proach of the ($xyz$) and $(\frac{1}{2}-x,\bar{y},\frac{1}{2}+z)$ molecules. It is not surprising that there should be no approximate mirror symmetry of the thermal vibration of the atoms in the molecule, because the intermolecular bonding is far from mirror-symmetrical (Fig. 2).

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# Descriptive Symbols for Crystal-Structure Types and Homeotypes Based on Lattice Complexes

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After a short historical review, a description of the invariant cubic lattice complexes according to C. Hermann is given. Besides the Bravais lattices only seven cubic lattice complexes and their splitting products into subgroups are needed. The description of variant cubic complexes, with the aid of coordination polyhedra and invariant complexes, is given for space group *Pm*3*m*. A crystal-structure type is symbolized by a list of lattice complexes, each of which is occupied by a set of equivalent atoms or coordination polyhedra.

## Introduction

Attempts have been made in the past to develop a satisfactory and comprehensive nomenclature of structure types.

In the *Strukturberichte* (1931–1943) P. P. Ewald and C. Hermann proposed a classification based on chemical composition. The symbol of a structure type consists of a capital letter followed by a number; it is not self-explanatory, and the authors considered this nomenclature to be only a preliminary solution. Later *Structure Reports* (from 1940 on) reported the results of structure determinations without any reference to structural types.

Laves (1930) published a nomenclature which is especially appropriate for $A_mB_n$ compositions but can also be expanded to $A_mB_nC_p$ compositions. The concept of 'connexion' is emphasized. Connexions in one, two, or three dimensions are symbolized by *I*(island), *C*(chain), *N*(net), or *L*(lattice). Besides these 'homogeneous' connexions (between equivalent atoms), 'heterogeneous' connexions (between dissimilar atoms) are also considered and are represented by small letters. In addition, coordination numbers and distances are also specified.

In six papers Wells (1954*a*–1956) discussed 'the geometrical basis of crystal chemistry', using the examples of regular polyhedra and *n*-connected nets. Wells's *n*-connected nets are special cases of lattice complexes.

Frank & Kasper (1958, 1959) described highly coordinated intermetallic compounds by means of 'triangulated coordination shells'. They have shown that these coordination shells have a number of representatives, but the triangulated coordination shells are not the only coordination polyhedra that are known in structures.

In 1957 a report of the Nomenclature Committee of the ASTM proposed a nomenclature for alloy phases. The symbols suggested consist of three parts; the first one gives the number of atoms in the cell, the last one designates the Bravais lattice by a new letter, and the middle part is a small letter, which distinguishes between different structure types that would otherwise have the same symbol; *e.g.* diamond–8*aF*, NaCl–8*bF*, ZnS(Sph)–8*cF*.

The first edition of the *International Tables (Internationale Tabellen zur Bestimmung von Kristallstrukturen*, 1935) included a good treatment of lattice complexes. C. Hermann redefined the concept, which had been introduced by P. Niggli. Each space-group description included the list of all the lattice complexes it contains. A lattice complex was designated by the symbol of the space-group of highest symmetry in which it occurs, followed by the Wyckoff letter of the position by which it is represented. Example: $Pm3m(a)$.

Hermann (1960) and Menzer (1960) published nomenclatures in which symbols are given to the few invariant lattice complexes and are modified for lattice complexes with degrees of freeedom.

In the present paper Hermann's symbolism will be used in a somewhat modified form, which was agreed on at an informal meeting of crystallographers held at Kiel, February 17–29, 1964 (Donnay, Hellner & Niggli, 1965).

## Lattice complexes

A lattice complex is defined as an arrangement of equivalent points (or equipoints) that are related by space-group symmetry operations, including lattice translations. One and the same lattice complex may occupy any one of several possible positions, in one or more space groups. The coordinates of the equivalent points for the various positions are tabulated in *International Tables for X-Ray Crystallography*. Besides invariant complexes there exist mono-, di-, and trivariant lattice complexes.

Niggli (1919, 1928, 1941) pointed out the importance of lattice complexes for the systematic description of crystal structures. He was convinced of the importance of lattice complexes not only for the description of structure types, but also as a guide to structure determination. Niggli failed to derive a simple symbolism for lattice complexes. He did not study the lattice complexes of the cubic system in detail. He considered as different those lattice complexes that can be represented by the same set of equivalent points with degrees of freedom, but have different values of the parameters.

Hermann, on the other hand, uses only one lattice-complex symbol for a set of equipoints in the whole parameter range in the asymmetric unit. Moreover, he considers two lattice complexes to be identical if one of them can be brought to coincidence with the other by a rotation. According to a proposal made by Donnay, Hellner & Niggli (1965), one and the same lattice complex may occur in both enantiomorphic representations.

An application of lattice complexes to the description of structure types becomes possible if Hermann's nomenclature be modified so as to take the *metrical* properties of lattice complexes into consideration. The following extensions are necessary:

(i) For invariant lattice complexes, the Hermann symbols will be used in a slightly revised form. To combine two or more complexes, it is important to know their positions with respect to the origin.

Example: In $F\bar{4}3m$ the $F$ complex may occur in four representations, corresponding to the following origins: $4(a)000$, $4(b)\frac{1}{2}\frac{1}{2}\frac{1}{2}$, $4(c)\frac{1}{4}\frac{1}{4}\frac{1}{4}$, and $4(d)\frac{3}{4}\frac{3}{4}\frac{3}{4}$. We distinguish between them by using primes, as $F$, $F'$, $F''$, $F'''$, or in a more explicit way, by means of superscripts, as $F$, $F^{444}$, $F^{222}$, $F^{666}$, where the three digits in superscript express eights of the cell edge.

In Table 1 all invariant cubic lattice complexes and their different representations are listed. Note that $P_2 = P_{abc}$ stands for a $P$ complex with each of the three cell edges $a$, $b$, $c$ halved, so that $P_2$ contains eight equipoints. We say that in $P_2$ the complex $P$ appears in the second order.

(ii) For complexes with degrees of freedom, one has to know the geometrical changes that take place when the parameters are allowed to range in the asymmetric unit.

Example: In $Pm3m$ consider the sixfold position $6(e): x00, \bar{x}00 \curvearrowright$. Hermann's symbol for the corresponding complex is $P6x$, in which $P$ stands for the point with the highest point symmetry, obtained for $x = 0{\cdot}0$; 6 is the multiplicity (or splitting number of the invariant complex $P$) when the parameter becomes larger than zero; $x$ indicates that there is only one degree of freedom in the direction [100].

For the metrical description, however, this information is not sufficient. It is necessary to know that the complex $P6x$ forms an octahedron around $P$ and a dumbbell around $J'$. In the parameter range $0 < x < 0{\cdot}293$ the shortest distances in the $P6x$ complex lie in the octahedron (abbreviation $6o$), therefore we describe this part as $P(6o)$. In the parameter range $0{\cdot}293 < x < 0{\cdot}5$ the complex $P6x$ has its shortest distance in the dumbbell around $J'$, which we describe (see Donnay, Hellner & Niggli (1964) as $J'(2l)$. For $x = 0{\cdot}293$ the distances in the coordination polyhedra $(6o)$ and $(2l)$ become equal and $P6x$ forms a sphere packing. An example of this sphere packing is found in $CaB_6$, where the B atoms occupy $P6x$ with $x = 0{\cdot}29$. Ca, located in $P'$, is surrounded by 24 B atoms, which form a cubo-octahedron described as $P'$ $(24co)$.

