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Uninodal 4-Connected 3D Nets. I. Nets without 3- or 4-Rings

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Abstract

A description is given of 4-connected nets with one kind of vertex in which the shortest rings containing each pair of edges are N-rings ($N>4$). Eleven uniform nets (6^6) are identified; seven of these are believed to be new. A further thirteen nets with one type of vertex and without 3- or 4-rings are described; nine of these are also believed to be new

Introduction

4-connected nets play an important role in crystal chemistry, notably as structures of elements and covalently bonded crystals and as the basis of the structures of hydrates, framework silicates and related materials. Considerable effort has been spent on enumerating possible structures and on characterizing their topologies; recent contributions that provide references to earlier work are those of Bosmans & Andries (1990) and Hansen (1990). In this series, some nets with all nodes congruent (uninodal) are described and analyzed topologically as a prelude to the development of a more complete topological theory of 4-connected nets than presently exists. With some reasonable geometrical restrictions (discussed below), the number of possible uninodal 4-connected nets is finite and we believe we have identified many of them. One motivation for this work is the belief that if we can discover how nature puts together simple nets, we can design more complicated nets by replacing single vertices by clusters of vertices (see, for example, Hansen, 1990).

Wells (1977) attached special significance to the uniform nets in which the shortest rings at every angle are equal in length. For uniform 4-connected nets, the rings at the six angles common to a vertex are all 6-rings (have six edges) and are symbolized 6^6. Wells in fact identified only three of these, of which two are the familiar diamond and lonsdaleite nets, and the third the structure of γ-silicon. Eleven are described here; we believe that seven of them have not been described before.

Most 4-connected nets found in crystal chemistry contain 3- or 4-rings. However, in addition to the uniform nets mentioned above, the familar nets of the quartz and NbO structures are examples of nets that contain only larger rings. Here we describe some other examples.

Terminology

A 4-connected net contains six angles defined by pairs of edges. Each angle has four others adjacent that share a common edge and one opposite that does not have a common edge. Each angle is contained in an N-circuit, which is a closed path (without retracing steps) of N edges from and returning to the reference vertex. A circuit is called a ring if, in addition, for every pair of vertices on the circuit, the path on the circuit between the vertices is a shortest path (*i.e.* there is no shortcut between them outside the circuit). Rings have been variously called 'fundamental circuits', 'primitive rings' and 'fundamental rings' by other authors. Goetzke & Klien (1991) have recently discussed nomenclature and different definitions used by different authors; their terminology is used here. For every net there is a finite number of rings for each vertex and their enumeration is of considerable

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interest (Marians & Hobbs, 1990; Stixrude & Bukowinski, 1990; Goetzke & Klien, 1991).

A net is often (partially) characterized by a 'Schläfli' symbol that indicates the shortest circuit contained in each angle (Wells, 1977; Smith, 1977). Thus, if for the six angles these were 4-, 4-, 6-, 6-, 6- and 8-circuits, the symbol (here called a short symbol) would be $4^2.6^3.8$. In this work we also give a related long symbol (O'Keeffe, 1991*a*) that is restricted to rings (as opposed to shortest circuits) and in which the angles are given as opposite pairs; thus if the edges are labeled *a*, *b*, *c*, *d*, the angles are grouped as (*ab cd*) (*ac bd*) (*ad bc*). The number of rings contained in each angle is given as a subscript if greater than unity. The hypothetical net referred to above might now have a symbol such as $4.6.4.6_2.8.8_5$ (one of the 6-circuits in the short symbol being rejected as not a ring). It is also useful for recognition of a symbol $U_u.V_v.W_w.X_x.Y_y.Z_z$ for the pairs of opposite angles to be ordered so that *UuVvWwXxYyZz*, considered as an integer written to some suitably large base,* be as small as possible. There are rare examples of nets that contain angles that do not contain any ring (O'Keeffe, 1991*a*).

