. Here this group is taken into consideration.

In example 3.2.2, Fig. 3 demonstrates that general chains between sets of $\mathcal{T}$-equivalent subgroups $\mathcal{U}_r$ and supergroups $\mathcal{G}_s$ may belong to different classes of $\mathcal{N}(\mathcal{G})$–$\mathcal{N}(\mathcal{U})$ relations, see also §3.1.

In example 3.2.3, possible implications on the underlying crystal structures are demonstrated which may occur if their space groups are equivalent under $\mathcal{T}(\mathcal{N}(\mathcal{M}))$, where $\mathcal{M}$ is Hermann's group. From Fig. 4, the group–subgroup relations may be taken. The symmetry relations are displayed in Figs. 5(*a*) to (*e*). The possibility of a transition from high to low as well as from low to high symmetry is suggested from Figs. 6(*a*) to (*e*). Such a transition would include *region formation* which has some similarity to the formation of antiphase domains in the usual phase transitions from high to low symmetry.

4. Conclusions

There are different methods, computer programs, tables and diagrams for the determination of the subgroups of a space group $\mathcal{G}$. Also when searching for the supergroups $\mathcal{G}_s > \mathcal{U}$ of a space group $\mathcal{U}$ it is usually easy to find a representative, say $\mathcal{G}_0$, of each type, *e.g.* by the inversion of available subgroup data. The equivalence under $\mathcal{N}(\mathcal{U})$ yields other groups $\mathcal{G}_k$ from $\mathcal{G}_0$. The main problem is then to determine all supergroups $\mathcal{G}_s > \mathcal{U}$ which are $\mathcal{T}$-equivalent to one of the groups $\mathcal{G}_k$. This problem can be solved now easily using the lemmata of §2.3. The tools are the normalizer $\mathcal{N}(\mathcal{M})$ of Hermann's group $\mathcal{M}$ and the