(iii) In crystal systems of low symmetry, the geometrical configuration of lattice complexes will vary with the axial ratios and the interaxialangles.

Example: Hermann proposed to add a small letter in front of the complex symbol to designate the crystal system; in English we propose to use $a$, $m$, $o$, $t$, $h$, $r$, $c$ for anorthic (=triclinic), monoclinic, orthorhombic, tetragonal, hexagonal, rhombohedral, and cubic. For example the $D$ complex in $Fddd$ is written $oD$.

For a metrical description, however, one has to know the axial ratios in addition; with $a{:}b{:}c \sim 1{:}1{:}1$ the geometrical configuration of the $D$ complex with its coordination number, distance, *etc.* will remain; with $a{:}b{:}c = 1{:}\sqrt{3}{:}2\sqrt{3}$ the same complex forms close-packed hexagonal nets perpendicular to $c$, which follow in a diamond sequence, with coordination number 10; in this case one may propose $(d)L$ for the geometrical description, where L stands for a close-packed hexagonal layer and $(d)$ for the diamond sequence as a four-layer type. The $\gamma$-Pu structure type is an example of this complex (Zachariasen & Ellinger, 1955); Laves & Wallbaum (1939) found $Si_2Ti$

Table 1. *The invariant cubic lattice complexes and their representations*

| Lattice complex | Coordinates of equipoints | Examples of possible space groups | | Representation of lattice complex | Multiplicity |
|---|---|---|---|---|---|
| | | Position | Point symmetry | | |
| $P$ | 000 | $Pm3m$ 1($a$) | m3m | $P$ | 1 |
| | | $Pm3m$ 1($b$) | m3m | $P'=\frac{1}{2}\frac{1}{2}\frac{1}{2}\,P=444/8\,P=P^{444}$ | 1 |
| | | $Fm3c$ 8($b$) | m3 | $P_2$ $(000, \frac{1}{2}\frac{1}{2}0 \frown)+000, \frac{1}{2}\frac{1}{2}\frac{1}{2}$ or $(000, \frac{1}{2}\frac{1}{2}\frac{1}{2})+000, \frac{1}{2}\frac{1}{2}0 \frown$ | 8 |
| | | $Ia3$ 8($a$) | $\bar{3}$ | | |
| | | $Fm3c$ 8($a$) | 432 | $P_2'=\frac{1}{4}\frac{1}{4}\frac{1}{4}\,P_2=222/8\,P_2=P_2^{222}$ | 8 |
| | | $Ia3$ 8($b$) | $\bar{3}$ | | |
| | | $Fm3m$ 8($c$) | $\bar{4}$3m | | |
| | | $Im3m$ 8($c$) | $\bar{3}$m | | |
| $I$ | $(000, \frac{1}{2}\frac{1}{2}\frac{1}{2})+000$ | $Im3m$ 2($a$) | m3m | $I$ | 2 |
| | | $Fd3c$ 16($a$) | 23 | $I_2$ $(000, \frac{1}{2}\frac{1}{2}0 \frown)+000, \frac{1}{2}\frac{1}{2}\frac{1}{2}, \frac{1}{4}\frac{1}{4}\frac{1}{4}, \frac{3}{4}\frac{3}{4}\frac{3}{4}$ or $(000, \frac{1}{2}\frac{1}{2}\frac{1}{2})+000, \frac{1}{2}\frac{1}{2}0, \frac{1}{4}\frac{1}{4}\frac{1}{4}, \frac{1}{4}\frac{1}{4}\frac{3}{4} \frown$ | 16 |
| | | $Ia3d$ 16($a$) | $\bar{3}$ | | |
| $F$ | $(000, \frac{1}{2}\frac{1}{2}0 \frown)+000$ | $Fm3m$ 4($a$) | m3m | $F$ | 4 |
| | | $Pa3$ 4($a$) | $\bar{3}$ | | |
| | | $Fm3m$ 4($b$) | m3m | $F'=\frac{1}{2}\frac{1}{2}\frac{1}{2}\,F=444/8\,F=F^{444}$ | 4 |
| | | $Pa3$ 4($b$) | $\bar{3}$ | | |
| | | $F\bar{4}3m$ 4($c$) | $\bar{4}$3m | $F''=\frac{1}{4}\frac{1}{4}\frac{1}{4}\,F=222/8\,F=F^{222}$ | 4 |
| | | $Pn3m$ 4($b$) | $\bar{3}$m | | |
| | | $F\bar{4}3m$ 4($d$) | $\bar{4}$3m | $F'''=\frac{3}{4}\frac{3}{4}\frac{3}{4}\,F=666/8\,F=F^{666}$ | 4 |
| | | $Pn3m$ 4($c$) | $\bar{3}$m | | |
| | | $Fd3c$ 32($b$) | 32 | $F_2''=F_2^{111}$ $(000, \frac{1}{2}\frac{1}{2}0 \frown)+\frac{1}{8}\frac{1}{8}\frac{1}{8}, \frac{1}{8}\frac{3}{8}\frac{3}{8}, \frac{3}{8}\frac{3}{8}\frac{1}{8}, \frac{3}{8}\frac{1}{8}\frac{3}{8}, \frac{5}{8}\frac{5}{8}\frac{5}{8}, \frac{5}{8}\frac{7}{8}\frac{7}{8}, \frac{7}{8}\frac{5}{8}\frac{7}{8}, \frac{7}{8}\frac{7}{8}\frac{5}{8}$ | 32 |
| | | $Fd3c$ 32($c$) | $\bar{3}$ | $F_2'''=\frac{1}{4}\frac{1}{4}\frac{1}{4}\,F_2''=333/8\,F_2^{333}$ | 32 |
| $J^*$ | $(000, \frac{1}{2}\frac{1}{2}\frac{1}{2})+\frac{1}{2}\frac{1}{2}0 \frown$ | $Im3m$ 6($b$) | 4/mmm | $J^*$ | 6 |
| | | $Fd3c$ 48($d$) | $\bar{4}$ | $J_2^*$ $(000, \frac{1}{2}\frac{1}{2}0 \frown)+\frac{1}{4}\frac{1}{4}0, \frac{1}{4}\frac{1}{4}\frac{1}{2}, 00\frac{1}{4}, 00\frac{3}{4} \frown$ | 48 |
| $J$ | $\frac{1}{2}\frac{1}{2}0 \frown$ | $Pm3m$ 3($c$) | 4/mmm | $J$ | 3 |
| | | $Pm3m$ 3($d$) | 4/mmm | $J'=\frac{1}{2}\frac{1}{2}\frac{1}{2}\,J=444/8\,J=J^{444}$ | 3 |
| | | $Fm3c$ 24($d$) | 4/m | $J_2$ $(000, \frac{1}{2}\frac{1}{2}0 \frown)+\frac{1}{4}\frac{1}{4}0, \frac{1}{4}\frac{1}{4}\frac{1}{2} \frown$ | 24 |
| | | $Fm3m$ 24($d$) | mmm | | |
| | | $Fm3c$ 24($c$) | $\bar{4}$m2 | $J_2'=\frac{1}{4}\frac{1}{4}\frac{1}{4}\,J_2=222/8\,J_2=J_2^{222}$ | 24 |
| $D$ | $(000, \frac{1}{2}\frac{1}{2}0 \frown)+000, \frac{1}{4}\frac{1}{4}\frac{1}{4}$ | $Fd3m$ 8($a$) | $\bar{4}$3m | $D$ | 8 |
| | | $Fd3m$ 8($b$) | $\bar{4}$3m | $D'=\frac{1}{2}\frac{1}{2}\frac{1}{2}\,D=444/8\,D=D^{444}$ | 8 |
| $W^*$ | $(000, \frac{1}{2}\frac{1}{2}\frac{1}{2})+\frac{1}{4}0\frac{1}{2}, \frac{3}{4}0\frac{1}{2} \frown$ | $Im3m$ 12($d$) | $\bar{4}$m2 | $W^*$ | 12 |
| $W$ | $\frac{1}{4}0\frac{1}{2}, \frac{3}{4}0\frac{1}{2} \frown$ | $Pm3n$ 6($c$) | $\bar{4}$m2 | $W$ | 6 |
| | | $Pm3n$ 6($d$) | $\bar{4}$m2 | $W'=\frac{1}{2}\frac{1}{2}\frac{1}{2}\,W=444/8\,W=W^{444}$ | 6 |
| $T$ | $(000, \frac{1}{2}\frac{1}{2}0 \frown)+\frac{1}{8}\frac{1}{8}\frac{1}{8}, \frac{3}{8}\frac{3}{8}\frac{1}{8} \frown$ | $Fd3m$ 16($c$) | $\bar{3}$m | $T$ | 16 |
| | | $Fd3m$ 16($d$) | $\bar{3}$m | $T'=\frac{1}{2}\frac{1}{2}\frac{1}{2}\,T=444/8\,T=T^{444}$ | 16 |
| $Y^{**}$ | $(000, \frac{1}{2}\frac{1}{2}\frac{1}{2})+\frac{1}{8}\frac{1}{8}\frac{1}{8}, \frac{7}{8}\frac{5}{8}\frac{3}{8}\, \frac{3}{8}\frac{3}{8}\frac{3}{8}, \frac{1}{8}\frac{5}{8}\frac{7}{8} \frown$ | $Ia3d$ 16($b$) | 32 | $Y^{**}$ | 16 |
| $^{+}Y^*$ | $(000, \frac{1}{2}\frac{1}{2}\frac{1}{2})+\frac{1}{8}\frac{1}{8}\frac{1}{8}, \frac{7}{8}\frac{5}{8}\frac{3}{8} \frown$ | $I4_132$ 8($a$) | 32 | $^{+}Y^*$ | 8 |
| | | $I4_132$ 8($b$) | 32 | $^{-}Y^*={}^{+}Y^*\,.\,\bar{1}$ | 8 |
| $^{+}Y$ | $\frac{1}{8}\frac{1}{8}\frac{1}{8}, \frac{7}{8}\frac{5}{8}\frac{3}{8}, \frown$ | $P4_332$ 4($a$) | 32 | $^{+}Y$ | 4 |
| | | $P4_332$ 4($b$) | 32 | $^{+}Y'=\frac{1}{2}\frac{1}{2}\frac{1}{2}\,{}^{+}Y=444/8\,{}^{+}Y={}^{+}Y^{444}$ | 4 |
| | | $P4_132$ 4($b$) | 32 | $^{-}Y={}^{+}Y\,.\,\bar{1}$ | 4 |
| | | $P4_132$ 4($a$) | 32 | $^{-}Y'=\frac{1}{2}\frac{1}{2}\frac{1}{2}\,{}^{-}Y=444/8\,{}^{-}Y={}^{-}Y^{444}$ | 4 |
| $S^*$ | $(000, \frac{1}{2}\frac{1}{2}\frac{1}{2})+\frac{3}{8}0\frac{1}{4}, \frac{1}{8}0\frac{3}{4}, \frac{7}{8}0\frac{1}{4}, \frac{5}{8}0\frac{3}{4} \frown$ | $Ia3d$ 24($d$) | $\bar{4}$ | $S^*$ | 24 |
| $S$ | $(000, \frac{1}{2}\frac{1}{2}\frac{1}{2})+\frac{3}{8}0\frac{1}{4}, \frac{1}{8}0\frac{3}{4} \frown$ | $I\bar{4}3d$ 12($a$) | $\bar{4}$ | $S$ | 12 |
| | | $I\bar{4}3d$ 12($b$) | $\bar{4}$ | $'S=S\,.\,\bar{1}$ | 12 |
| $V^*$ | $(000, \frac{1}{2}\frac{1}{2}\frac{1}{2})+\frac{1}{8}0\frac{1}{4}, \frac{3}{8}0\frac{3}{4}, \frac{5}{8}0\frac{1}{4}, \frac{7}{8}0\frac{3}{4} \frown$ | $Ia3d$ 24($c$) | 222 | $V^*$ | 24 |
| $^{+}V$ | $(000, \frac{1}{2}\frac{1}{2}\frac{1}{2})+\frac{1}{8}0\frac{1}{4}, \frac{3}{8}0\frac{3}{4} \frown$ | $I4_132$ 12($c$) | 222 | $^{+}V$ | 12 |
| | | $I4_132$ 12($d$) | 222 | $^{-}V={}^{+}V\,.\,\bar{1}$ | 12 |

