A further reason to consider the $W^*[4t_c]$ configuration as an important building unit within the intermetallic phases discussed above is the following: there exists an interesting relation to many inorganic crystal structures (Koch & Hellner, 1980), for which the anions form a framework $W^*[4t_c]$ with nearly ideal tetrahedra centered by Si, Al, Be, *etc.*

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Nested Polyhedra Units: A Geometrical Concept for Describing Complicated Cubic Structures*

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Abstract

A method for describing cubic giant cells is proposed. The structures may be regarded as arrangements of nested polyhedra units, isolated or linked, centred at sites of high point symmetry. Five basic types of nested polyhedra units, taken from well known cubic structures are defined: α-Mn (29 atoms), BCC (27), γ-brass (26), Ca_3Ag_8 (26) and Ti_2Ni (22) as well as variants of two of them, the non-centred α-Mn unit (28 atoms) and the centred Ca_3Ag_8 unit (27 atoms). All seven units have a cubo-octahedron as the outermost polyhedron. Sixteen structures are described in this paper, among which some have more than 400 atoms in the unit cell. This purely geometric description has the advantage that it can be easily obtained from the atom coordinates. It further makes structural similarities evident and simplifies the task of visualizing and memorizing complicated cubic structures.

Introduction

In the course of our structural studies of rare-earth (or Y, Sc) alloys we have recently solved three crystal structures with large cubic unit cells: $Sm_{11}Cd_{45}$, $a = 21{\cdot}699\,(3)$ Å (Fornasini, Chabot & Parthé, 1978), $Sc_{11}Ir_4$, $a = 13{\cdot}350\,(4)$ Å (Chabot, Cenzual & Parthé, 1980*a*), and $Sc_{44}Os_7$, $a = 20{\cdot}771\,(5)$ Å with $Mg_{44}Rh_7$ type (Chabot, Cenzual & Parthé, 1980*b*). The diffi-

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* *Editorial note:* The similarity between this paper, the preceding paper by Hellner & Koch [*Acta Cryst.* (1981), A**37**, 1–6] and the following paper by Nyman & Hyde [*Acta Cryst.* (1981), A**37**, 11–17] has been recognized and they have been published together to give an indication of the activity in the field with which they are concerned.

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culties we encountered in trying to interpret and understand these complicated structures with their large number of atoms in the unit cell motivated us to look for a simplified geometrical description. We wish to report here on a method of structure description which can be applied to certain cubic structures with between 44 and 448 atoms in the unit cell. Although not all the structural details can be reproduced, the gain in simplicity is such that the structure descriptions are easily memorized.

Disregarding the differences between atoms, thus concentrating only on structure sites, some structures can be imagined as being built up from a limited number of nested polyhedra units centred at points of high symmetry. This particular approach led us to define seven simple geometrical units consisting of various inscribed regular or semiregular polyhedra, the outermost polyhedron always being a cubo-octahedron. The task of visualizing and memorizing the atom arrangement in a complicated structure thus reduces to the much simpler problem of knowing the types of nested polyhedra units present and their mutual arrangement. The spatial arrangement of the geometrical units is always very simple, corresponding for example to the NaCl, NaTl structure types or their ternary or quaternary ordered versions.

Nested polyhedra units used as basic building blocks

Seven polyhedra units have been used in the description of the 16 structure types discussed in this paper. These geometric units are defined from well known cubic structure types and we use their names to label the different unit types. The nested polyhedra in a unit, as listed in the legend to Fig. 1, are ordered with increasing distances from the unit centre to their vertices. The outermost polyhedron is always a cubo-octahedron because all structures to be discussed here are characterized by cubo-octahedral positions. It should be mentioned that the word 'nested' does not imply that the vertices of a polyhedron are necessarily inside the faces of the following one.

α-Mn *unit with* 29 *atoms* (*Fig.* 1*a*)

The unit consists of a central atom (C) surrounded by a truncated tetrahedron (TT) of 12 atoms. Above each of the centres of the four hexagonal faces of the TT are the four atoms of a tetrahedron (T). The distances from the unit centre to the TT and T vertices are in most cases similar, resulting in a Friauf polyhedron of 16 atoms. The surrounding cubo-octahedron (CO) of 12 atoms is distorted so that the square faces become rectangular in such a way that the four large triangular faces cap the atoms of the tetrahedron (T). Two such isolated nested polyhedra units are found in the unit cell of the α-Mn structure (Oberteuffer & Ibers, 1970).

