(*Handbook of Mathematical Functions*, 1972, equation 22.9.15),

$$(1-Z)^{-\alpha-1}\exp[-XZ/(1-Z)]=\sum_{n=0}^{\infty}L_n^{\alpha}(X)Z^n, \quad (A3)$$

can be used with ($A1$) to rewrite ($A2$) as

$$F=\sum_{n=0}^{\infty}\left\{\int_0^{\infty}r^{l+2}\exp[-\gamma r(1+Z)/(1-Z)]j_l(Kr)\,dr\right\} \times Z^n/(1-Z)^{2l+3}. \quad (A4)$$

The integral in ($A4$) may be evaluated in simple closed form [Epstein & Stewart, 1977, equation ($A2$)]. With some algebraic rearrangements,

$$F=\frac{(2l+2)!(K/\gamma)^l}{(2l+1)!!\gamma^{l+3}[1+(K/\gamma)^2]^{l+2}} \times\sum_{n=0}^{\infty}\frac{(1+Z)}{(1-2tZ+Z^2)^{l+2}}Z^n, \quad (A5)$$

where

$$t=[(K/\gamma)^2-1]/[(K/\gamma)^2+1]. \quad (A6)$$

From the generating function for a Gegenbauer polynomial (*Handbook of Mathematical Functions*, 1972, equation 22.9.3), we can write ($A5$) as

$$F=\frac{(2l+2)!(K/\gamma)^l}{(2l+1)!!\gamma^{l+3}[1+(K/\gamma)^2]^{l+2}} \times\sum_{n=0}^{\infty}[C_n^{(l+2)}(t)+C_{n-1}^{(l+2)}(t)]Z^n. \quad (A7)$$

The Gegenbauer polynomial, $C_n^{(l+2)}(t)$, may be expressed as a Jacobi polynomial, $P_n^{(l+3/2,l+3/2)}(t)$ (*Handbook of Mathematical Functions*, 1972, equation 22.5.20). The sum of the two polynomials in ($A7$) then satisfies a recurrence relation for Jacobi polynomials (*Handbook of Mathematical Functions*, 1972, equation 22.7.19). Thus ($A7$) can be simplified to

$$F=(K/\gamma)^l\gamma^{-(l+3)}[1+(K/\gamma)^2]^{-(l+2)} \times\sum_{n=0}^{\infty}\frac{2^n(n+2l+2)!}{(2n+2l+1)!!}P_n^{(l+3/2,l+1/2)}(t)Z^n. \quad (A8)$$

In comparing ($A2$) to ($A8$), we have the desired result,

$$f_{n,l}(K)=\frac{(K/\gamma)^l 2^n(n+2l+2)!}{\gamma^{l+3}[1+(K/\gamma)^2]^{l+2}(2n+2l+1)!!} \times P_n^{(l+3/2,l+1/2)}(t). \quad (A9)$$

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The Implications of Normalizers on Group–Subgroup Relations Between Space Groups

By Elke Koch

Institut für Mineralogie, Lahnberge, D-3550 Marburg, Federal Republic of Germany

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Abstract

A hierarchy of classifications for subgroups of space groups by means of Euclidean and affine normalizers is introduced. The different levels of this classification scheme are illustrated in detail with examples and its usefulness for various problems is demonstrated. The Euclidean (or affine) normalizers of a space group G and of one of its subgroups U may either coincide [$N(G)=N(U)$], or form a group–subgroup pair [$N(G)\supset N(U)$ or $N(G)\subset N(U)$], or share only a common subgroup [$N(G)\not\supset N(U)$ and $N(G)\not\subset N(U)$]. The different implications of these cases on the equivalence classes of subgroups (or supergroups)

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are discussed. A procedure is given to calculate the number of equivalent subgroups or supergroups.

1. Introduction

The symmetry properties of any group G are completely described in a mathematical sense by the automorphism group of G. It may be appropriate for certain problems, however, to take into account only some of these symmetry properties. A typical example is formed by the crystallographic point group $2/m = \{1, \bar{1}, 2, m\}$. The group elements $\bar{1}$, 2 and m are mapped onto each other by outer automorphisms, *i.e.* from the group-theoretical point of view, the inversion, the twofold rotation and the reflection play an analogous role within this group. For most crystallographic problems, however, these symmetry operations have to be distinguished. In such a case it may be useful to embed G into a supergroup, and to consider the symmetry of G within this supergroup, instead of the automorphism group of G. This leads to the concept of normalizers.

The *normalizer* $N_H(G)$ of a group G with respect to any supergroup $H \supset G$ is defined as the set of all elements $h \in H$ that map G as a whole onto itself:

$$N_H(G) := \{h \in H | hGh^{-1} = G\}.$$

As $N_H(G)$ is always a supergroup of G, it is an advantage of normalizers against automorphism groups that the elements of G and the elements of any of its normalizers are elements from the same set and, therefore, necessarily have certain properties in common.

If G, for example, is a crystallographic group of motions, *i.e.* a space group or any subgroup of a space group, and if the group E of all Euclidean mappings is chosen as supergroup H then the group G and its Euclidean normalizer $N_E(G)$ may map the same objects (points, patterns, crystal structures *etc.*) onto another and define equivalence relations in this way. In the paper by Fischer & Koch (1983) this property is used for the definition of equivalent descriptions of a crystal structure and of equivalent crystallographic point configurations. Within that paper detailed tables of the Euclidean normalizers of all space groups are given. Additional tables contain the transformations needed for the derivation of all equivalent point configurations or all equivalent descriptions of a crystal structure. The following authors also give tables of the Euclidean and/or the affine normalizers or of the automorphism groups of the space groups: Hirshfeld (1968), Koch & Fischer (1975), Burzlaff & Zimmermann (1980), Gubler (1982*a*), Billiet, Burzlaff & Zimmermann (1982).

Within the present paper the problem of equivalent subgroups or supergroups of space groups will be discussed making use of affine and Euclidean normalizers. The same concept may be applied to other crystallographic groups without problems.

2. Classification of subgroups of space groups

Group–subgroup relationships are defined for space groups rather than for space-group types. This becomes obvious if group and subgroup belong to the same type. Nevertheless, some properties in connection with group–subgroup relations may be transferred to types of groups. In general, this is not the case for properties based on Euclidean normalizers (*cf. e.g.* Fischer & Koch, 1983): a space group of type $P222_1$ has a Euclidean normalizer of type *Pmmm*, if $a \neq b$, but of type $P4/mmm$, if $a = b$.