to be a superstructure of this type. In *Fmmm* one has the same properties for the *F* complex with the axial ratios $a:b:c=1:\sqrt{3}:\sqrt{3}$, which one can describe as $(f)L$ for a two-layer type with the coordination number 10. The $MoSi_2$ type forms a superstructure of this complex. (Note that a three-layer complex $(q)L$ exists; *q* is derived from the high-quartz structure, where the Si atoms occupy this complex in $P6_2 22$; the ideal type $(q)L$ is realized with the axial ratio $a:c=1:\frac{3}{2}\sqrt{3}$. $CrSi_2$ can be considered as a superstructure of this type).

In the following paragraphs we will deal only with the cubic lattice complexes, some of their relations and combinations, and their application to the nomenclature of cubic structure types.

## The invariant cubic lattice complexes

All invariant cubic lattice complexes and their representations are listed in Table 1. In the first column the revised Hermann symbols are tabulated. The second column gives the coordinates of the equipoints in the normal (unshifted) representation of the complex. In the third column the first line for each complex gives the notation used by Hermann in the first edition of the *International Tables*; example: *Pm*3*m* 1(*a*) was used to designate the *P* complex in its normal orientation. The third column also contains examples of other space groups, where the complex appears either in the same or in a higher order. For each example the fourth column gives the corresponding point symmetry, while the fifth column gives equipoint coordinates for non-normal (*e.g.* shifted) representations. In the last column the multiplicity of the complex, that is the number of equipoints in the cell, is noted. Niggli (1919) introduced the word *Punktner* (Hermann changed it to *Punkter*); in English one may use *pointer.*

Examples: *P* is a 1-pointer, *I* is a 2-pointer, $P_2$ is an 8-pointer.

In Figs. 1 to 3, each invariant cubic complex is drawn in its unit cell; the heights of the points are given in eighths of cell edge. In addition relations between the complexes are shown, which explain their derivation with the aid of subgroups and supergroups.

In *Pm*3*m* (Fig. 1) there exist two 1-pointers, *P* and *P′*, and two 3-pointers, *J* and *J′*. Several structure types can be described in terms of these complexes.

Examples:

| | | |
|---|---|---|
| CsCl type | $Cs_1Cl_1$ | *PP′* |
| $AuCu_3$ type (ordered) | $Au_1Cu_3$ | *PJ* |
| $ReO_3$ type | $Re_1O_3$ | *P′J* |
| $CaTiO_3$ type | $Ca_1Ti_1O_3$ | *PP′J* |
| $U_4S_3$ type | $U_1U_3S_3$ | *PJJ′* |

The structural formula in the second column explains the distribution of the atoms among the lattice complexes, which are listed in the third column.

