Acta Cryst. (1999). A**55**, 360–382

Enumeration of four-connected three-dimensional nets. III. Conversion of edges of three-connected two-dimensional nets into saw chains

Shaoxu Han and Joseph V. Smith*

Consortium for Theoretical Frameworks, Department of the Geophysical Sciences, University of Chicago, Chicago, IL 60637, USA. E-mail: smith@geo1.uchicago.edu

(*Received 3 April 1998; accepted 23 July 1998*)

Abstract

A three-repeat saw (*s*) chain has each vertical edge separated by a tooth composed of two tilted edges zig and zag. Some horizontal (*h*) edges from a parallel stack of three-connected two-dimensional (2D) nets can be converted into an *s* chain. Each resulting four-connected vertex in the three-dimensional (3D) net may be part of either one, two or three *s* chains. The first type of (*h*,*s*)* 3D net is related by a sigma-type mirror plane to a (*h*,*z*)* net listed in paper II [Han & Smith (1998). *Acta Cryst.* A**55**, 342–359]. The second type does not have an (*h*,*z*)* relative. Using the same three-connected 2D nets as in paper II, 174 four-connected 3D nets were selected from the first two types, including six in known structures: 'nepheline hydrate' (International Zeolite Association Structure Commission code JBW), $AlPO_4$-12-TAMU (ATT), offretite (OFF), Linde Type L (LTL), SUZ-4 (SZF) and ZSM-10 (ZST). The third type with three back-to-back *s* chains is represented by edingtonite (EDI), and systematic enumeration is in progress. The geometrical and topological properties of the 3D nets are given. Idealized unit-cell data and atomic coordinates for tetrahedral bonding were obtained for 40

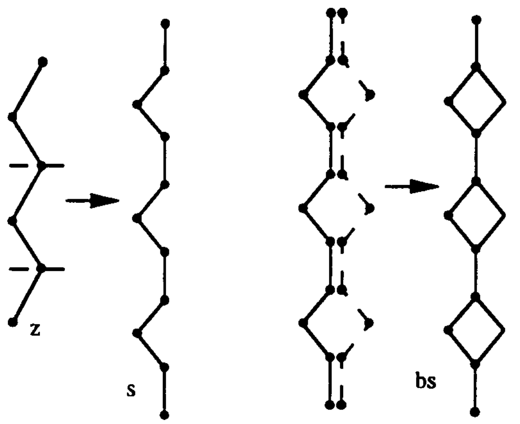


Fig. 1. Three simple 1D chains, *z*, *s* and *bs*. (*a*) Dashed lines through every other vertex of the *z* chain show the sigma-transformation to generate the *s* chain. (*b*) Two *s* chains forming the *bs* chain.

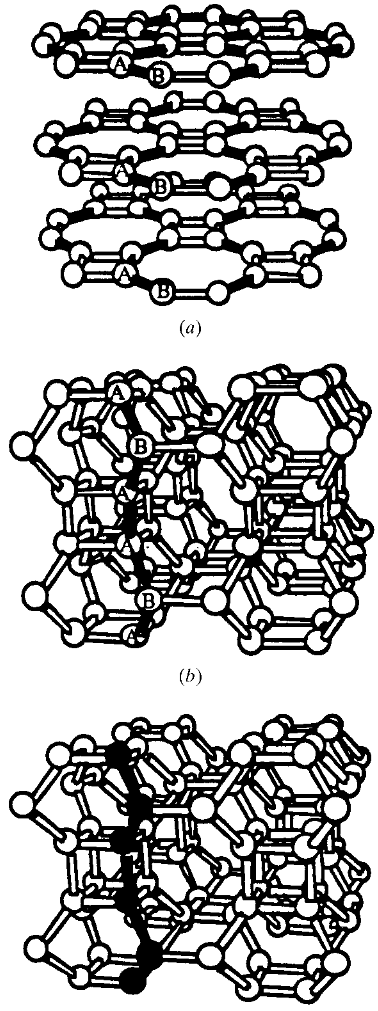


Fig. 2. Procedure for generation of 3D *s* nets by the first approach. (*a*) A vertical stack of horizontal congruent three-connected 2D nets (*fee* 48^2) with shaded edges becoming part of the *s* chain. (*b*) A four-connected 3D net (CTF number 99) obtained by converting the *h* edges in (*a*) into tilted and vertical edges of the *s* chain and making all the vertices four-connected. *A* and *B* represent two types of vertices. The *s* chain in the 3D net is indicated by the shaded edges. Each pair of tilted edges can be regarded as a saw tooth. This first type of *s** net can be obtained from a *z** net by a horizontal sigma-plus transformation through the vertical edge between vertices *A* in (*b*). (*c*) The 3D net after DLS refinement.

selected 3D nets by distance-least-squares (DLS) refinement.

1. Introduction

The first two papers in this series describe two enumerations of four-connected three-dimensional (3D) nets. In paper I (Han & Smith, 1998*a*), each edge of a congruent stack of horizontal three-connected two-dimensional (2D) nets is converted into a vertical four-repeat crankshaft (*c*) chain. In paper II (Han & Smith, 1998*b*), alternate edges are converted into a vertical two-repeat zigzag (*z*) chain.

This third paper considers the conversion of some edges of a congruent stack of horizontal three-connected 2D nets into a three-repeat zigzag-straight saw chain to yield a four-connected 3D net. Because this *s* chain can be described as a sigma-plus derivative (Shoemaker *et al.*, 1973) of the *z* chain, an obvious procedure for enumeration of 3D (*h*,*s*)* nets is to sigma-transform each 3D (*h*,*z*)* net from paper II. Another two sets of 3D nets arise because the *s* chain is a sigma-minus transform of the *c* chain.

2. Enumeration

The zigzag-straight repeat of the *s* chain is near 7.5 Å for silicates. It can be generated by a sigma-plus transformation through every other vertex of the *z* chain (Fig. 1*a*). Two back-to-back *s* chains generate a *bs* chain (Fig. 1*b*). Three *s* chains can also meet back-to-back, as in edingtonite (EDI). Various four-connected 3D nets were obtained by combining congruent stacks of some simple 2D nets with the *s* chain (Smith, 1979). We now examine congruent stacks of all the three-connected 2D nets in the catalog of the Consortium for Theoretical Frameworks (CTF) (Pluth & Smith, 1993).

Each 3D net in paper II was converted into a 3D (*h*,*s*)* net by simple addition of a vertical straight edge between each zigzag of the *z* chain (Fig. 2). Each 3D (*h*,*s*)* net contains two types of vertex: *A* with two *h* edges, one tilted and one vertical edge, and *B* with two *h* edges and two tilted edges. Transformation of a vertical zigzag *z* chain to a vertical zigzag-straight *s* chain by a

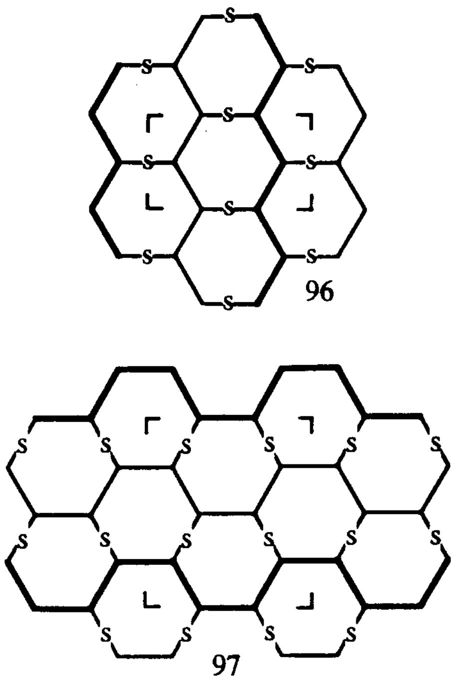


Fig. 3. Two 3D nets derived from the 2D *hex* net (6^3) by replacing *z* chains of CTF nets 1 and 2 (Han & Smith, 1998*b*) with *s* chains. Each tilted edge *s* is part of a vertical *s* chain. Different heights of the horizontal edges are shown by thick and thin lines. It is not necessary to specify the direction of the saw teeth in the projections of these nets, but the saw tooth must be shown by an arrow in certain nets illustrated later.

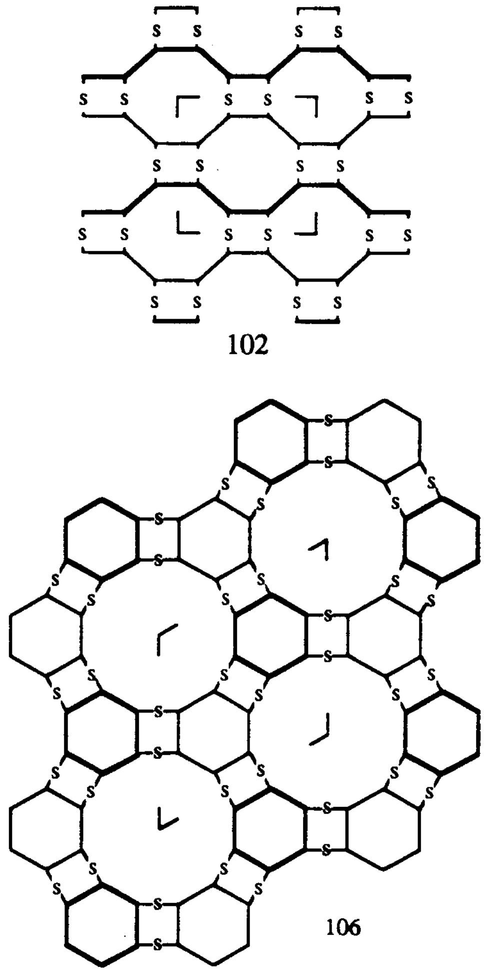


Fig. 4. Nets 102 (ATT) and 106 (offretite) projected down the *s* chains. The direction of the saw teeth need not be specified for these nets.

Table 1. *Geometrical properties of regular 3D nets obtained from conversion of edges of a parallel stack of three-connected 2D nets into a saw chain*

Three-connected 2D net		Four-connected 3D net									
	Circuit symbol	Label	Circuit symbol (Wells)	Z_c	Highest space group	a (Å)	b (Å)	c (Å)	γ (°)†	Space group for alternation	Structure type
hex	6^3	40‡§	$(4^26^28^2)_1(46^5)_1$	16	65:*Cmmm*	8.869	14.538	7.172	90	63:*Ccmm* (c = 14)	–
		96§	$(4^26^38)_2(6^6)_1$	6	51:*Pmcm*	7.556	8.270	5.323	90	59:*Pmnm* (a = 14)	JBW
		97§	$(4^26^38)_2(6^6)_1$	12	51:*Pmam*	8.965	9.865	7.466	90	57:*Pcam* (c = 15)	–
ttw	3.12^2	105§	$(34^26^28)_2(368^4)_1$	9	187:*P*$\bar{6}$*m*2	9.677	9.677	7.801	120	*i*	–
fee	48^2	99§	$(4^36^28)_2(468^4)_1$	12	123:*P*4/*mmm*	9.581	9.581	7.640	90	132:*P*4$_2$/*mcm* (c = 15)	–
		101§	$(4^36^3)_2(4^268^3)_1$	24	123:*P*4/*mmm*	13.802	13.802	7.676	90	124:*P*4/*mcc* (c = 15)	–
		324	$(4^36^3)_2(4^36^3)_2$ $(4^36^3)_2(4^36^3)_2$ $(4^268^3)_1(4^268^3)_1$ $(4^268^3)_1(4^268^3)_1$	96	123:*P*4/*mmm*	27	27	7.5	90	124:*P*4/*mcc* (c = 15)	–
		379§	$(4^36^3)_2(4^36^3)_2$ $(4^268^3)_1(4^268^3)_1$	48	65:*Cmmm*	13.787	27.577	7.680	90	72:*Ibam* (c = 15)	–
		387§	$(4^36^3)_2(4^36^3)_2$ $(4^268^3)_1(4^268^3)_1$	48	65:*Cmmm*	13.780	27.575	7.659	90	72:*Ibam* (c = 15)	–
		1035‡§	$(4^36^28)_2(4^38^3)_1$ $(4^28^4)_1$	32	65:*Cmmm*	9.496	28.541	7.212	90	72:*Ibam* (c = 15)	–
		102§	$(4^36^3)_2(4^268^3)_1$	12	51:*Pmam*	9.512	10.070	7.625	90	53:*Pcnm* (c = 14)	ATT
		893§	$(4^36^3)_2(4^36^3)_2$ $(4^268^3)_1(4^268^3)_1$	24	51:*Pmam*	13.811	13.822	7.644	90	57:*Pcam* (c = 15)	–
gml	4.6.12	376§	$(4^36^3)_2(4^36^3)_2$ $(4^26^38)_1(4^26^28^2)_1$	72	191:*P*6/*mmm*	26.681	26.681	7.681	120	192:*P*6/*mcc* (c = 15)	–
		386§	$(4^36^3)_2(4^36^3)_2$ $(4^26^38)_1(4^26^28^2)_1$	72	191:*P*6/*mmm*	26.734	26.734	7.628	120	192:*P*6/*mcc* (c = 15)	–
		106§	$(4^36^3)_2(4^26^28^2)_1$	18	187:*Pm*2	13.247	13.247	7.667	120	188:*Pc*2 (c = 15)	OFF
		919	$(4^36^3)_2(4^36^3)_2$ $(4^36^3)_2(4^26^38)_1$ $(4^26^38)_1(4^26^28^2)_1$	36	38:*Cm*2*m*	13	23	7.5	90	40:*Cc*2*m* (c = 15)	–
		918	12 types	36	25:*Pm*2*m*	13	23	7.5	90	28:*Pc*2*m* (c = 15)	–
		921	12 types	36	25:*P*2*mm*	13	23	7.5	90	28:*P*2*cm* (c = 15)	–
tfn	$(4^29)_1(4.9.12)_2$	314‡§	$(4^46^2)_1(4^38^210)_1$	24	191:*P*6/*mmm*	15.635	15.635	7.194	120	*i*	–
ffs	$(4^210)_1(4.10^2)_2$	48‡§	$(4^46^2)_1(4^38^210)_1$	16	65:*Cmmm*	8.974	14.534	7.270	90	63:*Ccmm* (c = 15)	–
		355	$(4^46^2)_2(4^36^3)_2$ $(4^36^3)_1(4^36^28)_2$ $(4^268^210)_1(468^4)_1$	36	51:*Pmam*	9	27	7.5	90	57:*Pcam* (c = 15)	–
		1034‡§	$(4^46^2)_1(4^36^28)_2$ $(4^28^4)_1$	16	38:*Cm*2*m*	8.860	14.524	7.263	90	40:*Cc*2*m* (c = 14)	–
tth	$(4^212)_1(4.8.12)_2$	1033‡§	$(4^46^2)_1(4^36^28)_2$ $(4^28^4)_1$	32	127:*P*4/*mbm*	16.526	16.526	7.265	90	135:*P*4$_2$/*mbc* (c = 14)	–
		357	$(4^46^2)_2(4^36^3)_1$ $(4^36^28)_2(4^36^28)_2$ $(4^268^3)_1(468^4)_1$	72	123:*P*4/*mmm*	23	23	7.5	90	124:*P*4/*mcc* (c = 15)	–
		302‡§	$(4^46^2)_1(4^38^3)_1$	16	123:*P*4/*mmm*	11.861	11.861	7.258	90	140:*I*4/*mcm* (a = 16.5, c = 15)	–
fos	$(4^212)_1(4.12^2)_1$-*a*	308§	$(4^46^2)_2(4^268^210)_1$	24	65:*Cmmm*	7.530	19.291	7.831	90	72:*Ibam* (c = 15)	–
		465§	$(4^36^3)_2(4^36^3)_1$	24	65:*Cmmm*	9.530	19.563	7.686	90	72:*Ibam* (c = 15)	–
		356§	$(4^46^2)_2(4^36^3)_1$ $(4^36^28)_2(468^4)_1$	24	38:*Cm*2*m*	9.403	19.384	7.679	90	46:*Ic*2*m* (c = 15)	–
twy	$(4^212)_1(4.12^2)_1$-*b*	292§	$(4^46^2)_2(4^268^210)_1$	36	191:*P*6/*mmm*	18.186	18.186	7.771	120	192:*P*6/*mcc* (c = 15)	–

Table 1 (*cont.*)