If G is a space group and if $U_1, U_2, U_3, \ldots, U_n$ are subgroups of G with the same finite index i, it is possible to define for these subgroups a hierarchy of classifications into equivalence classes.

(1) Two subgroups U_i and U_k of a space group G are called *isotypic* if they are conjugate subgroups of the group A of all affine mappings within R^3, *i.e.* if there exists an affine mapping $a \in A$ that transforms U_i into U_k by conjugation:

$$U_k = aU_ia^{-1} \text{ with } a \in A.$$

Isotypic subgroups always belong to one and the same class out of the 219 classes of isomorphic space groups, *i.e.* to the same space-group type.

(2) Two subgroups U_i and U_k of a space group G are called *equivalent with respect to the affine normalizer* (for short: *affine-equivalent* or N_A *equivalent*), if they are conjugate subgroups of the affine normalizer $N_A(G)$ of the space group G:

$$U_k = aU_ia^{-1}$$

with

$$a \in N_A(G)$$

and

$$N_A(G) = \{a \in A | aGa^{-1} = G\}, A = \text{affine group}.$$

Affine-equivalent subgroups necessarily are also isotypic.

(3) Two subgroups U_i and U_k of a space group G are called *equivalent with respect to the Euclidean normalizer* (for short: *Euclidean-equivalent* or N_E *equivalent*), if they are conjugate subgroups of the Euclidean normalizer $N_E(G)$ of the space group G:

$$U_k = eU_ie^{-1}$$

with

$$e \in N_E(G)$$

and

$$N_E(G) = \{e \in E | eGe^{-1} = G\}, E = \text{Euclidean group}.$$

Euclidean-equivalent subgroups necessarily are also affine-equivalent and, therefore, isotypic.

(4) Two subgroups U_i and U_k of a space group G are called *conjugate* if they are mapped onto each other by conjugation with an element $g \in G$:

$$U_k = gU_ig^{-1} \text{ with } g \in G.$$

Conjugate subgroups necessarily are also Euclidean- and affine-equivalent and, therefore, isotypic.

If the affine normalizer of a space group G coincides with its Euclidean normalizer the symbol $N(G)$ will be used instead of $N_A(G)$ or $N_E(G)$ in the following. In such a case 'equivalent subgroups' will be used instead of 'affine-equivalent' or 'Euclidean-equivalent subgroups'.

The different levels of classification will be illustrated by two examples. The derivation and the completeness of the lists of subgroups is not discussed here, but the existence of all the subgroups may easily be verified by the subgroup data in *International Tables of Crystallography* (1983) in connection with the symmetry diagrams.

Example (i): equivalence classes of the subgroups with index 2 of a space group of type $C222$ (basis vectors $\mathbf{a}, \mathbf{b}, \mathbf{c}$). There exist 15 subgroups of index 2 which belong to nine classes of isotypic subgroups:

$$C112(\mathbf{a}, \mathbf{b}, \mathbf{c}) \triangleq P2(\tfrac{1}{2}\mathbf{a}-\tfrac{1}{2}\mathbf{b}, \tfrac{1}{2}\mathbf{a}+\tfrac{1}{2}\mathbf{b}, \mathbf{c})$$
$$C211(\mathbf{a}, \mathbf{b}, \mathbf{c}) \triangleq B2(\mathbf{b}, \mathbf{c}, \mathbf{a})$$
$$C121(\mathbf{a}, \mathbf{b}, \mathbf{c}) \triangleq B2(\mathbf{a}, \mathbf{c}, -\mathbf{b})$$
$$P222(\mathbf{a}, \mathbf{b}, \mathbf{c})$$
$$P2_12_12(\mathbf{a}, \mathbf{b}, \mathbf{c})$$
$$P22_12(\mathbf{a}, \mathbf{b}, \mathbf{c}) \triangleq P222_1(\mathbf{c}, \mathbf{a}, \mathbf{b})$$
$$P2_122(\mathbf{a}, \mathbf{b}, \mathbf{c}) \triangleq P222_1(\mathbf{b}, \mathbf{c}, \mathbf{a})$$
$$C222(\mathbf{a}, \mathbf{b}, 2\mathbf{c}; 0, 0, 0)$$
$$C222(\mathbf{a}, \mathbf{b}, 2\mathbf{c}; 0, 0, \tfrac{1}{2})$$
$$C222_1(\mathbf{a}, \mathbf{b}, 2\mathbf{c}; 0, 0, 0)$$
$$C222_1(\mathbf{a}, \mathbf{b}, 2\mathbf{c}; 0, 0, \tfrac{1}{2})$$
$$I222(\mathbf{a}, \mathbf{b}, 2\mathbf{c}; 0, 0, 0)$$
$$I222(\mathbf{a}, \mathbf{b}, 2\mathbf{c}; 0, 0, \tfrac{1}{2})$$
$$I2_12_12_1(\mathbf{a}, \mathbf{b}, 2\mathbf{c}; 0, 0, 0)$$
$$I2_12_12_1(\mathbf{a}, \mathbf{b}, 2\mathbf{c}; 0, 0, \tfrac{1}{2}).$$

The two isotypic subgroups $C211$ and $C121$ ($B2$ in standard setting with c axis unique) differ from each other in the orientation of their symmetry elements. The same is true for $P22_12$ and $P2_122$ (standard setting $P222_1$). Within the other pairs of isotypic subgroups (space-group types $C222$, $C222_1$, $I222$, $I2_12_12_1$) the symmetry elements of both subgroups have the same orientation, but are shifted against each other by $\frac{1}{2}\mathbf{c}$ referred to the basis of the original group.

The affine normalizer $N_A(C222)$ is a group of affine mappings isomorphic to $P4/mmm$ and with basis vectors $\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$. The two subgroups of the pair $C211$–$C121$ and of $P22_12$–$P2_122$ are mapped onto each other by the affine analogue of the fourfold rotation, the two subgroups of the classes $C222$, $C222_1$, $I222$, and $I2_12_12_1$, respectively, by a translation of $\frac{1}{2}\mathbf{c}$, which also is an element of $N_A(C222)$. Consequently, the classes of isotypic subgroups with index 2 of a space group $C222$ coincide with the classes of affine-equivalent subgroups.

