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Structures Based on the 3-Connected Net 10^3-b*

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The net 10^3-b, one of the two simplest 3D 3-connected nets, is a periodic network of 3-connected points in which all the shortest circuits are 10-gons. Some configurations of this net are described, and examples are given of structures based on the net, in particular those formed from tetrahedral or octahedral coordination groups each joined to three other similar groups by sharing appropriate numbers of X atoms. Structures in which each X atom is 2-connected may be constructed from tetrahedral AX_4 groups (AX_2 and A_2X_5) and from octahedral AX_6 groups (AX_3, A_2X_7, AX_4, and A_2X_9). At present, however, examples are known only of A_2X_5 structures.

Introduction

In a periodic three-dimensional net in which each point is connected to the same number (p) of others the minimal value of p is 3 (3-connected net). A net may be described in terms of the shortest circuits which start from a point along any one link and return along another link. In a 3-connected net there are three ways of selecting two of the links which meet at any point, and we must therefore specify three circuits. If these are all n-gons ("uniform" net) the net symbol is n^3 (or n,3), and uniform nets are known in which $n = 7$, 8, 9, 10, or 12 (*1*). These nets are the 3D homologs of the regular solids, 3^3 (tetrahedron), 4^3 (hexahedron or cube), and 5^3 (pentagonal dodecahedron), and the plane net 6^3, but whereas for $n \lesssim 6$ there is a single solution this is not so for $n > 6$. Any periodic 3D net is generated by the repetition along three noncoplanar axes of a repeat unit which consists of Z_t points. In a 3-connected net Z_t must be an even number and the minimal value is 4. There are two 3-connected nets with this value of Z_t, 10^3-a and 10^3-b, and in their most symmetrical configurations both are referable to body-centered lattices and have 8 points (Z_c) in the unit cell. Table I also includes data for the net 10^3-c, to which we refer later.

A uniform net may be further characterized by the values of ${}^nx$, the number of different n-gon circuits to which a point belongs, and the values of ${}^ny$, the number of n-gon circuits to which a link belongs. The value of ${}^nx$ is not necessarily the same for all points of a uniform net, and ${}^ny$ may have different values for different links. The net 10^3-a is unique among 3D 3-connected nets in having not only all points equivalent but also all links equivalent (Table I). In 10^3-b all points are equivalent but one-third of the links, those parallel to the tetragonal c axis, have ${}^{10}y = 8$ while the remainder have ${}^{10}y =$

* Dedicated to Dr. M. J. Sienko.

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TABLE I

	Z_t	^{10}x	^{10}y	(y_{mean})	Most symmetrical configuration	Density as sphere packing
10^3-a	4	15	10	30/3	8(a) in $I4_132$, $(\frac{1}{8}\ \frac{1}{8}\ \frac{1}{8})$	0.185
10^3-b	4	10	8,6,6	20/3	8(a) in $I4_1/amd$, $(0\ 0\ \frac{1}{12})$	0.233
10^3-c	6	5	4,3,3	10/3	6(c) in $P3_112$, $(\frac{1}{3}\ \frac{1}{6}\ \frac{1}{9})$	0.269

6. We shall confine our attention here to the net 10^3-b, the most symmetrical configuration of which is shown in Fig. 1. We shall note compounds whose structures are based on this net and also a number of structures which have not yet been assigned to actual compounds.

Configurations of the Net 10^3-b

In the most symmetrical configuration (Fig. 1) all links have equal length and all interbond angles are 120°. As an open packing of equal spheres this has a density of only 0.233. Reduction of all the bond angles to 90° produces the configuration of Fig. 2d, in which the positions of the points are those of the simple cubic lattice, and the density is therefore 0.524. Taking account of the positions of the bonds the space group of this configuration is $C2/c$. This form of the net is obviously not of interest as the structure of an element since an atom would be equidistant from six others but bonded to only three, though we might note in this connection the structure of ice-VII (or -VIII) in which an oxygen atom is equidistant from 8 others in a body-centered structure but hydrogen-bonded to only 4 of them. However, this configuration is of interest as the form of the net underlying the structure of $La_2Be_2O_5$, which has this space group. Also of interest are a number of configurations with densities intermediate between those of the above configurations. The tetragonal form of the net can be "sheared" by rotations about one-third of the links, those parallel to the c axis. In this way the density, as a sphere packing, may be increased to 0.421, at which point the net is no longer 3- but 5-connected and has a density between those of the (4-connected) diamond net (0.338) and the (6-connected) simple cubic packing (0.524). In sheared forms the links meeting at any point remain coplanar and the bond angles remain 120°. The 8-point tetragonal cell becomes non-orthogonal but the net may be referred to an all-face-centered orthorhombic cell (Fig. 3). Just as cubic diamond (Z_c = 8, $Fd3m$) may be referred to a body-centered tetragonal cell (Z_c = 4, $I4_1/amd$) so conversely we may refer 10^3-b (Z_c = 8, $I4_1/amd$) to an all-face-centered orthorhombic cell (Z_c = 16, $Fddd$). We shall note later this relationship