Three-connected 2D net		Four-connected 3D net									
	Circuit symbol	Label	Circuit symbol (Wells)	Z_c	Highest space group	*a* (Å)	*b* (Å)	*c* (Å)	*γ* (°)†	Space group for alternation	Structure type
		916§	$(4^36^3)_2(4^36^3)_1$	36	191:*P*6/*mmm*	18.130	18.130	7.697	120	192:*P*6/*mcc* (*c* = 15)	–
		1032‡	$(4^46^2)_2(4^46^2)_1$ $(4^46^2)_1(4^36^28)_2$ $(4^38^210)_1(4^28^4)_1$	96	191:*P*6/*mmm*	30	30	7	120	192:*P*6/*mcc* (*c* = 14)	–
rho	$(4^216)_1(4.8.16)_1$	294§	$(4^46^2)_2(4^36^3)_1$ $(4^36^28)_2(468^4)_1$	48	127:*P*4/*mbm*	20.363	20.363	7.678	90	128:*P*4/*mnc* (*c* = 15)	–
		403§	$(4^46^2)_2(4^268^3)_1$	24	123:*P*4/*mmm*	14.291	14.291	7.809	90	124:*P*4/*mcc* (*c* = 15)	–
		463§	$(4^36^3)_2(4^36^3)_1$	24	123:*P*4/*mmm*	14.498	14.498	7.741	90	124:*P*4/*mcc* (*c* = 15)	–
eoo	$(4^218)_1(4.6.18)_2$	312‡	$(4^46^2)_1(4^368^2)_1$	24	191:*P*6/*mmm*	17	17	7.5	120	193:$P6_3$/*mcm* (*c* = 15)	–
tsv	$(4^224)_1(4.6.24)_1$	293§	$(4^46^2)_2(4^26^28^2)_1$	36	191:*P*6/*mmm*	20.700	20.700	7.828	120	192:*P*6/*mcc* (*c* = 15)	–
		917§	$(4^36^3)_2(4^36^3)_1$	36	191:*P*6/*mmm*	21.706	21.706	7.687	120	192:*P*6/*mcc* (*c* = 15)	–
ltl	$(468)_1(4.8.12)_1$	631§	$(4^36^3)_2(4^268^210)_1$	36	191:*P*6/*mmm*	18.332	18.332	27.671	120	192:*P*6/*mcc* (*c* = 15)	LTL
		902§	$(4^36^3)_2(4^26^28^2)_1$	36	191:*P*6/*mmm*	18.339	18.339	7.732	120	192:*P*6/*mcc* (*c* = 15)	–
fsy	$(468)_1(6^28)_1$	358§	$(4^36^28)_2(6^48^2)_1$	24	65:*Cmmm*	9.231	19.198	7.632	90	72:*Ibam* (*c* = 15)	–
		366§	$(4^26^38)_2(46^38^2)_1$	24	65:*Cmmm*	9.144	19.350	7.573	90	72:*Ibam* (*c* = 15)	–
		396§	$(4^36^3)_2(4^26^38)_2$ $(4^26^38)_1(6^48^2)_1$	24	51:*Pbmm*	8.622	20.665	7.629	90	57:*Pbcm* (*c* = 15)	–
		383§	$(4^36^3)_2(4^26^38)_2$ $(4^26^28^2)_1(6^58)_1$	24	38:*Cm*2*m*	8.726	19.161	7.699	90	46:*Ic*2*m* (*c* = 15)	–
brw	$(468)_2(68^2)_1$	38‡§	$(4^26^28^2)_1$	8	131:$P4_2$/*mmc*	7	7	8.5	90	138:$P4_2$/*ncm* (*a* = 10)	–
		369§	$(4^36^3)_4(4^26^38)_4$ $(6^28^4)_1$	9	115:$P\bar{4}m2$	7.775	7.775	8.703	90	111:$P\bar{4}2m$ (*a* = 10.5)	–
		295	$(4^36^3)_2(4^36^28)_2$ $(4^26^38)_2(4^26^28^2)_1$ $(46^38^2)_1(6^38^3)_1$	36	47:*Pmmm*	8.5	28	7.5	90	49:*Pccm* (*c* = 15)	–
		52‡	$(4^36^28)_2(4^368^2)_1$ $(46^28^3)_1$	8	25:*P*2*mm*	7	8.5	7	90	39:*B*2*cm* (*a* = 14, *c* = 14)	–
bor	$(47^2)_2(7^3)_1$	993‡	$(4^26^28^2)_1(4^27^4)_1$	16	127:*P*4/*mbm*	11	11	7.5	90	*i*	–
		360	$(4^36^3)_2(4^36^3)_2$ $(4^26^38)_2(4^267^3)_1$ $(4^267^28)_1(67^5)_1$	18	26:$Pb2_1m$	11	11	7.5	90	*i*	–
bik	$(5^28)_2(58^2)_1$	992‡	$(4^26^28^2)_1(45^38^2)_1$	16	65:*Cmmm*	7.5	17	7	90	*i*	–
		668‡	$(4^25^27^2)_2(45^38^2)_1$ $(45^28^3)_1$	16	51:*Pmmb*	7	16.5	6.5	90	*i*	–
		894	$(4^25^267)_2(4^256^27)_2$ $(4^256^27)_2(5^468)_1$ $(5^368^2)_1(5^268^3)_1$	36	51:*Pbmm*	14	17.5	7.5	90	*i*	–
		895	$(4^25^267)_4(4^256^28)_2$ $(5^468)_2(568^4)_1$	18	38:*Cm*2*m*	8	17.5	7.5	90	*i*	–
		929	$(4^25^267)_2(4^25^267)_2$ $(4^256^27)_2(5^468)_1$ $(5^368^2)_1(5^268^3)_1$	18	10:*P*112/*m*	9.5	14	7.5	105	*i*	–
fsv	$(4^210)_1(4.6.10)_2$ $(6.10^2)_1$	1038‡	$(4^46^2)_1(4^46^2)_1$ $(4^36^28)_2(4^368^2)_1$ $(4^26^28^2)_1(4^26^28^2)_1$ $(46^28^210)_1$	32	47:*Pmmm*	8.5	28	7	90	51:*Pcmm* (*c* = 14)	–
		405§	$(4^36^28)_2(4^26^4)_2$ $(4^26^28^2)_1(6^38^210)_1$	12	25:*Pm*2*m*	8.638	9.577	7.686	90	28:*Pc*2*m* (*c* = 15)	–
		407§	$(4^36^3)_2(4^36^3)_1$ $(4^26^38)_2(46^38^2)_1$	12	25:*Pm*2*m*	9.107	9.738	7.665	90	28:*Pc*2*m* (*c* = 15)	–

Table 1 (*cont.*)

Three-connected 2D net		Four-connected 3D net									
	Circuit symbol	Label	Circuit symbol (Wells)	Z_c	Highest space group	*a* (Å)	*b* (Å)	*c* (Å)	γ (°)†	Space group for alternation	Structure type
ttv	$(4^2 10)_1(4.8.10)_2$ $(8^2 10)_2$	1040‡	$(4^4 6^2)_1(4^4 6^2)_1$ $(4^3 6^2 8)_2(4^3 6^2 8)_2$ $(4^3 8^3)_1(4^3 8^2 10)_1$ $(4^2 8^4)_1(4^2 8^4)_1$	40	47:*Pmmm*	8.5	35	7	90	67:*Acmm* (*b* = 70, *c* = 14)	–
ooo	$(4^2 10)_2(4.8.10)_2$ $(8^2 10)_1$	582	$(4^4 6^2)_4(4^3 6^3)_4$ $(4^3 6^3)_2(4^2 6^3 8)_2$ $(4^2 6 8^3)_2(6 8^4 10)_1$	30	47:*Pmmm*	7	27.5	7.5	90	67:*Bmcm* (*a* = 14, *c* = 15)	–
ree	$(4^2 12)_1(4.6.12)_1$ $(4.12^2)_1$	1039‡	$(4^4 6^2)_2(4^3 6 8^2)_1$ $(4^3 8^2 10)_1$	48	191:*P*6/*mmm*	22	22	7	120	192:*P*6/*mcc* (*c* = 14)	–
fix	$(4^2 12)_1(4.6.12)_1$ $(6^2 12)_1$	1037‡	$(4^4 6^2)_1(4^3 6^2 8)_2$ $(4 6^3 8^2)_1$	32	65:*Cmmm*	8.5	29	7	90	72:*Ibam* (*c* = 14)	–
		377	$(4^4 6^2)_2(4^3 6^3)_1$ $(4^3 6^2 8)_2(4^2 6^3 8)_2$ $(4 6^3 8^2)_1(6^4 8^2)_1$	36	51:*Pmam*	8.5	27.5	7.5	90	57:*Pcam* (*c* = 15)	–
		373	$(4^4 6^2)_2(4^3 6^3)_2$ $(4^3 6^3)_1(4^2 6^3 8)_2$ $(4^2 6^2 8^2)_1(6^5 10)_1$	36	47:*Pmmm*	8.5	28.5	7.5	90	49:*Pccm* (*c* = 15)	–
		1036‡	$(4^4 6^2)_2(4^4 6^2)_1$ $(4^3 6 8^2)_1(4^2 6^2 8^2)_2$ $(4^2 6^2 8^2)_1(4 6^4 10)_1$	32	38:*Cm*2*m*	8.5	28	7	90	40:*Ic*2*m* (*c* =)	–
vvv	$(4^2 12)_1(4.8.12)_1$ $(4.8.12)_1$	408	$(4^4 6^2)_2(4^3 6^3)_2$ $(4^3 6^3)_2(4^3 6^3)_1$ $(4^2 6 8^3)_1(4^2 6 8^2 10)_1$	36	47:*Pmmm*	9	28.5	7.5	90	49:*Pccm* (*c* = 15)	–
		409	$(4^3 6^3)_2(4^3 6^3)_1$ $(4^3 6^2 8)_2(4^3 6^2 8)_2$ $(4 6 8^4)_1(4 6 8^4)_1$	36	47:*Pmmm*	9	28.5	7.5	90	49:*Pccm* (*c* = 15)	–
		1041‡	$(4^4 6^2)_1(4^3 6^2 8)_2$ $(4^2 8^4)_1$	16	47:*Pmmm*	8.5	14	7	90	49:*Pccm* (*c* = 14)	–
		1042‡	$(4^4 6^2)_2(4^4 6^2)_1$ $(4^3 6^2 8)_2(4^3 8^3)_1$ $(4^3 8^2 10)_1(4^2 8^4)_1$	16	25:*Pm*2*m*	9	14	7	90	28:*Pc*2*m* (*c* = 14)	–
fef	$(4 5 8)_2(5 8^2)_2$ $(5 8^2)_1$	411	$(4^3 5 6^2)_4(4^2 5 6^2 8)_4$ $(4^2 5 6^2 8)_2(4^2 5 6 7^2)_2$ $(5 6 8^4)_2(5 6 8^4)_1$	30	51:*Pbmm*	13	14	7.5	90	*i*	–
		410	$(4^3 5 6 7)_4(4^2 5 6^2 7)_4$ $(4^2 5 6^2 8)_2(4 5^2 6 7^2)_2$ $(5^2 6 8^3)_2(5 6 8^4)_1$	30	47:*Pmmm*	8	25	7.5	90	*i*	–
bks	$(4.5.12)_2(4.5.12)_2$ $(5.12^2)_1$	397	$(4^3 5 6^2)_4(4^3 5 6^2)_4$ $(4^2 5 6^2 8)_2(4^2 5 6 7^2)_2$ $(4^2 5 6 7^2)_2(5 6 8^4)_1$	30	38:*Cm*2*m*	11.5	18.5	7.5	90	*i*	–
		404	$(4^3 5 6^2)_4(4^3 5 6^2)_4$ $(4^2 5^2 6 7)_2(4^2 5^2 6 7)_2$ $(4^2 5 6^2 8)_2(5 6 8^4)_1$	30	38:*Cm*2*m*	12.5	19	7.5	90	*i*	–
eus	$(4.5.18)_6(5^3)_1$ $(5^2 18)_3$	897	12 types	60	47:*Pmmm*	18	29.5	7.5	90	*i*	–
ffv	$(4 6 8)_2(4 8^2)_2$ $(6 8^2)_1$	466	$(4^3 6^3)_4(4^3 6^3)_4$ $(4^2 6^3 8)_2(4^2 6^3 8)_2$ $(4^2 6 8^3)_2(6^2 8^4)_1$	30	51:*Pbmm*	8.5	24	7.5	90	59:*Pnmm* (*c* = 15)	–
fto	$(4 6 8)_1(4 8^2)_1$ $(6^2 8)_1$	378	$(4^3 6^2 8)_2(4^3 6^2 8)_2$ $(4^2 6^3 8)_2(4 6^3 8^2)_1$ $(4 6 8^4)_1(6^4 8^2)_1$	36	51:*Pmam*	9	28	7.5	90	57:*Pcam* (*c* = 15)	–
		380	$(4^3 6^3)_2(4^3 6^3)_2$ $(4^2 6^3 8)_2(4^2 6^2 8^2)_1$ $(4^2 6 8^3)_1(6^5 8)_1$	36	51:*Pmam*	9	28	7.5	90	57:*Pcam* (*c* = 15)	–
		1048‡	$(4^3 6^2 8)_2(4^3 6 8^2)_1$ $(4^2 6^2 8^2)_2(4^2 6^2 8^2)_1$ $(4^2 8^4)_1(4 6^4 8)_1$	16	25:*Pm*2*m*	8.5	13.5	7	90	28:*Pc*2*m* (*c* = 14)	–
		381	$(4^3 6^3)_2(4^3 6^3)_1$ $(4^2 6^3 8)_2(4^2 6^3 8)_1$ $(4^2 6 8^3)_2(6^4 8^2)_1$	18	10:*P*112/*m*	9	15	7.5	90	11:$P112_1/m$ (*c* = 15)	–
apd	$(4 6 8)_1(6^3)_1$ $(6^2 8)_1$	1044‡	$(4^2 6^2 8^2)_2(4^2 6^2 8^2)_1$ $(4 6^5)_1$	32	65:*Cmmm*	8.5	27.5	7	90	72:*Ibam* (*c* = 14)	–

Table 1 (*cont.*)

Three-connected 2D net		Four-connected 3D net									
	Circuit symbol	Label	Circuit symbol (Wells)	Z_c	Highest space group	*a* (Å)	*b* (Å)	*c* (Å)	γ (°)†	Space group for alternation	Structure type
		371	$(4^36^3)_2(4^26^38)_2$ $(4^26^38)_2(4^26^38)_1$ $(6^6)_1(6^48^2)_1$	36	51:*Pbmm*	8.5	31	7.5	90	57:*Pbcm* (*c* = 15)	–
		372	$(4^36^3)_2(4^26^38)_2$ $(4^26^38)_2(4^26^28^2)_1$ $(6^6)_1(6^58)_1$	36	51:*Pmam*	8.5	29	7.5	90	57:*Pcam* (*c* = 15)	–
		368	$(4^36^28)_2(4^26^38)_2$ $(4^26^38)_2(46^38^2)_1$ $(6^6)_1(6^48^2)_1$	36	47:*Pmmm*	8.5	27.5	7.5	90	49:*Pccm* (*c* = 15)	–
feo	$(468)_2(6^3)_1$ $(6^28)_2$	937	$(4^36^3)_4(4^26^38)_4$ $(4^26^38)_2(4^26^38)_2$ $(6^6)_1(6^48^2)_2$	15	25:*P*2*mm*	8	12.5	7.5	90	35:*A*2*mm* (*b* = 25, *c* = 15)	–
nos	$(5^26)_1(568)_2$ $(58^2)_1$	900	$(4^256^27)_2(4^256^27)_2$ $(5^36^3)_1(5^26^28^2)_1$	48	65:*Cmmm*	14.5	23	7.5	90	*i*	–
		913	$(4^25^267)_2(4^256^27)_2$ $(5^26^38)_1(5^268^3)_1$	48	65:*Cmmm*	14	22	7.5	90	*i*	–
		901	10 types	48	47:*Pmmm*	11.5	27.5	7.5	90	*i*	–
vnv	$(5^27)_1(57^2)_2$ $(57^2)_1$	938	10 types	48	51:*Pmam*	11.5	27	7.5	90	*i*	–
urg	$(56^2)_2(568)_2$ $(58^2)_1$	942	$(4^256^27)_4(4^256^27)_4$ $(4^256^28)_2(5^26^38)_2$ $(5^26^38)_2(568^4)_1$	30	51:*Pmam*	7.5	26	7.5	90	*i*	–
fsf	$(4^210)_1(4.6.10)_1$ $(4.10^2)_1(6^210)_1$	880	$(4^46^2)_2(4^36^28)_2$ $(4^268^210)_1(6^48^2)_1$	24	51:*Pmam*	9.5	20	7.5	90	57:*Pcam* (*c* = 15)	–
		881	$(4^36^3)_2(4^36^3)_1$ $(4^26^38)_2(46^38^2)_1$	24	51:*Pmam*	9	19.5	7.5	90	57:*Pcam* (*c* = 15)	
ftn	$(4^210)_1(4.6.10)_2$ $(6^3)_1(6^210)_2$	1047‡	$(4^46^2)_1(4^368^2)_1$ $(4^26^28^2)_1(46^410)_1$	16	47:*Pmmm*	8.5	14.5	7	90	51:*Pcmm* (*c* = 14)	–
		883	12 types	36	25:*Pm*2*m*	8.5	28.5	7.5	90	28:*Pc*2*m* (*c* = 15)	–
uiv	$(4^212)_2(4.5.12)_2$ $(58^2)_1(5.8.12)_2$	941	$(4^46^2)_4(4^3567)_4$ $(4^36^3)_2(4^256^27)_4$ $(4^256^28)_2(45^267^2)_2$ $(5^268^3)_2(568^4)_1$	21	25:*Pm*2*m*	7.5	17.5	7.5	90	*i*	–
vss	$(4^212)_1(468)_1$ $(4.6.12)_1(6.8.12)_1$	879	$(4^46^2)_2(4^36^3)_2$ $(4^36^3)_2(4^36^3)_1$ $(4^26^38)_2(4^26^28^2)_1$ $(4^26^28^2)_1(6^28^4)_1$	96	65:*Cmmm*	17	37	7.5	90	66:*Cccm* (*c* = 15)	–
		878	$(4^46^2)_2(4^36^3)_2$ $(4^36^3)_1(4^36^28)_2$ $(4^26^38)_2(4^26^28^2)_1$ $(46^38^2)_1(6^38^3)_1$	24	25:*Pm*2*m*	9	19.5	7.5	90	28:*Pc*2*m* (*c* = 15)	–
bsh	$(4^212)_1(4.6.12)_1$ $(6^3)_1(6^312)_1$	896	$(4^46^2)_2(4^36^3)_1$ $(4^36^28)_2(4^26^38)_2$ $(4^26^38)_2(46^38^2)_1$ $(6^6)_1(6^48^2)_1$	48	38:*Cm*2*m*	9	38	7.5	90	46:*Ic*2*m* (*c* = 15)	–
fvo	$(4^214)_2(4^214)_1$ $(4.6.14)_2(6.14^2)_1$	1049‡	$(4^46^2)_1(4^46^2)_1$ $(4^26^28^2)_1(4^26^28^2)_1$	16	47:*Pmmm*	8.5	14.5	7	90	51:*Pcmm* (*c* = 14)	–
		882	12 types	36	25:*Pm*2*m*	8.5	28.5	7.5	90	28:*Pc*2*m* (*c* = 15)	–
mor	$(458)_1(4.5.12)_1$ $(5^212)_1(5.8.12)_1$	898	$(4^356^2)_2(4^25^267)_2$ $(4^25^267)_1(5^268^3)_1$	48	65:*Cmmm*	18	19	7.5	90	*i*	–
		899	$(4^356^2)_2(4^25^267)_1$ $(4^256^27)_2(5^368^2)_1$	48	65:*Cmmm*	18	18.5	7.5	90	*i*	
		911	$(4^25^267)_2(4^256^27)_2$ $(45^267^2)_1(45^267^2)_1$	48	65:*Cmmm*	17.5	19.5	7.5	90	*i*	–
		912	$(4^3567)_2(4^3567)_2$ $(5^48^2)_1(5^268^210)_1$	48	65:*Cmmm*	17.5	19.5	7.5	90	*i*	
		935	$(4^356^2)_2(4^356^2)_2$ $(4^25^267)_2(4^25^267)_1$ $(4^25^267)_1(4^256^28)_2$ $(5^468)_1(568^4)_1$	48	38:*C*2*mm*	18	19	7.5	90	*i*	–
dac	$(4.5.10)_1(4.5.10)_1$ $(5^210)_1(5.10^2)_1$	616	$(4^25^267)_2(4^256^27)_2$ $(45^267^2)_1(45^267^2)_1$	12	10:*P*112/*m*	9.5	10.5	7.5	108	*i*	–