Another characteristic of a net is its coordination sequence (Brunner, 1979; Meier & Moeck, 1979). This is the sequence n_k of *k*th neighbors, a *k*th neighbor in turn being one that is separated from the reference vertex by a shortest path of *k* edges. Coordination sequences are readily enumerated for quite large values of *k* (say 50) for structures once the neighbors of a vertex are identified. It is found in practice that the sequence for $k \leq 10$ is adequate for most purposes. One use is for rapid computer recognition of a possible topology in a structure as it transpires that only very rarely do different nets have the same coordination sequence. The nets in this paper all have different coordination sequences that serve as useful 'fingerprints'. A useful measure of topological density is

$$\rho_k = \sum_{i=1}^{k} n_i/k^3; \qquad (1)$$

we arbitrarily use ρ_{10} ($1000\rho_{10}$ is the number of neighbors in the first ten coordination shells).

Enumeration methods

Based on purely topological criteria (connectivity), the number of uninodal 4-connected nets is surely very large. However, in application to crystal chemistry, a useful restriction is to those nets that can be realized geometrically with each vertex having only four equidistant nearest neighbors and with the lines joining these neighbors corresponding to the edges of the net. We call such nets realizable. The number of such realizable uninodal 4-connected nets is certainly finite (we believe it to be some hundreds). Some of these are not of great interest, however, as they represent just small distortions of nets of higher connectivity. We have eliminated these from consideration by a method described below.

The nets were found in an empirical computer search. In the method used, a point was moved in small increments throughout the asymmetric unit of the unit cell of all the cubic, hexagonal, tetragonal and orthorhombic space groups in turn. All the equivalent points in the cell generated by the group-symmetry operations were then identified. The topology of the net defined by the four nearest neighbors of the initial point was then characterized by its coordination sequence as described above.

If the net had a new coordination sequence, the next step was to allow the structure to relax to maximum volume subject to the constraint of equal edge lengths. If in that form there were still only four nearest neighbors of a given vertex and these corresponded to the edges of the net as originally identified, the net was retained. Nets consisting of rods or layers were identified by the volume increasing without limit and were eliminated. These criteria eliminated a lot of interesting topologies, but it was felt that the rejected nets were less likely to occur in crystal structures (but for a counter-example, we cite net number 23, described below, as an exception to the rule; it occurs in the $CdSO_4$ structure). For some nets, the parameters were subsequently adjusted to maximize the next-nearest-neighbor distance (as indicated for the specific net below).

For each orthorhombic space group, the calculations involved examination of about 10^6 different combinations of axial ratios (b/a and c/a) and positional coordinates (x, y and z), and took about a week on a VAX 3700 computer. As the orthorhombic space groups (five variables) yielded only ten new nets, the monoclinic and triclinic space groups (six and eight variables respectively) were not examined.

No claim of completeness is made; indeed the criteria for selection given above are somewhat arbitrary and may exclude some nets of potential interest in crystal chemistry. It is possible (but rather unlikely) that two different nets could have the same coordination sequence and space group, which would result in our missing one of them. It is also possible that we missed some nets that are triclinic or monoclinic in their most symmetrical forms, but no uninodal example of such a net is known. However, it should be remarked that we did not miss any previously known uninodal net. Of the nets that were identified, over one-half of them do not appear to have been described before.

* The number of smallest rings contained in an angle can exceed 1000.

Table 1. *Crystallographic data for uniform nets with edge length of unity*

The parameters are those which maximize the next-nearest-neighbor distance, d_2, except for 10 and 11, which are the maximum-volume configuration. r is the number of vertices per unit volume. In all centrosymmetric structures, the origin is chosen on a center.

Net	Space group	a, (b, c) (Å)	x, y, z	r	d_2
1	$Fd\bar{3}m$	$4/3^{1/2}$	1/8, 1/8, 1/8	0.650	1.633
2	$P6_3/mmc$	$(8/3)^{1/2}$, 8/3	1/3, 2/3, 1/16	0.650	1.633
3	$P6_122$	3.5369, 1.6507	0.1363, 0.4322, 0	0.671	1.381
4	$R\bar{3}m$	4.495, 1.504	0.1243, 2x, 1/12	0.683	1.504
5	$P4_122$	2.030, 1.414	0, 0.3258, 0	0.686	1.414
6	$Ia3d$	$(32/3)^{1/2}$	3/8, 0, 1/4	0.689	1.528
7	$I4_1/acd$	4.060, 1.412	0.0871, 0, 1/4	0.687	1.414
8	$Ia3$	$2/(6^{1/2}-3^{1/2})$	$(2^{1/2}-1)/4$, $y=x$, $z=x$	0.739	1.414
9	$Fddd$	4.644, 3.061, 1.531	0.3057, 1/8, 1/8	0.735	1.442
10	$R\bar{3}$	2.6045, 3.6464	0.3764, 0.0737, 0.0598	0.842	1.246
11	$P\bar{3}1c$	2.6133, 2.4733	0.3866, 0.0886, 0.0808	0.820	1.175

