Acta Cryst. (1999). A**55**, 332–341

Enumeration of four-connected three-dimensional nets. I. Conversion of all edges of simple three-connected two-dimensional nets into crankshaft chains

Shaoxu Han and Joseph V. Smith*

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

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

Abstract

Various topological approaches to mathematical analysis, classification and enumeration of four-connected three-dimensional (3D) nets are listed. Four-connected 3D nets are being generated systematically by conversion of edges of a vertical stack of congruent three-connected two-dimensional (2D) nets into chains. This paper describes 57 3D nets obtained by converting into crankshaft chains all edges of the simpler 2D nets in the catalog of the Consortium of Theoretical Frameworks. Atomic coordinates are given for distance-least-squares modeling in the highest space group. Nine nets occur in known structures: tridymite, $Zn_2P_2O_8 \cdot$ organic, aluminophosphates AlPO-5 (International Zeolite Association Structure Commission code AFI), AlPO-8 (AEI), AlPO-11 (AEL), AlPO-25 (ATV), AlPO-41 (AFO), AlPO-54 (VFI) and AlPO-H2 (AHT).

1. Introduction

Decomposition of four-connected three-dimensional (3D) nets in frameworks of known structures into subunits [3D polyhedra and cages; two-dimensional (2D) nets and layers; one-dimensional (1D) chains and columns] allows topochemical classification using mathematical principles (Smith, 1988, 1999). This introduction is deliberately concise. Many concepts and details are given by O'Keeffe & Hyde (1996). A comprehensive bibliography is available privately from JVS.

Comparison of subunits in phases that crystallize under similar conditions allows speculation on crystallization mechanisms that can be tested by observation of stacking faults, twin mechanisms and other growth indicators (Smith & Andries, 1993). Many natural and synthetic framework structures have been solved by (*a*) assembling subunits into new four-connected 3D nets, (*b*) comparing the highest space group, cell dimensions and calculated powder diffraction pattern for optimized geometry of the theoretical nets with experimental data for unknown structures, and (*c*) testing potential matches by structure refinement. Theoretical nets, as yet unrepresented in known materials, provide potential targets for synthesis of phases with interesting properties.

The Consortium of Theoretical Frameworks (CTF) at the University of Chicago maintains systematic databases of subunits invented from the decomposition of four-connected 3D nets in known framework structures and theoretical nets (Smith, 1989). This information has allowed recognition of geometrical similarities important for mineralogy and industrial chemistry, particularly for zeolites and other microporous materials. Perspective drawings and topological indexes are being published (Smith, 1999).

A single algorithm for derivation of the infinity of four-connected 3D nets is not known. A practical approach is (*a*) classify subunits from known structures into topological groups, (*b*) enumerate each topological group, and (*c*) assign all the subunits to an accessible unique position in a single database. The next step is (*a*) examine how the subunits are linked together in 3D nets of known structures, (*b*) use these linkage types to invent new four-connected 3D nets systematically from all known subunits, and (*c*) incorporate them into an active database of 3D nets and subunits. Assignment of a unique topogeometric signature, accessible by computer search, permits (*a*) rigorous search for nets and subunits with specific topological and geometric properties, and (*b*) identification of duplicates obtained from enumeration of different types of linkages.

New 3D nets built from known subunits and linkages reveal yet further subunits and types of linkages that extend the usefulness of the growing databases. By exploring new subunits and new types of linkages, more 3D nets will be enumerated. Is this an automatic procedure for generating the topogeometry of all four-connected nets? Are some nets inaccessible by this procedure, and discoverable only by random methods or solution of new crystal structures?

The current CTF catalog also contains 3D nets from known framework structures, including zeolites, clathrates, anhydrous silicates, borates *etc.*, together with theoretical nets enumerated by crystallographers at the University of Chicago. Each 3D net has a number assigned chronologically in the CTF catalog.