Table 1 (*cont.*)

Three-connected 2D net		Four-connected 3D net									
	Circuit symbol	Label	Circuit symbol (Wells)	Z_c	Highest space group	a (Å)	b (Å)	c (Å)	γ (°)†	Space group for alternation	Structure type
		933	$(4^{3}56^{2})_2(4^{3}56^{2})_2$ $(4^{2}5^{2}67)_2(4^{2}5^{2}67)_1$ $(4^{2}5^{2}67)_1(4^{2}56^{2}7)_2$ $(5^{3}68^{2})_1(5^{2}68^{2}10)_1$	24	10:*P*112/*m*	9.5	19.5	7.5	105	*i*	–
		934	$(4^{3}567)_2(4^{3}567)_2$ $(5^{3}68^{2})_1(5^{2}68^{2}10)_1$	12	10:*P*112/*m*	9.5	10.5	7.5	105	*i*	–
		914	$(4^{3}56^{2})_2(4^{3}56^{2})_2$ $(4^{2}5^{2}67)_2(4^{2}5^{2}67)_1$ $(4^{2}5^{2}67)_1(4^{2}56^{2}8)_2$ $(5^{4}68)_1(568^{4})_1$	12	6:*P*11*m*	9.5	10	7.5	105	*i*	–
dao	$(4.5.10)_1(4.5.10)_1$ $(5^{2}10)_1(5.10^{2})_1$	617	$(4^{2}5^{2}67)_2(4^{2}56^{2}7)_2$ $(45^{2}67^{2})_1(45^{2}67^{2})_1$	24	51:*Pbmm*	10	17	7.5	90	*i*	–
		930	$(4^{3}567)_2(4^{3}567)_2$ $(5^{3}68^{2})_1(5^{2}68^{2}10)_1$	24	51:*Pbmm*	10	17.5	7.5	90	*i*	–
		932	$(4^{3}56^{2})_2(4^{2}5^{2}67)_1$ $(4^{2}56^{2}7)_2(5^{3}68^{2})_1$	24	51:*Pbmm*	9	19.5	7.5	90	*i*	–
		931	$(4^{3}56^{2})_2(4^{3}56^{2})_2$ $(4^{2}5^{2}67)_2(4^{2}5^{2}67)_1$ $(4^{2}5^{2}67)_1(4^{2}56^{2}8)_2$ $(5^{4}68)_1(568^{4})_1$	24	25:*P*2*mm*	9.5	19.5	7.5	90	*i*	–
sxn	$(4.5.10)_1(4.5.10)_1$ $(5^{2}10)_1(5.10^{2})_1$	628	$(4^{2}5^{2}67)_2(4^{2}56^{2}7)_2$ $(45^{2}67^{2})_1(45^{2}67^{2})_1$	24	51:*Pbmm*	9.5	19	7.5	90	*i*	–
		939	$(4^{3}56^{2})_2(4^{3}56^{2})_2$ $(4^{2}5^{2}67)_2$ $(4^{2}5^{2}67)_1(4^{2}5^{2}67)_1$ $(4^{2}56^{2}7)_2(5^{3}68^{2})_1$ $(5^{2}68^{2}10)_1$	48	51:*Pmam*	17.5	19	7.5	90	*i*	–
		943	$(4^{3}567)_2(4^{3}567)_2$ $(5^{3}68^{2})_1(5^{2}68^{2}10)_1$	24	51:*Pbmm*	9	19	7.5	90	*i*	–
		940	$(4^{3}56^{2})_2(4^{3}56^{2})_2$ $(4^{2}5^{2}67)_2(4^{2}5^{2}67)_1$ $(4^{2}5^{2}67)_1(4^{2}56^{2}8)_2$ $(5^{4}68)_1(568^{4})_1$	24	26:*Pb*2$_1$*m*	10	17.5	7.5	90	*i*	–
fes	$(4.5.10)_2(56^{2})_1$ $(5.6.10)_2(6^{2}10)_1$	926	$(4^{3}567)_4(4^{2}56^{2}7)_4$ $(4^{2}56^{2}8)_2(4^{2}6^{3}8)_2$ $(45^{2}67^{2})_2(5^{2}6^{2}8^{2})_2$ $(56^{5})_1(6^{5}10)_1$	36	47:*Pmmm*	10	24.5	7.5	90	*i*	–
		925	12 types	36	25:*P*2*mm*	9	26.5	7.5	90	*i*	–
bab	$(4.5.12)_2(4.6.12)_2$ $(56^{2})_1(5.6.12)_2$	388	14 types	84	47:*Pmmm*	13.5	46	7.5	90	*i*	–
		927	$(4^{3}567)_4(4^{3}6^{3})_4$ $(4^{2}56^{2}7)_4(4^{2}56^{2}8)_2$ $(4^{2}6^{3}8)_2(45^{2}67^{2})_2$ $(5^{2}6^{2}8^{2})_2(56^{5})_1$	42	47:*Pmmm*	12.5	25.5	7.5	90	*i*	–
uss	$(46^{2})_1(4.6.12)_1$ $(4.6.12)_1(6^{2}12)_1$	837	$(4^{3}6^{3})_2$ $(4^{3}6^{3})_2(4^{3}6^{2}8)_2$ $(4^{2}6^{4})_1(4^{2}6^{3}8)_2$ $(4^{2}6^{3}8)_1(46^{3}8^{2})_1$ $(6^{4}8^{2})_1$	48	47:*Pmmm*	14	26	7.5	90	49:*Pccm* (c = 15)	–
sse	$(467)_2(478)_2$ $(67^{2})_1(78^{2})_1$	477‡	$(4^{2}6^{2}7^{2})_1(4^{2}6^{2}8^{2})_1$ $(4^{2}6^{2}8^{2})_1(4^{2}7^{2}8^{2})_1$	16	47:*Pmmm*	7.5	15	7	90	*i*	–
tva	$(468)_2(48^{2})_1$ $(48^{2})_1(68^{2})_1$	892	$(4^{3}6^{3})_4(4^{3}6^{2}8)_2$ $(4^{3}6^{2}8)_2(4^{2}6^{3}8)_2$ $(4^{2}6^{2}8^{2})_2(468^{4})_1$ $(468^{4})_1(6^{2}8^{4})_1$	30	47:*Pmmm*	14.5	15.5	7.5	90	65:*Ammm* (b = 31, c = 15)	–
stg	$(468)_2(48^{2})_2$ $(48^{2})_2(68^{2})_1$	884	$(4^{3}6^{3})_4(4^{3}6^{3})_4$ $(4^{3}6^{3})_4(4^{2}6^{3}8)_2$ $(4^{2}6^{2}8^{2})_2(4^{2}68^{3})_2$ $(4^{2}68^{3})_2(6^{2}8^{4})_1$	42	47:*Pmmm*	17	18	7.5	90	67:*Bmcm* (a = 34, c = 15)	–
		885	$(4^{3}6^{3})_4(4^{3}6^{3})_4$ $(4^{3}6^{3})_4(4^{2}6^{3}8)_2$ $(4^{2}6^{3}8)_2(4^{2}68^{3})_2$ $(4^{2}68^{3})_2(6^{2}8^{4})_1$	21	25:*P*2*mm*	9.5	17	7.5	90	35:*A*2*mm* (b = 34, c = 15)	–

Table 1 (*cont.*)

Three-connected 2D net		Four-connected 3D net									
	Circuit symbol	Label	Circuit symbol (Wells)	Z_c	Highest space group	a (Å)	b (Å)	c (Å)	γ (°)†	Space group for alternation	Structure type
fst	$(468)_1(48^2)_1$ $(6^3)_1(6^28)_1$	887	$(4^36^3)_2(4^26^38)_2$ $(4^268^3)_1(6^58)_1$	24	51:*Pmam*	9	19	7.5	9	57:*Pcam* (c = 15)	–
		888	$(4^36^28)_2(4^36^28)_2$ $(4^26^38)_2(4^26^38)_2$ $(46^38^2)_1(468^4)_1$ $(6^6)_1(6^48^2)_1$	24	25:*Pm*2*m*	8.5	19	7.5	90	28:*Pc*2*m* (c = 15)	–
		886	$(4^36^3)_2(4^36^3)_2$ $(4^26^38)_2(4^26^38)_2$ $(4^26^38)_1(4^268^3)_1$ $(6^6)_1(6^48^2)_1$	24	10:*P*112/*m*	9	21.5	7.5	90	11:*P*112$_1$/*m* (c = 15)	–
rxt	$(468)_2(568)_2$ $(568)_2(58^2)_1$	903	$(4^36^3)_4(4^256^27)_4$ $(4^256^28)_4(4^256^28)_2$ $(4^26^28^2)_2(5^26^38)_2$ $(5^26^38)_2(568^4)_1$	21	25:*Pm*2*m*	7.5	18	7.5	90	*i*	–
fss	$(468)_2(6^3)_2$ $(6^3)_1(6^28)_2$	891	$(4^36^3)_4(4^26^38)_4$ $(4^26^38)_4(4^26^38)_2$ $(4^26^38)_2(6^6)_2$ $(6^6)_1(6^48^2)_2$	21	25:*P*2*mm*	8.5	18	7.5	90	35:*A*2*mm* (b = 36, c = 15)	–
uhi	$(478)_2(478)_2$ $(478)_2(78^2)_1$	904	$(4^36^3)_4(4^36^3)_4$ $(4^36^3)_4(4^26^38)_2$ $(4^267^28)_2(4^267^28)_2$ $(4^2678^2)_2(678^4)_1$	21	25:*Pm*2*m*	7.5	17.5	7.5	90	*i*	–
fer	$(5^26)_1(5^210)_2$ $(5^210)_1(5.6.10)_2$	624§	$(4^25^267)_4(4^25^267)_2$ $(5^46^2)_1(5^26^28^2)_2$	36	65:*Cmmm*	14.56	19.28	7.66	90	*i*	–
		928§	$(4^25^267)_2(4^256^27)_4$ $(5^468)_1(5^368^2)_2$	36	65:*Cmmm*	14.594	19.126	7.622	90	*i*	SZF?
		689‡§	$(4^25^27^2)_1(4^25^27^2)_1$ $(45^38^2)_1(45^26^29)_1$	32	65:*Cmmm*	13.25	20.59	7.24	90	*i*	–
		798§	$(4^25^267)_4(4^25^267)_2$ $(4^25^267)_2(4^256^28)_4$ $(5^46^2)_1(5^468)_2$ $(5^468)_1(56^38^2)_2$	36	38:*Cm*2*m*	14.62	19.23	7.73	90	*i*	–
een	$(5^27)_1(57^2)_1$ $(57^2)_1(57^2)_1$	946	$(4^25^267)_2(4^256^27)_2$ $(5^267^3)_1(5^267^3)_1$	24	55:*Pbam*	9.5	17	7.5	90	*i*	–
		947	$(4^256^27)_2(4^256^27)_2$ $(5^367^2)_1(5^267^3)_1$	24	55:*Pbam*	10	17	7.5	90	*i*	–
		953	$(4^25^267)_2(4^256^27)_2$ $(4^256^27)_2(4^256^28)_2$ $(5^467)_1(5^267^3)_1$ $(5^267^3)_1(568^4)_1$	24	26:*Pb*2$_1$*m*	8.5	18.5	7.5	90	*i*	–
biz	$(5^28)_2(5^28)_1$ $(5^28)_1(5^28)_2$	910	$(4^25^267)_2(4^256^27)_4$ $(5^468)_1(5^368^2)_2$	18	51:*Pbmm*	9	14	7.5	90	*i*	–
		920	$(4^25^267)_4(4^25^267)_2$ $(5^468)_1(5^268^3)_2$	18	51:*Pbmm*	9	14	7.5	90	*i*	–
		686‡§	$(4^25^27^2)_1(4^25^27^2)_1$ $(45^38^2)_1(45^28^3)_1$	16	51:*Pbmm*	10.36	12.84	7.01	90	*i*	–
		922	$(4^25^267)_4(4^25^267)_2$ $(4^25^267)_2(4^256^28)_4$ $(5^468)_2(5^468)_1$ $(5^468)_1(568^4)_2$	18	18:*P*2*mm*	9.5	14	7.5	90	*i*	–
fex	$(5^28)_1(56^2)_1$ $(568)_2(6^28)_1$	923	$(4^25^267)_2(4^256^27)_4$ $(4^26^38)_4(5^468)_1$ $(5^26^4)_2(56^38^2)_2$	15	25:*P*2*mm*	9.5	11	7.5	90	*i*	–
		924	$(4^25^267)_2(4^256^27)_4$ $(4^256^28)_4(5^468)_1$ $(5^26^38)_2(6^48^2)_2$	15	25:*P*2*mm*	9.5	10	7.5	90	*i*	–
exn	$(56^2)_1(567)_2$ $(57^2)_2(6^27)_1$	906	$(4^256^27)_4(4^256^27)_4$ $(4^256^28)_2(4^26^38)_2$ $(5^26^27^2)_2(5^267^3)_2$ $(56^5)_1(6^57)_1$	36	51:*Pmam*	10	24	7.5	90	*i*	–
		905	12 types	36	25:*Pm*2*m*	9	27	7.5	90	*i*	–

Table 1 (*cont.*)