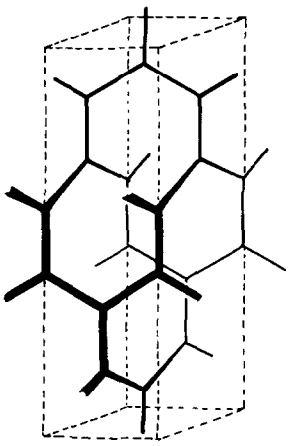


FIG. 1. The most symmetrical configuration of the net 10^3-b.

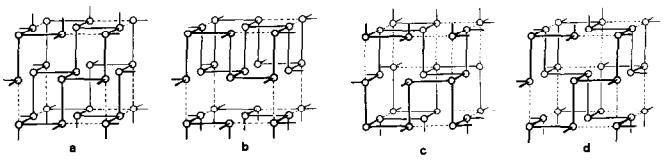


FIG. 2. (a) and (b) Relation of As and black P layers to the primitive cubic lattice; (c) and (d) relation of 90° configurations of 10^3-a and 10^3-b to the same lattice.

in connection with the structures of P_2O_5, $(Zn_2Cl_5)(H_5O_2)$, and GeS_2.

One configuration of the sheared 10^3-b net, with interaxial angle 109.5° instead of 90°, has the special property that its points are in one-third of the positions of cubic closest packing, corresponding to the breakdown of the cubic F net into three interpenetrating 10^3-b nets. Hexagonal closest packing also breaks down into three interpenetrating 10^3-b nets, but in this case the links from each point are not coplanar. The density of these configurations of the net is accordingly 0.247, one-third of that of closest packing of equal spheres; they are shown in projection in Fig. 4.

Structures Based on the Net 10^3-b

Since a structure consisting only of single atoms at the points of the net is unlikely to be formed owing to its very low density we have to consider how the density may be increased. This could be done in a number of ways, for example, by shearing the structure, by reducing the interbond angles, by the interpenetration of two or more nets, or by incorporating other atoms in the interstices of the net. The first possibility has been briefly explored for a hypothetical "metallic" form of carbon (*2*), this type of structure being suggested by the close relation of the 6^3 layer of graphite to the 10^3-b net. The polymorphs of elementary phosphorus exhibit a considerable range of interbond angles (down to 60°, assuming linear P–P bonds in the tetrahedral molecule of white P). If the 6^3 layer structures of As and black P are represented with interbond angles of 90° they are related to the simple cubic lattice as shown in Figs. 2a and b. Both the 10^3-a and 10^3-b nets may be derived from the same lattice in a similar way (Figs. 2c and d) by omitting different sets of

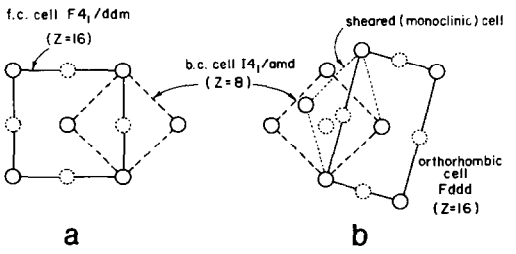


FIG. 3. (a) Relation between F and I cells of 10^3-b projected on (001). Dotted circles represent points c/2 above (below) the plane of the paper. (b) Relation of the body-centered cell of the sheared configuration of 10^3-b (broken lines) to the all-face-centered orthorhombic cell (full lines).