The complexes *P* and *J*, which are distinct in *Pm*3*m*, unite in the supergroup *Fm*3*m* to form the *F* complex, $P+J=F$ [Fig. 1(*a*)]. Likewise $P'+J'=F'$. In addition *Fm*3*m* contains the 8-pointer $P_2'$ and the 24-pointer $J_2$ (which can be derived from $P_2m3m$, as *Fm*3*m* is one of its hemisymmetric* subgroups).

Examples:

| | | |
|---|---|---|
| Cu type | $Cu_4$ | *F* |
| $AuCu_3$ type (disordered) | $\{Au_{1/4}Cu_{3/4}\}_4$ | *F* |
| NaCl type | $Na_4Cl_4$ | *FF′* |
| $CaF_2$ type | $Ca_4F_8$ | $FP_2'$ |
| $BiF_3$ type | $Bi_4F_4F_8$ | $FF'P_2'$ |

Note the braces enclosing the fractional atoms that together occupy each equipoint of the *F* complex in a statistical way.

In the hemisymmetric subgroup $F\bar{4}3m$ of *Fm*3*m*, the 8-pointer $P_2'$ splits into two representations of the *F*

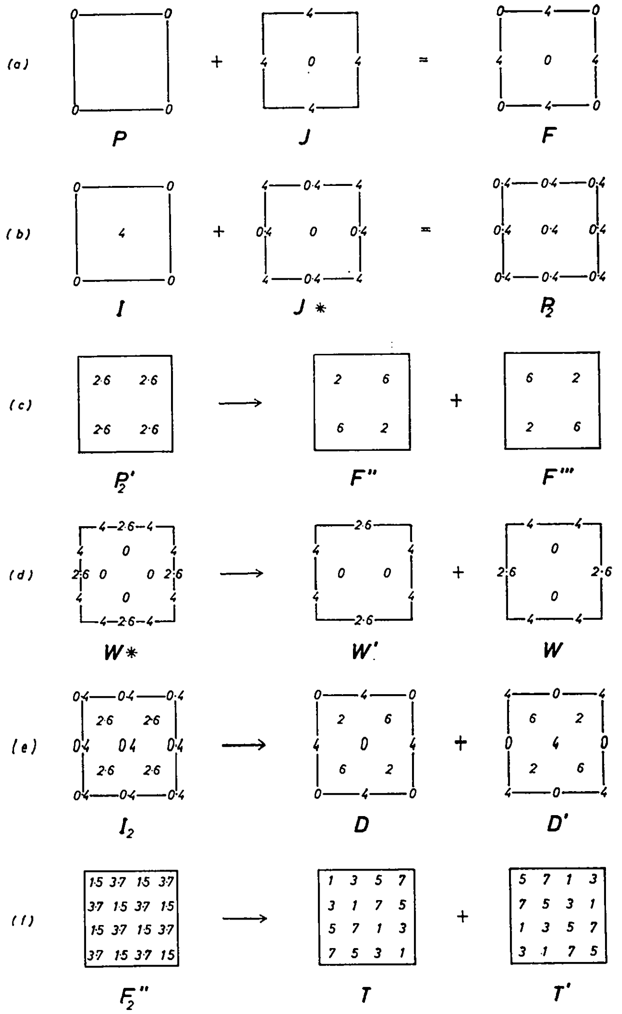

Fig. 1. Relations between the cubic complexes *P*, *I*, *F*, *J*, *J**, *W*, *W**, *D* and *T* (the numbers indicate the heights of the points in eighths).

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* The use of the term *merosymmetry* rather than *merohedry* was advocated by Rogers (1938) in the case of point-group symmetry. In space groups, it is impossible to speak of *merohedry*, since no planes are involved.

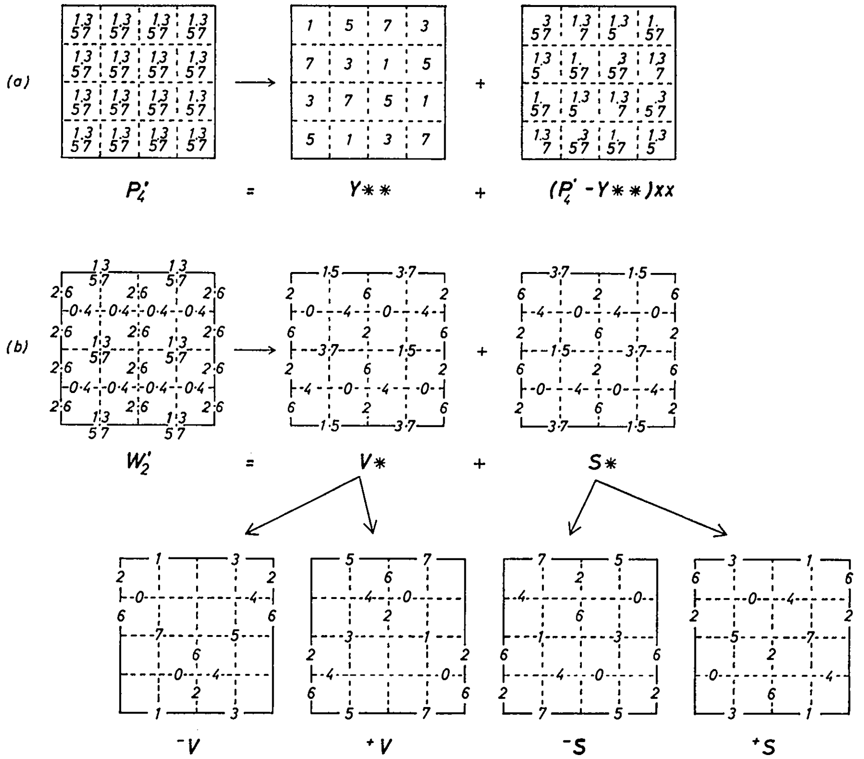

Fig. 2. Relations between the cubic lattice complexes $P_4'$, $Y^{**}$, $W_2'$, $V^*$, $S^*$, $^-V$, $^+V$, $^-S$, and $^+S$ (the numbers indicate the heights of the points in eighths).

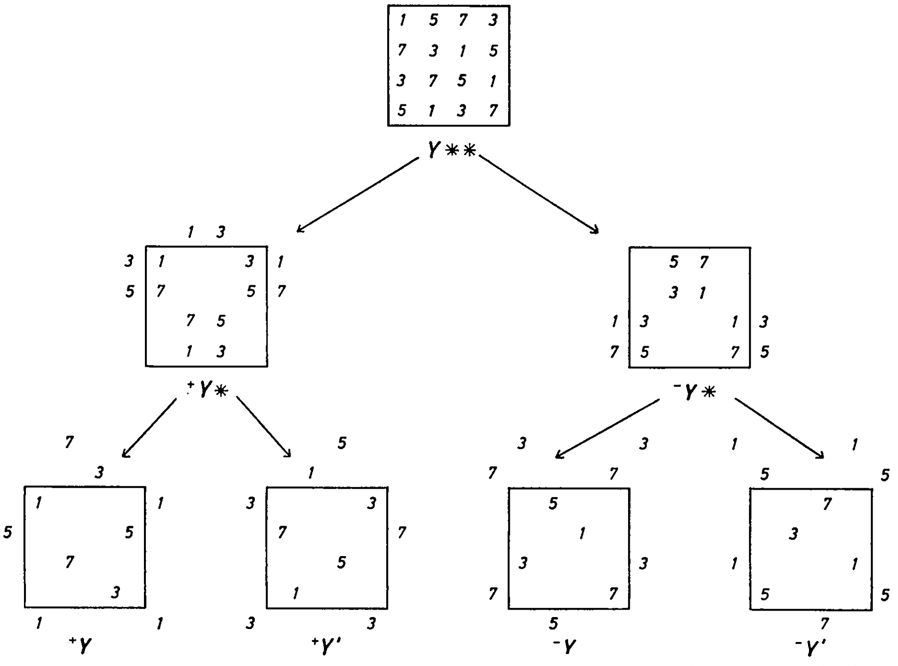

Fig. 3. Relations between the cubic lattice complex $Y^{**}$ and its splitting products (the numbers indicate the heights of the points in eighths).