Three-connected 2D net		Four-connected 3D net									
	Circuit symbol	Label	Circuit symbol (Wells)	Z_c	Highest space group	*a* (Å)	*b* (Å)	*c* (Å)	γ (°)†	Space group for alternation	Structure type
exe	$(56^2)_1(567)_2$ $(57^2)_2(6^27)_1$	907	$(4^256^27)_4(4^256^28)_2$ $(4^2567^2)_4(4^26^38)_2$ $(5^26^27^2)_2(5^267^28)_2$ $(56^5)_1(6^57)_1$	36	51:*Pmam*	10	24	7.5	90	*i*	–
		908	12 types	18	6:*P*11*m*	9	13.5	7.5	90	*i*	–
fis	$(56^2)_2(568)_2$ $(58^2)_1(6^3)_1$	1000‡	$(4^26^28^2)_1(45^268^2)_1$ $(456^4)_1(456^28^2)_1$	16	47:*Pmmm*	7.5	15	7	90	*i*	–
eig	$(4^210)_1(4.6.10)_2$ $(6^3)_2(6^3)_1$ $(6^210)_2$	889	$(4^46^2)_2(4^36^28)_2$ $(4^26^38)_2(4^26^38)_2$ $(4^26^28^2)_1(6^6)_1$ $(6^510)_1(6^48^2)_1$	24	25:*Pm*2*m*	8.5	18.5	7.5	90	28:*Pc*2*m* (*c* = 15)	–
		890	$(4^36^3)_2(4^36^3)_1$ $(4^26^38)_2(4^26^38)_2$ $(4^26^38)_2(46^38^2)_1$ $(6^6)_1(6^6)_1$	24	25:*Pm*2*m*	9	19.5	7.5	90	28:*Pc*2*m* (*c* = 15)	–
api	$(4^214)_1(46^2)_2$ $(4.6.14)_2(4.6.14)_2$ $(6^214)_2$	1045‡	$(4^46^2)_1(4^36^28)_2$ $(4^36^28)_1(4^368^2)_1$ $(46^410)_1$	48	65:*Cmmm*	14	31	7	90	63:*Ccmm* (*c* = 14)	–
eug	$(4.5.14)_2(5^3)_1$ $(5^214)_2(5^214)_2$ $(5^214)_1$	949	10 types	48	47:*Pmmm*	14	26.5	7.5	90	*i*	–
tvt	$(468)_2(468)_2$ $(6^3)_1(6^28)_2$ $(68^2)_1(6^6)_1$ $(6^48^2)_1(6^38^3)_1$	862	$(4^36^3)_2(4^36^28)_2$ $(4^36^28)_2(4^26^38)_2$ $(4^26^28^2)_1$	24	25:*Pm*2*m*	9	20	7.5	90	28:*Pc*2*m* (*c* = 15)	–
		876	$(4^36^3)_2(4^26^38)_2$ $(4^26^38)_2(4^26^38)_2$ $(4^26^28^2)_1(46^38^2)_1$ $(46^38^2)_1(6^58)_1$	24	25:*Pm*2*m*	9.5	20.5	7.5	90	28:*Pc*2*m* (*c* = 15)	–
		877	$(4^36^3)_4(4^36^3)_4$ $(4^26^38)_4(4^26^38)_2$ $(4^26^38)_2(4^26^38)_2$ $(4^26^38)_2(6^6)_1$ $(6^48^2)_1(6^28^4)_1$	24	25:*P*2*mm*	9	21.5	7.5	90	25:*P*2*mm* (*c* = 15)	–
fsm	$(468)_2(6^3)_2$ $(6^3)_2(6^3)_1$ $(6^28)_2$	1046‡	$(4^26^28^2)_2(4^26^28^2)_1$ $(4^26^28^2)_1(46^5)_1$ $(46^5)_1$	24	47:*Pmmm*	8.5	21	7	90	67:*Acmm* (*b* = 42, *c* = 14)	–
		915	10 types	27	25:*P*2*mm*	8.5	22.5	7.5	90	35:*A*2*mm* (*b* = 45, *c* = 15)	–
fev	$(4.5.10)_1(4.5.10)_1$ $(56^2)_1(5.6.10)_1$ $(5.6.10)_1(6^210)_1$	955	12 types	36	26:$Pb2_1m$	14.5	16	7.5	90	*i*	–
zsm	$(468)_1(468)_1$ $(4.6.12)_1(48^2)_1$ $(4.8.12)_1(4.8.12)_1$	1177	$(4^36^3)_2(4^36^3)_2$ $(4^36^3)_2(4^268^3)_1$ $(4^268^3)_1(4^268^210)_1$	108	191:*P*6/*mmm*	31.5	31.5	7.5	120	192:*P*6/*mcc* (*c* = 15)	ZSM-10
		1178	$(4^36^3)_2(4^36^3)_2$ $(4^36^3)_2(4^26^28^2)_1$ $(4^26^28^2)_1(4^26^28^2)_1$	108	191:*P*6/*mmm*	31.5	31.5	7.5	120	192:*P*6/*mcc* (*c* = 15)	–
nee	$(468)_2(5^28)_2$ $(5^28)_2(58^2)_1$ $(58^2)_1(68^2)_1$	1051‡	$(4^26^28^2)_1(4^26^28^2)_1$ $(4^26^28^2)_1(4^26^28^2)_1$ $(45^38^2)_1(45^38^2)_1$	24	47:*Pmmm*	7.5	26.5	7	90	*i*	–
		936	12 types	27	25:*Pm*2*m*	7.5	25	7.5	90	*i*	–
		1050‡	$(4^36^28)_2(4^368^2)_1$ $(4^25^27^2)_2(4^25^27^2)_2$ $(45^38^2)_1(45^38^2)_1$ $(45^28^3)_1(45^28^3)_1$ $(46^28^3)_1$	24	25:*P*2*mm*	7.5	26.5	7	90	*i*	–
eon	$(4.6.10)_2(5^26)_1$ $(5^210)_1(568)_2$ $(568)_2(5.6.10)_2$	952	12 types	30	25:*Pm*2*m*	11.5	18	7.5	90	*i*	–
mfv	$(4.5.10)_2(56^2)_1$ $(5.6.10)_2(6^3)_2(6^3)_1$ $(6^3)_1(6^210)_1$	944	10 types	30	25:*P*2*mm*	9	22	7.5	90	*i*	–

Table 1 (*cont.*)

Three-connected 2D net		Four-connected 3D net									
	Circuit symbol	Label	Circuit symbol (Wells)	Z_c	Highest space group	*a* (Å)	*b* (Å)	*c* (Å)	γ (°)†	Space group for alternation	Structure type
bta	$(4.5.12)_1(4.5.12)_1$ $(5^26)_1(5^212)_1$ $(5^212)_1(5.6.12)_1$ $(5.6.12)_1$	948	14 types	42	25:*P*2*mm*	12	25	7.5	90	*i*	–
btb	$(4.5.12)_1(4.5.12)_1$ $(5^26)_1(5^212)_1$ $(5^212)_1(5.6.12)_1$ $(5.6.12)_1$	951	14 types	42	10:*P*112/*m*	12	26	7.5	105	*i*	–
smt	$(467)_2(478)_2$ $(56^2)_2(568)_2$ $(58^2)_1(6^27)_2$ $(78^2)_1$	1054‡	$(4^26^27^2)_1(4^26^28^2)_2$ $(4^26^28^2)_1(4^26^28^2)_1$ $(4^27^28^2)_1(45^268^2)_1$ $(456^4)_1$	32	38:*Cm*2*m*	7.5	30	7	90	*i*	–
mtt	$(5^26)_2(5^210)_2$ $(5^210)_2(5^210)_1$ $(5^210)_1(5.6.10)_2$ $(5.6.10)_2$	954	14 types	36	25:*P*2*mm*	11	22	7.5	90	*i*	–
sma	$(5^27)_2(567)_2$ $(567)_2(57^2)_2$ $(6^27)_2(6^27)_1$ $(6^27)_1$	1053‡	$(4^26^28^2)_2(4^26^28^2)_1$ $(4^26^28^2)_1(45^37^2)_1$ $(45^2678)_1(456^27^2)_1$ $(46^378)_1$	32	51:*Pmam*	14.5	15	7	90	*i*	–
sft	$(5^28)_2(5^28)_2$ $(5^28)_2(5^28)_1$ $(5^28)_1(5^28)_2$ $(5^28)_2$	1052‡	$(4^25^27^2)_2(4^25^27^2)_1$ $(4^25^27^2)_1(45^38^2)_1$ $(45^38^2)_1(45^28^3)_1$ $(45^28^3)_1$	32	51:*Pbmm*	9.5	25	7	90	*i*	–
		950	14 types	36	25:*P*2*mm*	9	27	7.5	90	*i*	–
mln	$(458)_1(4.5.12)_1$ $(468)_1(468)_1$ $(4.6.12)_1(568)_1$ $(5.6.12)_1(58^2)_1$ $(6^28)_1(6^28)_1$	385	20 types	120	47:*Pmmm*	20	42	7.5	90	*i*	–
		945	20 types	60	25:*P*2*mm*	18.5	22.5	7.5	90	*i*	–

† $\alpha = 90°$, $\beta = 90°$. ‡ Nets generated by second approach. Nets from the third approach to be reported later. § Nets with DLS refinement.

horizontal mirror operation (sigma-plus transformation in Fig. 1) retains the parity restrictions given in paper II: namely, closure of a horizontal ring requires an even number of *s* edges (tilted), and the *s* edges must be separated by *h* edges (Smith, 1979).

Fig. 3 shows the two $(h,s)^*$ nets 96 and 97 generated from the 2D *hex* (6^3) net *via* the 3D $(h,z)^*$ nets 1 and 2. Net 96 represents the topology of structure type JBW (Smith, 1979; Hansen & Falth, 1981); the three-letter code refers to zeolite type J of Barrer & White. The JBW net also occurs in a synthetic phase, known to ceramists as 'nepheline hydrate'; primary references in Meier *et al.* (1996). In Fig. 4, net 102 from aluminophosphate $AlPO_4$-12-TAMU (Rudolf *et al.*, 1986) is derived from the 2D *fee* (48^2) net, and net 106 from offretite (Bennett & Gard, 1967; Gard & Tait, 1972) is based on the 2D *gml* (4.6.12) net (both from Smith, 1979).

Reversal of the saw direction is illustrated in Fig. 5. Nets 631 and 902 are both built from congruent stacks of the 2D *ltl* net $(468)_1(4.8.12)_1$. For the saw tooth pointing to the 12-ring, net 631 (Linde Type L: Barrer & Villiger, 1969; Smith, 1979) has superimposed hexagonal prisms (*hpr*) and *can* cages (Fig. 10 of paper II) alternating in projection down each six-ring. For the saw tooth pointing to the hexagon, net 902 has *gme* cages down the six-rings and dodecagonal prisms down the 12-rings. Nets 624 and 928 (SUZ-4; Lawton *et al.*, 1993) are similarly generated from the 2D *fer* net $(5^26)_1$-$(5^210)_2(5^210)_1(5.6.10)_2$. Net 928, with the saw tooth pointing away from the hexagon, has hexagonal prisms, whereas net 624, with the saw tooth pointing to the hexagon, has double bands (thin line).

The structure of ZSM-10 (Higgins & Schmitt, 1996) is based on net 1177. Its projection down the *s* chain shows the 2D net *zsm* $(468)_1(468)_1(46.12)_1(48^2)_1(48.12)_1$-$(48.12)_1$ (Fig. 6), which is an expansion of the *ltl* 2D net in net 631 (Fig. 5). Net 1177 contains superimposed *hpr* and *can* polyhedral units at the six-rings of the *zsm* net, and *pau* at the eight-rings. Its alternate, net 1178, has *gme* at the six-rings, and *opr* and *ocn* at the eight-rings (for *pau*, *opr* and *ocn*, see Fig. 14).

The second type of 3D s^* nets is related to the *bs* chain. The key feature is that two *s* chains meet back-to-back at a vertex of the 2D net to form a *bs* chain (Fig.

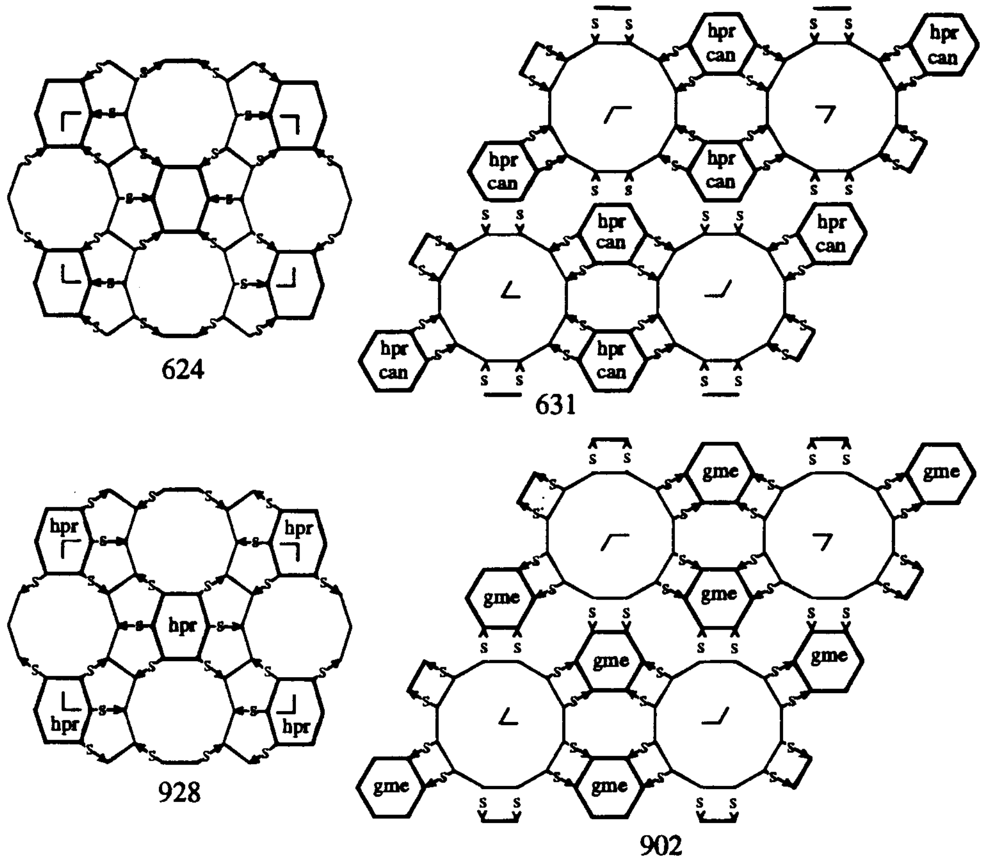


Fig. 5. Projections of pairs of 3D nets with saw teeth (arrow) pointing in opposite directions: 631 and 902 from 2D net *ltl* $(468)_1(4.8.12)_1$, and 624 and 928 from *fer* $(5^26)_1(5^210)_2(5^210)_1(5.6.10)_2$.