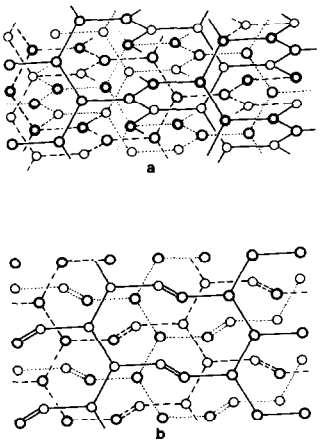


FIG. 4. Breakdown of (a) cubic and (b) hexagonal closest packing of equal spheres into three interpenetrating 10^3-b nets.

links. However, although the layer structures are known the 3D structures of this type with (3 + 3)-coordination are geometrically impossible; in fact, phosphorus has a high-pressure (high-temperature) form with the arsenic structure and also a metallic cubic form, with (3 + 3)- and 6-coordination, respectively.

The tetragonal structure of Fig. 1 (or a slightly distorted variant) forms the framework of Si atoms in a number of 4*f* and 5*f* disilicides and also in HP forms of $CaSi_2$ and $SrSi_2$; the metal atoms (ions) occupy the large interstices at (000), $(\frac{1}{2}\ \frac{1}{2}\ \frac{1}{2})$, $(\frac{1}{2}\ 0\ \frac{3}{4})$, and $(0\ \frac{1}{2}\ \frac{1}{4})$. The alkaline-earth disilicides form an interesting group, for including their HP polymorphs they provide examples of the simplest finite, 2D, and 3D 3-connected structures:

	3^3	6^3	10^3-a	10^3-b
$CaSi_2$		x		x
$SrSi_2$			x	x
$BaSi_2$	x	x	x	

Of these compounds $SrSi_2$ is of special interest as crystallizing with both of the two simplest 3D 3-connected nets, though in each case the structure is slightly distorted from the most symmetrical configuration. Although there are 4_1 axes in both 10^3-a and 10^3-b the helix in 10^3-a is a simple one, repeating after 4 atoms, whereas in 10^3-b the screw axis operates on a pair of atoms so that there are 8 atoms in the repeat unit. Conversion of one net into the other therefore involves not only rearrangement of the atoms within a helix but also the breaking and reforming of one-third of the links, those connecting the helices (*3*). A recent addition to the list of structures based on 10^3-b is that of LaPtSi (and the isostructural Ce, Pr, Nd, Sm, and Gd compounds), in which Pt and Si atoms occupy alternate positions in the net (*4*). This structure is possible because Pt–Si, 2.43 Å (mean) is virtually the same as Si–Si in the disilicides, in fact identical to the value in $BaSi_2$-II.

The ordered version of the net for a compound AX is unlikely to form because of its low density; accordingly BN forms the same 6^3 layer as graphite but, like carbon, adopts the 4-connected diamond type of net instead of a 3D 3-connected net. We shall now show that the whole range of structures: A_2X_3, AX_2, A_2X_5, AX_3, A_2X_7, AX_4, and A_2X_9, can be built from coordination groups AX_3, AX_4, or AX_6 which have their A atoms at the points of the 10^3-b net. In all the tetrahedral and octahedral structures to be described the coordination groups share some or all of their *X* atoms with other groups, and a shared *X* atom is common to *two* such groups only. If a shared *X* atom is common to *three* coordination groups both *A* and *X* are 3-connected and must be treated as together forming a 3-connected net. The simplest example is the BN layer, and the PtSi framework of LaPtSi is the simplest example of a 3D structure regarded as formed from AX_3 (here $PtSi_3$) groups in this way. The structures formed from tetrahedral AX_4 or octahedral AX_6 groups each having three *X* atoms common to three such groups would have the formulas AX_2 or AX_4, since the $X:A$ ratios would be $(1 + 3(\frac{1}{3}))$ and $(3 + 3(\frac{1}{3}))$, respectively. The (layer) structure of AlOCl (and GaOCl) is of this kind, but we have not been able to build the corresponding 3D AX_2 or AX_4 structures from regular tetrahedral or octahedral groups based on the 10^3-b net. We therefore confine our attention here to structures in which all *X* atoms are 2-coordinated.

Structures of composition A_2X_3 arise by the sharing of each *X* atom of each AX_3 group with one other group, which is equivalent to placing an *X* atom on each link of a 3-connected net of *A* atoms. Layer structures include those of As_2O_3 and As_2S_3, but the only 3D structure appears to be that of B_2O_3. This is based, not on one of the two

simplest 3D 3-connected nets but on 10^3-c, while the sulfide, B_2S_3, crystallizes with a layer structure. Here also the structure is not of the simplest possible topological type, for some of the BS_3 groups share edges to form 4-membered B_2S_2 rings.

