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Enumeration of 4-connected 3-dimensional nets and classification of framework silicates, III. Combination of helix, and zigzag, crankshaft and saw chains with simple 2D nets

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Abstract

Combination of a helix with the 3.6.3.6 2D net yields the quartz and NbO types of 3D nets. The latter cannot occur as the basis of a framework of linked tetrahedra. Combination of a helix with the 4^4 2D net yields the cristobalite net.

Zigzag, crankshaft and saw chains yielded interesting 3D nets when combined with simple 2D nets. Crankshafts can condense to give a hexagonal sheet, and a crankshaft combines with a saw to give a band of linked 5-rings.

Replacement of some horizontal branches of the 6^3 2D net with a zigzag chain gives the tridymite and cristobalite nets; for the 4.8^2 net, the *SCCSCC* and *SSCSSC* up-down combination on the 6^3 net, plus a tetragonal analog to cancrinite; for the 4.6.12 net, the cancrinite net. Nets with crankshaft chains were given in Part II.

Of 12 theoretical nets based on replacement of horizontal branches by saws or saws plus crankshafts, the nets for bikitaite (6^3 net + saw + crankshaft), scapolite (4.8^2 net + saw + crankshaft), and offretite (4.6.12 net + saw) are particularly interesting. Bikitaite contains hexagonal sheets, and scapolite and bikitaite contain 5-rings. Bikitaite can also be described as the combination of zigzags and the $(5^2.8)_2(5.8^2)_1$2D net.

Introduction

Following the enumeration of 4-connected 3D frameworks obtained by adding perpendicular or near-perpendicular branches to each node of 3-connected 2D nets (Part I, Smith, 1977; Part II, Smith, 1978), this paper describes the combination of either a helix or simple chains with 2D nets. Basic ideas on nets are summarized in Wells (1977), and detailed descriptions of the many types of chains of linked tetrahedra were given by F. Liebau over the past decade (references in Liebau, 1978).

Helix plus 2D net

Although 2D nets with four branches emanating from each node cannot be linked together by new branches to form 4-connected 3D nets, they can be turned into 3D nets by converting horizontal branches into tilted ones.

The 3.6.3.6 2D net yields the quartz-type net (Table 1, no. 90) when the 3- and 6-rings are turned into infinite helices. All helices have the same sense, resulting in a sequence of 012012 for the height of nodes around each 6-turn helix (Fig. 1). Two choices of clockwise or anticlockwise counting yield left-handed and right-handed enantiomorphs.

A second net with opposite sense for adjacent 3-turn helices has sequences 010101, 121212, and 202020 around the 6-turn helices. Wells (1977, Fig. 9.3ef) displayed the relationship between the two nets, and noted that the second one represents the structure of NbO if Nb and O are placed on alternate nodes. This NbO net (Table 1, no. 91) cannot occur as the basis of a framework of linked tetrahedra. Whereas in quartz the oxygens can be placed in a tetrahedral arrangement about the silicon atoms (Fig. 1), in the NbO net they cannot be so placed because of the geometrical restriction placed by the opposite chirality of adjacent helices. The hypothetical structure in Figure 1 has oxygens in square planar coordination about the nodes. For congruent nodes, net 91 has space group *Im*3*m* for highest symmetry, and Figure 1 shows a projection down [111]. The net can be constructed easily by linking with plastic spaghetti only four out of the six spokes of octahedral "stars."

The tetrahedral framework of an intergrowth of left- and right-handed quartz cannot be continuous unless the oxygens at the interface have non-tetrahe-

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Table 1. Simpler structures based on simple 2D nets and either helices or chains

Arbitrary number	2D net	Perpendicular element	Z_t	Circuit symbol	Z_c	Highest space group	a	b	c
90	6^3	spiral	3	$6^4.8^2$	3	$P6_222$; $P6_422$	5	-	~5.5
91	6^3	spiral	6	$6^4.8^2$	3	Im3m	6	-	-
92	6^3	spiral	3	3.7^5	3	R3	5 (α~100°)		
93	4.8^2	zigzag	8	$4^2.6^3.8$	16	I4/mmm	12	-	5
94	3.12^2	zigzag	6	3.6^5	6	$P6_3/mmc$	9	-	5
95	4.6.12	zigzag	12	$4^2.6^4$	12	$P6_3/mmc$	12	-	5
96	6^3	saw	6	$(4^2.6^3.8)_2(6^6)_1$	6	Pmcm	~6.5	8	5
97	6^3	saw	12	$(4^2.6^3.8)_2(6^6)_1$	12	Pmam	~8.5	9	~6.5
98	6^3	saw, crankshaft	6	$(5^4.6.8)_2(5.6^5)_1$	12	Cmcm	7	15	5
99	4.8^2	saw	12	$(4^3.6^2.8)_2(4.6.8^4)_1$	12	P4/mmm	9	-	7
100	4.8^2	saw, crankshaft	12	$(4.5^4.8)_2(4.5.8^4)_1$	24	I4/mmm	13	-	7
101	4.8^2	saw	24	$(4^3.6^3)_2(4^2.8^3.6)_1$	24	P4/mmm	13	-	7
102	4.8^2	saw	12	$(4^3.6^2.8)_2(4^2.6.8^3)_1$	12	Pmam	8	9	7
103	4.8^2	saw	12	$(4^2.5^2.6.7)_2(4^2.5.8^3)_1$	12	$P112_1/m$	a7,b9,c8,γ~110°		
104	4.8^2	saw, crankshaft	24	$(4^2.5^2.6.7)_2(4^2.5.8^3)_1$	48	I4/mmm	18	-	7
105	3.12^2	saw	9	$(3.4^2.6^2.8)_2(3.6.8^4)_1$	9	$P\bar{6}m2$	9	-	7
106	4.6.12	saw	18	$(4^3.6^3)_2(4^2.6^2.8^2)_1$	18	$P\bar{6}m2$	13	-	~7.5
107	4.6.12	saw, crankshaft	18	$(4^3.6^3)_2(4^2.5^2.6^2)_2(4^2.5^2.6.8)_2$ $(4^2.5.6.8^2)_2(4^2,6^2,8^2)_1$	36	Im2m	13	22	~7.5

Observed structures

Type	Name	Reference	Space Group	a	b	c
90	quartz(high) [low]	Bragg et al. (1965)	($P6_222$; $P6_422$) [$P3_121$; $P3_221$]	4.9	-	5.4
90	β-eucryptite	Tscherry et al. (1972)	$P6_222$; $P6_422$	5.24	-	5.59
95	cancrinite	Jarchow (1965)	$P6_3$	12.7	-	5.1
98	bikitaite	Kocman et al. (1974)	$P112_1$ (γ114°)	7.60	8.61	4.96
100	scapolite	Levien and Papike (1976)	I4/m; complexities	12.2	-	7.6
106	offretite	Gard and Tait (1972)	$P\bar{6}m2$	13.3	-	7.6

Note: other pertinent structures are listed in Parts I and II: see text.

dral coordination around the silicons. Mechanical deformation cannot change the sense of the quartz structure by a displacive transformation. Intergrowths of left- and right-handed quartz could have formed only by separate nucleation, perhaps involving epitaxy.