Table 2. *Alternative topological description, subunits and pore space of theoretical nets derived from conversion of edges of a parallel stack of three-connected 2D nets into a saw chain*

CTF no.	Alternative topological description	Rings providing access to pores	1D subunits including chains, columns, tubes	2D three-connected nets	3D polyhedra and cages (*sensu lato*)	Pores, channels and access
40	(*bhs,h*)**fee*	4,6,8	bhs,c,for,kbb,kbf,kpb	*brw,fee,hex*	kah,lov	2D-channel-nearcircular-8, rocker-8,8
96	(*h,z*)**brw*	4,6,8	fhe,kei,kox,kua,kub,s, sao,ton,z,zz	*brw,hex*	hes,kdq,lai,vvs	1D-channel-chair-8
97	(*c,h*)**brw*	4,6,8	afv,c,cc,for,kpb,niv,s	*brw,hex*	afi,afs,kah	1D-channel-nearcircular-nonplanar-8; afs sidepockets
105		3,4,6,8	hth,off,ppt,s	*brw,ttw*	htp,stp,tpr	3D-channel-doublecrown-12, nearplanar-8,8
99	(*c,h*)**brw*	4,6,8	c,chf,kad,kbi,s,sta,thr	*brw,fee*	cub,lau,ste	3D-channel-rocker-8,8,8
101		4,6,8	kbi,oon,ss,too	*fee,ooo*	kaa,ocn,opr,pau,ste	3D: pau cages *via* circular-8 and ste cages *via* hammock-8
324		4,6,8	kbi,kdf,kqj,oon,ss,too	*fee*	gsm,kaa,kdq,ocn,opr, oto,pau,phi,ste	1D-channel of pau *via* circular-8; 1D-channel of ocn & opr *via* circular-8; 3D-channel *via* nonplanar-8,8,8
379		4,6,8	kbi,kqj,oon,ss	*fee*	kaa,ocn,opr,phi,ste	1D-channel-circular-8 through opr & ocn; 3D-channel-distorted-8,8,8
387		4,6,8	kbi,ksh,ss,too	*fee*	oto,pau,ste	2D-channel, cages & sidepockets: circular & distorted-8
1035	(*c,h*)**fee*	4,6,8	bs,c,chf,kad,s,ss	*fee* (two types)	kaa,kdt,kuo,ste,sti	3D-channel-sofa-8, rocker-8 & distorted-8
102	(*c,h*)**brw*	4,6,8	c,cc,kdf,kei,ker,kfd,ss	*brw,fee*	gsm,kdq	2D-channel-nearcircular-8, chair-8
893		4,6,8	kqj,ksh,ss	*fee*	oto	2D-channel-sofa-8, rocker-8

Table 2 (*cont.*)

CTF no.	Alternative topological description	Rings providing access to pores	1D subunits including chains, columns, tubes	2D three-connected nets	3D polyhedra and cages (*sensu lato*)	Pores, channels and access
376		4,6,8,12	kow,koz,kpn,ofr,ss	*gml*	can,dpr,eni,hpr,tti	1D-channel-circular-12; 3D-channel-nearcircular bifurcated-12, near elliptical-8,8
386		4,6,8,12	koy,kpm,lel,ss,tix	*gml*	afs,gme,lil,oth	1D-channel-circular-12 *via* lil; 3D-channel-distorted-12 & -8
106		4,6,8,12	kgd,off,ofr,ss,tix	*gml,kyn″, ooo*	can,gme,hpr,kno	3D-channel-double-crown-12 connected *via* rocker-8 through gme cages
919		4,6,8,12	koy,koz,ksk,ss	*gml*	afs,kah,oth,tti	2D-channel, cages & sidepockets-nearcircular-sofa-12, irregular-8
918		4,6,8,12	koy,koz,ofr,ss,tix	*gml*	afs,can,gme,hpr,kah, oth,tti	3D-channel & cages-nonplanar-12, nearcircular-8,8
921		4,6,8,12	koy,koz,ss	*gml*	afs,kah,oth,tti	2D-channel with sidepockets-sofa-12, irregular-8
314		4,8,9,12	dbs,let,s,tof	*tfn*	cub,lil	1D-circular-12 thru lil cages; also very nonplanar - 9,8,8
48	(*c,cub,h*)**fee*	4,8,10	bs,c,dbs,ssf	*ee,ffs*	cub	3D-channel-elliptical-nonplanar-10, nearcircular-8,8
355	(*c,h*)**brw*	4,6,8,10	c,hii,s,ss	*brw,ffs*	baf,cub,oto	2D-channel-distorted-10, nearcircular-8
1034	(*c,h*)**fee*	4,6,8,10	bs,c,s,ss	*fee,ffs*	oto,sti	3D-channel-irregular-elongated-10, nearcircular-8 & rocker-8
1033		4,6,8,12	bs,kbi,s,ss,tot	*tth*	kaa,kuo,oto,ste,sti	3D-channel-square-crown-12 & nearcircular-8,8
357		4,6,8,12	hii,kbi,off,oon,s,ss,too	*tth*	baf,cub,ocn,opr,oto, pau,ste	3D-complex channel & cages; doublecrown-12,nonplanar-8, etc.
302		4,8,12	dbs,ss,too,tot	*brw,tth*	cub,pau	3D-channel and pau cages-crown-12, circular-8 & hammock-8,8
308		4,6,8,12	c,kpn,ss,tsx	*brw,fos*	cub,hpr	3D-channel-nonplanar-elliptical-12, near planar-elliptical-8
465	(*c,h*)**brw*	4,6,8,12	bre,cc,kpm,oih,ss	*brw,fos*	opr	2D-channel-elliptical-nonplanar-12, circular-8
356	(*c,h*)**brw*	4,6,8,12	c,hii,off,s,ss	*brw,fos*	baf,cub,oto	3D-channel-doublecrown-elliptical-12, nonplanar-8, rocker-8
292		4,6,8,12	lel,off,ss,tsx	*twy*	cub,hpr,lil	3D-channel: circular-12 & triangular-doublecrown-12, hammock-8,8
916		4,6,8,12	kow,off,oih,ss	*twy*	dpr,eni,opr	1D-channel-circular-12 with circular sidepockets; 3D-channel-doublecrown-12, circular-8,8
1032		4,6,8,12	bs,dbs,lel,off,oih,s,ss, tot	*twy*	cub,lil,opr,oto,sti	3D-channel-circular-12 through lil cages, triangular-crown-12 & hammock-8,8
294		4,6,8,16	hii,kbi,s,ss,tox	*brw,rho*	baf,cub,kaa,kql,oto, ste	3D-channel & cage: doublecrown-16 & rocker-8 *via* rocker- & chaise-longue-8
403		4,6,8,16	ss,too,tox,tsx	*rho*	cub,hpr,pau	3D-channel-square-doublecrown-16 & circular-8, rocker-8,8
463		4,6,8,16	oih,oon,ss,tox	*ooo,rho*	ocn,opr	3D-channel-square-doublecrown-16, circular-8,8; 1D-circular-8
312		4,6,8,18	dbs,ss,tix,tow	*eoo*	cub,gme	3D-channel-circular-nonplanar-18; gme cages *via* hammock-8,8
293		4,6,8,24	ss,tix,tsi,tsx	*tsv*	cub,gme,hpr	3D-channel & cage: doublecrown-24 *via* rocker-8,8 of gme cages
917		4,6,8,24	ofr,oih,ss,tsi	*tsv*	can,hpr,opr	3D-channel-doublecrown-24, circular-8,8
631		4,6,8,12	bre,kbi,lel,ofr,ss	*ltl*	can,hpr,kaa,lil,ste	3D-channel through lil cages: main access *via* circular-12; subsidiary *via* hammock-8,8
902		4,6,8,12	kbi,kow,ss,tix	*ltl*	dpr,eni,gme,kaa,ste	1D-kow column *via* circular -12; 3D-channel *via* hammock- & rocker-8
358	(*c,h*)**brw*	4,6,8	c,kbi,kpb,s,sta	*brw,fsy*	cub,kaa,kah,lau,ste	3D-channel-rocker-8,8, irregular-8
366	(*c,h*)**brw*	4,6,8	afv,c,cc,chf,kbi,niv,s	*brw,fsy*	afs,ste,stt	2D-channel-rocker-8,8 with sidepockets

Table 2 (*cont.*)

CTF no.	Alternative topological description	Rings providing access to pores	1D subunits including chains, columns, tubes	2D three-connected nets	3D polyhedra and cages (*sensu lato*)	Pores, channels and access
396	(*h,p*)**brw*	4,6,8	kdf,kox,ksf,ksg,p,pp,s,ss	*brw,fsy*	gsm,kdq,vvs	2D-channel-chair-8, sofa-8
383	(*c,h*)**brw*	4,6,8	c,cc,koy,koz,kph,s,ss	*brw,fsy*	afs,oth,tti	2D-channel-nearcircular-irregular-8, chair-8
38	(*bhs,h*)**fee*	4,6,8	bhs,c,chf,kba,kbb,kbf, kbi,s	*brw,fee*	lov,ste	3D-channel-nearcircular-8 & rocker-8,8
369	(*h,s*)**brw*	4,6,8	kdf,kox,s,ss	*brw*	gsm,hes,kdq	2D-channel-chair-8,8
295	(*c,h*)**brw*	4,6,8	c,cc,chf,kad,kbi,koy,koz, kph,s,ss,sta,thr	*brw*	cub,kaa,kab,lau,oth, ste	2D-channel: rocker-, chair-8 & irregular-8
52	(*c,h*)**fee*	4,6,8	c,s,ss	*brw,fee*	ohc,sti,tti	3D-channel-nearcircular-8, rocker-8 & distorted-8
993		4,6,7,8	bs,kad,kbf,s	*bor,tva*	lov,sig,ste	2D-channel-boat-8,8
360		4,6,7,8	s,ss	*bor*	-	2D-channel-nearcircular-nonplanar-8, nonplanar-7; sidepockets
992	(*c,h,s*)**brw*	4,5,6,8	bs,c,kbf,kbi,s	*bik,brw,fee*	euo,kaa,lov,ste	3D-channel-circular-8, boat-8 & twisted-8
668	*bru**T [010]Dm	4,6,8	abf,brs,kcr,kng,s	*bik,brw,fee*	bru,lov,ygw	3D-channel-nonplanar-8,8,8
894		4,5,6,8	kcr,kng,kpa,s,slv	*bik,brw*	eun,oto,pes	2D-complex channels & sidepockets, nonplanar-8,8
895	(*c,h,s*)**brw*	4,5,6,8	c,kcr,kpa,kph,s,ss	*bik,brw*	kdk,pes	2D-channel & sidepockets, chair-8,8
929	(*h,h′,n*)**brw*	4,5,6,8	kcr,kng,kpa,kph,n,nn,s, slv	*bik,brw*	eun,kdk,pes,ygw	2D-channel with sidepockets, chair-8, irregular-8
1038	(*c,h*)**fee*	4,6,8,10	bhs,bs,c,dbs,kbb,kbf,s, ss	*fee,fsv*	cub,lov,ohc,oto,tti	3D-channel-irregular-elongated-10, circular-8 & rocker-8
405	(*c,h*)**brw*	4,6,8,10	c,hii,koz,s,ss	*brw,fsv*	baf,cub,kah,tti,xio	3D-channel-nearelliptical-nonplanar-10, near circular-8, hammock-8
407	(*c,h*)**brw*	4,6,8,10	c,cc,koy,s,ss	*brw,fsv*	afs,oth,twe	2D-channel-nearelliptical-nonplanar-10, near circular-8
1040	(*c,h*)**fee*	4,6,8,10	bs,c,chf,dbs,kad,s,ss	*fee,ttv*	cub,kaa,kuo,oto,ste, sti	3D-channel-elongated-10, sofa-8 & rocker-8
582	(*h,s*)**brw*	4,6,8,10	kdf,kpk,kpo,oih,s,ss,tsx	*brw,ooo*	cub,gsm,hpr,kdq, opr	2D-channel-very elliptical-nonplanar-10 & chair-8, circular & nearcircular-8
1039		4,6,8,12	bs,dbs,lel,s,ss,tix,tot	*ree*	cub,gme,lil	3D-channel-circular-12, nonplanar-12 & rocker-8
1037	(*c,h*)**fee*	4,6,8,12	bs,c,for,kpb,oih,s,ss	*fee,fix*	kal,ohc,opr,sti	3D-channel-elongated-12, circular & nearcircular-8, & rocker-8
377	(*c,h*)**brw*	4,6,8,12	afv,c,cc,hii,kpb,niv,off, s,ss	*brw,fix*	afi,baf,cub,oto,twe, xio	2D-channel-doublecrown-elliptical-12, irregular-nearcircular -8 & -8
373	(*c,h*)**brw*	4,6,8,12	c,cc,koy,koz,kqf,kqg,oih, s,ss,tsx	*brw,fix*	cub,hpr,opr,oth,tti	2D-channel-elliptical-rocker-12, circular- & nearcircular -8
1036	(*c,h*)**fee*	4,6,8,12	bhs,bs,c,dbs,kbb,kbf, koz,s,ss	*fee,fix*	cub,loh,lov,oto,tti	3D-channel-elongated-12, nearcircular-8 & rocker-8
408	(*c,h*)**brw*	4,6,8,12	c,cc,kdf,kpm,kpn,oih,ss, tsx	*brw,vvv*	cub,gsm,hpr,kdq, opr	2D-channel-rocker-12, circular- & nearcircular-8
409	(*c,h*)**brw*	4,6,8,12	c,chf,hii,kad,kbi,off,s, ss,sta,thr	*brw, vvv*	baf,cub,kaa,lau,oto, ste	2D-channel-elliptical-doublecrown-12, nearcircular-nonplanar-8 & rocker-8
1041	(*c,h*)**fee*	4,6,8,12	bs,c,chf,kad,kbi,oih, s,ss	*fee,vvv*	kaa,kuo,opr,ste,sti	3D-channel-elongated-12, planar- & rocker-8; circular- & rocker-8; rocker-8
1042	(*c,h*)**fee*	4,6,8,12	bs,c,dbs,s,ss	*fee,vvv*	cub,oto,sti	3D-channel-irregular-elongated-12 & bifurcated-8; circular-8 & rocker-8
411		4,5,6,8	kbi,s,ss	*fef*	hsp,kaa,ppr,ste	3D-channel-very distorted-8,8,8
410	(*c,h,s*)**brw*	4,5,6,8	c,eca,kbi,kcr,kpa,kph, kpl,s,ss	*brw,fef*	cub,kaa,mtw,pes,sel, ste	2D-channel-sofa- & rocker-8
397		4,5,6,8,12	ksp,ksq,off,s,ss	*bks*	hvx,kso,ppr	3D-channel-doublecrown-elliptical-12, nearcircular- & distorted-8
404		4,5,6,8,12	kcr,kpa,ksk,s,ss	*bks*	kdk,pes	2D-channel-sofa-12, near chair-8
897		4,5,6,8,18	eca,kcr,kng,kpa,kpl,s, slv,ss	*eus*	cub,eun,kdk,mtw,pes, sel,ygw	2D-channel & sidepockets, nearcircular-18 with four bifurcations, near elliptical-8
466	(*d,h*)**brw*	4,6,8	d,dd,kdf,kox,ksx,ksy, s,ss	*brw,ffv*	gsm,hes,kdq	2D-channel-chair-8,8
378	(*c,h*)**brw*	4,6,8	c,cc,chf,kad,kax,kbi, kpb,niv,s,sta,thr	*brw,fto*	cub,kaa,kal,lau,ste	2D-channel-nearcircular- & rocker-8, rocker-8

Table 2 (*cont.*)

CTF no.	Alternative topological description	Rings providing access to pores	1D subunits including chains, columns, tubes	2D three-connected nets	3D polyhedra and cages (*sensu lato*)	Pores, channels and access
380	(*c,h*)**brw*	4,6,8	c,cc,koy,koz,kpr,s,ss	*brw,fto*	afs,gsm,oth,tti	2D-channel-nearcircular- & rocker-8, rocker-8
1048	(*c,h*)**fee*	4,6,8	bhs,bs,c,chf,kad,kbb, kbf,kbi,koz,s	*fee,fto*	loh,lov,ste,sti	3D-channel-nearcircular-8, rocker-8 & irregular-8
381	(*h,n*)**brw*	4,6,8	kdf,kox,ksm,ksn,n,nn, s,ss	*brw,fto*	gsm,hes,kdq,vvs	2D-channel-chair-8,8
1044	(*c,h*)**fee*	4,6,8	bhs,bs,c,chf,for,kad,kbb, kbf,kbi,kpb,s	*apd,fee*	kal,loh,lov,ste	3D-channel-nearcircular-8 & rocker-8,-8
371	(*h,l*)**brw*	4,6,8	kdf,kox,ksv,ksw,ll,s,ss	*apd,brw*	gsm,hes,kdq,vvs	2D-channel-chair-8,8
372	(*c,h*)**brw*	4,6,8	afv,c,cc,koy,koz,kpb,kph, niv,s,ss	*apd,brw*	afi,afs,oth,tti	2D-channel-chair-8, irregular-8
368	(*c,h*)**brw*	4,6,8	afv,c,cc,for,kad,kbi,kpb, niv,s,sta,thr	*apd,brw*	afi,afs,cub,kaa,kah, kal,lau,ste	2D-channel-rocker-8, irregular-8
937	(*f,h*)**brw*	4,6,8	f,ff,kdf,kox,kpu,kpv,s,ss	*brw,feo*	gsm,hes,kdq,vvs	2D-channel-sofa-8,8
900		4,5,6,8	kbi,kcr,kng,kni,kpb,s	*knh,nos*	kah,kal,kdk,jar,opr, ste,ygw	3D-channel-planar- & rocker-8, nonplanar-8,8
913		4,5,6,8	kbi,kpa,niv,s,slv	*nos*	afi,eun,koi,pes,ste	2D-channel with sidepockets, planar- & rocker-8,rocker-8
901		4,5,6,8	kbi,kcr,kox,kpa,kph,s	*brw,nos*	hes,hpr,pes,son,ste, stf	2D-channels with sidepockets, irregular-8,8
938		4,5,6,7,8	kcr,kpa,kpc,kpd,kpx, kpy,s	*brw,vnv*	ccs,kdk,koi,kpw,pes, zsv	2D-channels with sidepockets, irregular-8,7
942	(*c,h,h′,s*)**brw*	4,5,6,8	afv,c,cc,kcr,kpa,kpb,kph, niv,s,ss	*brw,urg*	afs,kah,kdk,kqb,kqc, pes	2D-channel & sidepockets, nearcircular-8 & irregular-8, near sofa-8
880	(*c,h*)**brw*	4,6,8,10	c,hii,kpb,s,ss	*brw,fsf*	baf,cub,kal,xio	3D-channel-elliptical-nonplanar-10, nearcircular-nonplanar-10 &10, rocker-8
881	(*c,h*)**brw*	4,6,8,10	afv,c,cc,niv,s,ss	*brw,fsf*	afi,afs,oto	2D-channel-elliptical-nonplanar-10, nearcircular- nonplanar-8
1047	(*c,h*)**fee*	4,6,8,10	bhs,bs,c,dbs,kbb,kbf,koz, s,ss	*fee,ftn*	bog,cub,loh,lov,tti	3D-channel-elongated-bifurcated-10, nearcircular- & rocker-8
883	(*c,h*)**brw*	4,6,8,10	afv,c,cc,hii,koy,koz,kpb, s,ss	*brw,ftn*	afi,baf,cub,kah,oth, oto,tti,xio	2D-channel-elliptical-nonplanar-10, nearcircular-8 & -8 & -8
941	(*c,h,s*)**brw*	4,5,6,8,12	c,hii,kcr,kpa,kph,off,s,ss	*brw, uiv*	cub,kdk,kpz,kqa,pes	2D-channel & sidepockets, elliptical-nonplanar-12 & sofa-8, nearcircular-8 & sofa-8
879		4,6,8,12	kbi,kst,ksu,off,oih,s, ss,tsx	*vss*	cub,hpr,kaa,kss,opr, ste,xib	3D-channel-elliptical-doublecrown-12 & 8, elliptical-planar- & boat-8,8
878	(*c,h*)**brw*	4,6,8,12	c,cc,hii,koy,koz,kph, off,s,ss	*brw,vss*	afs,baf,cub,oth,oto, tti,xio	2D-channel-elliptical-doublecrown-12 & chair-8, nearcircular-nonplanar-8 & -8
896	(*c,h*)**brw*	4,6,8,12	afv,c,cc,hii,kpb,niv,off, s,ss	*brw,bsh*	afi,cub,twe,xio	2D-channel-doublecrown-elliptical-12, nonplanar-8
1049	(*c,h*)**fee*	4,6,8,14	bhs,bs,c,dbs,kbb,kbf, s,ss	*fee,fvo*	cub,lov,oto	3D-channel-veryelongated-bifurcated-14, nearcircular-8 & rocker-8
882	(*c,h*)**brw*	4,6,8,14	c,cc,hii,koy,koz,oih,s, ss,tsx	*brw,fvo*	baf,cub,hpr,opr,oto, tti,twe	2D-channel-elliptical-nonplanar-14, circular-8 & nearcircular-nonplanar-8 & -8
898		4,5,6,8,12	kpm,s,slv,ss,uee	*brw,mor*	eun,pes	2D-channel and sidepockets, sofa-12 & elliptical-8, rocker-8
899		4,5,6,8,12	kng,kpn,s,ss	*brw,mor*	kdk,opr,xic,ygw	3D-channel & sidepockets, boat-12 & elliptical-8, sofa-8, 8
911	(*h,h′,pp*)**brw*	4,5,6,8,12	kbi,kpa,kqg,pp,s,slv	*brw,mor*	eun,kaa,koi,pes,sel, ste	2D-channel-rocker-12 & rocker-8, nearplanar-8
912	(*h,h′,p*)**brw*	4,5,6,8,12	eca,kbi,kcr,kng,p,s	*brw,mor*	cub,kdk,mtw,ygw	3D-channel-rocker-12, rocker-8 & sofa-8
935		4,5,6,8,12	kcr,kdf,kpa,kpq,s,ss	*brw,mor*	kdk,koi,pes	2D-channels with sidepockets, sofa-12 & sofa-8, irregular-8
616	(*h,h′,z′*)**brw*	4,5,6,8,10	kpa,kpl,kpo,s,slv,zz	*brw,dac*	eun,pes,sel	2D-channel-near hammock-10, near elliptical-8
933		4,5,6,8,10	kcr,kpa,s,slv,ss	*brw,dac*	eun,kdk,koi,pes,ygw	2D-channel-near sofa-10, irregular-8
934	(*h,h′,z′*)**brw*	4,5,6,8,10	eca,kcr,kng,kpk,s,z	*brw,dac*	cub,kdk,mtw,ygw	3D-channel-near rocker-10, irregular-8,8