Non-centred α-Mn *unit with* 28 *atoms* ['α-Mn(−C)']

Same as above; however, as a consequence of the absence of a central atom the tetrahedron becomes smaller than in the α-Mn unit.

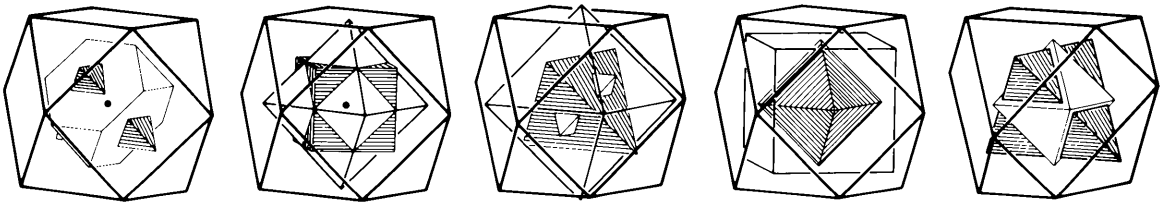
BCC unit with 27 *atoms* (*Fig.* 1*b*)

The atom at the unit centre (C) is surrounded by a cube (CB), which is occasionally split up into two tetrahedra of similar size (rotated by 90° from each other). Further away is an octahedron (OH) and still further a cubo-octahedron (CO). This sequence of nested polyhedra is typical for the body-centred-cubic structure of tungsten (BCC).

γ-*Brass unit with* 26 *atoms* (*Fig.* 1*c*)

This unit can be related to the BCC unit. Here there is no atom at the unit centre and, as a consequence, instead of an inner cube one finds a small inner tetrahedron (IT) and a larger outer tetrahedron (OT). Further away from the centre are the OH and the CO. The cubo-octahedron has square faces when a cube is present, as in the BCC unit, whereas it is deformed to have rectangular faces when two tetrahedra of different size replace the cube, as in the γ-brass unit.

Bradley & Jones (1933) first recognized this geometric unit in γ-brass phases and called it a cluster.



α-Mn unit
29 atoms
C+TT+T+CO
(*a*)

BCC unit
27 atoms
C+CB+OH+CO
(*b*)

γ-Brass unit
26 atoms
IT+OT+OH+CO
(*c*)

Ca_3Ag_8 unit
26 atoms
OH+CB+CO
(*d*)

Ti_2Ni unit
22 atoms
OH+T+CO
(*e*)

Fig. 1. Polyhedron construction of the five basic nested polyhedra units. For abbreviations used for different polyhedra see text.

Today, chemical significance having been attached to this term, it seems preferable to use the expression 'nested polyhedra unit'.

Ca_3Ag_8 *unit with* 26 *atoms* (*Fig.* 1*d*)

An OH is inscribed in a cube (CB) and the surrounding CO is undistorted. In Ca_3Ag_8 (Calvert & Rand, 1964) there are two identical units per body-centred cubic unit cell sharing corners of the cube along the cube diagonal.

Centred Ca_3Ag_8 *unit with* 27 *atoms* ['$Ca_3Ag_8(+C)$']

The addition of a central atom to the Ca_3Ag_8 unit does not seriously affect the relative distances from the unit centre to the surrounding polyhedra. This unit contains the same type of polyhedron as the BCC unit, but the order of the inner polyhedra is reversed.

Ti_2Ni *unit with* 22 *atoms* (*Fig.* 1*e*)

A central octahedron is surrounded by a tetrahedron and the enveloping CO thus has rectangular faces. This unit is one of the two fused units found in the Ti_2Ni structure type (Yurko, Barton & Parr, 1959).

It appears from this paragraph that only a small number of polyhedra types are necessary to define the seven nested polyhedra units. Five polyhedra have been used in all, among which three are regular polyhedra (tetrahedron, octahedron and cube), and two are Archimedean semi-regular polyhedra (truncated tetrahedron and cubo-octahedron). Each of these five types of polyhedra is formed by atoms belonging to one equipoint. The regular polyhedra are never distorted because they are always defined with only one adjustable parameter (tetrahedron or cube: xxx; octahedron: $x00$). The xxz equipoints define a perfect cubo-octahedron when $z = 0$ and a perfect truncated tetrahedron when $z = 3x$. As mentioned above, significant distortions occur for the cubo-octahedra in some units. Indeed, each time a tetrahedron or a truncated tetrahedron is present among the nested polyhedra the CO is distorted so that the square faces become rectangular ($z \neq 0$).