complex: $P_2' = F'' + F'''$ [Fig. 1(*c*)]. It follows that we can describe the sphalerite type in four different ways:

Sphalerite type ZnS $Zn_4S_4$ $FF''$ or $FF'''$
or $F'F''$ or $F'F'''$ .

Likewise the NaCl type can be described as $FF'$ or as $F''F'''$.

In *Im*3*m*, a supergroup of *Pm*3*m*, the complexes $PP'$ and $JJ'$ unite in the following way: $P+P'=I$ and $J+J'=J^*$ (pronounced 'J star'). $I$ is a 2-pointer and $J^*$ a 6-pointer; together they form an 8-pointer, $P_2=I+J^*$ [Fig. 1(*b*)]. Two other invariant complexes, $P_2'$ and $W^*$ exist in *Im*3*m* with point symmetries $\bar{3}m$ and $\bar{4}m2$, respectively. Complex $W^*$ is a 12-pointer. In the subgroup *Pn*3*m*, $P_2'$ splits into $F''$ and $F'''$ [Fig. 1(*c*)], and in *Pm*3*n*, $W^*$ splits into $W$ and $W'$ [Fig. 1(*d*)].

Examples:

| | | | |
|---|---|---|---|
| $Pt_3O_4$ type | in *Im*3*m* | $Pt_6O_8$ | $J^*P_2'$ |
| $Mg_3P_2$ type | in *Pn*3*m* | $Mg_6P_4$ | $J^*F''$ |
| $Cu_2O$ type | in *Pn*3*m* | $O_2Cu_4$ | $IF''$ |
| β-W type | in *Pm*3*n* | $W_2W_6$ | $IW$ |
| $NaPt_3O_4$ type | in *Pm*3*n* | $Na_2Pt_6O_8$ | $IWP_2'$ |

While $W^*$, like all the other complexes discussed above, is a three-dimensional network, $W$ and $W'$ consist of sets of mutually perpendicular linear chains, which do not intersect. The shortest interatomic distance occurs along the chains; a larger interatomic distance is needed to go from chain to chain.

In *Fd*3*m* there exist $D$ and $T$ complexes; the two $D$ representations together form an $I_2$ $(=D+D')$ complex [Fig. 1(*e*)], whereas the two $T$ representations form an $F_2''$ $(=T+T')$ complex [Fig. 1(*f*)].

Examples:

| | | |
|---|---|---|
| Diamond type | $C_8$ | $D$ |
| NaTl type | $Na_8Tl_8$ | $DD'$ |
| Cristobalite type | $Si_8O_{16}$ | $DT$ |
| $MgCu_2$ type | $Mg_8Cu_{16}$ | $DT'$ |
| PtCu type | $Pt_{16}Cu_{16}$ | $TT'$ |
| Spinel type | $Mg_8Al_{16}O_{32}$ | $DT'F_2'''xxx$ |

In the spinel type the complex $F_2'''$ has one degree of freedom in the direction of the body diagonal, as indicated by $xxx$; the value of $x$ is close to $\frac{3}{8}$, which justifies this way of describing it.

Space group *Ia*3*d*, in which the four threefold axes do not intersect and, consequently, no cubic point symmetry occurs, is the last holosymmetric space group and has four invariant complexes. Three of them are new ones. Besides an $I_2$ in 16(*a*), we find another 16-pointer designated $Y^{**}$ and two 24-pointers, which get the symbols $S^*$ and $V^*$. The 16 equipoints of $Y^{**}$ constitute part of a theoretical $P_4'$ complex, which does not appear in space groups of the first order. The remaining part of $P_4'$ is $[P_4'-Y^{**}]$, which in *Ia*3*d* can occupy position 48(*g*) $\frac{1}{8}, x, \frac{1}{4}-x$, with $x=\frac{5}{8}=0{\cdot}625$. This splitting of the $P_4'$ is shown in Fig. 2(*a*).

Examples:

High-leucite type
$K[AlSi_2O_6]$ $K_{16}\{(Al_{1/3}Si_{2/3})O_{4/2}\}_{48}$
$Y^{**}[P_4'-Y^{**}]xx({\cdot}4g_c)$

Analcime type
$\left\{\begin{array}{l} Na[AlSi_2O_6]\,.\,H_2O \\ \{H_2O\}_{16}\{(Al_{1/3}Si_{2/3})O_{4/2}\}_{48}\{Na_{16/24}\}_{24} \end{array}\right.$
$Y^{**}[P_4'-Y^{**}]xx({\cdot}4g_c)V^*$

Garnet type
$Al_2Ca_3[SiO_4]_3$ $Al_{16}Ca_{24}\{SiO_4\}_{24}$ $I_2V^*S^*({\cdot}4s)$

Note that the $Y^{**}$ and the $[P_4'-Y^{**}]$ complexes are occupied by K and (Al, Si) in the high-leucite type, whereas in the analcime type the $H_2O$ and (Al, Si) fill these positions. In both structure types the O atoms form connected, distorted tetrahedra around the (Al, Si) atoms. The distorted and connected tetrahedra are symbolized by $({\cdot}4g_c)$†. The dot in front of the symbol indicates the presence of an atom inside the tetrahedron. In analcime the 16 Na atoms are located statistically on the 24-pointer $V^*$.

Note also that $S^*+V^*=W_2'$ [Fig. 2(*b*)]. Both positions are occupied in the garnet structure, one by Si and the other by Ca. Adding $I_2$, which is occupied by Al, we can consider the garnet structure a superstructure of the second order of the β-W type, which has the symbol $IW$. In addition, the O atoms form isolated tetrahedra around $S^*$, designated by $4s$† in view of the point symmetry $\bar{4}$ of $S^*$, forming a sphere packing by itself. The splitting of $V^*$ and $S^*$ into $^+V$, $^-V$, and $^+S$, $^-S$, respectively, is shown in Fig. 2(*b*). Fig. 3 explains the splitting of $Y^{**}$.

The few examples given above should show that lattice complexes are useful not only for the study of space groups, but also as a basis for a nomenclature of structure types.

## Derivation of cubic invariant lattice complexes

All space groups other than hexagonal can be derived as merosymmetric subgroups of $I_2m3m$. The invariant cubic complexes, which we have described above, occur in various space groups. As example let us consider (Table 2) all the space groups that can be derived from $I_2m3m$ by keeping the same holohedral point group *m*3*m* and changing the translation group from $I_2$ (16 points per cell) to $P_2$(8 points), $F$(4 points), $I$ (2 points), and $P$ (1 point). For all space groups the invariant complexes are listed, showing the splittings from one line to the next. In the third, fourth, and fifth row of Table 2, all ten space groups of the first order are listed, together with their lattice complexes.

