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Uninodal 4-Connected 3D Nets. II. Nets with 3-Rings

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Abstract

A description is given of nineteen 4-connected nets with one kind of vertex and containing 3-rings. Many of them are believed to be new.

Introduction

This paper continues the systematic description and analysis of three-dimensional 4-connected nets with one kind of vertex ('uninodal') begun in paper I (O'Keeffe & Brese, 1992), which should be consulted for terminology and references. In this paper, 4-connected nets with at least one 3-ring are discussed; it follows a similar format to paper I: crystallographic descriptions are given in Table 1, coordination sequences in Table 2 and ring statistics in Table 3. Descriptions of some individual nets follow.

Nets with three 3-rings at a vertex

Nets 25 *to* 29. These nets all have three 3-rings meeting at a vertex. For such a three-dimensional net with equal edges, the vertices must be at the vertices of a regular tetrahedron and can be derived from simpler 4-connected nets by replacing a vertex by such a tetrahedron. For this to result in a uninodal net, the edges of the original net must all be equivalent (the net must be quasiregular). The procedure and the resulting nets (which are also of interest as rare sphere packings) have been described in some detail elsewhere (O'Keeffe, 1991). Net 25 appears to be the rarest known uninodal 4-connected net (Fischer, 1974).

Nets with two 3-rings at a vertex

Net 34. This is known as the lattice complex ^+V (Fischer & Koch, 1985) and is illustrated in Fig. 1. It is the only net of this compilation with two 3-rings meeting at a vertex. It is not difficult to see that such a uninodal net must have the 3-rings at opposite angles. The centers of the triangles formed by the 3-rings will fall on a 3-connected net and the vertices of the 4-connected net at the mid-points of the edges of the 3-connected net. As Wells (1977) has pointed out, for the 4-connected net to be uninodal, the edges of the 3-connected net must all be equivalent. The only such 3-connected net appears to be that of the Si atoms in $SrSi_2$ (lattice complex $^+Y^*$) from which this net is derived, so it is likely that there is only one uninodal net with two 3-circuits meeting at a vertex.†

† The two-dimensional net 3.6.3.6 (kagomé) is related to 6^3 (honeycomb) in an analogous way.

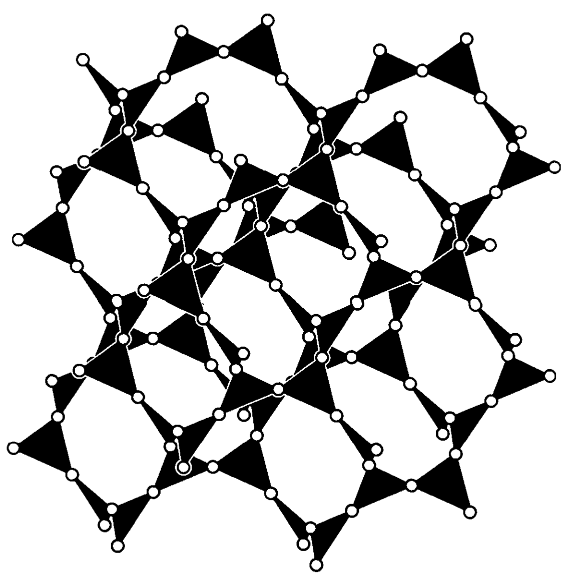

Fig. 1. Net 34 shown as corner-sharing triangles.

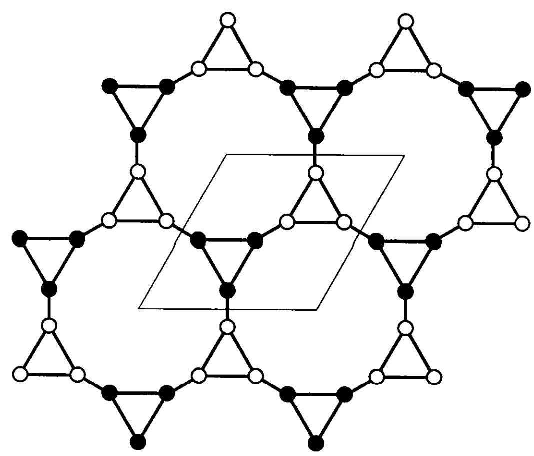

Fig. 2. Net 36 projected on (001). Open and filled circles are at $z = 0$ and $z = 1/2$. This drawing also serves to illustrate net 30 if the open circles are interpreted as superimposed points at $z = 0.09$ and 0.41 and filled circles as points at $z = 0.59$ and 0.91.