Wells (1977, Fig. 9.15b) invented the net in Figure 2, in which triangular helices are cross-linked by equilateral triangles. The sequence around the hexagons of the original 3.6.3.6 2D net is 001122, and all the triangular helices must have the same chirality which is opposite to the chirality of the hexagonal helices. Change of chirality is equivalent to choosing new axes rotated 60° about the 3-fold rotation axis (*International Tables for X-ray Crystallography*, vol. 1, p. 251). Triangular helices cannot be intermixed without destroying the equilateral triangles.

Conversion of the 4^4 2D net into a 3D net with 4-fold helices (Fig. 3) yields the cristobalite net already described in Part I on the basis of its 6^3 2D nets oriented perpendicular to [111].

No other simple 4-connected 2D nets exist.

Chain types

Out of the infinity of possible chain types, three are chosen here (Fig. 4). The zigzag and crankshaft chains were used by Wells (1977, Chapter 8). The saw type of chain, which can be regarded as a hybrid of the zigzag and crankshaft chains because of the alternation of a zigzag with a crank, was chosen because it is important in several zeolites with 5-rings. Particularly important is the geometrical flexing of the chains: thus the crankshaft can change from the compressed rectilinear configuration (Fig. 4b) to the extended configuration (Fig. 4c). Crankshafts can condense together to form a hexagonal sheet (Fig. 4e),

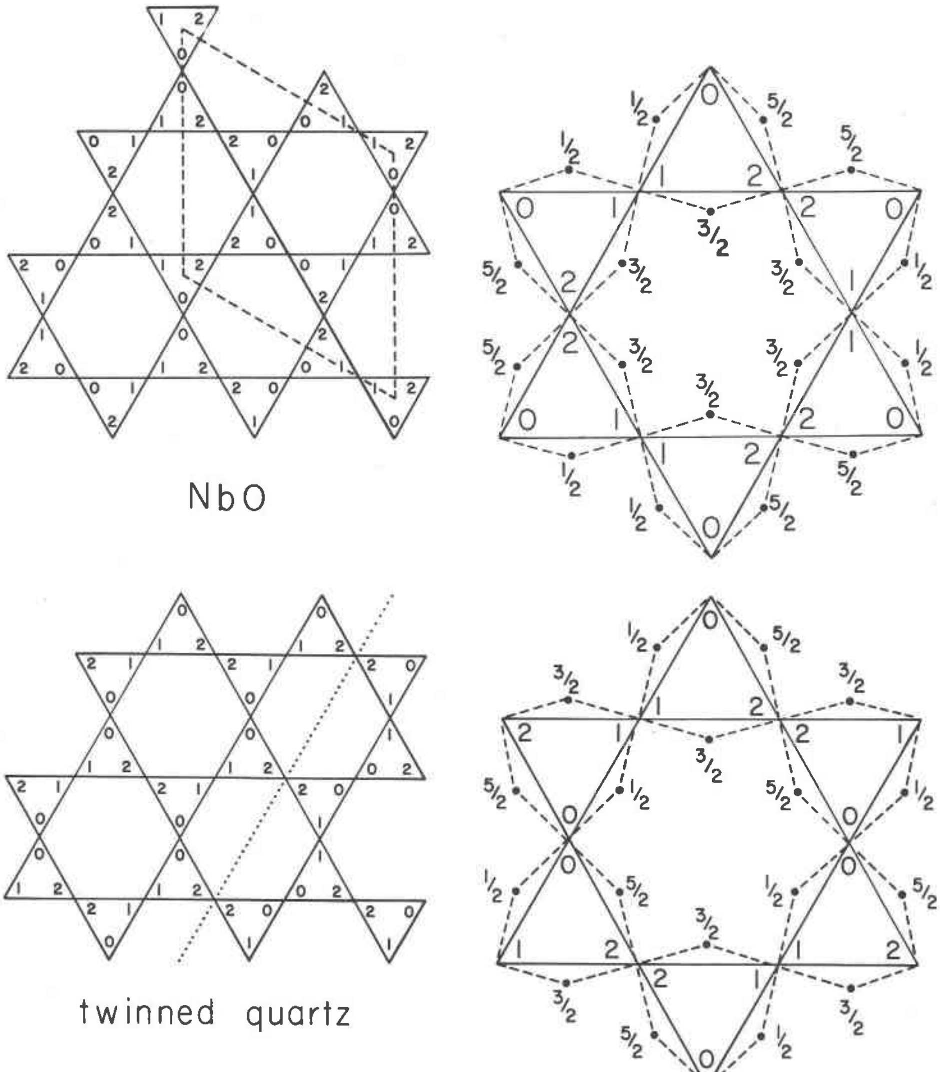


Fig. 1. *Left.* Projections on to a 3.6.3.6 2D net of the 3D nets of quartz (Table 1, no. 90) and NbO (Table 1, no. 91). The infinite helices are shown by the heights 0,1,2 which repeat perpendicular to the plane of the paper. Left- and right-handed varieties of quartz are shown related by a hypothetical twin boundary (dotted line)—but see text. *Right.* Diagrams showing how the same sense of adjacent helices in quartz (lower right) allows oxygen atoms (dots) to lie in tetrahedral configuration about silicon atoms, whereas the opposite sense of adjacent helices in net 91 (upper right) forbids a tetrahedral configuration and allows a square configuration tilted from the horizontal.

while a crankshaft and a saw condense to form 5-rings (Fig. 4f), and saws condense to give interconnected 4-rings (Fig. 4g).

3D nets based on zigzag chains and simple 2D nets

Conversion of a horizontal branch of a 6^3 2D net into a zigzag chain converts two nodes from 3-connected to 4-connected. The adjacent branches must be horizontal. Adjacent nodes of the zigzag chain have different heights, and closure of each 6-ring requires an even number of inclined branches from zigzag chains. Hence only two horizontal branches can be converted into zigzag chains. These branches cannot be adjacent and only two sequences are possible: *zhhzhh* and *zhzhhh*, where *z* and *h* are zigzag and horizontal branches respectively. Only two 3D nets (cristobalite and tridymite) result when these sequences are not intermixed (Fig. 5), and these nets were already described in Part I. Mixing of the sequences gives polytypes.