Descriptions of uniform nets

For each net we give, in Table 1, an arbitrary identification number, a crystallographic description for equal edges of unit length, r = number of vertices per unit volume and the next-nearest-neighbor distance, d_2. Table 2 gives the coordination sequences n_k for $k \leq 10$ and ρ_{10}. Table 3 gives the Schläfli symbol and the numbers of rings at a vertex for each net. Note that as an N-ring has N vertices, the number of rings per vertex is $1/N$ times the number given here. Further comments on the individual nets follow.

Nets 1 *and* 2: *diamond and lonsdaleite.* These are entirely familiar nets. We simply note that the diamond net is the only regular 4-connected three-dimensional net (with all vertices, edges and angles equivalent). It also has the lowest topological density of any uniform net. Simple analytical expressions for n_k have been given before (O'Keeffe, 1991*b*). These nets (and all their polytypes) have symbol $6_2.6_2.6_2.6_2.6_2.6_2$.

Net 6. This structure is known as the invariant lattice complex S^*. It has been described and illustrated elsewhere (O'Keeffe, 1991*a*). It is the only uniform net other than diamond with all edges equivalent (quasiregular). It occurs in nature as the Si positions in the garnet grossular ($Ca_3Al_2Si_3O_{12}$) and as the Ag positions in Ag_3AuTe_2 (Frueh, 1959). The midpoints of the edges are positions 48(g) (1/8, y, 1/4 − y *etc.*) of $Ia\bar{3}d$ with $y = 5/16 = 0.3125$. This suggests an attractive possible metastable structure for SiO_2 with Si in 24(d) and O in 48(g). The two parameters of the structure, a and y, can be determined from the Si–O bond length and the Si–O–Si bond angle. For these to be the same as in α-quartz (Levien, Prewitt & Wiedner, 1980), $a = 9.989$ Å and $y = 0.2771$. The density is 91% that of quartz and the O–Si–O bond angles are 105.1 (2×) and 111.7° (4×).

Net 8. This net is familiar as the γ-Si structure and is illustrated by Wells (1977). The structural parameters are determined by the requirement of equal edge lengths.

Table 2. *Numbers of kth neighbors, n_k, for uniform nets*

$n_1 = 4$, $n_2 = 12$ in every case. The net number is the same as in Table 1.

Net	n_3	n_4	n_5	n_6	n_7	n_8	n_9	n_{10}	ρ_{10}
1	24	42	64	92	124	162	204	252	0.980
2	25	44	67	96	130	170	214	264	1.026
3	24	40	64	96	134	176	221	272	1.043
4	25	44	69	100	135	176	223	276	1.064
5	26	48	74	104	144	186	234	292	1.124
6	26	48	76	110	146	192	244	302	1.160
7	26	46	72	106	148	194	248	308	1.164
8	27	49	77	109	148	194	244	301	1.165
9	27	50	77	112	152	200	252	312	1.198
10	27	52	87	132	182	242	309	386	1.433
11	27	52	87	132	185	250	317	392	1.458

Table 3. *Numbers of rings meeting at a vertex in uniform nets and Z_t, the number of vertices in the topological repeat unit*

The net number is the same as in Table 1.