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† $4s$ symbolizes a tetragonal distorted tetrahedron (tetragonal disphenoid) with the point symmetry $\bar{4}$.

$4g$ symbolizes a rhombical distorted tetrahedron (rhombic disphenoid) with the point symmetry 222.

Subindex $c$ indicates that the polyhedra are connected, having corners in common.

*Pm*3*m* can be derived as a hemisymmetric subgroup of *Im*3*m* and as a tetartosymmetric subgroup of *Fm*3*m*. In the first case, complexes *I* and $J^*$ split into *PP*′ and *JJ*′, whereas $P_2'$ and $W^*$ become the monovariant lattice complexes $8(g)xxx$ and $12(h)x\frac{1}{2}0$, which are not listed. With $x=\frac{1}{4}$ the latter become the configuration of $P_2'$ and $W^*$, respectively. In the second case (going from *Fm*3*m* to *Pm*3*m*), *F* and *F*′ split into *PJ* and *P*′*J*′ respectively; while $P_2'$ and $J_2$ acquire degrees of freedom: $P_2'$ in the same way as in the transition from *Im*3*m* to *Pm*3*m*, $J_2$ becoming $12(i)0xx$ and $12(j)\frac{1}{2}xx$, two monovariant complexes which coalesce in $J_2$ for $x=\frac{1}{4}$.

Consider now the other system-symorphic subgroups of *Im*3*m*, namely *Pn*3*m*, *Pm*3*n*, and *Pn*3*n*. The *I* complex remains *I* in all three. Besides, all the invariant complexes are the same in *Pn*3*n* as in *Im*3*m*†. In *Pn*3*m*, $P_2'$ splits into *F*″ and *F*‴, while in *Pm*3*n*, $W^*$ splits into *W* and *W*′. Important structures crystallize in these two space groups.

For the derivation of the *F* and *I* space groups in the holohedral point group (Table 2, row 2), we use $P_2m3m$, $P_2n3m$, and $P_2m3n$, which are subgroups of $I_2m3m$. With increasing order of the space groups, the order of the lattice complexes increase too.

In the hemisymmetric transition from $P_2m3m$ to *Fm*3*m*, the invariant complex $P_2$ splits into *F* and *F*′, $P_2'$ and $J_2$ remain unchanged, while $J_2'$ becomes a com-

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† In consequence we shall not find, in *Pn*3*n*, any structure type that occupies invariant or (and) monovariant complexes only. Only the trivariant complex $48(i)xyz$ is characteristic of the space group.

Table 2. *Space groups of the holohedral point group m3m derived from $I_2m3m$ and their invariant complexes*

Solid lines indicate hemisymmetry, dotted lines tetartosymmetry

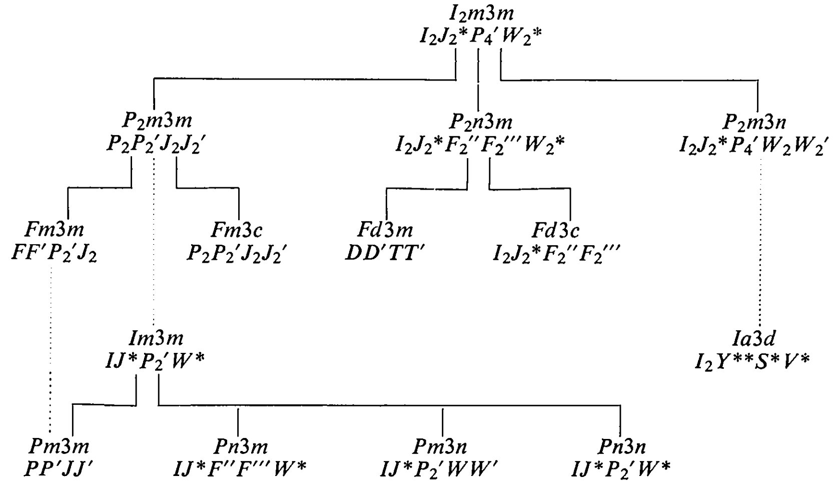

Table 3. *Coordination number N for different lattice complexes*

Each equipoint of a complex shown in the left column is surrounded by *N* equipoints of a complex given on the top row

| | *P* | *P*′ | *J* | *J*′ |
|---|---|---|---|---|
| *P* | 6 | 8 | 12 | 6 |
| *P*′ | 8 | 6 | 6 | 12 |
| *J* | 4 | 2 | 8 | 4 |
| *J*′ | 2 | 4 | 4 | 8 |

in *Pm*3*m*

| | *I* | $J^*$ | $P_2'$ | $W^*$ |
|---|---|---|---|---|
| *I* | 8 | 6 | 8 | 24 |
| $J^*$ | 2 | 4 | 8 | 4 |
| $P_2'$ | 2 | 6 | 6 | 6 |
| $W^*$ | 4 | 2 | 4 | 4 |

in *Im*3*m*

| | *D* | *D*′ | *T* | *T*′ |
|---|---|---|---|---|
| *D* | 4 | 4 | 4 | 12 |
| *D*′ | 4 | 4 | 12 | 4 |
| *T* | 2 | 6 | 6 | 6 |
| *T*′ | 6 | 2 | 6 | 6 |

in *Fd*3*m*

Table 4. *Examples of structure types and homeotypes*

| Chemical composition | Space group | Structural formula | Structure-type symbol |
|---|---|---|---|
| Cu | *Fm*3*m* | $Cu_4$ | *F* |
| $CO_2$ | *Pa*3 | $\{CO_2\}_4$ | $F(\cdot 2l)$ |
| NaCl | *Fm*3*m* | $Na_4Cl_4$ | *FF*′ |
| $FeS_2$ | *Pa*3 | $Fe_4\{S_2\}_4$ | $FF'(2l)$ |
| $Co(NH_3)_6TlCl_6$ | *Pa*3 | $\{Co(NH_3)_6\}_4\{TlCl_6\}_4$ | $F(\cdot 6o)\ F'(\cdot 6o)$ |
| $CaF_2$ | *Fm*3*m* | $Ca_4F_8$ | $FP_2'$ |
| $Zn(BrO_3)_2 . 6H_2O$ | *Pa*3 | $\{Zn(H_2O)_6\}_4\{BrO_3\}_8$ | $F(\cdot 6o)\ P_2'\ xxx(\cdot 3y)$ |
| $BiF_3$ | *Fm*3*m* | $Bi_4F_4F_8$ | $FF'P_2'$ |
| $KAl(SO_4)_2 . 12H_2O$ | *Pa*3 | $\{K(H_2O)_6\}_4\{Al(H_2O)_6\}_4\{SO_4\}_8$ | $F(\cdot 6o)\ F'(\cdot 6o)\ P_2'\ xxx(\cdot 4t)$ |

plex with one degree of freedom $24(e)x00$. Many structures crystallize in this space group (see Table 4). In $Fm3c$, on the other hand, all invariant complexes of $P_2m3m$ remain unchanged, as do four monovariant complexes, which are not listed in Table 2. This fact explains why $Fm3c$ is of minor importance in crystal chemistry.

In the hemisymmetric transition from $P_2n3m$ to $Fd3m$, two important splittings take place: $I_2=D+D'$ and $F_2''=T+T'$. Important structures, such as diamond, NaTl, PtCu, cristobalite, $MgCu_2$, and spinel crystallize in $Fd3m$, as shown above. In going from $P_2m3m$ to $Fd3c$, the complexes $I_2$, $J_2^*$, $F_2''$, and $F_2'''$ remain unchanged.