Spatial arrangement of nested polyhedra units in cubic structures

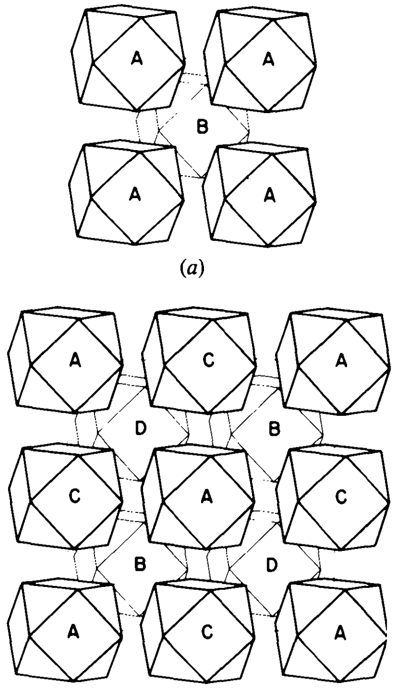
It is possible to distinguish between two groups of cubic structures depending on whether the structures can be described by means of an arrangement of isolated nested polyhedra units or an arrangement of linked units. In the first group the units have no atoms in common and consequently the number of atoms in the unit cell is equal to the sum of the number of atoms in each unit in the cell. In the second group, polyhedra of neighbouring units share atoms and in this case the calculation of the number of atoms in the unit cell is not straightforward.

Structures with isolated units

The spatial arrangements of the nested polyhedra units, presented by their outer cubo-octahedra only, are shown in Fig. 2.

A structure with only one type of unit will be body-centred cubic and will contain only two units in the cell. If the units are of different types or if they differ in atom distribution on the polyhedron sites, the unit cell may be (*a*) primitive with the same volume as above (Fig. 2*a*) or (*b*) face-centred cubic with a volume eight times as great (Fig. 2*b*). The units are centred at the points of high symmetry ($\bar{4}3m$, $m3m$ or 23) in the structure, *viz* at 0,0,0 and $\frac{1}{2},\frac{1}{2},\frac{1}{2}$ in the smaller I and P cells and at 0,0,0; $\frac{1}{4},\frac{1}{4},\frac{1}{4}$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$; $\frac{3}{4},\frac{3}{4},\frac{3}{4}$ [$+\frac{1}{2}\frac{1}{2}0$ ↻] in the larger F cell. With the Bravais lattice translations the whole structure can be easily derived from the sequence of the geometric units along the cube diagonal. The characteristic sequences (AB in Fig. 2*a* and $ABCD$ in Fig. 2*b*) for nine structures are given in Table 1.

V_5Al_8, Cu_9Al_4 and $Cu_{41}Sn_{11}$ are all γ-brass phases and are built up exclusively from γ-brass units. Their



(*a*)

(*b*)

Fig. 2. Arrangement of isolated nested polyhedra units in cubic structures with (*a*) P (I when $A = B$) and (*b*) F Bravais lattices. Only the outer cubo-octahedra are shown. In (*b*) only units in front (heavy lines) and those $\frac{1}{4}$ of a translation behind (thin lines) are drawn.

only difference lies in the site occupation of the nested polyhedra units which leads to structures with *I*, *P* and *F* Bravais lattices respectively.

Considering the nested polyhedra units like pseudo-atoms we can further characterize the structures by the structure-type name of the pseudo-atom arrangement, for example W or CsCl type for the structures with small unit cells or NaTl, BiF_3 or Cu_2MnAl type for structures with larger face-centred unit cells.

Structures with linked units

Structures described by means of linked nested polyhedra units are listed in Table 2. Phases with an *F* Bravais lattice contain eight geometric units per cell while only two are present in the *I* cell of Ca_3Ag_8. For each of the face-centred structures the characteristic sequence of nested polyhedra units can be found along the cube diagonal as well as in the direction parallel to the crystallographic axes. The units are in general linked along ⟨100⟩. The unit symbols which describe a sequence are joined by a hyphen to indicate connections between polyhedra. Two polyhedra, shared between neighbouring units, are always of the same type.