Table 2 (*cont.*)

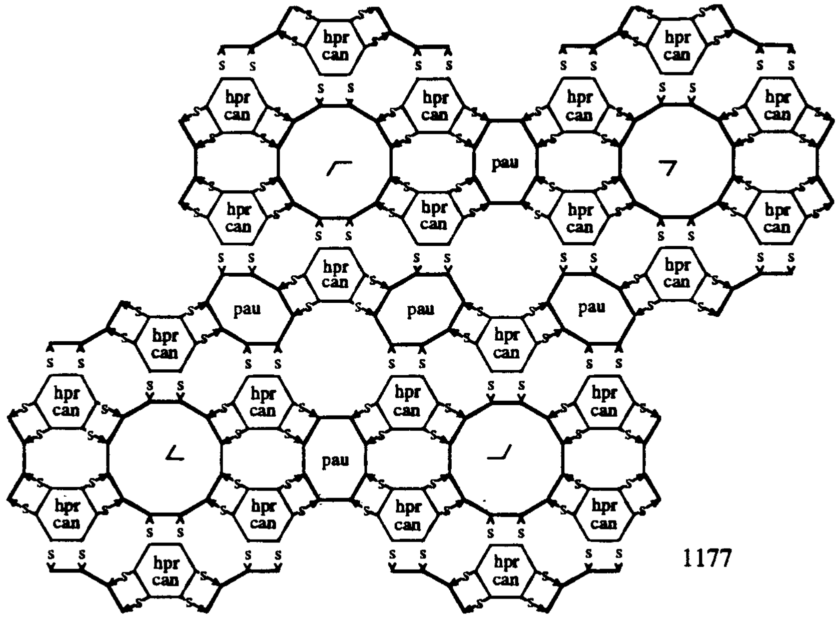
CTF no.	Alternative topological description	Rings providing access to pores	1D subunits including chains, columns, tubes	2D three-connected nets	3D polyhedra and cages (*sensu lato*)	Pores, channels and access
914		4,5,6,8,10	kcr,kpa,s,ss	*brw,dac*	kdk,pes	2D-channel with sidepockets, sofa-10, chair-8
617	(h,h',z')**brw*	4,5,6,8,10	kpa,kpl,kpo,s,slv,zz	*brw,dao*	eun,pes,sel	2D-channel-chair-10, near elliptical-8
930	(h,h',z')**brw*	4,5,6,8,10	eca,kcr,kng,kpk,s,z	*brw,dao*	cub,kdk,mtw,ygw	3D-channel-rocker-10, irregular-8,8
932		4,5,6,8,10	kcr,kng,s,ss	*brw,dao*	kdk,ygw	2D-channel-sofa-10, irregular-8
931		4,5,6,8,10	kcr,kpa,s,ss	*brw,dao*	kdk,koi,pes	2D-channel-sofa-10, irregular-8
628		4,5,6,8,10	kpa,kpl,pp,s,slv	*brw,sxn*	eun,pes,sel	2D-channel-nonplanar-10, nearcircular-8 through sel cages
939		4,5,6,8,10	kcr,kng,kpa,s,slv,ss	*brw,sxn*	eun,kdk,koi,pes	2D-channel-chaiselongue-10, irregular-8
943		4,5,6,8,10	eca,kcr,kng,s	*brw,sxn*	cub,kdk,mtw,ygw	3D-channel-near hammock-10, near sofa-8, near rocker-8
940		4,5,6,8,10	kcr,kpa,s,ss	*brw,sxn*	kdk,koi,pes	2D-channel-sofa-10, chair-8
926	(h,h',z')**brw*	4,5,6,8,10	eca,kcr,kox,kpa,kpk, kpl,s,z	*brw,fes*	cub,hes,kdk,kdq, mtw,pes,sel	2D-channel with bifurcation-rocker-10, irregular-8
925		4,5,6,8,10	kcr,kpa,kpb,niv,s,ss	*brw,fes*	afi,kal,kdk,koi,pes	2D-channel with sidepockets-sofa-10, irregular-8
388		4,5,6,8,12	kad,kcr,koy,koz,kpa, kpb,kpm,kpn,kpq, niv,s,ss,sta	*bab,brw*	afi,afs,cub,kab,kal, kdk,lau,oth,stt,xve	2D-channels & sidepockets: boat- & sofa-12,distorted-8
927	(f,h,h')**brw*	4,5,6,8,12	eca,f,ff,kcr,kox,kpa,kpl, kpm,kpn,s,ss	*bab,brw*	cub,hes,kdk,mtw,pes, sel	2D-channel with bifurcation-rocker-12, irregular-8
837		4,6,8,12	kad,kox,koy,kpm,kpn,s, ss,sta	*brw,uss*	afs,cub,hes,lau,oth, ste,stt,tti	2D-channel-rocker-12, irregular-8
477	(c,h,s)**tva*	4,6,7,8	bhs,bs,c,kad,kbb,kbi,s	*brw,fee, sse,tva*	kaa,lov,ste	3D-channel-circular-8, rocker-8 & distorted-8
892		4,6,8	kad,kbi,kst,ksu,s,ss,sta	*tva*	cub,hpr,kaa,kss,lau, ste,xib	3D-channel-various nonplanar-8,8,8
884		4,6,8	kbi,kst,ksu,oon,s,ss,too	*stg*	hpr,kaa,kss,ocn,opr, pau,ste, xib	3D-channel-circular-8 & rocker-8, rocker-8,8
885	(h,v)**brw*	4,6,8	kdf,kox,ksr,ksz,s,ss,v,vv	*brw,stg*	gsm,hes,kdq	2D-channel-nearcircular-chair-8,8
887	(c,h)**brw*	4,6,8	c,cc,koy,kpb,ksl,s,ss	*brw,fst*	afs,kal,oth	2D-channel-nearcircular-chair & irregular-8, chair-8
888	(c,h)**brw*	4,6,8	afv,c,cc,chf,for,kad,kbi, kpb,niv,s,sta	*brw,fst*	afi,cub,kaa,kal,lau, ste	2D-channel-rocker- & irregular-8, rocker-8
886	(e,h)**brw*	4,6,8	e,ee,kdf,kox,kta,ktb, s,ss	*brw,fst*	gsm,hes,kdq,lai	2D-channel-nearcircular-chair-8, chair-8
903	(c,h,s)**brw*	4,5,6,8	c,cc,kcr,koy,koz,kpa, kph,s,ss	*brw, rxt*	afs,kdk,oth,pes,tti	2D-channels with sidepockets, two types, both irregular-8
891	(h,w)**brw*	4,6,8	kdf,kox,ktc,ktd,s,ss, w,ww	*brw,fss*	gsm,hes,kdq,vvs	2D-channel-nearcircular-8, chair-8
904	(c,h,s)**brw*	4,6,7,8	c,cc,kdf,kpf,kpg,s,ss	*brw,uhi*	gsm,kdq,zfs,zsv	2D-channel with sidepockets, two types, both irregular-8
624		4,5,6,8,10	kpa,kpi,kpo,s,slv,sss	*brw,fer*	eun,pes,stf	2D-channel-hammock-10, rocker-8 through stf cages
928		4,5,6,8,10	kcr,kng,kpk,kpp,s,szf	*brw,fer*	hpr,kdk,son,ygw	3D-channel-hammock-10, irregular-8,8
689	*bru**T [010]Em, (h',p,4)**fee*	4,5,6,8,10	abf,brt,kcr,kng,p,s	*fee,fer*	bru,lov,ygw	3D-channel-nearcircular-10 with two bifurcations, chair-8 & hammock-8
798		4,5,6,8,10	kcr,kox,kpa,kqh,s,sss	*brw,fer*	pes	2D-channel-near circular-sofa-10, non-planar-8
946	(c,h',z')**brw*	4,5,6,7,8	c,kpa,kpd,s,slv,zz	*brw,een*	eun,koi,pes,zsv	2D-channel & sidepockets-irregular-8, irregular-7
947	(c,h',z')**brw*	4,5,6,7,8	cc,kcr,kng,kpc,s,z	*brw,een*	kdk,kqd,kqe,ygw	2D-channel & sidepockets-sofa-8, irregular-7
953		4,5,6,7,8	kcr,kpa,kpc,kqi,s	*brw,een*	kdk,koi,kqd,pes,zsv	2D-channel & sidepockets-sofa-8 & chair-7
910		4,5,6,8	kcr,kng,kpe,s	*biz,brw*	kdk,ygw	2D-channel with sidepockets, irregular-8,7
920		4,5,6,8	kpa,kpj,s,slv	*biz,brw*	eun,koi,pes	2D-channel with sidepockets-sofa-8, lounger-8
686	*bru**T [010]Et, (partial z)**fee*	4,5,8	abf,brt,kcr,kng,s,z	*biz,fee*	bru,lov,ygw	3D-channel-various distorted-8,8,8

Table 2 (*cont.*)

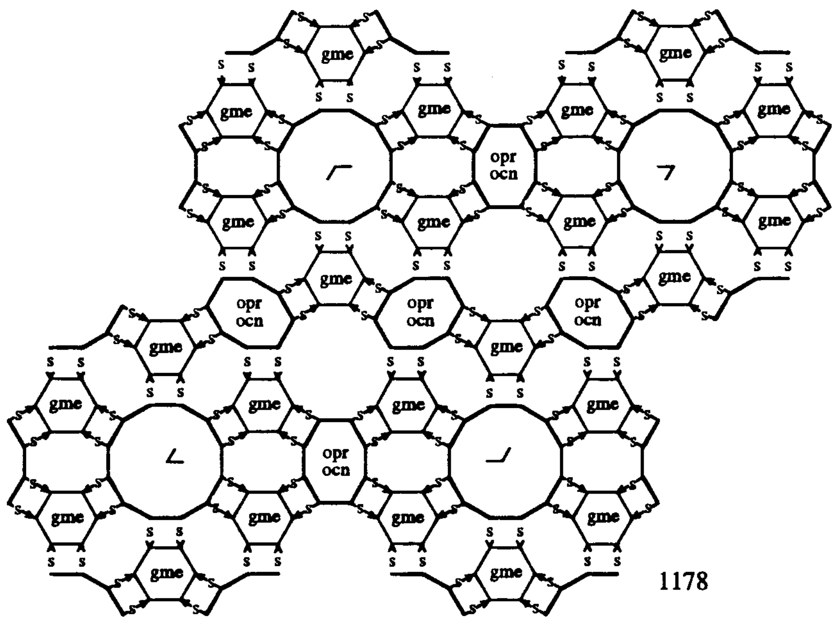
CTF no.	Alternative topological description	Rings providing access to pores	1D subunits including chains, columns, tubes	2D three-connected nets	3D polyhedra and cages (*sensu lato*)	Pores, channels and access
922		4,5,6,8	kcr,kpa,kpe,kpj,s	*biz,brw*	kdk,koi,pes	2D-channel with sidepockets-sofa-8, irregular-8
923		4,5,6,8	kcr,kpb,kpe,niv,s	*brw,fex*	afi,kdk,vvn	2D-channel with sidepockets-sofa-8, irregular-8
924		4,5,6,8	kpa,kpb,kpi,kpj,niv,s	*brw,fex*	afi,pes,vvn	2D-channel with sidepockets-sofa-8, irregular-8
906	(*c,h,h′,z′*)**brw*	4,5,6,7,8	c,cc,kcr,kox,kpa,kpc, kpd,kqi,s,z,zz	*brw,exn*	hes,kdk,kdq,pes,zsv	2D-channel with sidepockets, two types, both irregular-7,8
905		4,5,6,7,8	kbk,kcr,kpa,kpb,kpc, kpd,kqi,niv,s	*brw,exn*	afs,kdk,pes,vvn,zsv	2D-channel with sidepockets, irregular-8, chair-7
907	(*c,h,h′,z′*)**brw*	4,5,6,7,8	c,cc,kcr,kox,kpa,kpc, kpd,kqi,s,z,zz	*brw,exe*	hes,kdk,kdq,koi,pes	2D-channel with sidepockets, three types, all irregular-7,8
908		4,5,6,7,8	kcr,kpa,kpb,kpc,kpd, kqi,niv,s	*brw,exe*	afs,kdk,koi,pes,vvn, zsv	2D-channel with sidepockets, irregular-8,7
1000	(*c,h,s*)**tva*	4,5,6,8	bhs,bs,c,kad,kbb,kbf, kbi,s	*brw,fee, fis,tva*	bog,euo,kaa,lov,ste	3D-channel-circular-8, distorted-8 & rocker-8
889	(*c,h*)**brw*	4,6,8,10	afv,c,cc,for,hii,kpb,niv, s,ss	*brw,eig*	afi,baf,cub,kal,tti	2D-channel-near elliptical-near boat-10, nearcircular-nonplanar-8 & -8
890	(*c,h*)**brw*	4,6,8,10	afv,c,cc,for,koy,kpb,niv, s,ss	*brw,eig*	afi,afs,kal,oth,oto	2D-channel-near elliptical-near boat-10, nearcircular-nonplanar-8 & -8
1045		4,6,8,14	bs,dbs,kbb,koz,s,ss	*api,fee*	cub,lov,ohc,sti,tti	3D-channel-elliptical-14 with 2 bifurcations, nearcircular-8 & collapsed-8
949		4,5,6,8,14	eca,kcr,kng,kpa,kpl, s,slv	*brw,eug*	cub,eun,kdk,koi, mtw,pes,sel,ygw	2D-channel & sidepockets-near elliptical-14 with 4 bifurcations, irregular-8 & 8
862	(*c,h*)**brw*	4,6,8	c,cc,kbi,koy,koz,kpb, kph,s,ss,sta,thr	*brw,tvt*	cub,kaa,kal,lau,oth, ste,tti	2D-channel-nonplanar-nearcircular-8, rocker- & chair-8
876	(*c,h*)**brw*	4,6,8	afv,c,cc,kad,kbi,koy,koz, kph,niv,s,ss	*brw,tvt*	afi,afs,kah,oth,ste, stt,tti	2D-channel-nearcircular-rocker & irregular-8, rocker- & chair-8
877	(*g,h*)**brw*	4,6,8	g,gg,kdf,kox,ksi,ksj,s,ss	*brw,tvt*	gsm,hes,kdq,lai,vvs	2D-channel-chair-8, sofa-8
1046	(*c,h*)**fee*	4,6,8	bhs,bs,c,for,kad,kbb,kbf, kbi,kpb,s	*fee,fsm*	bog,kal,loh,lov,ste	3D-channel-nearcircular-8 & rocker-8,8
915	(*h,i*)**brw*	4,6,8	i,ii,kdf,kox,s,ss	*brw,fsm*	gsm,hes,kdq,lai	2D-channel with sidepockets, sofa-8, sofa-8
955		4,5,6,8,10	kcr,kox,kpa,s,ss	*brw,fev*	hes,kdk,kdq,koi,lai, pes,vvs	2D-channel-sofa-10, near chair-8
1177		4,6,8,12	kbi,lel,off,ofr,ss,too	*zsm*	can,hpr,kaa,kno,lil, pau,ste	1D-channel-circular-12 *via* lil; 1D-channel-doublecrown -12; 3D *via* various-8
1178		4,6,8,12	kbi,kow,off,oon,ss,tix	*zsm*	dpr,eni,gme,kaa, kno,ocn,opr,ste	1D-channel-circular-12 *via* kow; 1D-channel-doublecrown -12; 3D *via* various-8
1051	(*c,h,s*)**brw*	4,5,6,8	bs,c,kad,kbb,kbf,kbi,s	*brw,fee,nee*	euo,lov,ste	3D-channel-circular-8, rocker-8 & irregular-8
936	(*c,h,s*)**brw*	4,5,6,8	c,kcr,kox,kpa,kph,kpr, kps,kpt,ksl,s,ss	*brw,nee*	hes,kdk,kdq,koi,pes	2D-channel-near sofa-8,8
1050		4,5,6,8	abf,bs,kbf,kcr,kng,koz, s,ss	*fee,nee*	bru,lov,ohc,tti	3D-channel-nearcircular-8, rocker-8 & irregular-8
952		4,5,6,8,10	kcr,kox,koy,koz,kpa, kph,kpi,kpp,kqh,s,ss	*brw,eon*	afs,hes,kdk,kdq, oth,pes,tti	2D-channel & sidepockets-sofa-10 & lounger-8, irregular-8 & -8
944		4,5,6,8,10	kpa,kpb,niv,s,ss	*brw,mfv*	afi,afs,kah,koi,pes,vvn	2D-channel-sofa-10, nearcircular-nonplanar-8
948	(*f,h,h′*)**brw*	4,5,6,8,12	eca,f,ff,kcr,kng,kox,kpa, kpl,kqf,kqg,s,slv	*brw,bta*	cub,eun,hes,kdk,kdq, mtw,pes,sel,ygw	2D-channel & sidepockets-rocker-12, sofa-8
951	(*f,h,h′*)**brw*	4,5,6,8,12	eca,f,ff,kcr,kng,kox,kpa, kpl,kqf,kqg,s,slv	*brw,btb*	cub,eun,hes,kdk, kdq,koi,mtw,pes, sel,ygw	2D-channel & sidepockets-rocker-12, elliptical- & irregular-8
1054	(*c,h,s*)**tva*	4,5,6,7,8	bhs,bs,c,kad,kbb,kbf,kbi, kpb,s	*smt,tva*	euo,kal,loh,lov,sig, ste	3D-channel-rocker-8, sofa-8 & complex circular-8
954		4,5,6,8,10	kcr,kox,kpa,s	*brw,mtt*	hes,kdk,kdq,pes	2D-channel-lounger-10, irregular-8
1053		4,5,6,7,8	bs,c,for,kbf,kpb,s	*fee,sma,tva*	bog,euo,kal,lov,sig	2D-channel-irregular-8,8
1052	(*h,z*)**fee*	4,5,8	abf,bs,kbf,kcr,kng,s,z	*fee,sft*	bru,lov,ygw	3D-channel-nearcircular-8,8 & double bifurcated-8