The Euclidean normalizer $N_E(C222)$ is a space group of type $Pmmm$ with basis vectors $\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$, provided that $a \neq b$ for $C222$. $N_E(C222)$ again maps the two subgroups of the types $C222$, $C222_1$, $I222$, and $I2_12_12_1$, respectively, onto each other because the translation of $\frac{1}{2}\mathbf{c}$ also belongs to $N_E(C222)$. $N_E(C222)$, however, contains no elements that map $C211$ onto $C121$ or $P22_12$ onto $P2_122$. Therefore, $C222$ has 11 classes of Euclidean-equivalent subgroups of index 2.

In this example there do not exist pairs of conjugate subgroups because all subgroups of index 2 are normal subgroups, *i.e.* each of the 15 subgroups of index 2 forms a class of conjugate subgroups by itself.

Example (ii): a space group of type $Pm3m$ and its subgroups of index 6 that belong to space-group type $I4/mcm$. In total there exist 12 such subgroups, four with tetragonal axes in each of the directions $\mathbf{a}$, $\mathbf{b}$ and $\mathbf{c}$. The corresponding vector bases are $\mathbf{b}-\mathbf{c}, \mathbf{b}+\mathbf{c}, 2\mathbf{a}$; $\mathbf{c}-\mathbf{a}, \mathbf{c}+\mathbf{a}, 2\mathbf{b}$; $\mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}, 2\mathbf{c}$, respectively. The four subgroups with their tetragonal axes in the same direction differ in the sites of their origins referred to the standard description of $I4/mcm$ (*cf.* Billiet, 1981). For example, the points $0, 0, 0$; $\frac{1}{2}, \frac{1}{2}, 0$; $0, 0, \frac{1}{2}$; and $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ (referred to the unit cell of $Pm3m$) are the origins of the four subgroups with fourfold axes in the $\mathbf{c}$ direction of $Pm3m$.

The 12 subgroups considered form four classes of conjugate subgroups. Each such class consists of three groups, the symmetry patterns of which are mapped onto each other by a threefold rotation out of $Pm3m$. In this case, the Euclidean normalizer $N_E(Pm3m) = Im3m$ (basis vectors $\mathbf{a}, \mathbf{b}, \mathbf{c}$) is identical with the affine normalizer. The translation by $\frac{1}{2}\mathbf{a}+\frac{1}{2}\mathbf{b}+\frac{1}{2}\mathbf{c}$ combines the four classes of conjugate subgroups into two classes of Euclidean- (and affine-) equivalent subgroups. The difference between the subgroups of these two classes becomes obvious by looking at Wyckoff position $4(c)$ $0, 0, 0$ of $I4/mcm$ (site symmetry $4/m$). For one class this Wyckoff position originates from Wyckoff positions $1(a)$ $0, 0, 0$ or $1(b)$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ of space group $Pm3m$ (site symmetry $m3m$), for the other class, however, it originates from Wyckoff positions $3(c)$ $0, \frac{1}{2}, \frac{1}{2}$ or $3(d)$ $\frac{1}{2}, 0, 0$ (site symmetry $4/mmm$). The subgroups from the two different equivalence classes, therefore, play different roles with respect to the structure of the original group.

The second example in addition illustrates a further general feature of the classification scheme. The subgroups $I4/mcm$ with index 6 are not maximal subgroups of $Pm3m$, but the four groups with the same direction of their fourfold axes stem from a common intermediate group of type $P4/mmm$ with the same unit cell as $Pm3m$. With respect to $P4/mmm$ these groups $I4/mcm$ are subgroups of index 2 and, therefore, normal subgroups. The Euclidean normalizer of $P4/mmm$ is a space group which also belongs to class $P4/mmm$, but with basis vectors $\frac{1}{2}\mathbf{a}-\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{a}+\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$. The additional translations of this normalizer map all four subgroups $I4/mcm$ of $P4/mmm$ onto each other, *i.e.* all four subgroups $I4/mcm$ are Euclidean-equivalent with respect to the intermediate group $P4/mmm$. This means that equivalence properties, as defined above, cannot be transferred within a chain of subgroups.

The different levels of the hierarchic classification of subgroups are of interest for different types of problems.

Under normal pressure the crystal structure of $K_2Zn(CN)_4$ belongs to the spinel type (CN dumbbells instead of oxygen atoms), but its symmetry $Fd3m$ decreases under high pressure to $R\bar{3}c$ (index 8) and quartets are formed (Ahsbahs, 1979). For each component of such a quartet the threefold axes parallel to another one of the four space diagonals of $Fd3m$ are preserved. The corresponding four subgroups $R\bar{3}c$ are conjugate in $Fd3m$.

The possibilities of a crystal structure to deform in the course of a phase transition may be discussed without distinguishing conjugate subgroups of the original group. Subgroups that are Euclidean-equivalent but not conjugate, however, have to be regarded separately because each class of conjugate subgroups corresponds to another type of deformation. This has recently been discussed by Billiet (1981) for the example of tetragonally distorted perovskite structures with symmetry $I4/mcm$ [*cf.* also example (ii)]. Each of the four classes of conjugate subgroups $I4/mcm$ of space group $Pm3m$ (index 6) corresponds to a specific kind of deformation of the perovskite structure.

For the derivation of types of colour groups with i different colours, classes of affine-equivalent subgroups of index i may be used. Each group–subgroup pair exactly corresponds to one colour group. If two subgroups are affine-equivalent, the two corresponding colour groups are not essentially different, *i.e.* they belong to the same type. If, on the contrary, the two subgroups cannot be mapped onto each other by the affine normalizer (or the automorphism group) of the group the corresponding group–subgroup pairs define two essentially different colour groups (*cf. e.g.* Jarratt & Schwarzenberger, 1980; Nabonnand & Billiet, 1983; Senechal, 1983).