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

r is the number of vertices per unit volume. For centrosymmetrical structures, the origin is chosen on a center.

Net	Space group	$a, (c)$	x, y, z	r
25	$I4_132$	$4+2\times2^{1/2}$	$x=y=2^{1/2}/8,\ z=0$	0.151
26	$Im\bar{3}m$	$2+3\times2^{1/2}$	$48(k),\ ay=1/2+2^{1/2},\ az=1/2+3/2^{1/2}$	0.197
27	$Fd\bar{3}m$	$2\times2+4/3^{1/2}$	$32(e),\ x=1/(8+4\times6^{1/2})$	0.236
28	$Ia\bar{3}d$	7.1678	0.0646, 0.2238, 0.4243	0.261
29	$P6_222$	3.5497	0.4579, 0.1150, 0.0910	0.283
30	$P6_3/mmc$	3.4536, 3.0875	$12(k),\ x=0.4299,\ z=0.0881$	0.376
31	$I4_132$	$[8/(9-6\times2^{1/2})]^{1/2}$	$24(h),\ x=(8^{1/2}-1)/8$	0.391
32	$R32$	3.3918, 4.4830	0.1917, 0.1335, 0.1048	0.403
33	$Fm\bar{3}m$	$2+3\times2^{1/2}$	$96(k),\ x=(1+2^{1/2})z,\ z=1/(4+6\times2^{1/2})$	0.395
34	$I4_132$	$(32/3)^{1/2}$	$12(c)$	0.344
35	$R\bar{3}c$	3.6720, 5.4911	0.1543, 0.5510, 0	0.561
36	$P6_3/mmc$	3.1196, 1.5260	$6(h),\ x=0.4402$	0.457
37	$Pm\bar{3}m$	$2/(3-6^{1/2})$	$24(j),\ x=(3-6^{1/2})/4$	0.501
38	$R32$	$5/3^{1/2}, 5^{1/2}$	$9(d),\ x=1/5$	0.558
39	$Pa\bar{3}$	3.5334	0.1046, 0.1709, 0.3295	0.544
40	$R\bar{3}c$	2.7736, 8.7009	0.1108, 0.4767, 0.0417	0.618
41	$I432$	$(32/3)^{1/2}$	$24(i),\ x=1/8$	0.689
42	$F4_132$	$4/(2\times3^{1/2}-6^{1/2})$	$48(g),\ x=0.0214$	0.783
43	$R\bar{3}c$	2.6373, 3.7637	$18(e),\ x=0.2192$	0.794

One can, of course, make a large number of binodal nets of this type. Perhaps the simplest is that derived from the Si net of the $ThSi_2$ structure (Wells, 1977); it has a compact crystallographic description: $I4_1/amd$, $a=2$, $c=4\surd3$ with vertices in $4(a)$ and $8(c)$. This last net is the net of the Ge atoms in GeS_2.

Nets with one 3-ring at a vertex

These nets fall into two categories: (a) hexagonal or rhombohedral nets with all 3-rings parallel and (b) cubic nets with 3-rings normal to the four threefold symmetry axes. The former are discussed first.

Nets 36 *and* 38. Net 36 (Fig. 2) and net 38 (Fig. 3) represent the two simplest ways of connecting triangles to have a two- or three-layer sequence, respectively. Nets 36 and 38 are, respectively, nos. 94 and 92 of Smith (1979); net 38 was also described by Wells (1977).

Nets 30 *and* 32. Net 30 is simply derived from net 36 by replacing the triangles by right triangular prisms

Table 2. *Numbers of kth neighbors, n_k; $n_1=4$ in every case*

$1000\rho_{10}$ is the total number of vertices in the first ten coordination shells.