Salts $MH_3(SeO_3)_2$ provide examples of structures based on 3-connected nets, for with a $H:SeO_3$ ratio of 3:2 each SeO_3 group can form hydrogen bonds to three others. The anion in the Li salt consists of chains in which each SeO_3 is hydrogen-bonded to *two* others, by a single and a double bridge, but the Na salt forms layers based on 6^3 while the structures of the Rb and NH_4 salts (5) are based on 10^3-b. The lengths of the Se–O bonds (1.66 and 1.75 Å) indicate nonequivalence of the Se atoms and formulation as $NH_4(H_2SeO_3)(HSeO_3)$.

We now come to structures formed from tetrahedral or octahedral groups sharing some or all of their vertices (*X* atoms). The *highest* $X:A$ ratio for a tetrahedral structure based on a 3-connected net obviously results from the sharing of three 2-connected vertices, when the formula is A_2X_5; the corresponding limit for an octahedral structure is A_2X_9. The *lowest* $X:A$ ratio for an octahedral structure based on a 3-connected net is apparently 3, and AX_3 structures based on 10^3-b can be formed by the sharing of three edges or of one vertex, one edge, and one face. The tetrahedral and octahedral structures based on 10^3-b accordingly form the complete series of Table II, though examples appear to be known only of the A_2X_5 structure.

Tetrahedral Structures

In a short survey of AX_2 structures that can be built from tetrahedral AX_4 groups (6) the following restrictions were introduced. It must be possible to build a structure from regular tetrahedra all of which share their vertices or edges in the same way, and all distances between *X* atoms of different tetrahedra must be at least as great as *X*–*X* within an AX_4 group (i.e., the edge length). The structures were classified according to the coordination numbers (x) of the *X* atoms. If v_x is the number of *X* atoms of each AX_4 group that are bonded to x *A* atoms in a structure of composition A_mX_n then $\Sigma v_x = 4$ and $\Sigma(v_x/x) = n/m$. For some compositions (for example, AX_4, A_2X_7, and AX_3) there is

TABLE II

TETRAHEDRAL AND OCTAHEDRAL STRUCTURES BASED ON 10^3-b

	C.N. of *A*	Number of shared *X* atoms	Vertices (v), or edges (e) shared	Packing of *X* atoms	Figs. 9 and 10
AX_2	4	4	$2v$ $1e$		
A_2X_5		3	$3v$		
			Vertices (v), edges (e), or faces (f) shared		
AX_3	6	6	$3e$	c	a
			$1v$ $1e$ $1f$	hc	b
A_2X_7		5	$2v$ $1f$	h ($\frac{7}{8}$)	c
			$1v$ $2e$	c ($\frac{7}{8}$)	d
AX_4		4	$2v$ $1e$	c ($\frac{4}{8}$)	e
			$2v$ $1e$	c ($\frac{4}{8}$)	f
A_2X_9		3	$3v$	c ($\frac{9}{16}$)	g

only one solution, but for others two or more. The next stage is to see how each solution can be realized by the sharing of vertices and/or edges; face-sharing is excluded as being unlikely to occur in actual structures. The only solutions leading to structures based on 3D 3-connected nets and involving only unshared vertices (v_1) or vertices shared between two tetrahedra (v_2) are AX_2 ($v_2 = 4$) and A_2X_5 ($v_1 = 1$, $v_2 = 3$). The solution for AX_2 corresponds to the sharing by each tetrahedron of one edge and two vertices, and that for A_2X_5 to the sharing of three vertices of each tetrahedron.

AX_2 structures. Structures of all four main types, finite, one-, two-, and three-dimensional are possible if each tetrahedron shares one edge and two vertices, with all X atoms 2-connected. Structures of the first three types have been described and illustrated (*6*); the only known example appears to be one layer structure. There are two layers in which the A atoms occupy one-half of the tetrahedral interstices between a pair of close-packed layers of X atoms. These are the layers based on the 6^3 and 4.8^2 nets, and it is interesting that the latter is found in $GaPS_4$ (*7*), alternate positions of tetrahedral coordination being occupied by Ga and P atoms. (In layers based on the other two semiregular 3-connected plane nets, 3.12^2 and 4.6.12, the X atoms occupy, respectively, two-thirds and three-quarters of the positions of closest packing.) It was noted (*6*) that structures based on 3D 3-connected nets should be possible, but this field was not further explored. It has now been ascertained, by constructing models, that structures can indeed be built which are based on each of the nets 8^3-a, 8^3-b, 9^3-a, 10^3-b, and 10^3-c, and the last two will now be described. The following descriptions refer to the configurations of structures with collinear A–X–A bonds; structures with smaller A–X–A bond angles, which conceivably result in closer packing of the X atoms, have not been studied.