3. Types of group–subgroup relationships between space groups

Each group–subgroup relationship between a space group G and one of its subgroups U with finite index i corresponds to one of the following four cases defined by the Euclidean (or the affine) normalizers $N(G)$ and $N(U)$ of both groups:

(1) the normalizers of G and U coincide:

$$N(G)=N(U);$$

(2) the normalizer of G is a supergroup of the normalizer of U:

$$N(G)\supset N(U);$$

(3) the normalizer of G is a subgroup of the normalizer of U:

$$N(G)\subset N(U);$$

(4) there does not exist a group–subgroup relationship between the normalizers of G and U:

$$N(G)\not\supset N(U) \text{ and } N(G)\not\subset N(U).$$

For the cubic space groups, Fig. 1 gives a group–subgroup diagram in which in addition the Euclidean normalizer (identical with the affine normalizer within the cubic system) of each group is indicated. The diagram is complete in the sense that it contains the maximal subgroups (except the infinitely many isomorphic ones) for one representative of each cubic space-group class. It has to be noticed, however, that each class of Euclidean-equivalent subgroups is represented only once. The colour of a space-group symbol characterizes the corresponding normalizer, the space-group symbol of which is framed in that colour. The position of the space-group symbols within the diagram indicates the subgroup index: consecutive levels correspond to index 2. The relation between the unit cells of a group–subgroup pair follows directly from the index and the Bravais types of both groups.

Within the cubic crystal family only cases (1), (2) and (3) occur if only maximal subgroups are considered. If group and subgroup have the same normalizer (case 1), the corresponding line in the diagram has been drawn in the colour of that normalizer. If the normalizer changes the corresponding line is black, a full line representing case (2), a broken line case (3).

Only the space groups of classes $Im3m$ and $Ia3d$ coincide with their own Euclidean and affine normalizers. According to a theorem by Bieberbach (1912), each automorphism of a space group corresponds to at least one affine mapping of the space group onto itself. As a consequence, space groups of

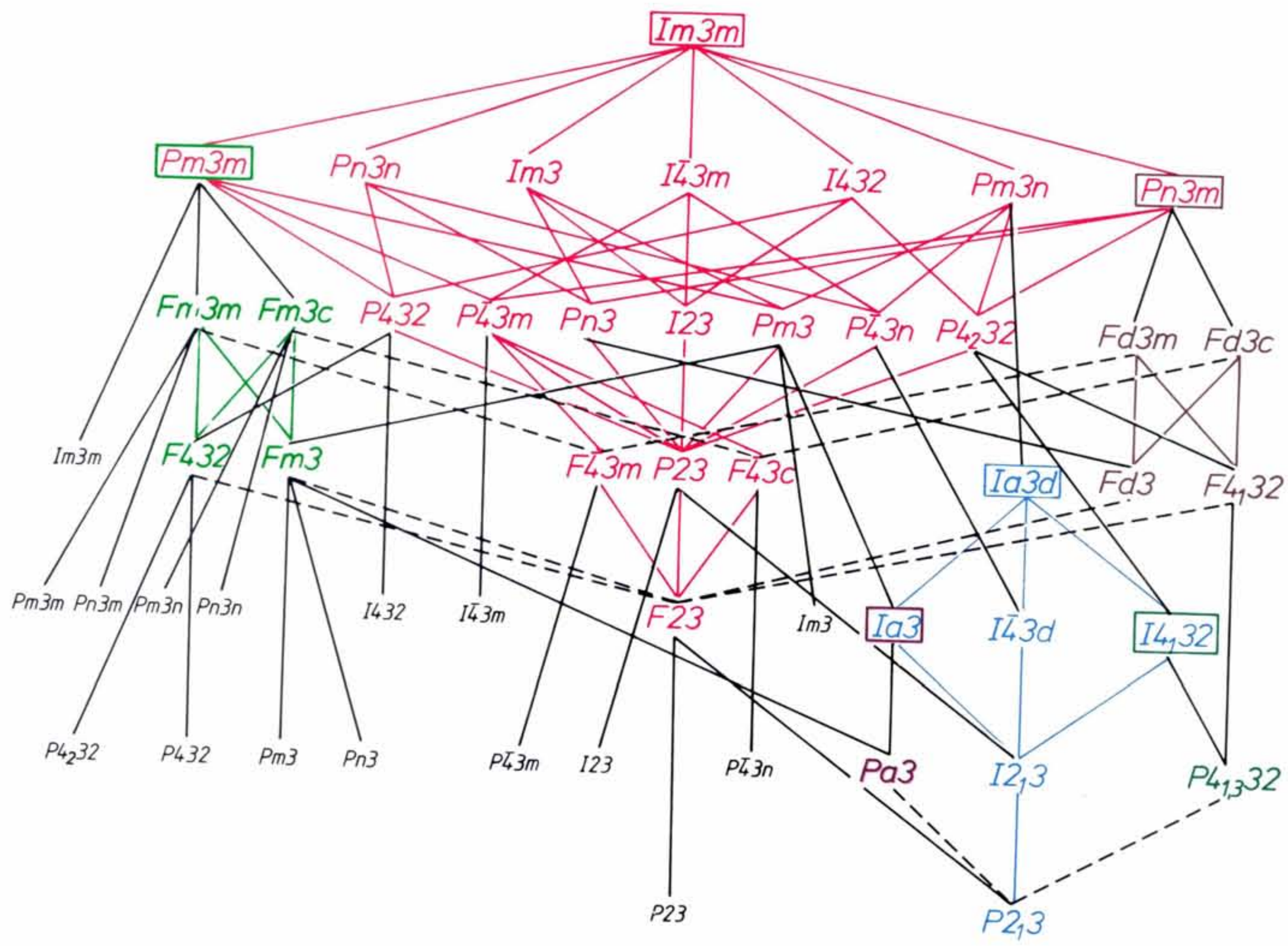

Fig. 1. Group–subgroup diagram for cubic space groups: Euclidean normalizers are marked by coloured frames. The normalizer of each space group is indicated by the same colour for the space-group symbol and the frame of the normalizer symbol: red symbolizes the normalizer $Im\bar{3}m$, blue $Ia\bar{3}d$, green $Pm\bar{3}m$, and brown $Pn\bar{3}m$: $Ia\bar{3}$ is the normalizer of $Pa\bar{3}$ (purple), and $I4_132$ the normalizer of the enantiomorphic pair $P4_132$, $P4_332$ (dark green).

classes $Im3m$ and $Ia3d$ have no outer automorphisms, *i.e.* they are the only *complete groups* among all space groups (*cf. e.g.* Gubler, 1982*a*, *b*).