Systematic examination of theoretical nets published by other scientists is proceeding slowly, partly because of

ISSN 0108-7673 © 1999

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

Three-connected 2D net			Four-connected 3D net							
	Circuit symbol	CTF number	Circuit symbol (Wells)	Z_c	Highest space group	*a* (Å)	*b* (Å)	*c* (Å)	Space group for alternation	Structure type
hex	(6^3)	2	(6^6)	4	194($P6_3/mmc$)	5	5	8.5	186($P6_3mc$)	Tridymite
fee	(48^2)	39	(46^5)	16	140(*I4/mcm*)	10	10	8.5	108(*I4cm*)	$Zn_2P_2O_8$-organic
gml	(4.6.12)	81	(46^5)	24	192(*P6/mcc*)	13.5	13.5	8.5	184(*P6cc*)	AFI
ffs	$(4^210)_1(4.10^2)_2$	418	$(4^26^4)_1(46^5)_2$	24	63(*Ccmm*)	9.5	15	8.5	36($Ccm2_1$)	AHT
tth	$(4^212)_1(4.8.12)_2$	417	$(4^26^4)_1(46^5)_2$	48	140(*I4/mcm*)	18	18	8.5	108(*I4cm*)	
fos	$(4^212)_1(4.12^2)_1-a$	456	$(4^26^4)_1(46^5)_1$	32	72(*Ibam*)	9.5	21	8.5	45(*Iba2*)	
twy	$(4^212)_1(4.12^2)_1$-b	854	$(4^26^4)_1(46^5)_1$	48	192(*P6/mcc*)	18.5	18.5	8.5	184(*P6cc*)	
rho	$(4^216)_1(4.8.16)_1$	455	$(4^26^4)_1(46^5)_1$	32	124(*P4/mcc*)	15	15	8.5	103(*P4cc*)	
eoo	$(4^218)_1(4.6.18)_2$	520	$(4^26^4)_1(46^5)_2$	36	193($P6_3/mcm$)	18	18	8.5	185($P6_3cm$)	VFI
tsv	$(4^224)_1(4.6.24)_1$	531	$(4^26^4)_1(46^5)_1$	48	192(*P6/mcc*)	23	23	8.5	184(*P6cc*)	
ltl	$(468)_1(4.8.12)_1$	656	$(46^5)_1(46^5)_1$	48	192(*P6/mcc*)	18.5	18.5	8.5	184(*P6cc*)	
fsy	$(468)_1(6^28)_1$	657	$(46^5)_1(6^6)_1$	32	72(*Ibam*)	9.5	20	8.5	45(*Iba2*)	
brw	$(468)_2(68^2)_1$	651	$(46^5)_2(6^6)_1$	24	67(*Abmm*)	9.5	15	8.5	39(*Abm2*)	ATV
eee	$(4^28)_1(48^2)_2(8^3)_1$	701	$(4^26^4)_1(46^5)_2$ $(6^6)_1$	64	69(*Fmmm*)	15	24.5	8.5	42(*Fmm2*)	
twl	$(4^210)_1(4.6.10)_2$ $(6^210)_2$	702	$(4^26^4)_1(46^5)_2$ $(6^6)_2$	40	63(*Ccmm*)	9	26.5	8.5	36($Ccm2_1$)	
fsv	$(4^210)_1(4.6.10)_2$ $(6.10^2)_1$	703	$(4^26^4)_1(465)_2$ $(6^6)_1$	16	51(*Pcmm*)	9	10.5	8.5	26($Pcm2_1$)	
ttv	$(4^210)_1(4.8.10)_2$ $(4.8.10)_2$	532	$(4^26^4)_1(46^5)_2$ $(46^5)_2$	40	67(*Abmm*)	10	26	8.5	39(*Abm2*)	