Net	n_2	n_3	n_4	n_5	n_6	n_7	n_8	n_9	n_{10}	ρ_{10}
25	6	11	12	22	24	44	48	88	91	0.350
26	6	12	17	28	38	52	64	84	104	0.409
27	6	12	18	36	48	60	78	108	126	0.496
28	6	12	18	36	49	68	88	124	147	0.552
29	6	12	18	36	51	84	103	124	156	0.594
30	8	16	28	42	64	89	110	141	178	0.680
31	8	13	22	38	64	89	112	150	196	0.696
32	8	16	32	49	67	93	123	149	188	0.729
33	9	18	30	47	69	91	125	160	191	0.744
34	8	16	32	54	70	102	128	158	212	0.784
35	8	16	32	49	70	101	135	166	212	0.793
36	10	20	34	58	82	108	144	186	222	0.868
37	9	20	38	59	84	114	148	187	230	0.893
38	10	26	40	66	90	126	160	206	250	0.978
39	10	25	40	69	92	132	165	218	261	1.016
40	10	26	43	74	106	149	194	256	308	1.170
41	10	23	43	76	108	156	206	270	335	1.231
42	10	22	42	78	118	166	232	292	374	1.338
43	10	26	46	82	120	176	230	302	366	1.362

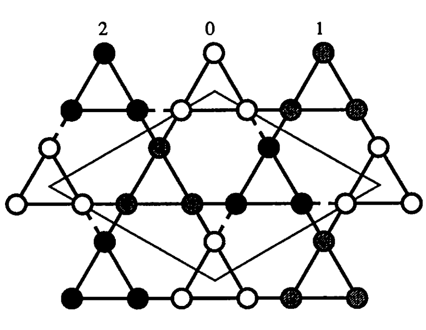

Fig. 3. Net 38 projected on (001) of the hexagonal cell. Numbers represent elevations in multiples of $c/3$.

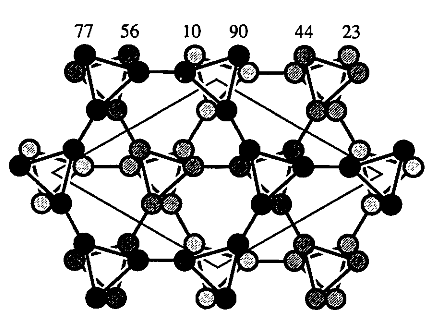

Fig. 4. Net 32 projected on (001) of the hexagonal cell. Numbers represent elevations in multiples of $c/100$.

Table 3. *Rings in nets with* 3-*rings*

N_i is the number of i-rings meeting at each vertex. 'Short' and 'long' refer to Schläfli symbols defined in paper I of this series (O'Keeffe & Brese, 1992).

Net	Z_t	Short	Long	N_3	N_4	N_6	N_7	N_8	N_9	N_{10}	N_{12}	N_{14}	N_{16}	N_{18}	N_{20}	N_{24}
25	24	$3^3.6.7^2$	$3.6.3.20_2.3.20_3$	3	0	1	0	0	0	0	0	0	0	0	5	0
26	24	$3^3.8.9^2$	$3.8.3.12.3.12$	3	0	0	0	1	0	0	2	0	0	0	0	16
27	8	$3^3.12^3$	$3.12_2.3.12_2.3.12_2$	3	0	0	0	0	0	0	6	0	0	0	0	0
28	48	$3^3.12^3$	$3.12.3.12_2.3.12_2$	3	0	0	0	0	0	0	3	0	0	0	0	0
29	12	$3^3.12^2.13$	$3.12.3.12_2.3.16_7$	3	0	0	0	0	0	0	3	0	20	0	0	0
30	12	$3.4^2.8^3$	$3.8_2.4.8.4.8$	1	2	0	0	4	0	0	2	0	0	0	0	0
31	12	$3.4^2.5^2.7$	$3.14_{75}.4.4.14_{30}.14_{30}$	1	2	0	0	0	0	0	0	175	0	0	0	0
32	6	$3.4^2.9^3$	$3.9_3.4.9_2.4.9_3$	1	2	0	0	0	9	0	2	0	0	0	0	0
33	24	$3.4.6^2.8^2$	$3.4.6.8.6.8$	1	1	2	0	2	0	0	2	0	0	36	0	0
34	6	$3^2.10^4$	$3.3.10_2.10_2.10_3.10_3$	2	0	0	0	0	0	10	0	0	0	0	0	0
35	12	$3.4^2.9^3$	$3.9_3.4.9_2.4.9_3$	1	2	0	0	0	9	0	2	0	0	0	0	0
36	6	3.6^5	$3.6_2.6.6.6.6$	1	0	6	0	0	0	0	40	0	0	0	0	0
37	24	$3.4.8^4$	$3.4.8.8.8_2.8_2$	1	1	0	0	6	0	10	4	0	0	0	0	0
38	3	3.7^5	$3.7.7.7.7_2.7_2$	1	0	0	7	0	0	0	0	0	0	0	0	0
39	24	$3.6.7^4$	$3.6.7.7.7_2.7_2$	1	0	1	7	0	0	5	0	0	0	0	0	0
40	12	3.7^5	$3.7.7.7.7_2.7_2$	1	0	0	7	0	0	5	0	0	0	0	0	0
41	12	$3.6^3.7^2$	$3.6.6.6.8.8$	1	0	3	0	4	0	10	4	0	0	0	0	0
42	12	$3.6^4.9$	$3.9.6.6.6.6$	1	0	4	0	0	3	0	0	0	0	0	0	0
43	12	3.7^5	$3.7.7.7.7_2.7_2$	1	0	0	7	0	0	10	0	0	0	0	0	0