$N(G)=N(U)$: Group–subgroup relationships of type (1) occur between class-equivalent groups as well as between translation-equivalent groups (*cf.* Fig. 1). Examples are the pairs $I\bar{4}3m$–$P\bar{4}3m$ with the common normalizer $Im3m$ and $I\bar{4}3d$–$I2_13$ with normalizer $Ia3d$. Group–subgroup relationships of this kind may also exist between space groups from different crystal systems. Each space group $Fm3$ has a translation-equivalent maximal subgroup of type $Fmmm$, but with specialized cubic unit cell. The normalizer of $Fm3$ is $Pm3m$ with lattice constants $\frac{1}{2}a$; the Euclidean normalizer of such a subgroup $Fmmm$ is identical with its affine normalizer and coincides with the normalizer of $Fm3$. In contrast to this, the normalizers of the 'analogous' pair $Pm3$–$Pmmm$ differ from each other: $N_E(Pm3)=Im3m(\mathbf{a},\mathbf{b},\mathbf{c})$, but $N_E(Pmmm)=Pm3m(\frac{1}{2}\mathbf{a},\frac{1}{2}\mathbf{b},\frac{1}{2}\mathbf{c})$. A different aspect is demonstrated by a group of type $Cmmm$ and its four isotypic subgroups of index 4 with the same unit cell: $P2/m11$, $P12/m1$, $P112/m$ (origin at 0, 0, 0), and $P112/m$ (origin at $\frac{1}{4},\frac{1}{4}$, 0). $Cmmm$ and all these four subgroups have the Euclidean normalizer $Pmmm(\frac{1}{2}\mathbf{a},\frac{1}{2}\mathbf{b},\frac{1}{2}\mathbf{c})$ in common, *i.e.* all four subgroup relationships belong to type (1). Therefore, no two of these isotypic subgroups are Euclidean-equivalent.

$N(G)\supset N(U)$: Group–subgroup relationships of type (2) seem to be confined to class-equivalent subgroups, if only maximal subgroups are considered. Examples are the group–subgroup pairs $Pm3$–$Fm3(2\mathbf{a},2\mathbf{b},2\mathbf{c})$ and $P432$–$I432(2\mathbf{a},2\mathbf{b},2\mathbf{c})$ with the corresponding normalizers $N(Pm3)=Im3m$, $N(Fm3)=Pm3m$ and $N(P432)=Im3m$, $N(I432)=Im3m(2\mathbf{a},2\mathbf{b},2\mathbf{c})$. The second example shows a remarkable feature: though the normalizers of group and subgroup belong to the same space-group type $Im3m$, they differ because the basis vectors of $N(I432)$ are twice as long as the basis vectors of $N(P432)$. The orthorhombic pair $Cmmm$–$Immm(\mathbf{a},\mathbf{b},2\mathbf{c})$ forms a similar example: the Euclidean normalizers $N_E(Cmmm)=Pmmm(\frac{1}{2}\mathbf{a},\frac{1}{2}\mathbf{b},\frac{1}{2}\mathbf{c})$ and $N_E(Immm)=Pmmm(\frac{1}{2}\mathbf{a},\frac{1}{2}\mathbf{b},\mathbf{c})$ differ in their translation periods parallel to $\mathbf{c}$ only. Additional examples are most isomorphic subgroups. In this case the normalizers of group and subgroup obviously belong to the same type but have different translation periods. Exceptions may either be caused by specialized metric of group or subgroup or by enlargement of a translation period in a degenerate direction (*cf.* Fischer & Koch, 1983) of the normalizers.

$N(G)\subset N(U)$: Group–subgroup relations of type (3) are less frequent than those of types (1) and (2). In the case of maximal subgroups they occur mostly in connection with translation-equivalent subgroups. Typical examples from the cubic crystal system are the pairs $Fm3$–$F23$ and $P4_132$–$P2_13$ with normalizers $N(Fm3)=Pm3m(\frac{1}{2}\mathbf{a})$, $N(F23)=Im3m(\frac{1}{2}\mathbf{a})$ and $N(P4_132)=I4_132$, $N(P2_13)=Ia3d$, respectively. A somewhat different example is supplied by the pair $P6/mmm$–$P6mm$. The Euclidean (and affine) normalizer of $P6/mmm$ is an isomorphic supergroup with half the translation period in the $\mathbf{c}$ direction, $N(P6/mmm)=P6/mmm(\mathbf{a},\mathbf{b},\frac{1}{2}\mathbf{c})$. The normalizer of $P6mm$ has infinitesimally short translations in the $\mathbf{c}$ direction and, therefore, is no space group but a supergroup of a space group, $N(P6mm)=Z^16/mmm(\mathbf{a},\mathbf{b},\mu\mathbf{c})\supset P6/mmm(\mathbf{a},\mathbf{b},\frac{1}{2}\mathbf{c})$. One of the exceptional examples for a group–subgroup relationship of type (3) between class-equivalent groups is the pair $R3$–$P3$ with

$$N(R3)=Z^1\bar{3}1m(\tfrac{2}{3}\mathbf{a}+\tfrac{1}{3}\mathbf{b}+,\ -\tfrac{1}{3}\mathbf{a}+\tfrac{1}{3}\mathbf{b},\ \mu\mathbf{c})$$

and

$$N(P3)=Z^16/mmm(\tfrac{2}{3}\mathbf{a}+\tfrac{1}{3}\mathbf{b},\ -\tfrac{1}{3}\mathbf{a}+\tfrac{1}{3}\mathbf{b},\ \mu\mathbf{c}),$$

where $N(R3)$ is a true subgroup of $N(P3)$. Such exceptions seem to be connected with a change of the Bravais system within a crystal family (for the terms Bravais system and crystal family see Wondratschek, 1983).

$N(G)\not\supset N(U)$ *and* $N(G)\not\subset N(U)$: Group–subgroup relationships of type (4) are frequently but not necessarily connected with a change of the crystal family. The following examples illustrate two different situations (affine groups are symbolized in analogy to the isomorphic space groups).