Table 2 (*cont.*)

CTF no.	Alternative topological description	Rings providing access to pores	1D subunits including chains, columns, tubes	2D three-connected nets	3D polyhedra and cages (*sensu lato*)	Pores, channels and access
950		4,5,6,8	kcr,kpa,kpe,kph,kpj,s	*brw,sft*	kdk,koi,pes	2D-channel & sidepockets-irregular-8, 8 (several types)
385	(h,h',p)**brw*	4,5,6,8,12	eca,kbi,kcr,kdf,kox,kpa, kpl,kpm,kpn,kpr,ksf, ksg,p,pp,s,ss	*brw,mln*	cub,hes,kdq,lai,mtw, pes,sel	Complex channel & cage system: distorted-12 & -8
945		4,5,6,8,12	kcr,kdf,koy,koz,kpa,kph, kpq,s,ss	*brw,mln*	kah,kdk,oth,pes,tti	2D-channels-sofa-12, nearcircular-nonplanar-8



1177



1178

Fig. 6. Projections of 3D nets 1177 and 1178 based on 2D *zsm* net $(468)_1(468)_1(46.12)_1(48^2)_1(48.12)_1(48.12)_1$.

1). This connectivity in the 3D net enforces two types of vertex: *B* with two *h* and two tilted edges, and *A* with one *h*, one vertical and two tilted edges (Fig. 7). This type of $(h,s)^*$ net cannot be converted into a $(h,z)^*$ net by removal of a vertical edge. On the projection of this second type of 3D s^* nets (Fig. 8), the shared back of two *s* chains meet at one *h* edge, and all the saw teeth must point outwards. Net 40, obtained from 2D *hex* net (6^3), contrasts with nets 96 and 97 in Fig. 3. Net 1035 is generated from the 2D *fee* net (48^2) and net 314 from the 2D *tfn* net $(4^29)_1(4.9.12)_2$. The stricter topological requirement for the second type of $(h,s)^*$ net allows fewer possibilities in general than for the first type. Net 314 illustrates an exception (Fig. 8), in which the 2D *tfn* net yields an $(h,s)^*$ net only by the second approach.

As for the first type of 3D $(h,s)^*$ nets, pairs of 3D nets can be generated by the second procedure with different arrangement of *h* and *s* edges from the parent 2D net. For the 2D *ffs* net $(4^210)_1(4.10^2)_2$, net 48 has the *s* edges at the branches of the square with the higher symmetry, and net 1034 has one pair of *s* edges at the

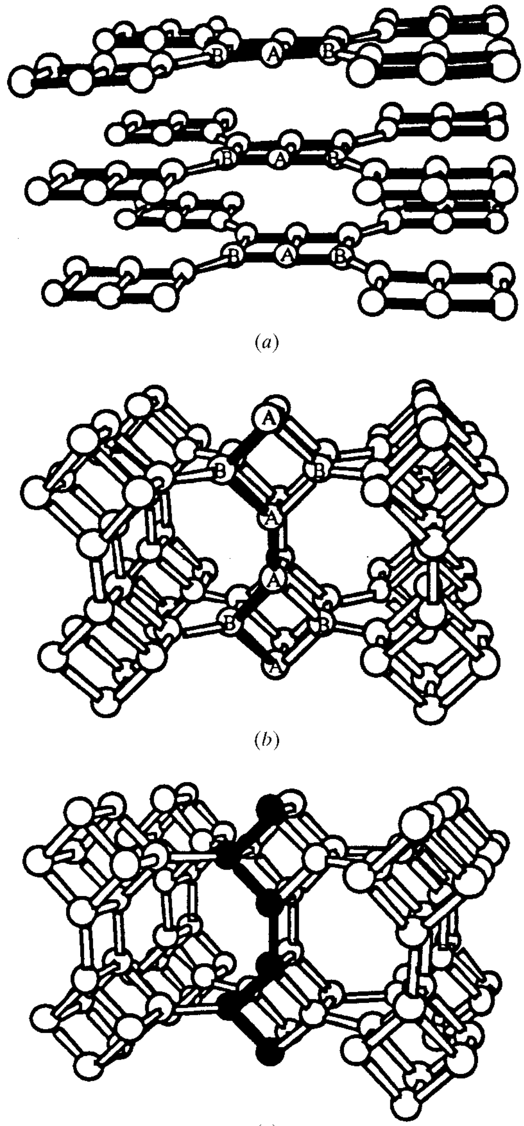


Fig. 7. Procedure for generation of *s* chains by the second approach. (*a*) A vertical stack of congruent three-connected 2D nets *ffs* $(4^210)_1(4.10^2)_2$. (*b*) Adjacent vertices from the horizontal 2D nets are linked by vertical and tilted edges to generate saw chains (shaded edges) which fit together back-to-back to form a *bs* chain. (*c*) The 3D net after DLS refinement: net 48 in Fig. 9.

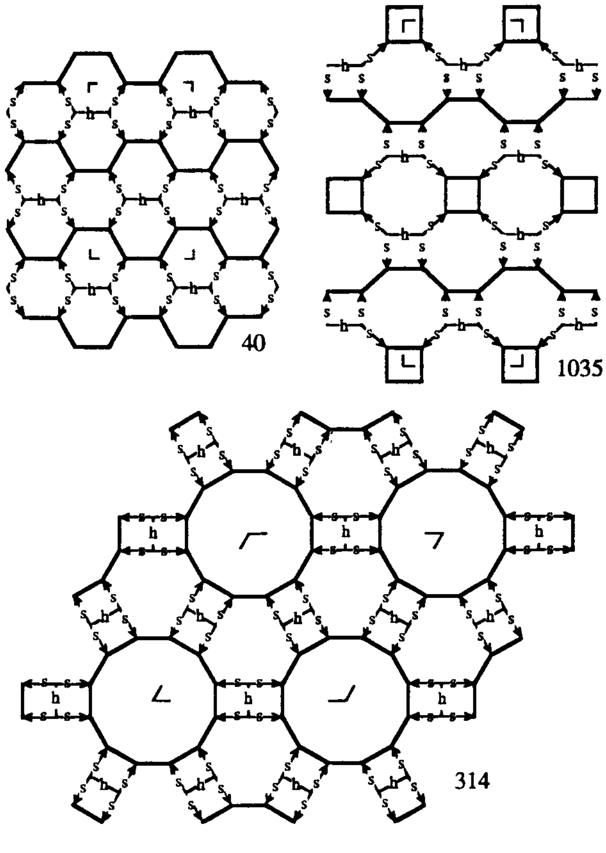


Fig. 8. Projection of 3D nets 40, 314 and 1035 from the second approach. The downward projection of net 40, which derives from 2D *hex* net (6^3), shows how the pairs of *s* chains are linked by horizontal edges. Unlabeled edges are horizontal. Edges marked specifically with *h* join vertices from adjacent *s* chains. The vertices at the saw head (arrow) have two horizontal edges, whereas those at the back of the saw have one horizontal and one vertical edge. 3D net 1035 is obtained from the *fee* net (482), and net 314 from *tfn* $(4^29)_1(5.9.12)_2$. The *bs* chain is nonplanar in 3D nets 40 and 1035, but planar in 314.

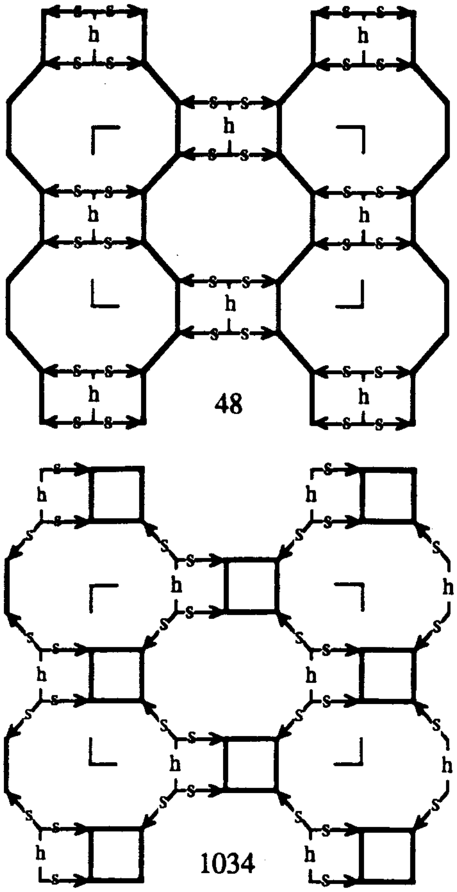


Fig. 9. Two 3D nets with same unit cell but different symmetry derived from the 2D *ffs* net $(4^2 10)_1(4.10^2)_2$.

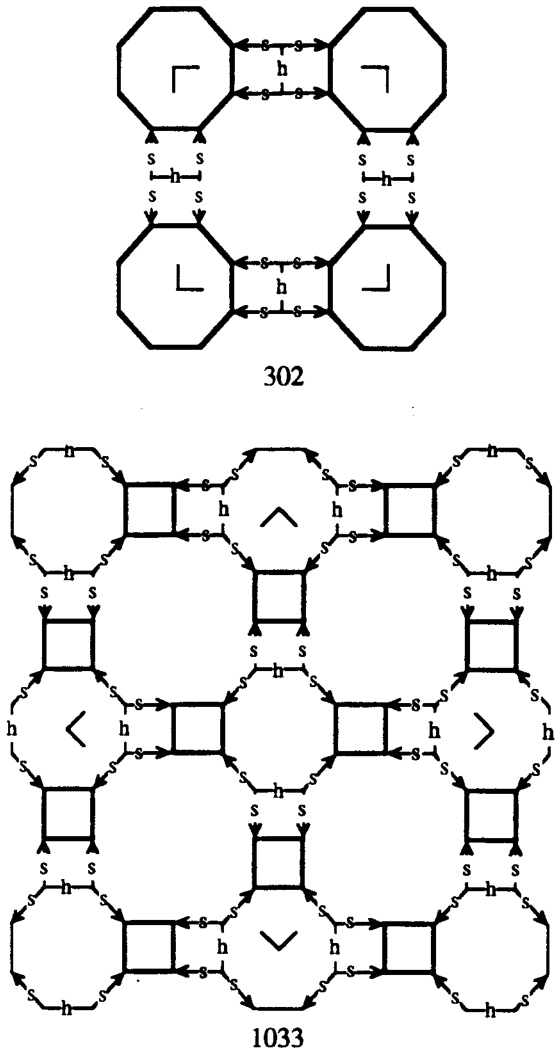


Fig. 10. Two 3D nets with different unit cell and symmetry derived from the 2D *tth* net $(4^2 12)_1(4.8.12)_1$ by the second approach.

branches of the square and the other pair at the branches shared by two ten-rings, leaving one square horizontal (Fig. 9). These two nets have different symmetries but the same unit cell. Nets 302 and 1033 are both built from the 2D *tth* net $(4^2 12)_1(4.8.12)_2$ (Fig. 10); they have different symmetry and unit-cell constants.

The 136 3D nets generated by sigma-plus expansion from their (h,z)*-net counterparts, plus the 38 nets from the second approach (marked with †) add up to 174 nets (Table 1). The EDI net from the third approach raises the total to 175, which will increase after systematic enumeration.

Alternation of two chemical types of T atoms, allowed only for even-numbered rings, results in doubling of the c axis of the unit cell and change in the space-group symmetry of the 3D (h,s)* net (Table 1). Subunits are given in Table 2.

3. DLS refinement

40 3D nets with higher symmetry and small unit cell were chosen for DLS refinement (Baerlocher *et al.*, 1977). Atomic coordinates are given in Table 3† and cell constants in Table 1 marked with §. The ideal values for T—O, O—O and T—T distances were set to 1.63, 2.6618 and 3.1258 Å with weights of 2.0, 1.0 and 0.1, respectively. The residuals for the DLS refinements (mostly

† Table 3 has been deposited and is available from the IUCr electronic archives (Reference: BR0077). Services for accessing these data are described at the back of the journal.

0.001 to 0.002) are smaller than for the $(h,z)^*$ nets because some T atoms in the $(h,s)^*$ nets have the extra freedom of a general position.

The sigma-expanded $(h,s)^*$ nets have a longer repeat along the zigzag-straight chain (~7.6–7.7 Å) than the second type (7.2 Å) because the vertical four-rings of the *bs* chain cannot open up as much as the 'free' edges of the *s* chain (Fig. 1).