(see the caption for Fig. 2). Net 32 is analogously obtained from net 38. In its maximum-volume form (illustrated in Fig. 4), the prisms are somewhat distorted. Nets 30 and 32 are, respectively, nos. 64 and 65 of Smith (1978). Net 32 was also described by Wells (1977).

Nets 35, 40 *and* 43. These nets (all with symmetry $R\bar{3}c$) continue the series started with nets 36 and 38. Nets 35 (Fig. 5) and 43 (Fig. 6) have a six-layer repeat and net 40 (Fig. 7) has a twelve-layer repeat. I have not found these nets described elsewhere.

Net 33. This is familiar as the net of a space filling by truncated tetrahedra, truncated cubes and truncated cuboctahedra (Andreini, 1907); for an illustration see, for example, Wells (1977).

Nets 31, 37, 39 *and* 41. These nets form a closely related group. They all have 24 vertices in a cubic unit cell in which eight triangles are perpendicular to the four threefold axes. Net 31 is difficult to illustrate satisfactorily owing to the large rings (see Table 3). The others (see Figs. 8–10) are simpler. Net 39 (Fig. 9) occurs as the net of the tetrahedrally coordinated cations in CaB_2O_4, SrB_2O_4, $BaAl_2S_4$ and

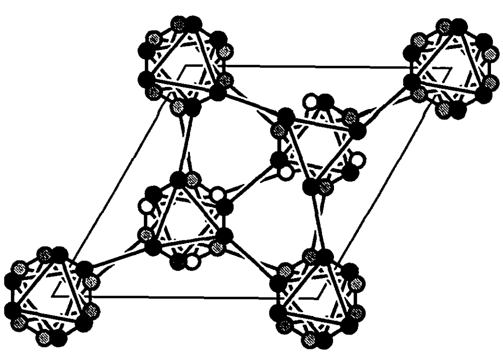

Fig. 5. Net 35 projected on (001) of the hexagonal cell. Progressively darker shading represents increasing elevations from $z = 0$ (open circles), 1/6, 2/6, 3/6, 4/6 and 5/6 (filled circles).

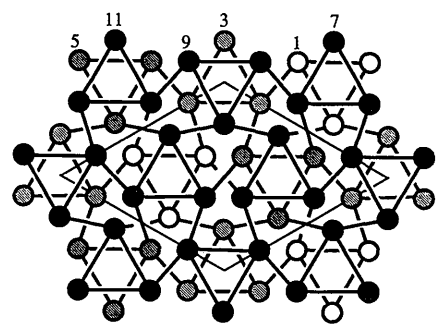

Fig. 6. Net 43 projected on (001) of the hexagonal cell. Numbers represent elevations in multiples of $c/12$.