Net	Z_t	Symbol	N_6	N_8	N_{10}	N_{12}	N_{14}
1	2	$6_2.6_2.6_2.6_2.6_2.6_2$	12	0	0	0	0
2	4	$6_2.6_2.6_2.6_2.6_2.6_2$	12	0	0	0	0
3	12	$6.6_2.6_2.6_4.6_3.6_3$	15	0	0	6	7
4	6	$6.6_2.6_2.6_3.6_2.6_3$	13	0	10	0	0
5	4	$6.6.6_2.6_2.6_3.6_3$	12	8	10	0	0
6	12	$6.6.6_2.6_2.6_2.6_2$	10	0	0	0	0
7	8	$6.6.6_2.6_2.6_3.6_3$	12	12	0	0	0
8	8	$6.6_2.6.6_2.6.6_2$	9	12	15	0	0
9	4	$6.6.6.6_2.6_2.6_2$	9	8	0	0	0
10	6	$6.6.6.6_2.6_2.6_2$	9	0	10	0	0
11	12	$6.6.6.6_2.6_2.6_2$	9	0	10	0	0

Nets 3, 4, 5, 7 *and* 9. These nets are simply derived from planar 3-connected nets by replacing some of the edges by zigzag chains as illustrated in Figs. 1–5. Net 3 (Fig. 1) is derived from 4.6.12 by replacing the edges common to hexagons and dodecagons by zigzags running parallel to **c**. Net 4 (Fig. 2) is similarly derived from 6^3 [compare also net 14 (Fig. 9)].

Nets 5 and 7 (Figs. 3 and 4) illustrate two ways in which the plane net 4.8^2 can be converted to uniform nets by replacing the edges between octagons by zigzags. Net 5 contains 4_1 helices of vertices (and has an enantiomorph with 4_3 helices), net 7 contains 4_1

and 4_3 helices in equal numbers. It might be noted that these nets can also be considered as made of puckered 6^3 nets [parallel to (110)]. In Smith's (1977) notation, the pattern of linkages between the 6^3 layers is *SCCSCC*. With vertical linkages between the layers, one obtains the well known net of the atoms in the β-BeO structure, net no. 3 of Smith (1977). In nets 5 and 7, the linkages between the 6^3 layers are neither perpendicular to the layers nor all parallel (*cf.* net 9 below).

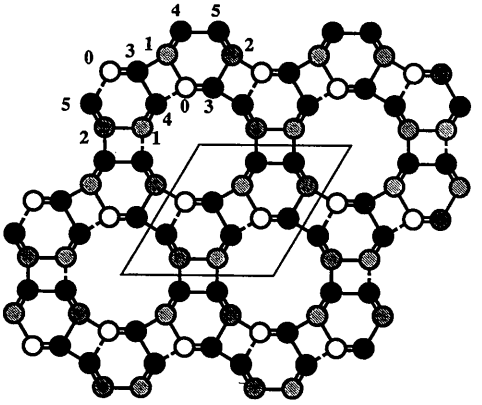

Fig. 1. Net 3 shown as a projection on (001). Numbers are elevations in multiples of $c/6$. Double lines represent zigzags parallel to c.

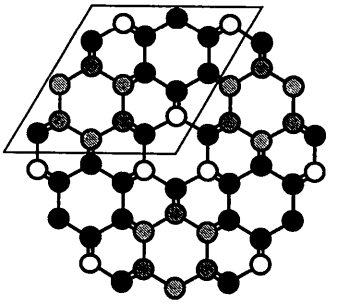

Fig. 2. Net 4 shown as a projection on (001) of the hexagonal cell. Elevations are shown by successively darker shading: $c/12$ (open circles), $3c/12$, $5c/12$, $7c/12$, $9c/12$, $11c/12$ (filled circles). Double lines represent zigzags parallel to c.

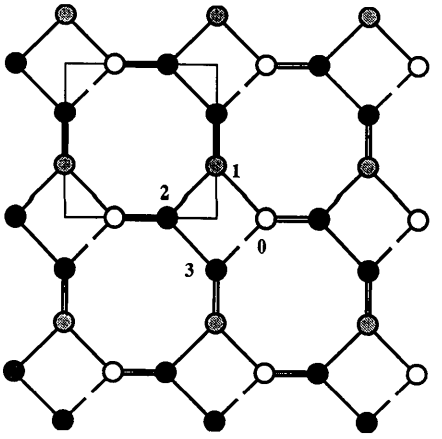

Fig. 3. Net 5 shown as a projection on (001). Numbers are elevations in multiples of $c/4$. Double lines represent zigzags parallel to c.