The tetrahedral structure based on the tetragonal configuration of 10^3-b and constructed with collinear A–X–A bonds projects on (100) as shown in Fig. 5a, which illustrates one ring of 10 tetrahedra. There are unacceptably short X–X distances of 0.73 times the length of a tetrahedron edge between the chains (dotted lines), and these are also seen in Fig. 5b which shows two chains projected on (001). This difficulty is overcome by shearing the structure (Fig. 5c), when the X atoms in the bases of the tetrahedra form a close-packed (cp) layer, and the remaining X atoms occupy one-third of the positions of closest packing on each side of the cp layer. These "layers," strictly sets of parallel chains, may be stacked in various ways and joined by sharing the X atoms which are not shared in the chains. Stacking of the layers vertically above one another gives a set of discrete layers based on 6^3 perpendicular to the projection of Fig. 5c. Alternatively, successive layers may be rotated relative to one another through 60° (or 120°), the chains lying in the directions (i), (ii), or (iii), to form a family of 3D structures. There are two different structures which repeat after two layers (along c) because the sequences (i)(ii) and (i)(iii) result in c or hc packing of the X atoms, respectively. There is a similar pair of structures, with 3-layer repeats, based on 10^3-c, and a series of polytypic structures in all of which the X atoms occupy two-thirds of the positions of more complex types of closest packing. Since the positions of the X atoms in any one chain are those of cubic closest packing alternate layers must be c layers, from which it follows that the cp symbol must contain an *odd* number of consecutive c layers (for example, c, ch, ccch, but not cch or cccch, and so on.)

A_2X_5 structures. Neutral compounds with the formula A_2X_5 are few in number. It

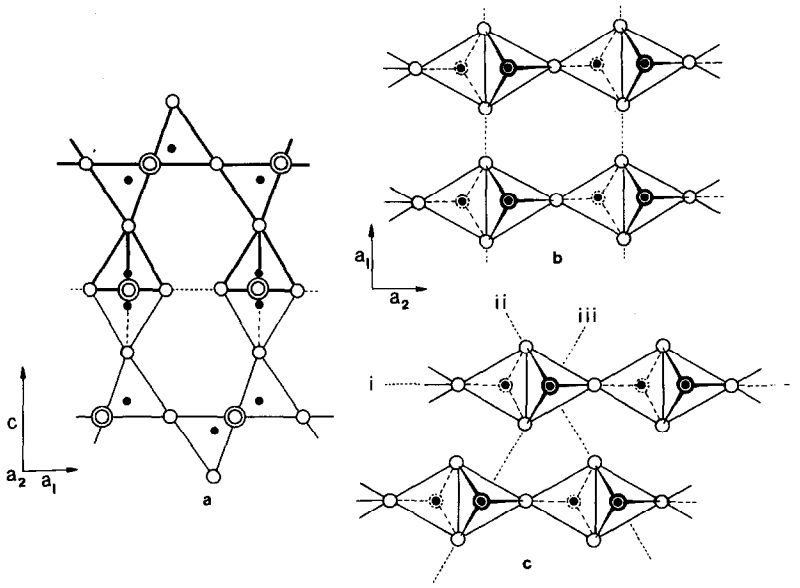
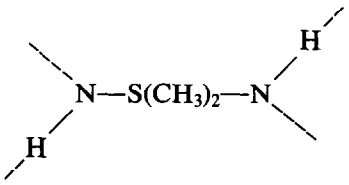


FIG. 5. (a) Projection on (100) of tetrahedral structure based on 10^3-b showing one ring of 10 tetrahedra. (b) and (c) Projections of two chains on (001) in the orthogonal and sheared forms of the net.