Except for Ca_3Ag_8, VAl_{10} and $Mg_3Cr_2Al_{18}$, the characteristic geometric units share square (or rectangular) faces of their cubo-octahedra (perpendicular to the crystallographic axes). This spatial arrangement of the cubo-octahedra – resulting in a cubo-octahedral framework – is shown in Fig. 3. Depending on the type of nested polyhedra units involved, other inner polyhedra are also shared with the corresponding polyhedra in their neighbouring units

Table 1. *Structures described by an arrangement of isolated nested polyhedra units*

Asterisks are used to differentiate, within a structure, between units which differ only in the atom distribution on the polyhedra sites.

Structure type	Pearson symbol	*a* (Å)	Space group	Point symmetry at unit centres	Unit sequence along the cube diagonal *A*	*B*	*C*	*D*	Reference
V_5Al_8	*cI*52	9·23	$I\bar{4}3m$	$\bar{4}3m$	γ-brass,	γ-brass			(*a*)
Cu_9Al_4	*cP*52	8·70	$P\bar{4}3m$	$\bar{4}3m$	γ-brass,	γ-brass*			(*b*)
Tl_7Sb_2	*cI*54	11·62	$Im3m$	$m3m$	BCC,	BCC			(*c*)
α-Mn	*cI*58	8·91	$I\bar{4}3m$	$\bar{4}3m$	α-Mn,	α-Mn			(*d*)
Mg_6Pd	*cF*396	20·11	$F\bar{4}3m$	$\bar{4}3m$	γ-brass,	Ti_2Ni,	α-Mn,	Ti_2Ni	(*e*)
$Mg_{44}Rh_7$	*cF*408	20·15	$F\bar{4}3m$	$\bar{4}3m$	γ-brass,	γ-brass*,	α-Mn (–C),	Ti_2Ni	(*f*)
$Cu_{41}Sn_{11}$	*cF*416	17·98	$F\bar{4}3m$	$\bar{4}3m$	γ-brass,	γ-brass*,	γ-brass**,	γ-brass***	(*g*, *h*)
$Li_{22}Pb_5$	*cF*432	18·75	$F23$	23	BCC,	BCC*,	BCC*,	BCC	(*i*)
$Sm_{11}Cd_{45}$	*cF*448	21·70	$F\bar{4}3m$	$\bar{4}3m$	BCC,	α-Mn,	α-Mn*,	BCC*	(*j*)

References: (*a*) Brandon, Pearson, Riley, Chieh & Stokhuyzen (1977). (*b*) Arnberg & Westman (1978). (*c*) Stokhuyzen, Chieh & Pearson (1977). (*d*) Oberteuffer & Ibers (1970). (*e*) Samson (1972). (*f*) Westin & Edshammar (1971). (*g*) Arnberg, Jonsson & Westman (1976). (*h*) Booth, Brandon, Brizard, Chieh & Pearson (1977). (*i*) Zalkin & Ramsey (1958). (*j*) Fornasini, Chabot & Parthé (1978).

Table 2. *Structures described by an arrangement of linked nested polyhedra units*

The link is symbolized by a hyphen and the superscript ^{m} is used to indicate that a unit is related to the preceding one by a mirror plane. In the case of Ti_2Ni, VAl_{10} and $Mg_3Cr_2Al_{18}$ the nested polyhedra units are centred on one half of each of the two eightfold point positions (8*a* and 8*b*) with $\bar{4}3m$ point symmetry. As for all other structures listed here the two characteristic units of a sequence are separated by $\frac{1}{2}\frac{1}{2}\frac{1}{2}$.