(i) The translation subgroup of the normalizer is more comprehensive for the subgroup than for the original group; the crystal class, however, is higher for the group than for the subgroup:
$Pm3m$–$P4/mmm$ with normalizers

$$N(Pm3m)=Im3m$$

and

$$N(P4/mmm)=P4/mmm(\tfrac{1}{2}\mathbf{a}-\tfrac{1}{2}\mathbf{b},\ \tfrac{1}{2}\mathbf{a}+\tfrac{1}{2}\mathbf{b},\ \tfrac{1}{2}\mathbf{c});$$

$Pmmm$–$Pmm2$ with affine normalizers

$$N_A(Pmmm)=Pm3m(\tfrac{1}{2}\mathbf{a},\tfrac{1}{2}\mathbf{b},\tfrac{1}{2}\mathbf{c})$$

and

$$N_A(Pmm2)=Z^14/mmm(\tfrac{1}{2}\mathbf{a},\tfrac{1}{2}\mathbf{b},\mu\mathbf{c}).$$

(ii) The translation subgroup of the normalizer is more comprehensive for the group than for the subgroup; the crystal class, however, is higher for the subgroup than for the group:
$Pmma$–$Pmmn(\mathbf{a},2\mathbf{b},\mathbf{c})$ with affine normalizers

$$N_A(Pmma)=Pmmm(\tfrac{1}{2}\mathbf{a},\tfrac{1}{2}\mathbf{b},\tfrac{1}{2}\mathbf{c})$$

and

$$N_A(Pmmn)=P4/mmm(\tfrac{1}{2}\mathbf{a},\mathbf{b},\tfrac{1}{2}\mathbf{c});$$

$R\bar{3}m$–$P\bar{3}m1$ with normalizers

$$N(R\bar{3}m) = R\bar{3}m(-\mathbf{a}, -\mathbf{b}, \tfrac{1}{2}\mathbf{c})$$

and

$$N(P\bar{3}m1) = P6/mmm(\mathbf{a}, \mathbf{b}, \tfrac{1}{2}\mathbf{c}).$$

The following theorem holds for group–subgroup relations between class-equivalent space groups.

Theorem: The normalizer $N(U)$ of a class-equivalent subgroup U of a space group G cannot contain translations other than those of the normalizer $N(G)$ of the group G itself.

Proof: If i is the subgroup index of U in G, then G may be subdivided into i cosets of U:

$$G = U \cup t_1 U \cup t_2 U \cup \ldots \cup t_{i-1} U.$$

As the groups G and U are class-equivalent each coset of U may be represented by a translation t_j. If $t \in N(U)$ also is a translation, it commutes with all elements $t_j \in G$:

$$\begin{aligned} tGt^{-1} &= t(U \cup t_1 U \cup t_2 U \cup \ldots \cup t_{i-1} U)t^{-1} \\ &= tUt^{-1} \cup tt_1 Ut^{-1} \cup tt_2 Ut^{-1} \cup \ldots \cup tt_{i-1} Ut^{-1} \\ &= tUt^{-1} \cup t_1 tUt^{-1} \cup t_2 tUt^{-1} \cup \ldots \cup t_{i-1} tUt^{-1} \\ &= U \cup t_1 U \cup t_2 U \cup \ldots \cup t_{i-1} U = G. \end{aligned}$$

Each translation from $N(U)$ maps the group G onto itself, *i.e.* also belongs to $N(G)$.

For crystal families other than the cubic one the relations between group–subgroup pairs and their normalizers cannot be represented as simply as in Fig. 1 for the following reasons: (1) the only complete space groups are the cubic groups $Im3m$ and $Ia3d$ and, therefore, natural 'summits' are lacking for the other crystal families; (2) for non-cubic space groups maximal isomorphic subgroups play a far more important role. As a consequence, each non-cubic subgroup diagram has to contain a large number of isomorphic subgroups (with different basis vectors) in order to be complete in the sense used above. This, however, results in diagrams that are difficult to survey and hardly representable at all.

4. Calculation of the number of conjugate, Euclidean- or affine-equivalent subgroups

For each subgroup U of a space group G the number of conjugate subgroups may be calculated with the aid of the Euclidean normalizer $N_E(U)$. The intersection of G with $N_E(U)$ exactly contains all those elements of G which map U onto itself, *i.e.* $G \cap N_E(U) = N_G(U)$. If $N_G(U) = G$, U is a normal subgroup of G. Otherwise, the index of $N_G(U)$ in G gives the number j of subgroups conjugate to U. *Example*:

$$G = F23, \qquad U = P23, \qquad N_E(U) = Im3m.$$

The subgroup U can be chosen such that the conventional unit cells (and origins) for all three groups are identical.

$$N_G(U) = Im3m \cap F23 = P23, \qquad j = 4.$$

There exist three further subgroups of type $P23$ (origins at $0, \tfrac{1}{2}, \tfrac{1}{2}$; $\tfrac{1}{2}, 0, \tfrac{1}{2}$ and $\tfrac{1}{2}, \tfrac{1}{2}, 0$, referred to the unit cell of $F23$) which are conjugate to U. In addition, four other subgroups of type $P23$ exist which are conjugate to each other but not conjugate to the first ones (origins at $\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}$; $\tfrac{1}{2}, 0, 0$; $0, \tfrac{1}{2}, 0$; $0, 0, \tfrac{1}{2}$).

The number of Euclidean- or affine-equivalent subgroups of a space group may easily be calculated if the normalizers of group and subgroup are known. For this, the types of group–subgroup relations defined in § 3 will be treated separately.

(1) $N(G) = N(U)$: Each element of the normalizer of G simultaneously is an element of the normalizer of U. Consequently no additional subgroups can exist which are equivalent to U with respect to $N(G)$, and U is a normal subgroup.

(2) $N(G) \supset N(U)$: If j is the index of $N(U)$ in $N(G)$, then $N(G)$ may be subdivided into j cosets of $N(U)$. Each of these cosets [except $N(U)$ itself] maps U onto another equivalent subgroup of G. *Examples*:

$G = Pm3$	$N(G) = Im3m$	
$U_1 = Fm3(2\mathbf{a})$	$N(U_1) = Pm3m$	$j_1 = 2$
$U_2 = Ia3(2\mathbf{a})$	$N(U_2) = Ia3d(2\mathbf{a})$	$j_2 = 8.$

Because of $j_1 = 2$, each space group $Pm3$ has two equivalent subgroups $Fm3$ with index 2; in the standard setting these two subgroups differ in the site of their origins ($0, 0, 0$ and $\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}$, referred to the unit cell of $Pm3$). As each subgroup of index 2 is a normal subgroup, these two subgroups are not conjugate. From $j_2 = 8$ it follows that there exist eight equivalent subgroups $Ia3$ of $Pm3$ with origins at $0, 0, 0$; $1, 0, 0$; $0, 1, 0$; $0, 0, 1$; $\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}$; $\tfrac{3}{2}, \tfrac{1}{2}, \tfrac{1}{2}$; $\tfrac{1}{2}, \tfrac{3}{2}, \tfrac{1}{2}$; $\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{3}{2}$ (referred to the unit cell of $Pm3$). The first four of these are mutually conjugate and so are the last four, as the index 4 of $N_G(U_2) = Ia3(2\mathbf{a})$ in G shows.