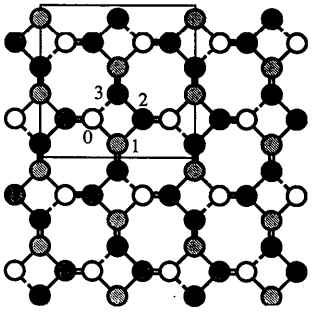

Fig. 4. Net 7 shown as a projection on (001). Numbers are elevations in multiples of $c/4$. Double lines represent zigzags parallel to c.

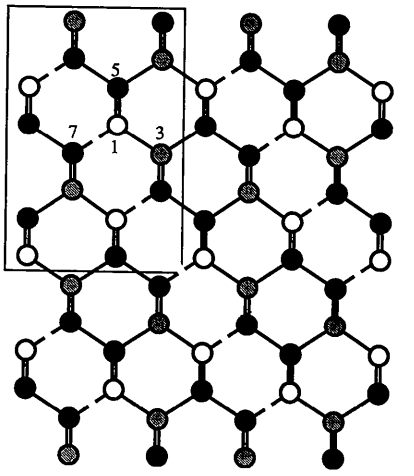

Fig. 5. Net 9 shown as a projection on (001). Numbers are elevations in multiples of $c/8$. Double lines represent zigzags parallel to c.

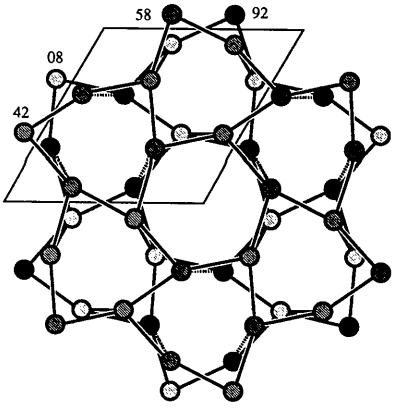

Fig. 6. Net 11 shown as a projection on (001). Numbers are elevations in multiples of $c/100$. Broken lines represent edges to vertices with $z<0$ or $z>1$.

Table 4. *Crystallographic data for non-uniform nets without 3- or 4-rings*

For centrosymmetric structures, the origin is chosen on a center.

Net	Space group	a, c (Å)	x, y, z	r	d_2
12	$R\bar{3}c$	5.3068, 1.3501	0, 0.4305, 1/4	0.547	1.268
13	$P6_122$	3.0621, 1.3501	0.4305, 2x, 1/4	0.547	1.268
14	$P6_122$	2.5255, 1.6027	0.3816, 0, 0	0.678	1.466
15	$P6_122$	2.2858, 2.2115	0.2348, 2x, 1/4	0.600	1.595
16	$I4_1/a$	2.8818, 2.5275	0.0888, 0.1010, 3/8	0.762	1.414
17	$Im\bar{3}m$	2.0	0, 1/2, 1/2	0.750	1.414
18	$P6_222$	1.6330, 1.7321	1/2, 0, 0	0.750	1.414
19	$R\bar{3}c$	4.6141, 2.2680	0.2309, 0.0435, 0.0433	0.861	1.180
20	$R\bar{3}c$	4.4420, 2.6648	0.1186, 0.5331, 0.0632	0.791	1.290
21	$P4_22_12$	1.8373, 2.6685	0.1342, 0.2632, 0.1765	0.888	1.086
22	$R\bar{3}c$	3.0984, 2.6833	1/4, 0, 1/4	0.807	1.265
23	$P4_2/mmc$	1.0, 2.0	0, 0, 0	1.0	1.0
24	$P6_222$	1.0, 3.0	0, 0, 0	1.155	1.0

Net 9 (Fig. 5) is of interest because of its close relationship to the diamond and lonsdaleite nets. The structure can be considered as made up of puckered 6^3 layers parallel to {110} with additional edges connecting the layers alternating up and down. In Smith's (1977) notation, the pattern of linkages between the 6^3 layers is *CCCCCC* as in diamond and lonsdaleite. The difference between those structures and the *Fddd* structure is that the linkages in the latter are no longer perpendicular to the layer but canted in two different directions. One can readily construct coherent intergrowths of the three structures with {111} of diamond or (001) of lonsdaleite parallel to {110} of the *Fddd* structure.