is therefore satisfactory to find that P_2O_5 has polymorphs with all of the three simplest possible types of structure, the 3-connected systems 3^3, 6^3, and 10^3-b, though the reason for the selection of 10^3-b in preference to the more symmetrical 10^3-a net is not obvious. We noted earlier that the most symmetrical configuration of a sheared 10^3-b net has the space group *Fddd*. The space group of P_2O_5 is *Fdd*2, and this is also the space group of (Zn_2Cl_5)–(H_5O_2), in which the 3-connected net is built of $ZnCl_4$ tetrahedra each sharing three vertices. The packing of the Cl atoms is a distorted hexagonal closest packing in which these atoms occupy $\frac{5}{6}$ of the cp positions. The distortion is necessary to accommodate the pairs of hydrogen-bonded water molecules ($H_2O\cdot\cdot H\cdot\cdot OH_2$), which are shown as shaded circles in Fig. 6.

It is convenient to mention here the structure of dimethyl sulfone diimine (*8*) which is based on 10^3-b and has the same space group as P_2O_5 and $(Zn_2Cl_5)(H_5O_2)$. In the crystal each N atom is hydrogen-bonded to N atoms of two other molecules:



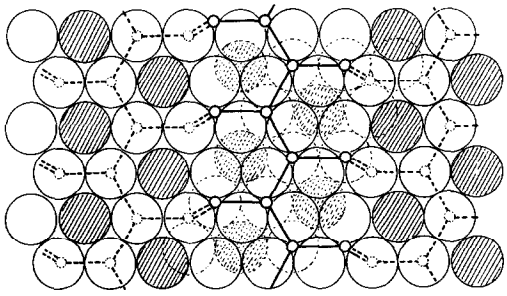


FIG. 6. The net 10^3-b in the structure of (Zn_2Cl_5) (H_5O_2) which is shown in idealized form with the Cl atoms in five-sixths of the positions of hexagonal closest packing. The shaded circles indicate the positions of the $(H_5O_2)^+$ ions.

The N atoms are situated at the points of the 3-connected net, two-thirds of the links represent N··H··N bonds, and $-S(CH_3)_2-$ groups are situated on the remaining links.

Also of interest in the present connection is an AX_2 structure which is related to 10^3-b in the following way. The unit cell of the 3-connected net contains 8 points and 12 links. Twelve A atoms are placed at the midpoints of the links and joined to form a 4-connected net (Fig. 7). An X atom is then placed on each of the 24 links of this net to form an AX_2 structure with 12 AX_2 in the unit cell. The structure consists of AX_4 tetrahedra each of which shares all four vertices (X atoms). The structure of GeS_2 is of this type, though it does not have the space group $Fdd2$ originally assigned to it but has a distorted version of the structure with $Z_c = 24$ and space group Pc (9).

Very few examples are known of structures which consist of two frameworks of the same composition which interpenetrate but are not connected by bonds of the type operating within the frameworks. Examples include the structures of Cu_2O (and Ag_2O) and ice-VII, β-quinol, edingtonite, and ice-VI. The mineral neptunite provides an example of a structure based on two interpenetrating 10^3-b nets. The full lines in Fig. 8 show a less familiar view of this net, drawn with one-third of the links much longer than the others. If tetrahedral AX_4 groups are situated at the points of the net, each sharing three vertices, the composition of the framework is $(A_4X_{10})_n$. The addition of two tetrahedra, each sharing only two vertices, along each of the long links of Fig. 8 is equivalent to adding $4AX_3$ for every 4 A atoms in the framework, giving the composition A_8X_{22}. Two such frameworks (full and broken lines) form the basis of the structure of neptunite, $M'_4M''_2(TiO)_2Si_8O_{22}$, where M' is an alkali

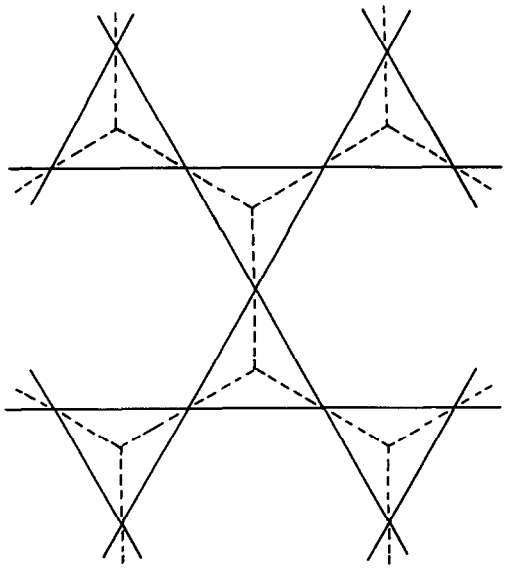


FIG. 7. Formation of 4-connected net by joining midpoints of links of a 3-connected net.