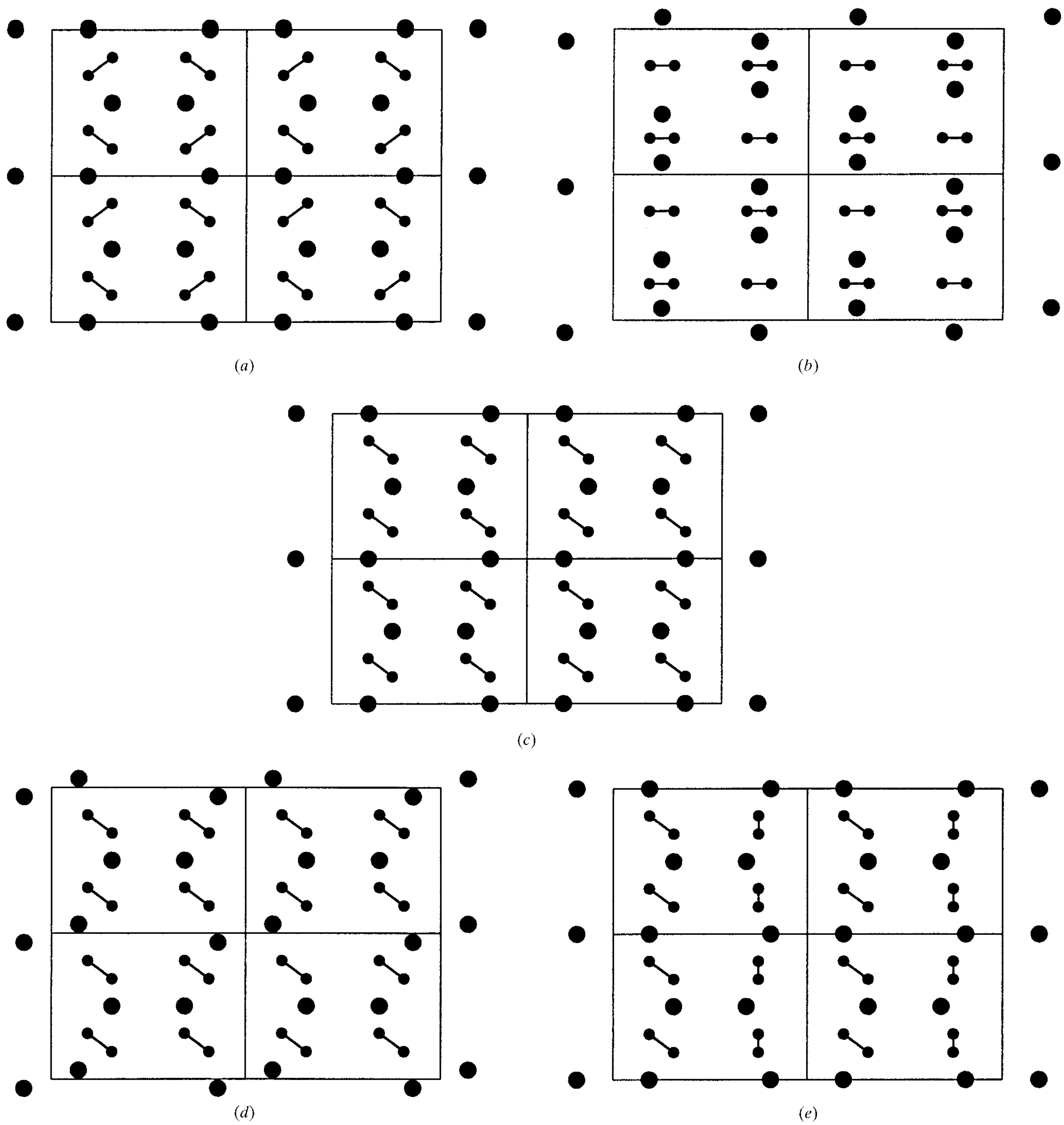

Figure 6
(*a*) Structure with plane group $\mathcal{G}_0$; four unit cells; origin in $\langle 00\rangle$. (*b*) Structure with plane group $\mathcal{G}_1$; four unit cells; origin in $\langle\frac{1}{4}\frac{1}{4}\rangle$. (*c*) Structure with plane group $\mathcal{M}$; four unit cells; origin in $\langle 00\rangle$. (*d*) Structure with plane group $\mathcal{U}_0$; four unit cells; origin in $\langle 00\rangle$. (*e*) Structure with plane group $\mathcal{U}_1$; four unit cells; origin in $\langle\frac{1}{4}\frac{1}{4}\rangle$.

coset decomposition of its translation group $\mathcal{T}(\mathcal{N}(\mathcal{M}))$ relative to $\mathcal{T}(\mathcal{N}(\mathcal{G}))$. The coset representatives are the translations $\mathsf{t}_s \in \mathcal{T}$ which transform the groups $\mathcal{G}_k$ into $\mathcal{G}_s$ by conjugation.

The lemma of §2.2 facilitates the search for subgroups. The analogy of the lemmata in §§2.2 and 2.3 reduces the difficulty of the search for supergroups to the level of the search for subgroups and thus makes supergroups of space groups much more accessible.

It is shown in example 3.2.3 of §3.2 how structural changes are possible in phase transitions from high to lower and from low to higher symmetry, which include a process called *region formation* in this paper. Region formation may resemble the well known formation of shift domains in transitions from high to lower symmetry.

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References

Billiet, Y. (1981*a*). *Acta Cryst.* A**37**, 649–652.
Billiet, Y. (1981*b*). *Acta Cryst.* A**37**, C354.
Boisen, M. B., Gibbs, G. V. & Wondratschek, H. (1990). *Acta Cryst.* A**46**, 545–552.
Giacovazzo, C. (1992). Editor. *Fundamentals of Crystallography. IUCr Texts on Crystallography*, No. 2. Oxford University Press.
Hermann, C. (1929). *Z. Kristallogr.* **69**, 533–555.
International Tables for Crystallography (1983). Vol. A, *Space-Group Symmetry*, edited by Th. Hahn, Part 8. Dordrecht: Kluwer Academic Publishers.
International Tables for Crystallography (2001). Vol. A, *Space-Group Symmetry*, 5th ed., edited by Th. Hahn, Part 15. Dordrecht: Kluwer Academic Publishers. In the press.
Koch, E. (1984). *Acta Cryst.* A**40**, 593–600.
Koch, E. & Müller, U. (1990). *Acta Cryst.* A**46**, 826–831.