3D nets with hexagonal *space-group* symmetry cannot be constructed because of parity problems, as illustrated by the impossible net in Figure 5. An attempt to integrate *zhzhhh* and *hhhhhh* sequences

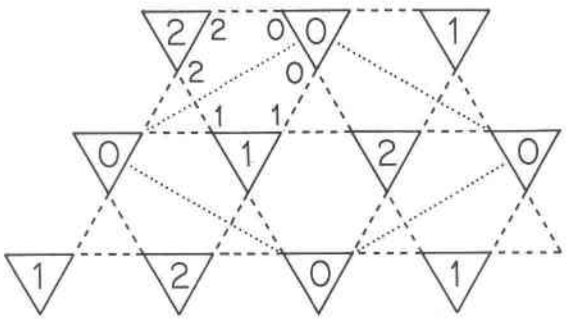


Fig. 2. Projection onto a 3.6.3.6 2D net of a 3D net (Table 1, no. 92) invented by Wells (1977, Table 9.2, no. 2). The infinite helices (dashed lines, height 012) are connected by equilateral triangles (solid lines, height 0, 1, or 2). The triply-primitive hexagonal cell is shown by dotted lines.

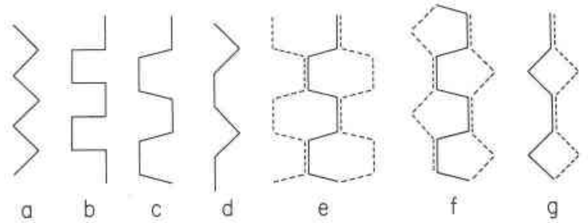


Fig. 4. Types of chains (*a*, zizag; *b* and *c*, rectilinear and extended configurations of crankshaft; *d*, saw) and three ways of combining chains into hexagonal sheet (*e*), band of 5-rings (*f*), and string of 4-rings (*g*).

results in 3-connected nodes at the end of the horizontal branches denoted by dashed lines. However, a remarkable net with radial hexagonal symmetry about a single line was invented by Wells (1977, Figs. 9.13 and 9.14); here, the parity problem was solved by the existence of a discontinuity at the starting line. This net does not have crystallographic symmetry.

For the 4.8^2 2D net, there are only 3 simple ways of converting horizontal branches into zigzag chains. Replacement of a single horizontal branch between two 8-rings by a zigzag chain leads inexorably to net 3 in Figure 6. This net is merely the *SCCSCC* variation of up and down linkages to the 6^3 2D net (Part I), and was described by Wells (1977, Fig. 9.17). Replacement of a branch between a 4-ring and an 8-ring leads to an infinity of nets, of which the simplest two are given here. The first net was already given as the *SSCSSC* variation of up and down linkages to the 6^3 2D net (Part I; Wells, 1977, net 8, Figs. 9.27a, b). The second net is new (Table 1, no. 93), and is characterized by horizontal 8-rings (*hhhhhhhh*) which form the top and bottom of cages whose sides are composed of four pairs of adjacent 4-rings alternating with non-planar 6-rings. This type of cage is the tetragonal analog of the cancrinite cage. The cages form channels with 8-ring windows, while a second set of narrower channels is spanned by non-planar 8-rings. Net

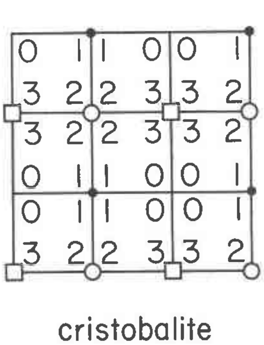


Fig. 3. Cristobalite net interpreted as the addition of 4-fold helices to a 4^4 2D net. Tetrahedral nodes lie at the relative heights 0,1,2, and 3.

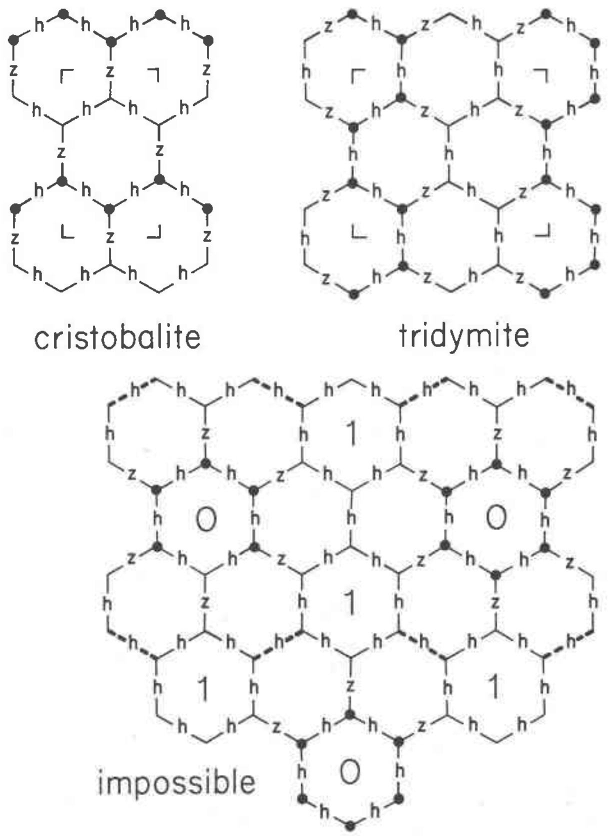
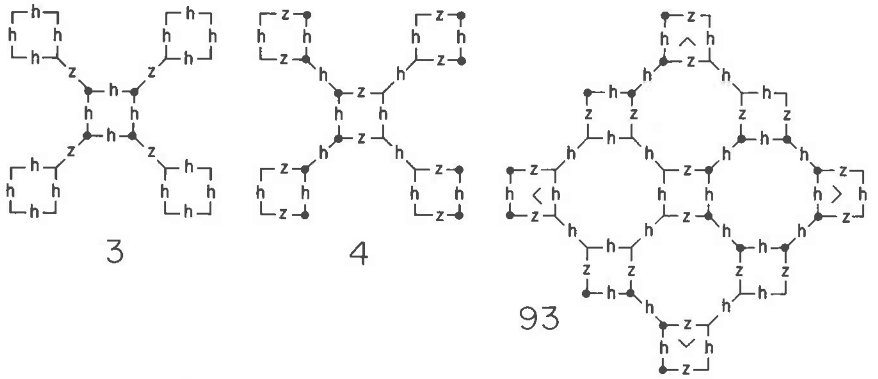


Fig. 5. One impossible and two possible 4-connected 3D nets formed by converting horizontal branches (*h*) of a 6^3 2D net into zigzag chains (*z*). Actually the projection of the *z* branches should be shorter than *h* branches for constant internodal distance, but hexagonal geometry is retained for convenience of drawing. Nodes marked by a dot have height halfway between unmarked nodes.