Structure type	Pearson symbol	*a* (Å)	Space group	Point symmetry at unit centres	Unit sequence along cube diagonal *A* *B*	Polyhedra sharing atoms with neighbouring units	Directions in which the units are linked	Number of interstitial atoms	Reference
Ca_3Ag_8	*cI*44	9·81	$Im3m$	$m3m$	$Ca_3Ag_8 - Ca_3Ag_8$	CB	⟨111⟩	–	(*a*)
Ti_2Ni	*cF*96	11·78	$Fd3m$	$\bar{4}3m$	Ti_2Ni – γ-brass	CO,OH	⟨100⟩	–	(*b*)
$Cr_{23}C_6$	*cF*116	10·65	$Fm3m$	$\bar{4}3m$	α-Mn – α-Mn^m	CO,TT	⟨100⟩	4	(*c*)
Th_6Mn_{23}	*cF*116	12·52	$Fm3m$	$\bar{4}3m$	γ-brass – γ-brass^m	CO,OH	⟨100⟩	4	(*d*)
				or					
				$m3m$	Ca_3Ag_8 – BCC	CO,OH		–	
$Sc_{11}Ir_4$	*cF*120	13·35	$Fm3m$	$\bar{4}3m$	γ-brass – γ-brass^m	CO,OH	⟨100⟩	8	(*e*)
				or					
				$m3m$	Ca_3Ag_8(+C) – BCC	CO,OH		–	
VAl_{10}	*cF*176	14·49	$Fd3m$	$\bar{4}3m$	[α-Mn(–C) –], Ti_2Ni	CO	⟨110⟩	–	(*f*)
$Mg_3Cr_2Al_{18}$	*cF*184	14·55	$Fd3m$	$\bar{4}3m$	(α-Mn –), Ti_2Ni	CO	⟨110⟩	–	(*g*)

References: (*a*) Calvert & Rand (1964). (*b*) Yurko, Barton & Parr (1959). (*c*) Westgren (1933). (*d*) Florio, Rundle & Snow (1952). (*e*) Chabot, Cenzual & Parthé (1980*a*). (*f*) Brown (1957). (*g*) Samson (1954).

(OH or TT, see Table 2). The octahedra share vertices in the ⟨100⟩ directions. In $Cr_{23}C_6$, neighbouring truncated tetrahedra share edges lying in the rectangular faces common to the linked cubo-octahedra. For some structures, two different descriptions have been given depending on the point-symmetry sets chosen as centres of the nested polyhedra units. Additional atoms may be necessary in some cases to describe the whole structure. These 'interstitial' atoms (see Table 2) are located in the octahedral holes formed in the cubo-octahedral framework.

In the Ca_3Ag_8 structure neighbouring Ca_3Ag_8 geometric units are shared only by the vertices of their CB polyhedron (see Table 2) along ⟨111⟩.

In VAl_{10} the characteristic sequence consists of α-Mn(−C) and Ti_2Ni units. In this structure the linkage does not occur between two different geometric units, as in the other compounds listed in Table 2, but between identical α-Mn(−C) units. Each unit is connected to twelve others along ⟨110⟩ by the 12 vertices of the outer CO resulting in a cubo-octahedral framework, which is exactly the same as the framework shown in Fig. 3. If from the drawing we assume the α-Mn(−C) units to be in *A* positions, the remaining *B* sites correspond to cubo-octahedral holes in which are the Ti_2Ni units. Due to the presence of the Ti_2Ni units in the holes, the cubo-octahedra forming the framework are strongly distorted. The polyhedron description of the structure of $Mg_3Cr_2Al_{18}$ is identical to the description of VAl_{10} except that the α-Mn(−C) units are replaced by α-Mn units.

Discussion

No grave difficulties have been encountered during the search for nested polyhedra units in the structures listed in Tables 1 and 2. As a general rule, all atoms inside the outer cubo-octahedron belong to the unit in question. However, the atoms situated in the space limited by the faces of the cubo-octahedron and the sphere circumscribing it are considered to belong to the unit only if they are needed to complete one of the basic nested polyhedra units, if not they belong to another unit. Except for four cases [the α-Mn(−C) unit in $Mg_{44}Rh_7$ and VAl_{10}, the α-Mn unit in Mg_6Pd and $Mg_3Cr_2Al_{18}$] all the atoms inside the sphere belong to the same unit.

It is of interest to compare the nested polyhedra units of the same type found in the different structures listed in Tables 1 and 2. For this purpose the relative distances from the vertices of the different polyhedra to the unit centre, normalized so that $r_{CO} = 1$, have been studied. As an example the r/r_{CO} values for some γ-brass units are shown in Fig. 4, three being found in structures with isolated nested polyhedra and three from structures with linked polyhedra units. Variations in the relative distances may be due to different site occupations, to differences in radii between atoms and to the environment of the unit itself. In the α-Mn unit, the distances from the T and TT to the unit centre are similar, the T in some structures being an inner and in others an outer tetrahedron. Such an inversion in the sequence of the internal polyhedra has only been found with the α-Mn unit.