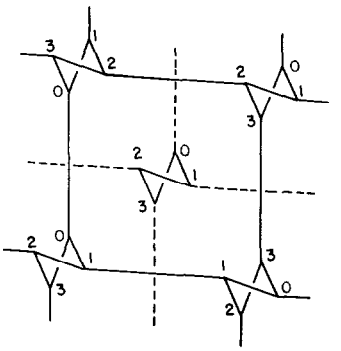


FIG. 8. Two interpenetrating 10^3-b nets which form the basis of the structure of neptunite.

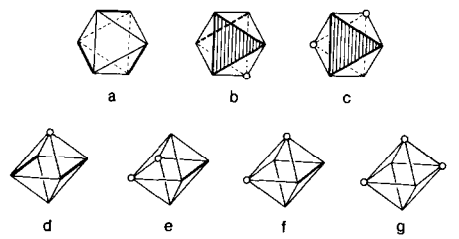


FIG. 9. Formation of structures based on 3-connected nets from octahedral groups sharing vertices (circles), edges (heavy lines), or faces (shaded); labeling as in Table II.

metal and M'' a doubly charged ion of Fe, Mg, or Mn. The additional O atoms, together with those of the frameworks, complete the coordination groups around the cations.

Octahedral Structures

Structures that can be built of octahedral AX_6 groups all of which share their X atoms in the same way may be classified, as in the