The two space groups $Im3m$ and $Ia3d$ are derived as tetartosymmetric subgroups from $P_2m3m$ and $P_2m3n$, respectively. The $P_2$ complex in $P_2m3m$ splits into $I$ and $J^*$ in $Im3m$, $P_2'$ remains unchanged, $J_2$ acquires one degree of freedom, and $J_2'$ splits into $W^*$ and the monovariant complex $12(e)x00$. During the tetartosymmetric reduction of $P_2m3n$ to $Ia3d$, the $I_2$ complex remains unchanged, $J_2^*$ gets one degree of freedom as $48(f)x0\frac{1}{4}$, $P_4'$ splits into $Y^{**}$ and a 48-pointer $48(g)\frac{1}{8}, x, \frac{1}{4}\text{-}x$; with $x=\frac{3}{8}$, $W_2$ can occur as the same 48-pointer with $x=\frac{1}{4}$, while $W_2'$ splits into two new invariant complexes $S^*$ and $V^*$.

The following rules hold true for a tetartosymmetric derivation of lattice complexes:

(1) If the number of equipoints of the complex remains the same in the subgroup as it was in the original group, the point symmetry has to be reduced in a tetartosymmetric way.

Example: Complex $I_2$ in $P_2m3n$ has point symmetry $m3$; in $Ia3d$ it has point symmetry $\bar{3}$.

(2) If the number $n$ of equipoints in the original group splits into $n/4+3n/4$ in the tetartosymmetric subgroup, the point symmetry remains unchanged in the $n/4$-pointer, but its order is divided by 3 in the $3n/4$-pointer.

Example: From $P_2m3n$ to $Ia3d$, the 64-pointer $P_4'$ with point symmetry 32 splits into the 16-pointer $Y^{**}$ with point symmetry 32 and the 48-pointer $[P_4'-Y^{**}]$ with point symmetry 2, which necessarily has one degree of freedom.

(3) If the number of equipoints is halved, the order of the point symmetry must also be halved.

Example: From $P_2m3n$ to $Ia3d$, the 48-pointer $W_2'$ with point symmetry $\bar{4}m2$ (order 8) splits into the 24-pointer $S^*$ with point symmetry $\bar{4}$ (order 4) and the 24-pointer $V^*$ with point symmetry 222 (order 4).

## Coordination number

C. Hermann gave the self-coordination (German: *Eigenkoordination*) of every invariant cubic complex, that is, the number of equipoints that surround any equipoint of the same complex: 12 for $F$, 8 for $I$, $J$, and $S$; 6 for $P$, $T$, and $Y$; 4 for $D$, $W^*$, $J^*$, $V$, and $S^*$; 3 for $Y^*$. We give examples of the coordination number of an equipoint of a complex surrounded by equipoints of the same complex or of another complex (Table 3).

## Coordination polyhedra

We will use the following symbols for coordination polyhedra needed in this paper:

| | |
|---|---|
| 2*l* | line segment collinear with the origin ('dumb-bell') |
| 3*y* | trigon (equilateral triangle), not coplanar with the origin |
| 4*t* | tetrahedron |
| 6*o* | octahedron |
| 8*c* | cube (hexahedron) |
| 8*r* | tetragonal prism + pinacoid |
| 8*l* | octagon coplanar with the origin |
| 12*co* | cuboctahedron (cube + octahedron, all edges equal) |
| 24*co* | truncated cube (cube truncated by octahedron) |
| 24*oc* | truncated octahedron (octahedron truncated by cube) |
| 24*cod* | rhombicuboctahedron (cube + octahedron + rhombdodecahedron) |

## Metrical description of the lattice complexes in a space group

Let us consider space group $Pm3m$. The first four positions can be defined by invariant complexes, as follows: $1(a)$: 000 by $P$, $1(b)$: $\frac{1}{2}\frac{1}{2}\frac{1}{2}$ by $P'$, $3(c)$: $\frac{1}{2}\frac{1}{2}0\curvearrowright$ by $J$, $3(d)$: $\frac{1}{2}00\curvearrowright$ by $J'$.

The next position is $6(e)$: $\pm x00\curvearrowright$, which is the normal representation of the monovariant complex $P6x$, discussed above with metrical description $P(6o)$ $J'(2l)$ and a sphere packing (SP) at $x=0{\cdot}293$. The next set of equivalent points, $6(f)$: $\pm x\frac{1}{2}\frac{1}{2}\curvearrowright$, has the same metrical properties as $6(e)$. The complex is $P6x$, but shifted by $\frac{1}{2}\frac{1}{2}\frac{1}{2}$; this fact could be emphasized by changing coordinates and writing $\frac{1}{2}+x'$ instead of $x$. Position $8(g)$ is named complex $P8xxx$, which forms a cube around $P$ or $P'$; and the sphere packing $P_2'$ at $x=0{\cdot}250$. In position $12(h)$: $\pm x\frac{1}{2}0\curvearrowright$, complex $J4x$ does not reach the origin as the parameter ranges from 0 to 0·5; a square (4*l*) appears as coordination polyhedron and the sphere packing $W^*$ is found at $x=0{\cdot}250$. In positions $12(i)$: $\pm 0xx\curvearrowright$, $\pm 0x\bar{x}\curvearrowright$ and $12(j)$: $\pm\frac{1}{2}xx\curvearrowright$, $\pm\frac{1}{2}x\bar{x}\curvearrowright$, complexes $P12xx$ and $P'12xx$ are related to each other like $P6x$ and $P'6x$; the new coordination polyhedron is a cuboctahedron (12*co*) around $P$ or $P'$; a sphere packing occurs at $x=0{\cdot}293$.

The metrical representation for the divariant lattice complex $P24yz$ in position $24(k)\,0yz$ is given in the plane $xy0$ in the asymmetric unit. The boundary lines of the two-dimensional asymmetric unit consist of representations of monovariant lattice complexes, explained in the drawing. The triangular two-dimensional asymmetric unit is divided by dashed lines into three parts, which are Niggli's symmetry regions (*Symmetrie-Bereiche*) around the three invariant complexes *P*, *J'*, and *J*. Sphere packing occurs at the point where the three symmetry regions meet, *i.e.* where the distances in the three different coordination polyhedra become equal; the parameters of this point are $x=0{\cdot}364$, $y=0{\cdot}186$. The coordination polyhedra, truncated octahedron (24*oc*), tetragonal prism and pinacoid (8*r*), and octagon (8*l*), surround the equipoints of *P*, *J'*, and *J*, respectively. The properties of position $24(l)\frac{1}{2}yz$ are identical with those of position $24(k)0yz$, except for a shift of $\frac{1}{2}\frac{1}{2}\frac{1}{2}$. This could be emphasized by changing coordinates and writing $y=\frac{1}{2}\pm y'$; $z=\frac{1}{2}\pm z'$, so that the position becomes $24(l)\frac{1}{2}$, $\frac{1}{2}+y'$, $\frac{1}{2}+z'$; this position does not appear on Fig. 4. The metrical representation for $24(m)P24xxz$ is quite different. The coordination polyhedra (8*r*) surround equipoints of *J* and *J'*. Two new polyhedra are around *P* (or *P'*), namely, the truncated cube (24*co*) and the rhombicuboctahedron (24*cod*). The parameters for sphere packing are $x=0{\cdot}146$, $z=0{\cdot}354$ and $x=0{\cdot}354$, $z=0{\cdot}146$.