Nets 10 *and* 11. These nets are closely related and represent yet another way of deriving uniform nets from 6^3. The 6^3 nets are considerably distorted and the linkages between them are far from vertical as illustrated for net 11 in Fig. 6. Net 10 is essentially a three-layer version of the two-layer net 11.

Descriptions of non-uniform nets

We follow a similar procedure for the description of non-uniform nets. For each net we give, in Table 4, an arbitrary identification number, a crystallographic description for equal edges of unit length, r = number of vertices per unit volume and the next-nearest-neighbor distance, d_2. Table 5 gives the coordination sequences n_k for $k \leq 10$ and ρ_{10}. Table 6 gives the Schläfli symbol and the numbers of rings at a vertex for each net. Further brief comments on the individual nets follow. Nets 18 and 19 are familiar as those of the Si atoms in quartz and of all the atoms in NbO, respectively: they need no further comment other than to remark that they are quasiregular and the only uninodal nets we know that are $6^4.8^2$.

Nets 12, 13 *and* 14. These nets continue the theme of deriving nets from plane nets by replacing edges by zigzags. In nets 12 and 13 (Figs. 7 and 8), the plane net is now 3.12^2 and the edges between dodecagons are replaced by zigzags. The triangles of the plane nets now become helices, of one hand in net 13 and of both hands in net 12. Net 14 (Fig. 9), derived from 6^3, is very closely related to net 4 (Fig. 2).

Table 5. *Numbers of kth neighbors, n_k, for non-uniform nets*

$n_1 = 4$, $n_2 = 12$ in every case. The net number is the same as in Table 4.

Net	n_3	n_4	n_5	n_6	n_7	n_8	n_9	n_{10}	ρ_{10}
12	22	40	66	98	126	168	216	262	1.014
13	22	40	66	102	128	168	218	268	1.028
14	26	46	70	100	136	178	224	276	1.072
15	26	44	72	104	138	178	228	282	1.088
16	25	50	75	106	150	190	241	303	1.156
17	28	50	76	110	148	194	244	302	1.168
18	30	52	80	116	156	204	258	318	1.230
19	29	58	88	124	169	222	280	346	1.332
20	29	54	86	128	173	228	291	360	1.365
21	30	56	89	129	177	233	295	364	1.389
22	26	50	86	128	182	240	310	382	1.420
23	30	58	94	138	190	250	318	394	1.488
24	36	72	122	188	264	354	456	570	2.078

Net 15. This net (Fig. 10) illustrates a second way of generating three-dimensional nets from plane nets. In the 4-connected plane net 3.4.6.4, the hexagons and triangles are converted into helices (which must all be of the same hand) to generate a three-dimensional structure. This procedure is analogous to the derivation of the quartz and NbO nets from 3.6.3.6 and the diamond net from 4^4 (Wells, 1977; Smith, 1979).

Net 16. This net (Fig. 11) is of interest because of its close resemblance to that of Si in the keatite form of SiO_2 (the keatite net is also found in a polymorph of Ge and in H_2O). It is one of only five uninodal nets that we have identified with shortest rings that are 5-rings.

Nets 19 *to* 24. Nets 19 to 22 are presented in their maximum-volume forms in Table 4. Nets 19 to 21 provide further examples of $6^5.8$ nets and net 22 (Fig. 12) provides a rare example of a net in which all shortest rings are odd. This last net also has a very simple description using a primitive rhombohedral

Table 6. *Numbers of rings meeting at a vertex in non-uniform nets*

The net number is the same as in Table 4 and Z_t is the number of vertices in the topological repeat unit. 'Short' and 'long' refer to the two ways of giving Schläfli symbols discussed in the text. '∞' in the symbol means that the angle in question does not contain a ring.