4. Topology

4.1. *1D subunits*

Some of the 100-plus one-dimensional (1D) subunits in the 3D nets, including chains, tubes and columns from the CTF database (Andries & Smith, 1993*a*), are shown in Fig. 11. Along the *c* axis each net has either an *s* chain or double saw chain (*ss*), or both, and the 3D nets obtained from the second method also have the *bs* bifurcated chain. Other simple chains occur along the *a* or *b* axis, including *c*, *d*, *e*, *f*, *g*, *i*, *n*, *p*, *v*, *w* and *z*. Some 1D subunits combine rings with the *s* chain, such as *kox* (six-ring) and *kdf* (eight-ring). Reversal of the saw tooth generates two distinct 1D subunits from the same ring: *kcr* and *kpa* units from a five-ring; *koy* and *koz*, six-ring; *kpc* and *kpd*, seven-ring; *kpr* and *ksl*, eight-ring; and *kqf* and *kqg*, 12-ring.

4.2. *2D subunits*

The three-letter code for each parent 2D net is listed in the first column of Table 1. The combination of a congruent stack of horizontal 2D nets with the *z* chain yields a vertical 2D *hex* net (6^3) (Han & Smith, 1998*b*).

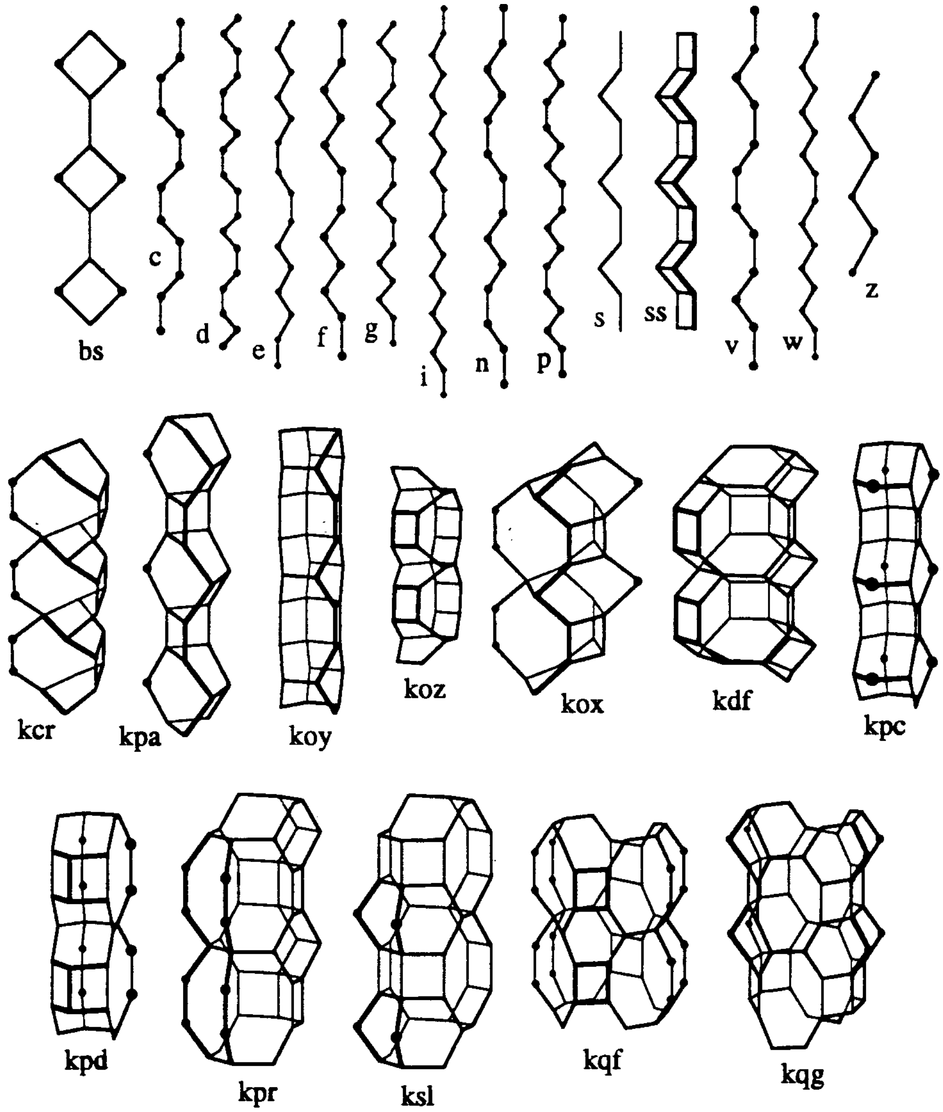
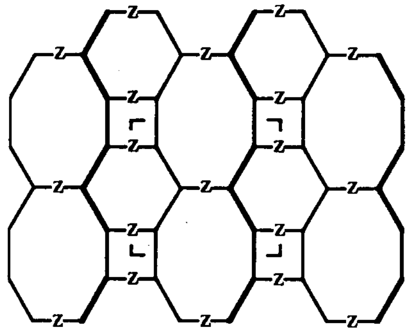


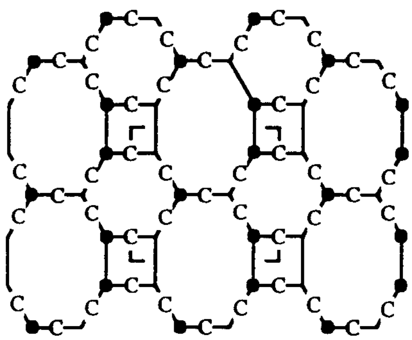
Fig. 11. Selected 1D subunits with CTF code.

Correspondingly, the *s* chain yields vertical 2D nets *brw* $(468)_2(68^2)_1$ and *fee* (48^2). Thus, some of the 3D nets can also be described as the combination of the vertical *brw* and *fee* 2D nets with a simple horizontal chain (Smith, 1979; column 2 in Table 2). Fig. 12 shows the combination of the vertical *brw* 2D net with horizontal *z* (net 96) and *c* (nets 97 and 102).

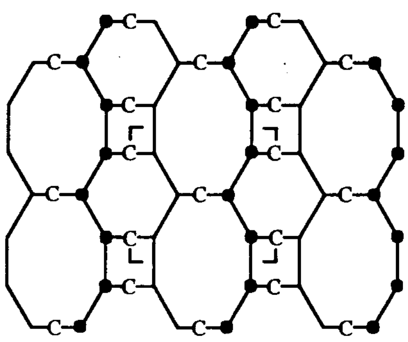
The second approach generates a vertical *fee* 2D net. Fig. 13 shows nets 38, 40, 48 and 1041 with different up–down sequences perpendicular to the *fee* 2D net.



96



97



102

Fig. 12. Projection of 3D nets with vertical *s** nets along a horizontal *c* or *z* chain showing the vertical 2D *brw* net $(468)_2(68^2)_1$. Unlabeled edges are horizontal. For nets 97 and 102, presence and absence of dots indicate opposite directions of linkages along the *c* chain.

4.3. *Polyhedral subunits*

74 polyhedral subunits (Andries & Smith, 1993*b*) were identified in the 174 3D nets. The following have been already found in the *c** and $(h,z)^*$ nets: *afi* 6^36^2, *baf* $4^24^26^26^1$, *eun* 5^46^2-*a*, *hes* 6^4, *hpr* 4^66^2, *kaa* 6^28^2, *kah* 6^3, *kdq* $4^26^28^2$-*b*, *lau* 4^26^4-*a*, *lov* 4^26^2-*a*, *mtw* $4^25^46^2$, *oth* $4^26^26^2$ and *pes* 5^26^2 (Han & Smith, 1998*a*,*b*). New ones (Fig. 14) are *afs* $(4^24^16^28^1)$, 1,2-open hexagonal prism; *cub* (4^6), cube; *gme* $(4^64^36^28^3)$, 1,2-3,4-5,6-doublehandle hexagonal prism; *gsm* $(4^44^28^4$-$a)$, 1,2-doublehandle,3,8-open octagonal prism; *kal* $(4^16^28^28^1)$, 1,2,4,7-open opr; *kdk* $(4^15^28^2)$, 1,3-open,2-handle pentagonal prism; *koi* $(4^25^28^1$-$b)$, 1′,1″-handle trigonal prism; *ocn* $(4^86^48^2)$, 1,2-3,4-5,6-7,8-double-stellated octagonal prism; *opr* (4^88^2), octagonal prism; *oto* $(4^24^24^18^28^1)$, 1,2-open octagonal prism; *pau* $(4^84^48^48^2$-$a)$, 1,2-3,4-5,6-7,8-doublehandle octagonal prism; *sel* $(4^44^25^48^2)$, 1,2-5,6-double-stellated octagonal prism; *ste* $(4^28^4$-$a)$, 1,2,3,4-handle cube; *sti* $(4^24^26^1)$, 1-open cube; *tti* $(4^24^14^16^28^2)$, 1,4-open octagonal prism; *ygw* $(4^25^48^2$-$a)$, 7,9,10′,12′-stellated hexagonal prism.

4.4. *Channel system*

Unlike the *c** and $(h,z)^*$ nets which are restricted to six-rings in the vertical planes, the $(h,s)^*$ nets contain eight-rings. Most of the $(h,s)^*$ nets have at least a 2D channel system, one channel along the *s* chain and the other one or two perpendicular to the *s* chain through eight-ring apertures. Although the $(h,s)^*$ nets tend to have more open space, the framework density is increased by the four-rings in the 3D net from the *bs* and *s* chains.

5. Conclusions

Seven of the 175-plus theoretical 3D $(h,s)^*$ nets occur in known structures, a smaller fraction than for the *c** and *z** nets. In general, the $(h,s)^*$ nets have larger pores and lower framework density than the *c** and $(h,z)^*$ nets. Five out of the seven known structures derive from simple 2D nets. The 2D *zsm* net $(468)_1(468)_1$-$(46.12)_1(48^2)_1(48.12)_1(48.12)_1$ in ZSM-10 has a rather large hexagonal unit cell, and contains two different 1D 12-ring channel systems. The $(h,s)^*$ net in SUZ-4 is based on the 2D *fer* net $(5^26)_1(5^210)_2(5^210)_1(5.6.10)_2$, and is related to the $(h,z)^*$ net in TON. Nets produced by the third approach will be reported later.

Direct financial support from UOP, Exxon Educational Foundation, Mobil Corporation and Chevron Corporation for preparation of the CTF databases is highly appreciated. Support from the University of Chicago and the State of Illinois Technology Challenge Grant for computer facilities was invaluable. Koen

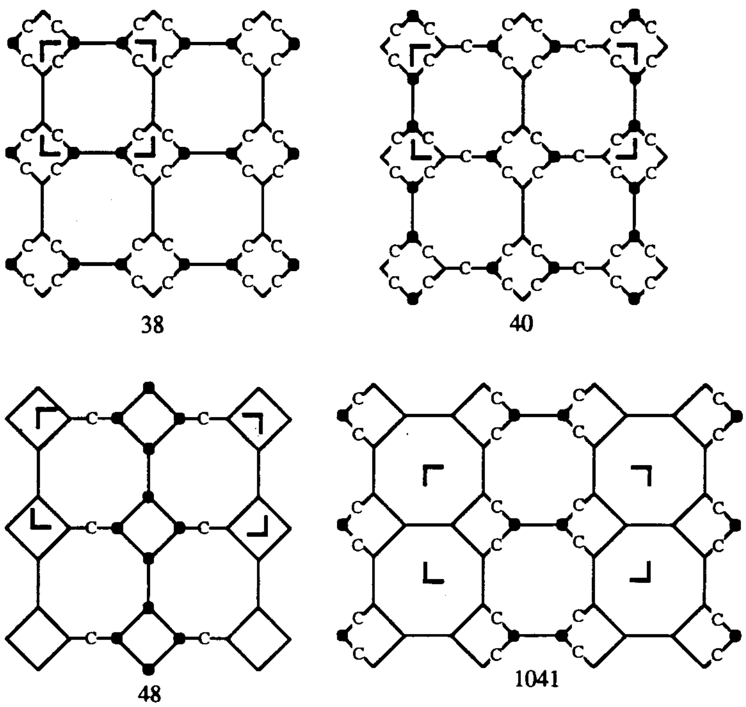


Fig. 13. Projection of 3D with vertical *s** nets along a horizontal *c* chain showing the 2D *fee* net (48^2) and different patterns of *c* and *h* linkages.

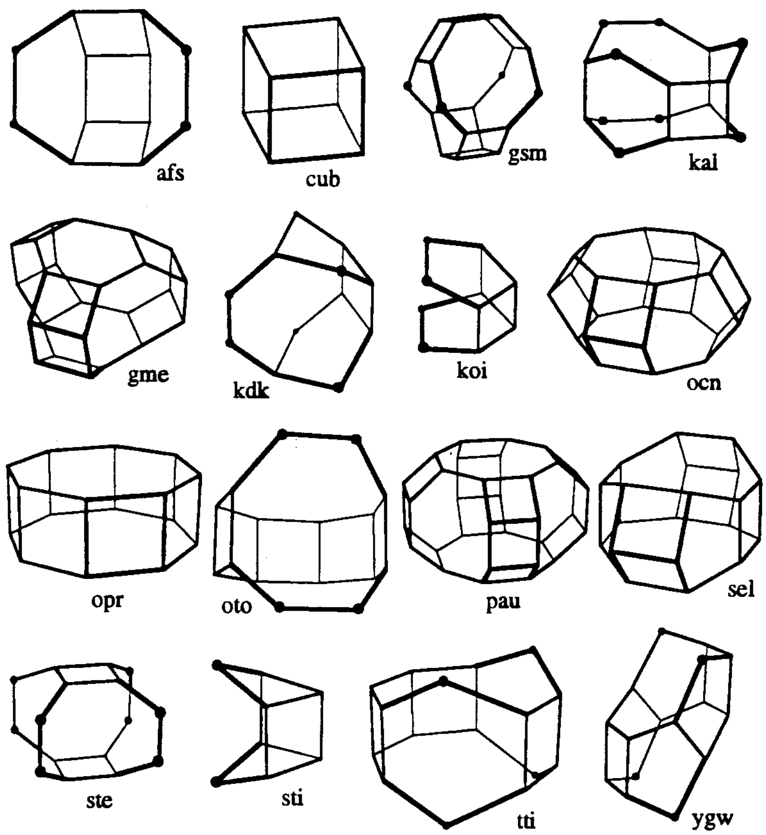


Fig. 14. Polyhedral subunits with CTF code arranged alphabetically.

Andries and Joseph J. Pluth generated the original graphics of most subunits in the CTF databases. The detailed advice of the Associate Editor was very helpful in clarifying mathematical matters.

References

Andries, K. J. & Smith, J. V. (1993*a*). *1D Building Units Related to 3D Frameworks.* Database, Consortium for Theoretical Frameworks, University of Chicago, Chicago, USA.

Andries, K. J. & Smith, J. V. (1993*b*). *Polyhedral Units and Cages Related To 3D Frameworks.* Database, Consortium for Theoretical Frameworks, University of Chicago, Chicago, USA.

Baerlocher, Ch., Hepp, A. & Meier, W. M. (1977). *DLS-76. A Program for the Simulation of Crystal Structures by Geometric Refinement.* Institut für Kristallographie und Petrographie, ETH, Zürich, Switzerland.

Barrer, R. M. & Villiger, H. (1969). *Z. Kristallogr.* **128**, 352–370.

Bennett, J. M. & Gard, J. A. (1967). *Nature (London)*, **214**, 1005–1006.

Gard, J. A. & Tait, J. M. (1972). *Acta Cryst.* B**28**, 825–834.

Han, S. & Smith, J. V. (1998*a*). *Acta Cryst.* A**55**, 332–341.

Han, S. & Smith, J. V. (1998*b*). *Acta Cryst.* A**55**, 342–359.

Hansen, S. & Falth, L. (1981). Recent Progress Reports, 5th International Zeolite Conference, Naples, Italy, pp. 9–12.

Higgins, J. B. & Schmitt, K. D. (1996). *Zeolites*, **16**, 236–244.

Lawton, S. L., Bennett, J. M., Schlenker, J. L. & Rubin, M. K. (1993). *J. Chem. Soc. Chem. Commun.* **11**, 894–896.

Meier, W. M., Olson, D. H. & Baerlocher, Ch. (1996). *Zeolites*, **17**, 1–230.

Pluth, J. J. & Smith, J. V. (1993). *2D Nets Related to 3D Frameworks.* Database, Consortium for Theoretical Frameworks, University of Chicago, Chicago, USA.

Rudolf, P. R., Saldarriaga-Molina, C. & Clearfield, A. (1986). *J. Phys. Chem.* **90**, 6122–6125.

Shoemaker, D. P., Robson, H. E. & Broussard, L. (1973). *Proceedings of the Third International Conference on Molecular Sieves*, edited by J. B. Uytterhoeven, pp. 138–143, Zürich, Switzerland. Leuven University Press, Belgium.

Smith, J. V. (1979). *Am. Mineral.* **64**, 551–562.