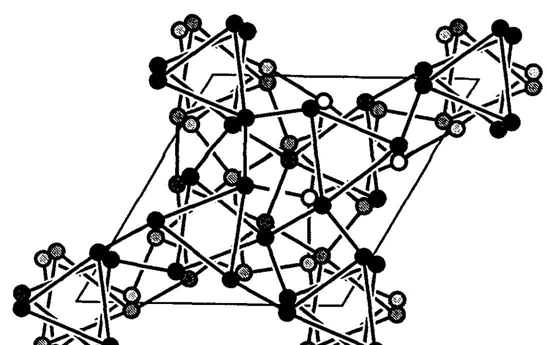

Fig. 7. Net 40 projected on (001) of the hexagonal cell. Progressively darker shading represent increasing elevations from $z = 1/24$ (open circles), 3/24, 5/24, 7/24, 9/24, 11/24, 13/24, 15/24, 17/24, 19/24, 21/24 and 23/24 (filled circles).

$BaGa_2S_4$. The others have not been identified elsewhere other than in Fischer's list of cubic sphere packings (Fischer, 1973, 1974) but might also be expected to occur in crystal structures.

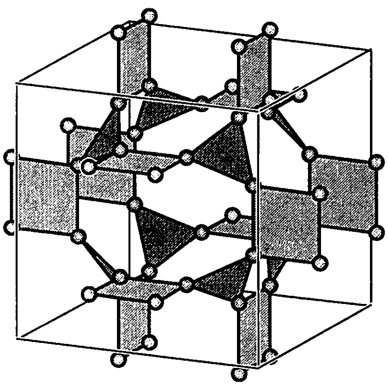

Fig. 8. Clinographic projection of net 37. The cubic unit cell is outlined.

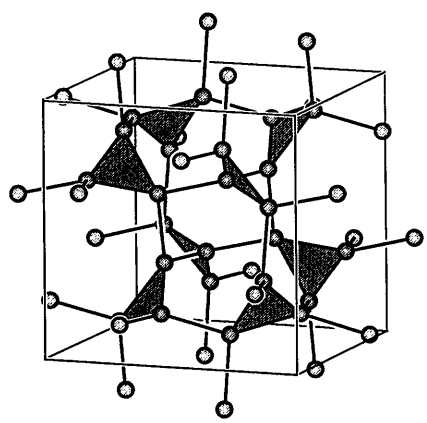

Fig. 9. Clinographic projection of net 39. The cubic unit cell is outlined.

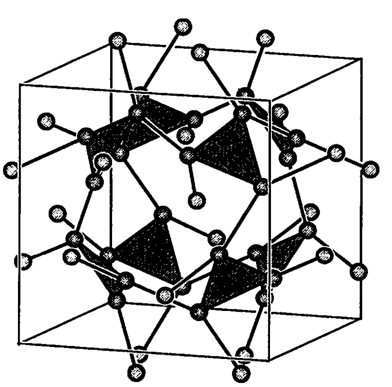

Fig. 10. Clinographic projection of net 41. The cubic unit cell is outlined.

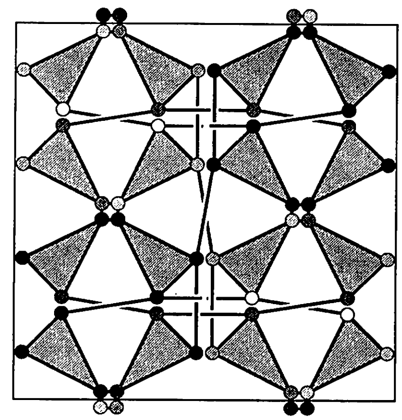

Fig. 11. Projection of net 42 on (001). Progressively darker shading indicates increasing elevation from $z = 0.02$ to $z = 0.98$ (all elevations are within ± 0.02 of multiples of 1/8).

Net 42. This net (Fig. 11) is of interest as a dense net with 3-rings. The structure is simply derived from the rods of the *A*15 structure [*i.e.* Cr of Cr_3Si (see O'Keeffe & Andersson, 1977)] by small displacements along ⟨110⟩ to produce a $2 \times 2 \times 2$ superstructure. The positional parameter ($x = 0.021$, Table 1) has to be changed to $x = 0$ to recover the *A*15 rods.

Discussion

Nets with 3-rings have a remarkably wide range of densities and ring sizes. The largest rings are 24-rings (in net 26). Strong rings (Goetzke & Klien, 1991) are those which cannot be decomposed into sums of smaller circuits. The largest of these are the 20-rings occurring in net 25. The very simple net 38 with only three vertices in the repeat unit appears to be the only uninodal net in which all the rings are odd.

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