Net	Z_t	Short	Long	N_5	N_6	N_7	N_8	N_9	N_{10}	N_{12}	N_{13}
12	6	$5^4.6^2$	$5.5.5.5_2.12_{10}.12_{10}$	5	0	0	0	0	0	40	0
13	6	$5^4.6^2$	$5.5.5.5_2.12.12$	5	0	0	0	0	0	12	13
14	6	$6^5.8$	$6_2.6_2.6_2.8_5.6_3.6_3$	0	12	0	8	0	0	0	0
15	6	$5^5.8$	$5.5.5.5.5.8_4$	5	0	0	8	0	0	0	0
16	8	$5^4.8^2$	$5.5_2.5.8.5.8$	5	0	0	4	0	5	0	0
17	3	$6^4.8^2$	$6_2.6_2.6_2.6_2.8_2.8_2$	0	8	0	8	0	0	0	0
18	3	$6^4.8^2$	$6_2.6_2.6_2.6_2.8_7.8_7$	0	6	0	40	0	0	0	0
19	12	$6^5.8$	$6.6_2.6.6_2.6.8_4$	0	7	0	12	0	35	0	0
20	12	$6^5.8$	$6.6_2.6.6_2.6.8_4$	0	7	0	24	0	0	0	0
21	8	$6^5.8$	$6.6.6.6_2.6.8_5$	0	6	0	32	0	0	0	0
22	8	$5^5.8$	$5.5.5.5.5.9$	5	0	0	0	9	10	0	0
23	2	$6^5.8$	$6.6.6.6.6_2.\infty$	0	6	0	24	0	0	0	0
24	3	$7^5.9$	$7_2.\infty.7_3.7_3.7_3.7_3$	0	0	14	0	0	0	0	0

cell for $R\bar{3}c$: $a=2$ and $\alpha=\cos^{-1}(-1/5)$, vertices in 6(*e*) with $x=0$. Half of the edges form linear rods running in three of the four directions of b.c.c. cylinder packing (O'Keeffe & Andersson, 1977). It is also closely related to a 5-connected net (obtained by inserting the fourth rod) described by Wells (1977, Fig. 16.28).

Nets 23 and 24 in their maximum-volume forms have vertices on a primitive cubic lattice (six nearest neighbors) and a primitive hexagonal lattice (eight nearest neighbors), respectively. They have been described before (O'Keeffe, 1991*a*) and are of interest because of the small numbers of vertices (two and three, respectively) in the topological repeat unit. Net

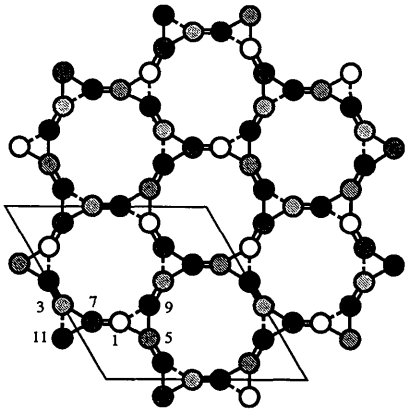

Fig. 7. Net 12 shown as a projection on (001). Numbers are elevations in multiples of $c/12$. Double lines represent zigzags parallel to **c**.

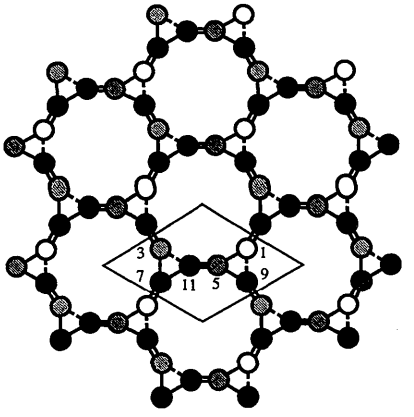

Fig. 8. Net 13 shown as a projection on (001). Numbers are elevations in multiples of $c/12$. Double lines represent zigzags parallel to **c**.

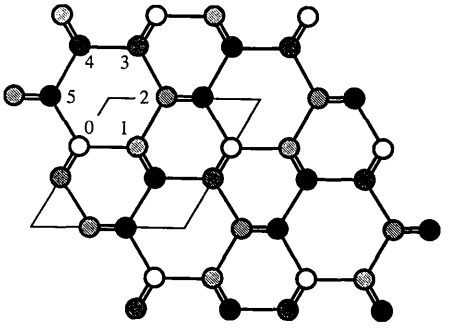

Fig. 9. Net 14 shown as a projection on (001). Numbers are elevations in multiples of $c/6$. Double lines represent zigzags parallel to **c**.