(3) $N(G) \subset N(U)$: As each element of $N(G)$ is also an element of $N(U)$, there cannot exist subgroups equivalent to U [*cf.* also (1)].

(4) $N(G) \not\supset N(U)$ *and* $N(G) \not\subset N(U)$: In such a case there always exists a largest common subgroup M of $N(G)$ and $N(U)$, $M = N(G) \cap N(U)$. The index of M in $N(G)$ gives the number of subgroups equivalent to U. *Example*:

$$\begin{aligned} G &= R\bar{3}m & N(G) &= R\bar{3}m(-\mathbf{a}, -\mathbf{b}, \tfrac{1}{2}\mathbf{c}) \\ U &= P\bar{3}m1 & N(U) &= P6/mmm(\mathbf{a}, \mathbf{b}, \tfrac{1}{2}\mathbf{c}) \\ & & M &= P\bar{3}m1(\mathbf{a}, \mathbf{b}, \tfrac{1}{2}\mathbf{c}). \end{aligned}$$

As the subgroup index j of M in $N(G)$ equals 3, $R\bar{3}m$ has three equivalent subgroups of type $P\bar{3}m1$ (origins at 0, 0, 0; $\frac{1}{3},\frac{2}{3},\frac{2}{3}$; $\frac{2}{3},\frac{1}{3},\frac{1}{3}$, referred to the unit cell of G). They are conjugate, because the index of $N_G(U)=U$ in G equals 3.

A subgroup U of a group G is called *characteristic* if U is mapped onto itself by each automorphism of G. G being a space group, U is characteristic if and only if U is mapped onto itself by all elements of $N_A(G)$, *i.e.* if the group–subgroup relation between G and U is of type (1) or (3) with respect to the affine normalizers.

The problem of characteristic subgroups of space groups has been treated in some detail by Gubler (1982*a*). A general statement by Gubler (1982*a*, pp. 114, 115) has to be corrected, however: If G is a space group with centered Bravais lattice and U is a class-equivalent subgroup of G with primitive Bravais lattice and the same conventional unit cell as G, then – in contrast to Gubler's statement – U need not be a characteristic subgroup of G. Gubler himself gives an example demonstrating the opposite (pp. 115, 120): $P3_1$ and $P3_2$ are affine-equivalent subgroups of $R3$. For the same reason Gubler's example on p. 115 is not appropriate: $P432$ and $P4_232$ are not characteristic subgroups of $F432$. From $N(F432)=Pm3m(\frac{1}{2}\mathbf{a})$, $N(P432)=N(P4_232)=Im3m$ and $j=4$ it follows immediately that $P432$ and $P4_232$ belong to a class of four equivalent subgroups each.

Gubler's example of space group $R3$ and its class-equivalent subgroups with index 3 is of special interest because the subgroup $P3$ has a normalizer other than $P3_1$ and $P3_2$:

$$G=R3 \quad N(G)=Z^1\bar{3}1m(\tfrac{2}{3}\mathbf{a}+\tfrac{1}{3}\mathbf{b},\,-\tfrac{1}{3}\mathbf{a}+\tfrac{1}{3}\mathbf{b},\,\mu\mathbf{c})$$

$$U_1=P3 \quad N(U_1)=Z^1 6/mmm(\tfrac{2}{3}\mathbf{a}+\tfrac{1}{3}\mathbf{b},\,-\tfrac{1}{3}\mathbf{a}+\tfrac{1}{3}\mathbf{b},\,\mu\mathbf{c})$$

$$\left.\begin{array}{l}U_2=P3_1\\ U_3=P3_2\end{array}\right\} N(U_2)=N(U_3)=Z^1 622(\tfrac{2}{3}\mathbf{a}+\tfrac{1}{3}\mathbf{b},\,-\tfrac{1}{3}\mathbf{a}+\tfrac{1}{3}\mathbf{b},\,\mu\mathbf{c}).$$

The translation periods parallel to $\mathbf{c}$ are infinitesimal for all three normalizers. As $N(U_1)\supset N(G)$, the group–subgroup relation $R3$–$P3$ is of type (3), *i.e.* $P3$ is a characteristic subgroup. On the contrary, the relations $R3$–$P3_1$ and $R3$–$P3_2$ refer to type (4). The common subgroup M of $N(G)$ and $N(U_2)$ is Z^1312 with the same basis vectors as the normalizers. The index j of M in $N(G)$ equals 2, *i.e.* there exist two equivalent subgroups, $P3_1$ and $P3_2$.

5. Equivalent supergroups

Equivalent supergroups of a space group may be defined in analogy to equivalent subgroups.

Two supergroups V_1 and V_2 of a space group G are called *Euclidean-equivalent* (*affine-equivalent*) if they are mapped onto each other by the Euclidean (affine) normalizer of G. *Examples*: Each group $F\bar{4}3m$ has two supergroups $Fm3m$ which differ with respect to their origins (0, 0, 0 and $\frac{1}{4},\frac{1}{4},\frac{1}{4}$, referred to the unit cell of $F\bar{4}3m$); they are mapped onto each other by the normalizer $Im3m(\frac{1}{2}\mathbf{a})$ of $F\bar{4}3m$. Each group $P222$ with general metric has three supergroups of type $Pccm$ which are not mapped onto each other by the Euclidean normalizer $N_E(P222)=Pmmm(\frac{1}{2}\mathbf{a},\frac{1}{2}\mathbf{b},\frac{1}{2}\mathbf{c})$, but by the affine normalizer $N_A(P222)=Pm3m(\frac{1}{2}\mathbf{a},\frac{1}{2}\mathbf{b},\frac{1}{2}\mathbf{c})$.