3 4 93

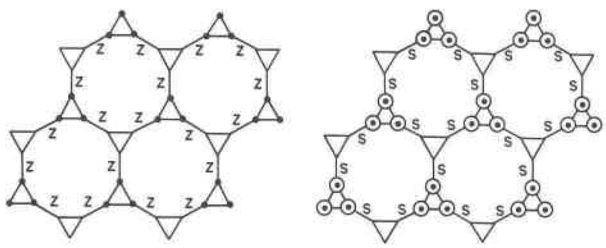
Fig. 6. Three nets derived by converting horizontal branches of the 4.8^2 2D net into zigzag chains (z). Actually the projection of the z branches should be shorter than the h branches. Nodes marked by a dot have height halfway between unmarked nodes. Horizontal branches are not labeled.

93 was described as net 8′ by Wells (1977, Figs. 9.27c and 9.29).

For the 3.12^2 2D net, parity restrictions result in only one net (Fig. 7, left; Table 1, no. 94) already described by Wells (1977, Figs. 9. 15a and 9.16).

For the 4.6.12 2D net, parity restrictions result in only one net (Fig. 8; Table 1, no. 95) already described by Wells (1977, Fig. 9.20b), and represented by cancrinite. The well-known cancrinite cage consists of two parallel hexagonal rings connected by three pairs of 4-rings. In net 95, the cancrinite cages share hexagonal rings, and pairs of 4-rings join up into a double zigzag chain which is shared between adjacent columns of cancrinite cages. The resulting framework has a 1-dimensional channel system with 12-ring windows.

All the nets in this section are based on cross-linking of vertical zigzag chains by horizontal branches. Although it is theoretically possible to combine zigzag chains with crankshafts or saw chains, it was decided not to enumerate the nets because the enforced presence of 3-rings and the complexity of the circuit symbols made them implausible as prototypes for chemical compounds.



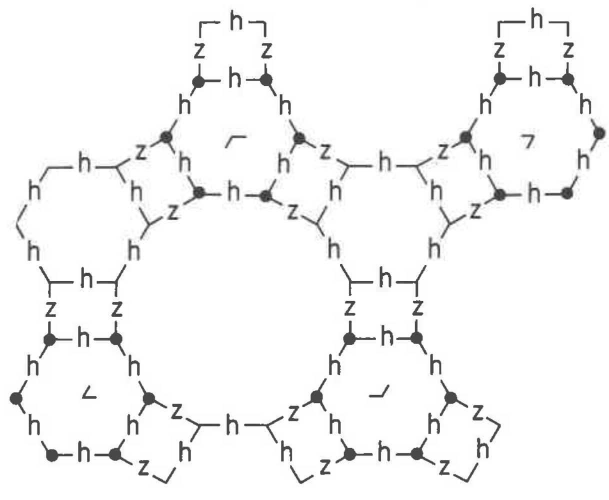
94 105

Fig. 7. The only nets formed by converting horizontal branches (h) of the 3.12^2 2D net into zigzag (z) or saw (s) chains. Nodes marked by a dot have height halfway between unmarked nodes. Unmarked branches are horizontal.

3D nets based on crankshaft chains and simple 2D nets

Crankshaft chains can be combined with horizontal linkages or saw chains, but the latter type is deferred until the next section.

A crankshaft chain is obtained whenever vertical linkages pointing in opposite directions are added to two adjacent nodes of a 2D net. Thus for the 6^3 2D



95 cancrinite

Fig. 8. The only net formed by converting horizontal branches (unlabeled) of the 4.6.12 2D net into zigzag chains (z). Nodes marked by a dot have height halfway between unmarked nodes.

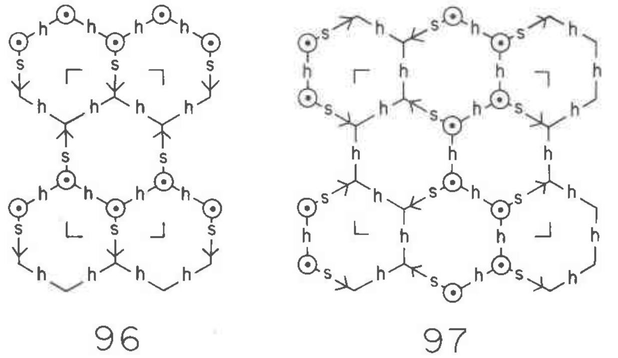


Fig. 9. The two ways of combining saw chains (s) with the 6^3 2D net. The arrow points to the tooth of the saw chain, and the circled dot denotes the back side.

net, every C in the diagrams in Part I represents a crankshaft chain. The *CCCCCC* net (tridymite) is obtainable solely from the condensation of crankshaft chains, but all other nets require horizontal linkages (denoted S) to crosslink the crankshafts. It is not possible to decompose the cristobalite net into crankshafts because of the rotation of adjacent hexagonal nets.

Combination of crankshaft chains with the 4.8^2 2D net was described in Part II, and both twisted and untwisted chains were utilized. Net 39 can be derived solely from condensation of crankshaft chains without addition of horizontal linkages (Part II, Fig. 1). Nets 6, 9a, 10a, 11–24 contain double crankshafts.

Parity restrictions make it impossible to form a 3D net with a 3.12^2 2D net as the guide for condensation of just crankshaft chains. All nets in Figure 4 of Part II have some horizontal linkages between crankshafts.

For the 4.6.12 2D net, only net 81 (Part II, Fig. 7) can be constructed merely from the condensation of crankshafts without addition of horizontal linkages.

3D nets based on saw chains and simple 2D nets

Parity restrictions for a saw chain are similar to those for a zigzag chain, but the saw chain can be combined with either horizontal branches or crankshaft chains or both to produce nets of which some are represented by chemical compounds.

For the 6^3 2D net, two horizontal branches must be replaced by saw chains in each 6-ring and the saws must be separated by at least one horizontal branch to yield the two nets numbered 96 and 97 (Fig. 9; Table 1). The back side of the saw combines with horizontal linkages to give either the double zigzag chain in net 96 (horizontal row of circles enclosing dots) or the double crankshaft in net 97 (vertical row of circles enclosing dots). When viewed along these chains (Fig. 10), nets 96 and 97 can be seen to be also describable in terms of condensation of either zigzag or crankshaft chains with a non-regular 2D net with circuit symbol $(4.6.8)_2(6.8^2)_1$. For net 96, the zigzags are connected by single horizontal branches, whereas for net 97 the horizontal linkages combine in pairs to give 4-rings separated like a row of stepping stones (denoted *s4s*).

Combination of crankshaft and saw chains with horizontal branches from the 6^3 net gives the 3D net for bikitaite (Fig. 11; Table 1, no. 98). Two horizontal branches must meet the arrow of the saw chain to give four branches for the node. Either one or two crankshafts can combine with the back side of each saw, as in Figure 4f. If one crankshaft is combined with a saw, the partial sequence *hsc* is produced in one hexagon and *hh* in an adjacent hexagon. For congruent hexagons, the only possible full sequence is *hhsccs* in which two crankshafts meet at the back of each saw. The resulting 3D net can also be described in terms of zigzag chains and horizontal branches placed on the $(5^2.8)_2(5.8^2)_1$ 2D net (Fig. 11 left). Furthermore, the crankshaft chains are condensed into corrugated hexagonal sheets which are joined by zigzag chains, as pointed out independently by Merlino (1975) and Meier (1978).