The structure description based on nested polyhedra units differs from a description of cubic structures proposed recently by Chieh (1979). This author divides the space of any cubic cell into congruent Archimedean truncated octahedra, centred at sites of high point symmetry, which fill the entire space. Only in exceptional cases are atoms at the vertices of these polyhedra, the division having been made strictly on geometrical grounds. The atoms inside a truncated octahedron are considered to form a geometric unit. Chieh's definition of which atoms belong to a given unit is precise but it is precisely this rigid definition of a unit which makes it difficult to recognize similarities between structures. Atoms close to the outer limit of Chieh's truncated octahedron may, after a small

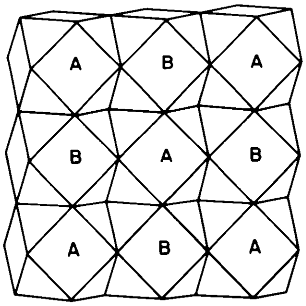


Fig. 3. Arrangement of linked nested polyhedra units for the structures listed in Table 2 except for Ca_3Ag_8, VAl_{10} and $Mg_3Cr_2Al_{18}$. Only the linked cubo-octahedra are drawn and only for the polyhedra units in the front half of the unit cell.

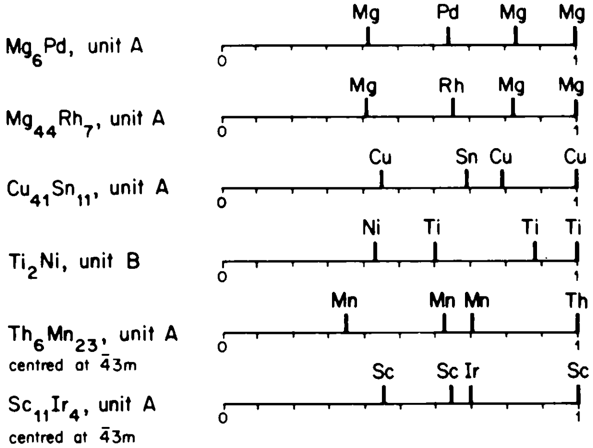


Fig. 4. r/r_{CO} values for six different γ-brass units from six different structures, three with isolated and three with linked nested polyhedra units. The sequence with increasing r/r_{CO} values is for all of them IT, OT, OH and CO.

change of their positional coordinates, have changed their affiliation, thus belonging to another unit.

Conclusion

It follows from this study that the notion of nested polyhedra units is a purely geometrical concept. It should be emphasized that the interatomic distances within a unit are not necessarily shorter than those between units. Further, the nested polyhedra units must not be confused with the coordination polyhedra which are defined around the atoms. This geometric description offers nevertheless great advantages for structures with high symmetry. As each polyhedron is formed by atoms from one equipoint, it is possible to find rapidly the type of polyhedron, as well as its centre, from the atom coordinates. Further, since all the nested polyhedra are simple and have the same centre, the structure can be visualized and memorized more easily than from descriptions based on arrangements of smaller polyhedra sharing vertices, edges and/or faces. The nested polyhedra concept can thus be useful to describe in a condensed way, and to compare, apparently complicated cubic structures containing a large number of atoms in the unit cell.

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The Related Structures of α-Mn, Sodalite, Sb_2Tl_7, *etc.**

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Abstract

The sodalite structure can be regarded as a three-dimensional framework of corner-connected tetrahedra. By tilting the tetrahedra through various angles equivalent frameworks in the structures of α-Mn, sodalite and Sb_2Tl_7 are obtained. The complete structures are obtained by filling the large interstices in these frameworks with various atom groups.

Introduction

In an earlier paper (Nyman, Andersson, Hyde & O'Keeffe, 1978) rather complicated structures, *e.g.* VAl_{10}, W_3Fe_3C and Ti_2Ni, were described as pairs of simple interpenetrating frameworks. By the same

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* *Editorial note:* The similarity between this paper and the two preceding papers, by Hellner & Koch [*Acta Cryst.* (1981), A**37**, 1–6] and by Chabot, Cenzual & Parthé [*Acta Cryst.* (1981), A**37**, 6–11], has been recognized and they have been published together to give an indication of the activity in the field with which they are concerned.

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