The metrical description of the trivariant lattice complex has not been attempted on Fig. 4.

## Homeotype structures

Any structure type can be described by listing the lattice complexes that are occupied by atoms. Table 4 shows the simple types *F*, *FF'*, $FP'_2$ and $FF'P'_2$ for Cu, NaCl, $CaF_2$, and $BiF_3$, respectively; under each of these, one or two other structure types are listed, which have coordination polyhedra around the equipoints of the invariant complexes, whether the latter are occupied or not. These structure types are homeotypes of the simple types.

In the $CO_2$ structure, the C atoms occupy an *F* complex. Around each C, two O atoms form a 'dumbbell' (2*l*), that is to say, they are collinear with the C atom and equidistant from it. We speak of a 'centered dumbbell' and symbolize it (·2*l*). The dot inside the parenthesis indicates that an atom (here, C) occupies the midpoint of the coordination polyhedron (here, a

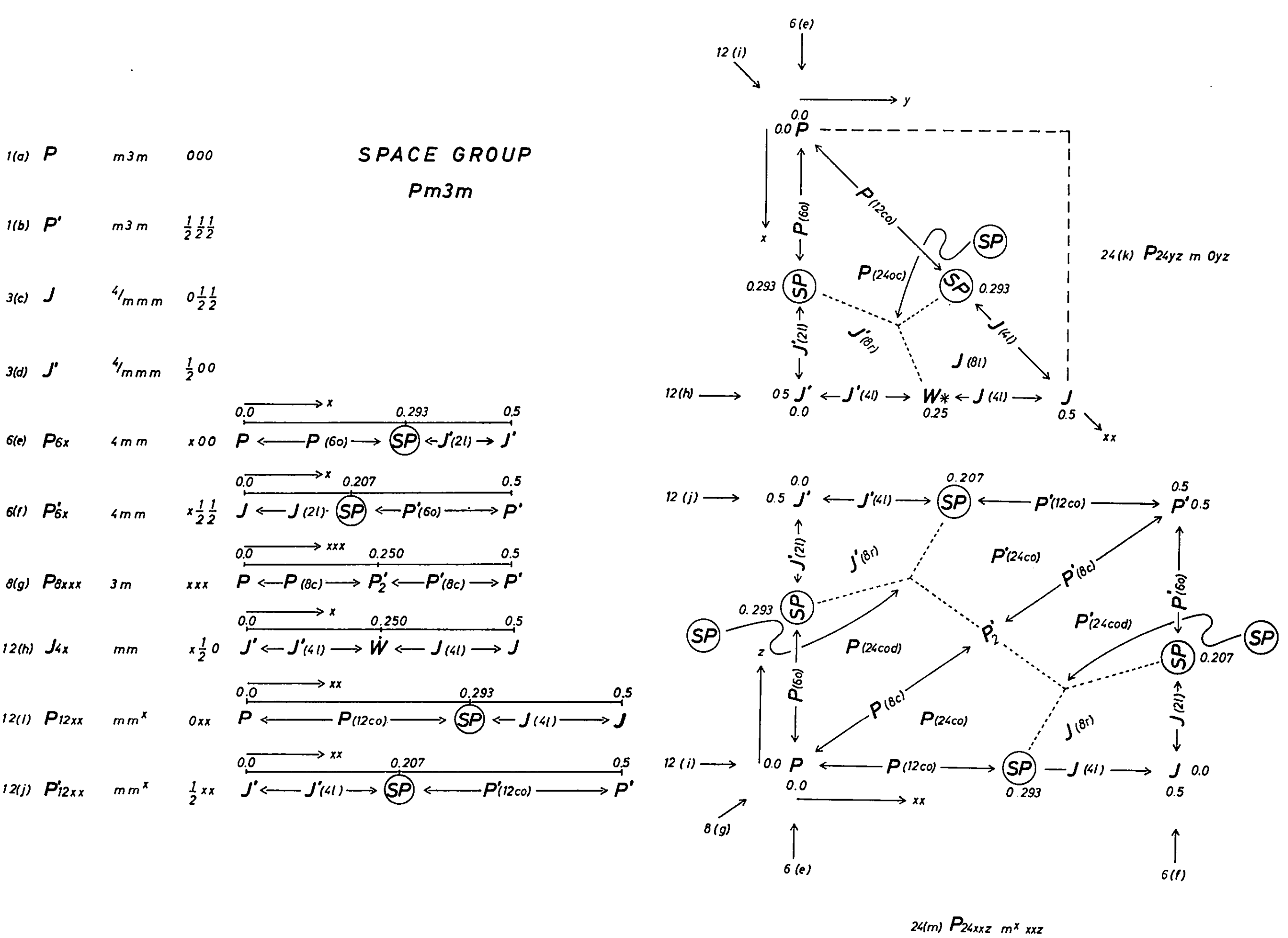

Fig. 4. Representation of the space group *Pm3m* including lattice complexes; the metrical description for mono- and divariant complexes is done with the aid of coordination polyhedra, which surround the invariant complexes. The special position for a sphere packing in each complex with degree of freedom is indicated by a circle labelled *SP*. ($\dot{W}\equiv W^*$).

line segment). The $CO_2$ structure type is designated $F(\cdot 2l)$; it is a homeotype of structure type $F$, in which Cu crystallizes. Likewise $FeS_2$ and $Co(NH_3)_6TlCl_6$ belong to homeotypes of the NaCl type, $FF'$. The $F$ complex occurs in two representations, both of which are occupied by isolated atoms in NaCl. In $FeS_2$ one of them is occupied by Fe atoms, the other by dumbbells formed by $S_2$ molecules. Note that the midpoint of the dumbbell is *not* occupied by any atom, so that the symbol is $F'(2l)$ and not $F'(\cdot 2l)$. In $Co(NH_3)_6TlCl_6$ both $F$ and $F'$ are occupied by 'centered octahedra' $(\cdot 6o)$.

In the structure of $Zn(BrO_3)_2 \,.\, 6H_2O$, which belongs to a homeotype of $FP'_2$ ($CaF_2$ type), six $H_2O$ molecules form an octahedron around Zn, while three O atoms form a trigon $(3y)$, which is not coplanar with Br, but together with Br makes a trigonal pyramid. The Br atom has one degree of freedom $xxx$, but the parameter $x=0{\cdot}259$ is only slightly different from the ideal $x=0{\cdot}250$.

Finally, the alum structure belongs to a homeotype of $FF'P'_2$ ($BiF_3$ type), with water octahedra around K and Al in $F$ and $F'$, and a tetrahedron around S in the $P'_2$ position, which is monovariant with $x=0{\cdot}310$ (instead of $x=0{\cdot}250$).

To the six rules of Laves & Wallbaum (1944) we may add the following: structures in which the same complexes, in the same representations, are occupied by discrete coordination polyhedra (centered or not) are homeotypes of the simpler structure in which the complexes are occupied by individual atoms.

The nomenclature proposed in this paper is the result of the many discussions I had with C. Hermann over a period of several years. It is a natural outgrowth of his work on lattice complexes. In a way it can also be regarded as a continuation of the nomenclature of Laves, whose 'connection concept' is used, now expressed in terms of lattice complexes and coordination polyhedra.

I am greatly indebted to Professor F. Laves for the help and encouragement he gave me when I was first a student, then an assistant in his Institute.

Professor J. D. H. Donnay was kind enough to revise my manuscript.

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