Replacement of all branches between two 8-rings of the 4.8^2 2D net leads to nets 99 and 100 (Fig. 12). In net 99 the remaining branches are horizontal, whereas in net 100 the backs of the saws are staggered to yield crankshafts. The teeth of the saws connect to single 4-rings in both nets. In net 99, the other side of the saws links up to form cubes at the corners of the tetragonal unit cell in which the center is occupied by a single 4-ring. This net can also be described as the combination of horizontal branches and crankshafts with the nonregular $(4.6.8)_2(6.8^2)_1$ 2D net (Fig. 10) when projected down a tetragonal a axis.

Net 100 is the basis of the scapolite family of minerals, for which Si,Al ordering on the nodes leads to symmetries lower than the topologic framework symmetry $I4/mmm$. The crankshafts change the relative height of the nodes in the 4-rings, as distinguished in Figure 12 by the dotted circles and squares. Instead of cubes in net 99, there are polyhedra composed of two twisted 4-rings connected by four 5-rings. Each 5-ring is connected by a vertical linkage to another 5-ring and by a zigzag to a third 5-ring. In the vertical direction, each crankshaft shares vertical edges with two saws to produce the 5-rings (Fig. 4f).

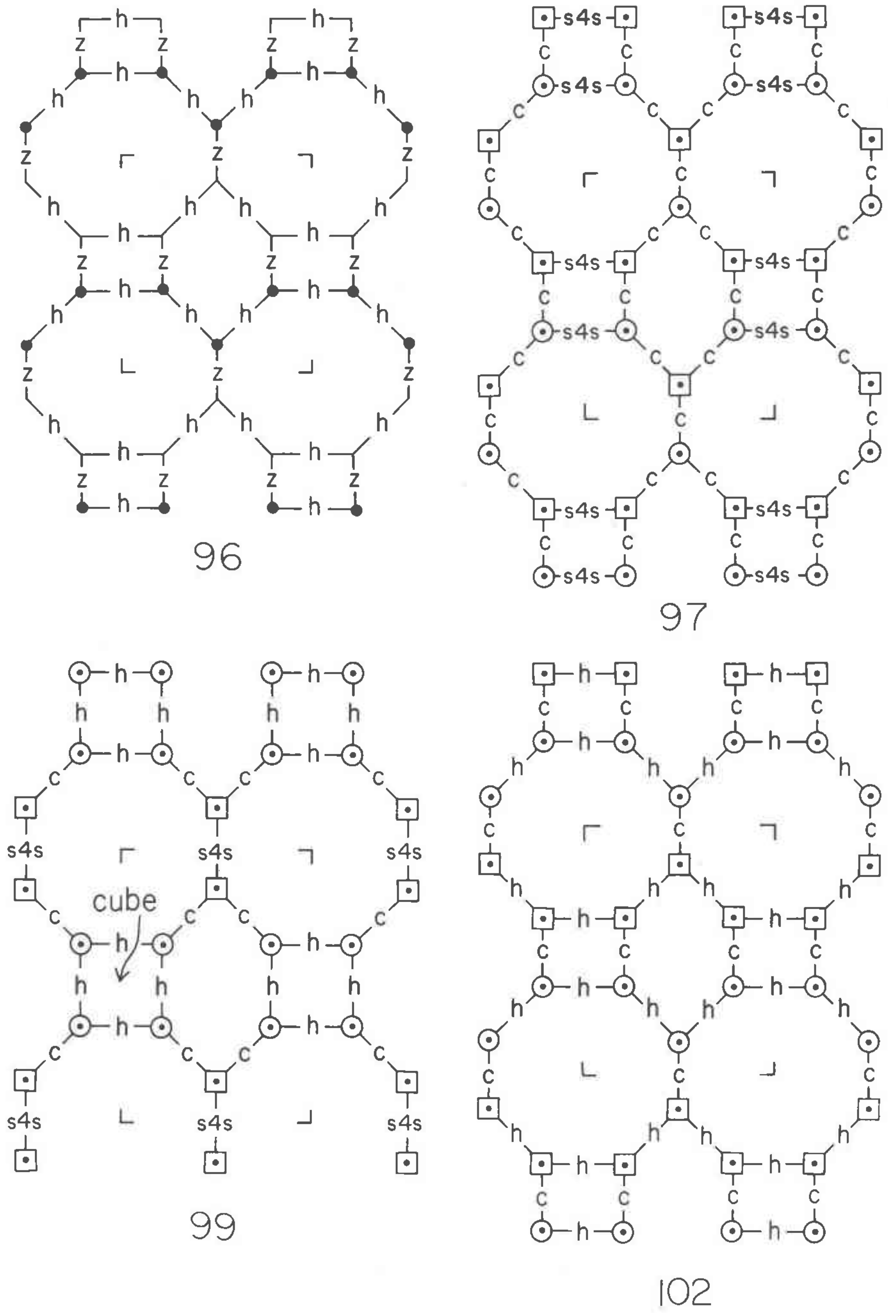
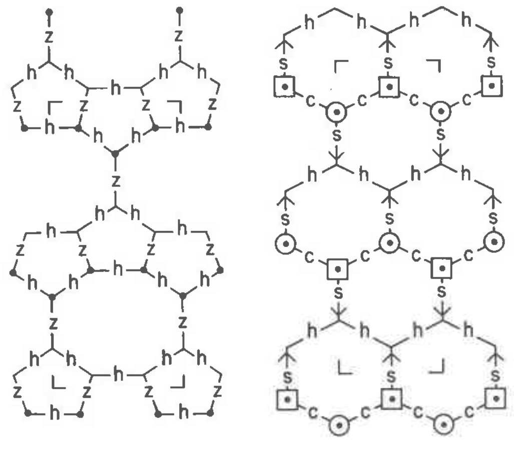


Fig. 10. Projection of four nets on the non-regular $(4.6.8)_2(6.8^2)_1$ 2D net. The symbols *c*, *h*, and *z* represent crankshafts, horizontal branches, and zigzags, while *s4s* represents a row of 4-rings lying perpendicular to the paper like stepping stones. Relative heights of the nodes are indicated by dots, circles, squares, or absence of symbol.