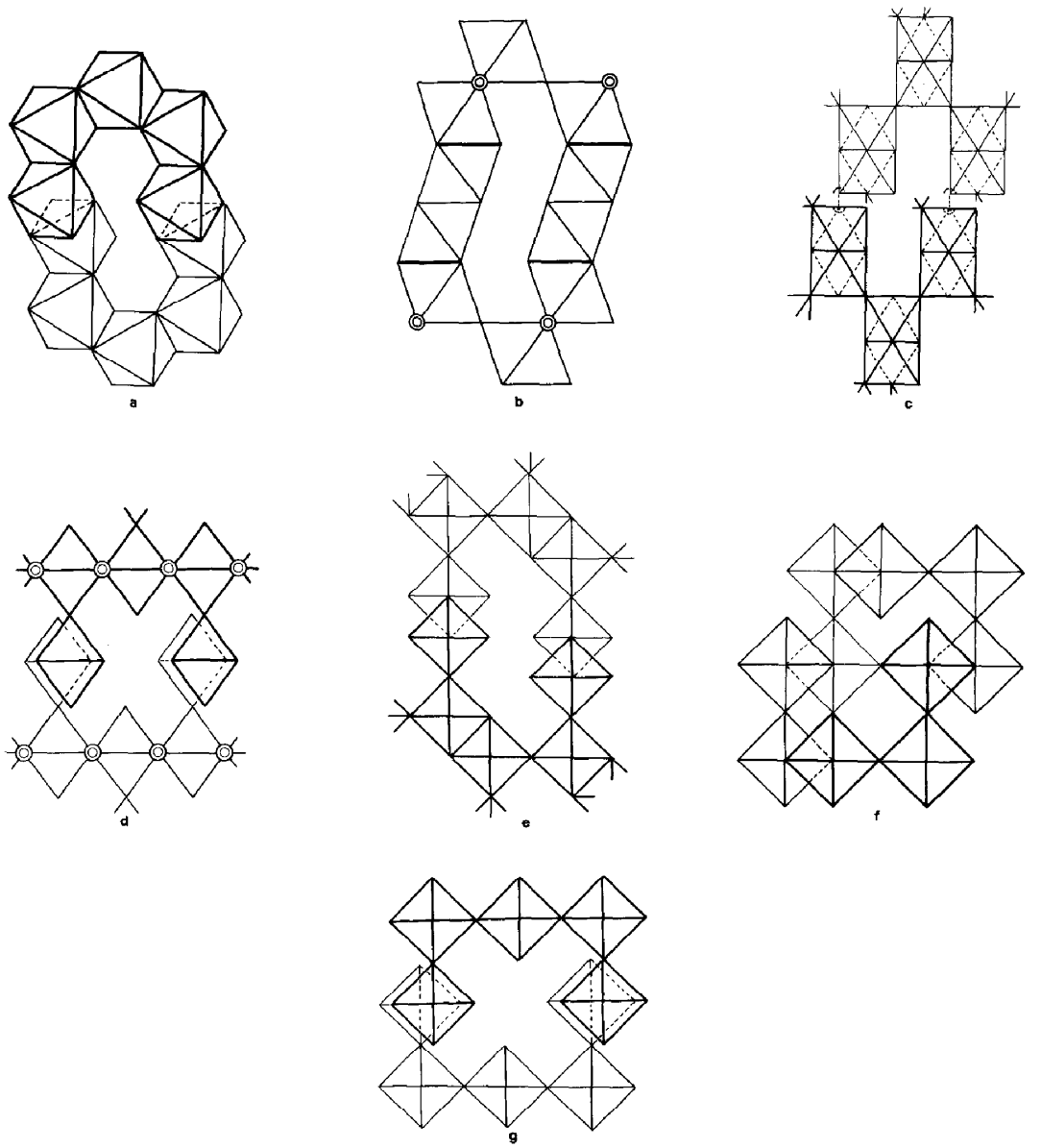


FIG. 10. Rings of 10 octahedra in structures based on 10^3-b sharing vertices, edges, and/or faces as in Fig. 9 and Table II. In (b) and (d) double circles indicate shared edges perpendicular to the plane of the paper and in (b) heavy lines indicate shared faces. In (c), (d), and (g) the lower half of the ring is displaced to avoid overlapping.

case of tetrahedral structures, in terms of the coordination numbers of the X atoms. The appropriate equations are $\Sigma v_x = 6$ and $\Sigma(v_x/x) = n/m$. The solutions of these equations are numerous, but the numbers of structures that are geometrically possible are much smaller if we insist that the octahedra are regular and that no distances between X atoms of different octahedra are less than the X–X distance within an octahedron (edge length of octahedron). These requirements limit the coordination number of X to 6. Structures extending indefinitely in three dimensions can be constructed for all the formulas A_2X_9, AX_4, A_2X_7, AX_3, A_2X_5, AX_2, A_2X_3, and AX, but structures based on 3D 3-connected nets have been found (*10*) only for the compositions A_2X_9, AX_4, A_2X_7, and AX_3. However, a particular solution of the above equations may be realizable in more than one way. For example, the sharing of each X atom between two octahedral AX_6 groups (the solution $v_2 = 6$ for composition AX_3) may be realized by sharing the following numbers of vertices (V), edges (E), and/or faces (F):

	V	E	F
(i)	6		
(ii)	4	1	
(iii)	2	2	
(iv)		3	
(v)			2
(vi)	3		1
(vii)	1	1	1

(For octahedral structures we must include face- as well as edge- and vertex-sharing.) Two of these combinations result in structures based on 3-connected nets, namely, (iv) and (vii). In (iv) the shared edges must have no vertices in common, and in (vii) the shared edge and face must have no vertex in common. Structures of both these types based on 10^3-b can be constructed. In Table II are listed examples of structures based on this net in which each octahedron shares the vertices, edges, and/or faces of Fig. 9, and one ring of 10 octahedra in each structure is illustrated in Fig. 10.

We have included in Table II the density of packing of the X atoms in each structure, as determined from models. This density is dependent on the interbond angles A–X–A. For shared edges or faces the A–X–A angle is fixed (90° or 70.5°) but for vertex-sharing it may range from 180° to 132° (*11*). The packing of the X atoms in Table II corresponds to models in which A–X–A has been made equal to 180°, except in the A_2X_7 model (c), where the hexagonal closest packing implies angles of 132° at the shared vertices. It is possible that by suitable rotations of the octahedra more densely packed configurations of some of these structures could be made; compare the relation of the ReO_3 structure, in which the O atoms occupy three-quarters of the positions of cubic closest packing, with the topologically similar RhF_3 structure, in which there is hexagonal closest packing of the F atoms.

Our object here has been to bring together in one place the somewhat scattered pieces of information concerning the net 10^3-b. References are given only to more recent structural papers, and octahedral structures have been dealt with only briefly since it is hoped that a fuller account will be published later.

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