The analogy between supergroup relations and subgroup relations is not complete, however.

(i) A group–supergroup relation, in general, cannot be transferred from single groups to the complete class of space groups (if one restricts the supergroups to space groups and does not include additional affine groups isomorphic to space groups). *Example*: Only if the metric of a group of type $Pmmm$ is cubic, has it a cubic supergroup $Pm3$. For each group $Pmmm$, however, there exists an affine analogue of $Pm3$ as supergroup.

(ii) The classes of affine equivalent supergroups may contain, in addition to space groups, affine groups isomorphic to these space groups. *Example*: $G=P222(a=b\neq c)$, $V=P422(a=b\neq c)$. The affine normalizer $Pm3m(\frac{1}{2}\mathbf{a},\frac{1}{2}\mathbf{b},\frac{1}{2}\mathbf{c})$ of $P222$ maps the three directions of the rotation axes onto each other. $N_A(G)$, therefore, generates from V two additional affine-equivalent supergroups with the affine analogues of the fourfold rotation axes running in the $\mathbf{a}$ or $\mathbf{b}$ direction.

According to the relation between the normalizers of group and supergroup four cases may be distinguished as for group–subgroup relations:*

(1) $N(G)=N(V)$.

(2) $N(G)\subset N(V)$.

In both cases each element of $N(G)$ is contained in $N(V)$. $N(G)$, therefore, maps V only onto itself and does not generate further equivalent supergroups. *Examples*:

(i) $G=Pmma$ $\quad N_E(G)=Pmmm(\frac{1}{2}\mathbf{a},\frac{1}{2}\mathbf{b},\frac{1}{2}\mathbf{c})$

$V=Cmma$ $\quad N_E(V)=Pmmm(\frac{1}{2}\mathbf{a},\frac{1}{2}\mathbf{b},\frac{1}{2}\mathbf{c})$

(ii) $G=P432$ $\quad N(G)=Im3m$

$V=F432$ $\quad N(V)=Pm3m(\frac{1}{2}\mathbf{a})$.

(3) $N(G)\supset N(V)$

* The main ideas of the present section and of this paper were first presented by the author on the occasion of the 23*rd Diskussionstagung der Arbeitsgemeinschaft Kristallographie* (Koch, 1983). In connection with the derivation of non-characteristic orbits, Engel (1983) distinguishes between cases (1) and (2) on one side and (3) on the other in order to restrict the number of minimal supergroups that have to be considered. In fact, however, no restriction is achieved, because in cases (1) and (2) additional equivalent supergroups do not exist anyhow. The existence of case (4) is not mentioned by Engel.

The normalizer of G is a supergroup with index j of the normalizer of V. Then $N(G)$ may be subdivided into j cosets of $N(V)$. Each of these cosets [except $N(V)$ itself] maps V onto another supergroup of G (*cf.* Engel, 1983). If $N(G)$ is the Euclidean normalizer and V is a space group, all equivalent supergroups are space groups again. If $N(G)$ is the affine normalizer, the supergroups equivalent to space group V may be affine groups (*cf.* example above).

Example (i) $G = F23 \qquad N(G) = Im3m(\frac{1}{2}\mathbf{a})$

$$V = Fd3 \qquad N(V) = Pn3m(\tfrac{1}{2}\mathbf{a}), \quad j = 2.$$

There exist two supergroups $Fd3$ which are mapped onto each other, *e.g.* by the centering translation of $N(G)$ with vector $(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$.

Example (ii)

$$G = Pmm2 \qquad N_E(G) = Z^1mmm(\tfrac{1}{2}\mathbf{a}, \tfrac{1}{2}\mathbf{b}, \mu\mathbf{c})$$

$$V = Pmmm \qquad N_E(V) = Pmmm(\tfrac{1}{2}\mathbf{a}, \tfrac{1}{2}\mathbf{b}, \tfrac{1}{2}\mathbf{c}).$$

The index of $N_E(G)$ in $N_E(V)$ is infinite. Accordingly, there exist an infinite number of different supergroups $Pmmm$ for each group $Pmm2$. The mirror planes perpendicular to the $\mathbf{c}$ axis may be inserted at any height z within the unit cell of $Pmm2$.

(4) $N(G) \not\subset N(V)$ *and* $N(G) \not\supset N(V)$

There exists a largest common subgroup M of $N(G)$ and $N(V)$. The index of M in $N(G)$ gives the number of supergroups equivalent to V.

Example (*cf.* § 3):

$$G = P\bar{3}m1 \qquad N(G) = P6/mmm(\mathbf{a}, \mathbf{b}, \tfrac{1}{2}\mathbf{c})$$

$$V = R\bar{3}m \qquad N(V) = R\bar{3}m(-\mathbf{a}, -\mathbf{b}, \tfrac{1}{2}\mathbf{c}).$$

The common subgroup M is $P\bar{3}m1(\mathbf{a}, \mathbf{b}, \frac{1}{2}\mathbf{c})$. The index of M in $N(G)$ is 2. Each group $P\bar{3}m1$, therefore, has two supergroups $R\bar{3}m$ which differ with respect to the setting of the rhombohedral lattice (reverse and obverse).

For the classification of crystal structures it is necessary to derive for each crystal structure the corresponding idealized structure type with highest possible symmetry. This has been called aristotype by Bärnighausen (1980). In this context the knowledge of all different but Euclidean- (or affine-) equivalent supergroups of a space group is of special interest, because such different supergroups may result in different aristotypes for a given crystal structure.

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A Method for the Systematic Comparison of the Three-Dimensional Structures of Proteins and Some Results

By Michael Levine,* David Stuart† and John Williams

Department of Biochemistry, University of Bristol, Bristol BS8 1TD, England

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Abstract

A new rapid method of comparing three-dimensional protein structures using the sequence of dihedral angles is described. Systematic screening of protein structures by this method followed by detailed analysis reveals in particular that the calcium-binding protein carp parvalbumin is similar to cytochrome C2 from *Rhodospirillum rubrum*, cytochrome C is similar to hen lysozyme, carboxypeptidase A is similar to phage lysozyme. These results are completely unexpected and show interesting correlation with the

* Present address: Department of Physiology, University of Bristol, England.

† Present address: Laboratory of Molecular Biophysics, Zoology Department, University of Oxford, England.

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