Replacement of a branch between a 4-ring and an 8-ring of the 4.8^2 2D nets yields an infinity of nets, but only the simpler ones with high symmetry are listed here. Replacement of opposite branches of the 4-rings leads to double-saw chains. The most symmetrical net (Table 1, no. 101; Fig. 13) has tetragonal symmetry like its relatives merlinoite (net 17) and net 93, which are based on the crankshaft and zigzag chains. Net 101 has two types of channels parallel to the tetrad axis, one formed from alternating octago-



98 bikitaite

Fig. 11. Topologic description of net 98 (bikitaite) as the combination of zigzag chains (z) and horizontal branches (h) with a $(5^2.8)_2(5.8^2)_1$ 2D net or the combination of crankshaft (c) and saw (s) chains with horizontal branches from a 6^3 2D net. The relative heights of nodes are shown by different symbols, and the teeth of the saws are shown by arrows.

nal prisms and the tetragonal analog of the cancrinite cage, and the other formed from the tetragonal analog of the gmelinite cage.

Of the infinity of less symmetrical nets, the simplest one (Table 1, no. 102; Fig. 13) is characterized by alternate direction of the saw teeth. This net can also be described as the combination of crankshaft chains with horizontal branches derived from the non-regular $(4.6.8)_2(6.8^2)_1$ 2D net (Fig. 10). A related net (Table 1, no. 103; Fig. 14, left) is obtained by connecting the double-saw chains with alternate crankshaft chains and horizontal branches from a 4.8^2 2D net. This results in a monoclinic cell, which is seen more clearly in the c-axis projection (Fig. 14, right). Here the net is seen to derive from a non-regular 2D net $(5^2.8)_2(5.8^2)_1$ by conversion of some horizontal branches into crankshafts. This 3D net can be derived from the bikitaite net (Fig. 11, left) by replacing zigzags by crankshafts. It is not possible to replace any other horizontal linkages of net 103 (Fig. 14, left) by crankshafts because of parity restrictions.

Returning to net 101 (Fig. 13, left), the horizontal branches connecting the backs of saws can be replaced by crankshafts to yield net 104 (Fig. 15). The tetragonal analog of the gmelinite cage occupies each corner and body center of the unit cell, and chains of linked 5-rings alternate with double saws around the channels which crosslink the tetragonal analog of the gmelinite cage.

The analog of net 94 with zigzag chains is net 105 with some branches of the 3.12^2 net replaced by saw chains (Fig. 7, right).

For the 4.6.12 2D net, replacement of alternate

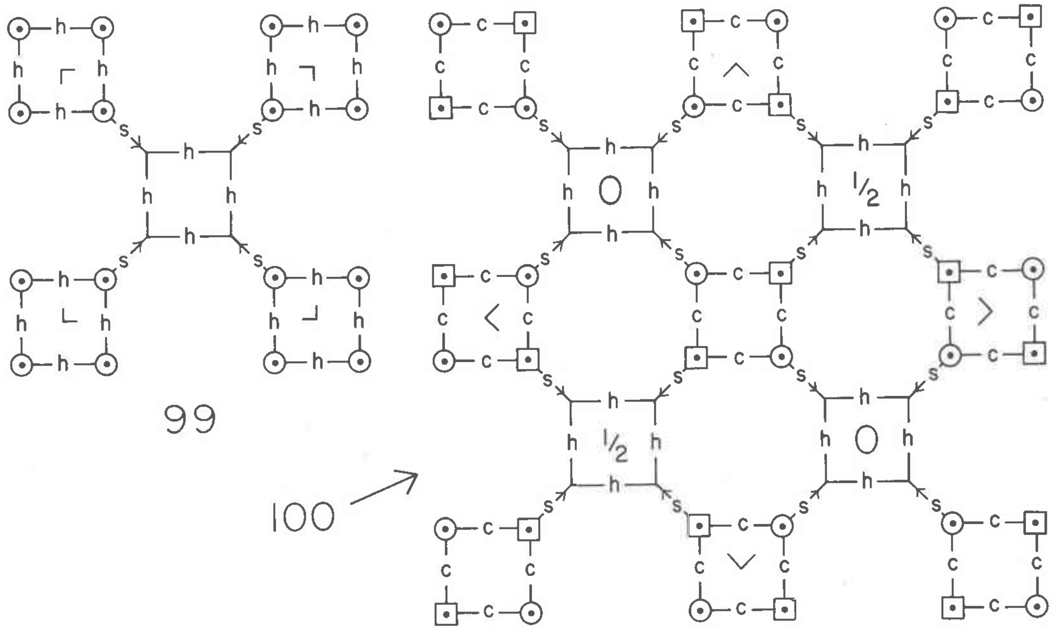
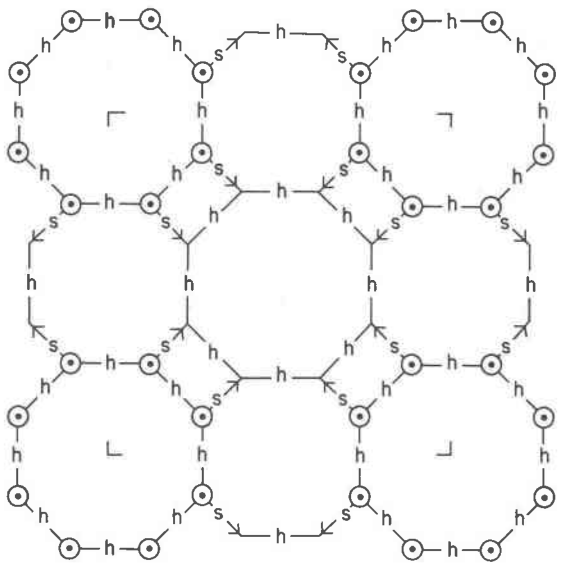


Fig. 12. Two nets formed by combination of saw chains (s) with the 4.8^2 2D net. In net 99 all the links are horizontal branches (h), whereas in net 99 some are crankshafts (c). The nodes lie at three different heights in net 99 and six in net 100 (pairs of nodes shown by dotted circle and dotted square, and nodes of single 4-rings at height 0 and 1/2).



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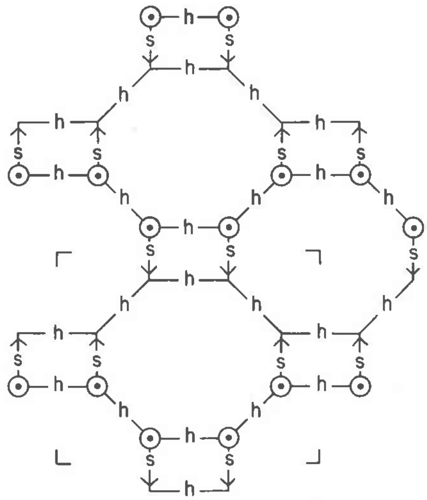

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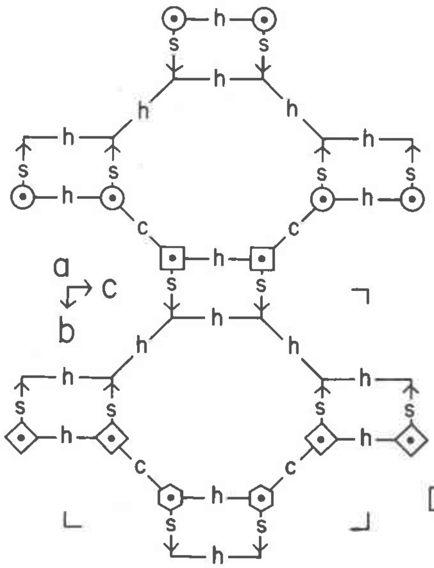
Fig. 13. Two simple nets formed by combination of saw chains (s) with the 4.8^2 2D net. Note octagonal prisms and octagons in net 100, formed respectively by joining the back side and teeth of eight saws. Net 102 has both double crankshafts and single crankshafts running east–west.