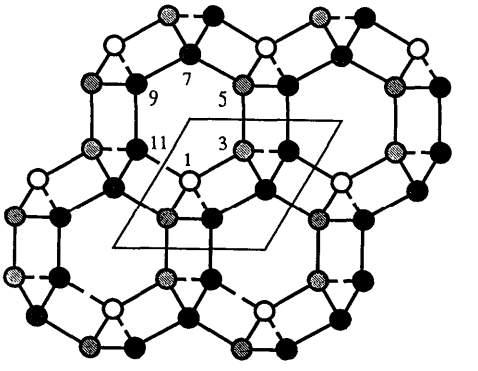

Fig. 10. Net 15 shown as a projection on (001). Numbers are elevations in multiples of $c/12$.

23 occurs in the $CdSO_4$ structure (O'Keeffe, 1991*a*). Net 24 is also of interest as being possibly the densest 4-connected net in the topological sense; it might be considered uniform in the sense that the rings are all 7-rings, but note that one angle is not contained on any ring.

Discussion

We are surprised, in view of the long interest in 4-connected nets, that some of the simpler nets described here do not appear to have been recognized before. This may be in part due to the prevalence of screw axes and glide planes and the absence of mirror planes in some of their symmetries. Two of the new nets have only four vertices in the repeat unit and a further six have only six in the repeat unit. Pleasing models of most of the nets are readily made with tetrahedral vertices and plastic tubing as edges, although net 22 is better made using four non-coplanar spokes of an octahedral 'star'. It is an interesting challenge either to identify these nets in crystal structures (this is most readily done using the coordination sequences) or to explain why they should not occur.

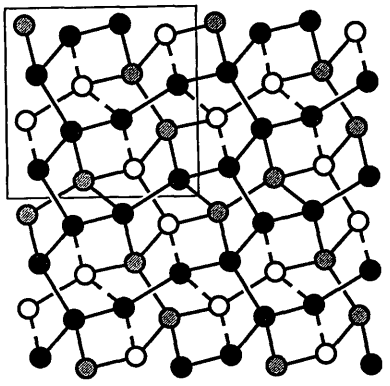

Fig. 11. Net 16 shown as a projection on (001). Open circles are at $z = 0$, lightly shaded at $z = 1/4$, darker shaded at $z = 1/2$ and filled circles are at $z = 3/4$.

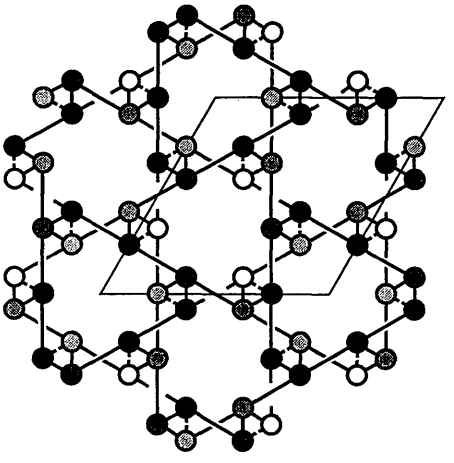

Fig. 12. Net 22 shown as a projection on (001) of the hexagonal cell. Elevations are shown by successively darker shading: $c/12$ (open circles), $3c/12$, $5c/12$, $7c/12$, $9c/12$, $11c/12$ (filled circles).

We have reported all the rings in the nets under discussion as these are considered most relevant to discussions of topology (Stixrude & Bukowinski, 1990). However, Goetzke & Klien (1991) further define 'strong rings', which are rings that cannot be decomposed into a sum of smaller rings. Nets 1, 2, 4 and 6 contain only six-membered strong rings and might be termed 'strongly' uniform. Uniform nets that can be realized with shortest distances corresponding to edges (realizable) are all 6^6, but we know of no proof that this must always be the case. Net 24 shows that if we remove the restriction to realizable nets, a net with only 7-rings (which are of course strong rings) exists. The chlorine hydrate net (Wells, 1977) contains vertices 5^6, but the two other kinds of vertex in the structure are $5^5.6$ and $5^4.6^2$.

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