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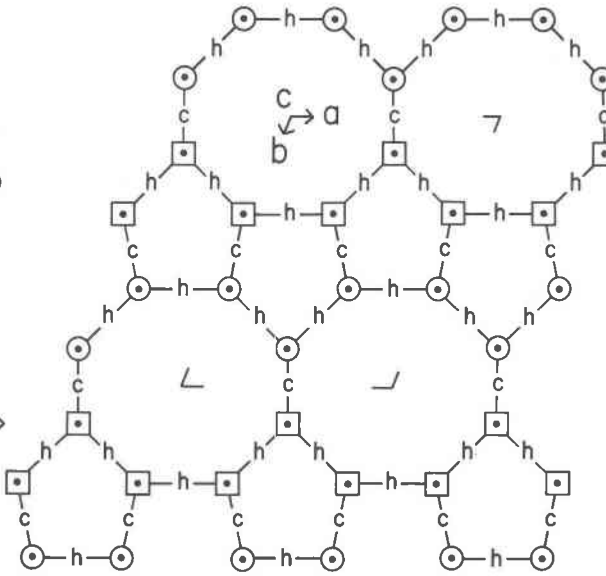
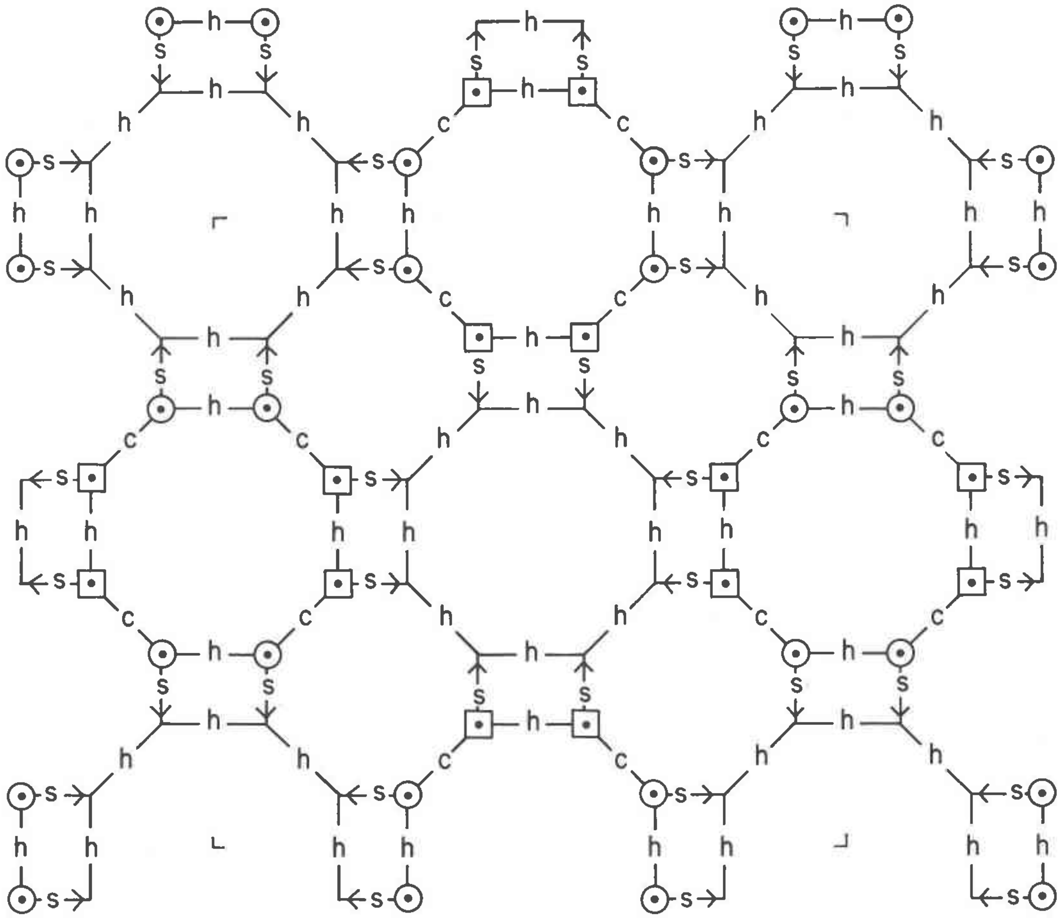


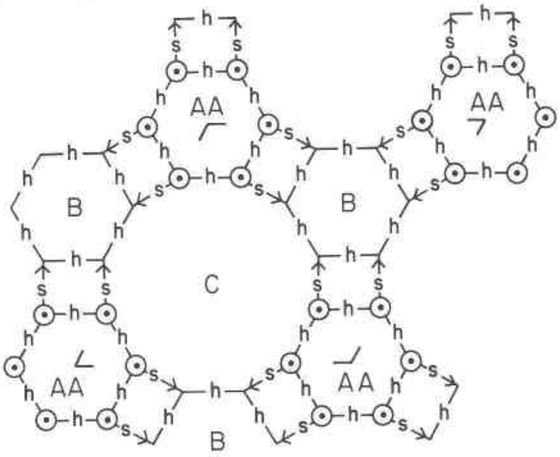
103

Fig. 14. Two projections of net 103 showing how it can be derived from the 4.8^2 (left) and $(5^2.8)_2(5.8^2)_1$ (right) nets by replacing horizontal branches (h) by crankshaft (c) or saw (s) chains. Relative heights of nodes are shown by different symbols, and the teeth of the saws are shown by arrows.



104

Fig. 15. Projection of net 104 on the 4.8^2 2D net shows how horizontal branches (h) are replaced by crankshaft (c) or saw (s) chains. Relative heights of nodes are shown by different symbols, and the teeth of saws are shown by arrows. The diagram is rotated 45° with respect to Fig. 13.

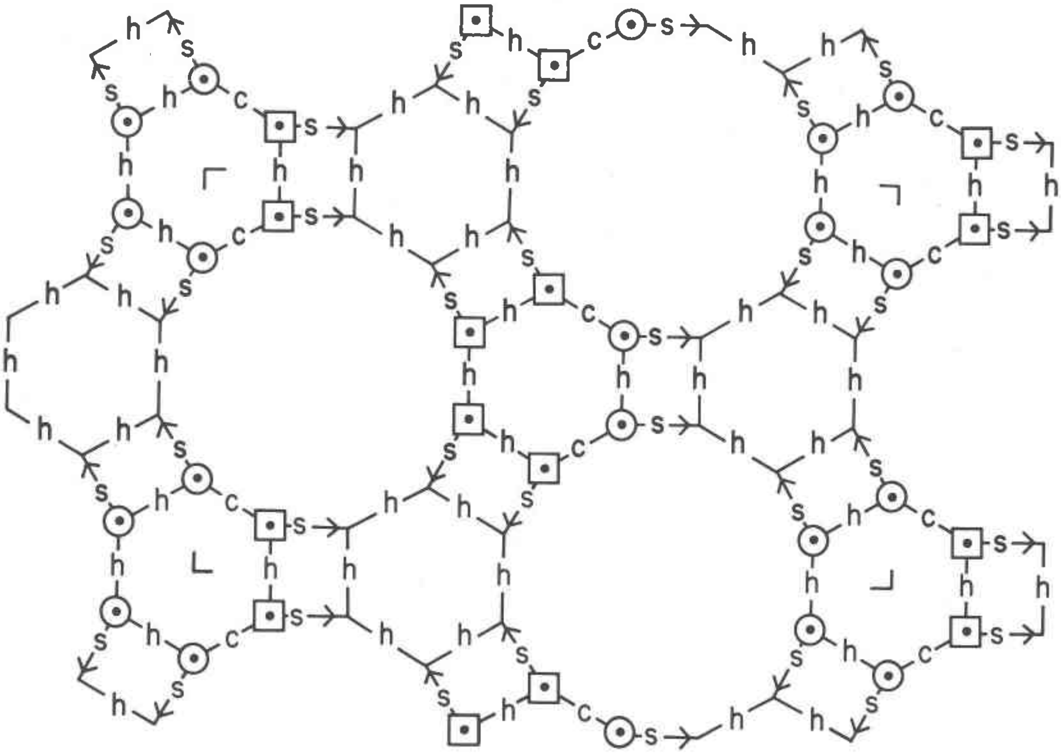


106 offretite

Fig. 16. Topologic description of net 106 (offretite) as the partial replacement of horizontal linkages (h) in the 4.6.12 2D net by saw chains (s). A and B show the horizontal positions of the 6-rings, and different symbols show the relative height of the nodes. Position C is used in the erionite net (see text).

horizontal branches around the rings with saw chains yields net 106 (Fig. 16; Table 1), found in offretite. This net can be obtained by replacing the crankshaft chains in gmelinite (Part II) by saws. Chabazite was related to gmelinite by staggering the 6-rings in an $\dot{A}ABBC\dot{C}$ sequence instead of the $\dot{A}AB\dot{B}$ sequence, and the erionite net ($\dot{A}ABAA\dot{C}$) is similarly related to the offretite net ($\dot{A}A\dot{B}$). Strictly speaking, the erionite net should not be described here, since the $\dot{A}ABAA\dot{C}$ sequence does not allow a saw chain with parallel teeth, and detailed description of it plus the $\dot{A}ABCC\dot{B}$ net will be deferred to a later paper which includes a section on nets with parallel 6-rings.

The offretite net has horizontal linkages for all six sides of each hexagon from the original 4.6.12 2D net, and two of them can be converted into crankshaft chains where the back sides of two saws are adjacent. Such a conversion yields net 107 (Fig. 17) with orthorhombic symmetry.



107

Fig. 17. Topologic description of net 17 as the partial replacement of horizontal linkages (*h*) in the 4.6.12 2D net by saw chains (*s*) and crankshafts (*c*). Different symbols show the relative height of the nodes which occur in pairs. Horizontal single 6-rings occur at relative height 0 and 1/2.

Conclusion

The present investigation reaffirms the conclusion in Part II that simple congruent nets are not the only types represented by natural or synthetic materials. Of the five minerals listed in Table 1, only quartz and cancrinite have nodes with just one type of circuit symbol. Several of the present set of theoretical nets have 5-rings, and bikitaite can be related to a 2D net with 5-rings. The next paper of the series will enumerate 3D nets based on complex 2D nets and yield several complex 3D nets containing a high proportion of 5-rings.

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References

Bragg, L., G. F. Claringbull and W. H. Taylor (1965) *Crystal Structures of Minerals.* Cornell University Press, Ithaca, New York.

Gard, J. A. and J. M. Tait (1972) The crystal structure of the zeolite offretite, $K_{1.1}Ca_{1.1}Mg_{0.7}[Si_{12.8}Al_{5.2}O_{36}]\cdot 15.2H_2O$. *Acta Crystallogr., B28,* 825–834.

Jarchow, O. (1965) Atomanordnung und Strukturverfeinerung von Cancrinit. *Z. Kristallogr., 122,* 407–422.

Kocman, V., R. I. Gait and J. Rucklidge (1974) The crystal structure of bikitaite, $Li(AlSi_2O_6)\cdot H_2O$. *Am. Mineral., 59,* 71–78.

Levien, L. and J. J. Papike (1976) Scapolite crystal chemistry: aluminum–silicon distributions, carbonate group disorder, and thermal expansion. *Am. Mineral., 61,* 864–877.

Liebau, F. (1978) Silicates with branched anions: a crystallochemically distinct class. *Am. Mineral., 63,* 918–923.

Meier, W. M. (1978) Constituent sheets in the zeolite frameworks of the mordenite group. In L. B. Sand and F. Mumpton, Eds., *Natural Zeolites,* p. 99–103. Pergamon, New York.

Merlino, S. (1975) Le strutture dei tettosilicati. *Soc. Ital. Mineral. Petrol. Rend., 31,* 513–540.

Smith, J. V. (1977) Enumeration of 4-connected 3-dimensional nets and classification of framework silicates, I. Perpendicular linkage from simple hexagonal net. *Am. Mineral., 62,* 703–709.

——— (1978) Enumeration of 4-connected 3-dimensional nets and classification of framework silicates, II. Perpendicular and near-perpendicular linkages from 4.8^2, 3.12^2 and 4.6.12 nets. *Am. Mineral., 63,* 960–969.

Tscherry, V., H. Schulz and F. Laves (1972) Average and superstructure of β-eucryptite ($LiAlSiO_4$). Part I. Average structure. Part II. Superstructure. *Z. Kristallogr., 135,* 161–174, 175–198.

Wells, A. F. (1977) *Three-dimensional Nets and Polyhedra.* Wiley, New York.

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