ooo	$(4^210)_2(4.8.10)_2$ $(8^210)_1$	855	$(4^26^4)_2(46^5)_2$ $(6^6)_1$	40	67(*Bmcm*)	14	15	8.5	39(*Bma2*)	
ree	$(4^212)_1(4.6.12)_1$ $(4.12^2)_1$	715	$(4^26^4)_1(46^5)_1$ $(46^5)_1$	72	192(*P6/mcc*)	23	23	8.5	184(*P6cc*)	
fix	$(4^212)_1(4.6.12)_1$ $(6^212)_1$	856	$(4^26^4)_1(46^5)_1$ $(6^6)_1$	48	72(*Ibam*)	9	30.5	8.5	45(*Iba2*)	
toh	$(4^212)_2(4.6.12)_2$ $(6.12^2)_1$	857	$(4^26^4)_2(46^5)_2$ $(6^6)_1$	40	67(*Abmm*)	9	26	8.5	39(*Abm2*)	
vvv	$(4^212)_1(4.8.12)_1$ $(4.8.12)_1$	533	$(4^26^4)_1(46^5)_1$ $(46^5)_1$	24	49(*Pccm*)	10	15	8.5	27(*Pcc2*)	
krp	$(46^2)_1(4.6.12)_2$ $(6^212)_1$	343	$(46^5)_2(46^5)_1$ $(6^6)_1$	32	132($P4_2/mcm$)	14.5	14.5	8.5	101($P4_2cm$)	
wek	$(468)_3(48^2)_3$ $(8^3)_1$	344	$(46^5)_3(46^5)_3$ $(6^6)_1$	28	190($P\bar{6}2c$)	14	14	8.5	159(*P31c*)	
fto	$(468)_1(48^2)_1$ $(6^28)_1$	705	$(46^5)_1(46^5)_1$ $(6^6)_1$	24	57(*Pcam*)	9.5	15	8.5	29($Pca2_1$)	
ffv	$(468)_2(48^2)_2$ $(68^2)_1$	842	$(46^5)_2(46^5)_2$ $(6^6)_1$	40	63(*Ccmm*)	9.5	25.5	8.5	36($Ccm2_1$)	
apd	$(468)_1(6^3)_1$ $(6^28)_1$	706	$(46^5)_1(6^6)_1$ $(6^6)_1$	48	72(*Ibam*)	9.5	32	8.5	45(*Iba2*)	
feo	$(468)_2(6^3)_1$ $(6^28)_2$	707	$(46^5)_2(6^6)_2$ $(6^6)_1$	40	67(*Abmm*)	9.5	25.5	8.5	39(*Abm2*)	
ael	$(4.6.10)_2(4.6.10)_2$ $(6^210)_1$	263	$(46^5)_2(46^5)_2$ $(6^6)_1$	40	74(*Icmm*)	13.5	18.5	8.5	46(*Ibm2*)	AEL
ftf	$(4^210)_1(4^212)_2$ $(4.10.12)_2$ $(4.10.12)_2$	535	$(4^26^4)_2(4^26^4)_1$ $(46^5)_2(46^5)_2$	56	67(*Abmm*)	9.5	36	8.5	39(*Abm2*)	
fsf	$(4^210)_1(4.6.10)_1$ $(4.10^2)_1(6^210)_1$	708	$(4^26^4)_1(46^5)_1$ $(46^5)_1(6^6)_1$	32	57(*Pcam*)	9	21	8.5	29($Pca2_1$)	
ftn	$(4^210)_1(4.6.10)_2$ $(6^3)_1(6^210)_2$	709	$(4^26^4)_1(46^5)_2$ $(6^6)_2(6^6)_1$	24	51(*Pcmm*)	9	15.5	8.5	26($Pcm2_1$)	
vss	$(4^212)_1(468)_1$ $(4.6.12)_1(6.8.12)_1$	858	$(4^26^4)_1(46^5)_1$ $(46^5)_1(6^6)_1$		49(*Pccm*)	9	20	8.5	27(*Pcc2*)	
bsh	$(4^212)_1(4.6.12)_1$ $(6^3)_1(6^212)_1$	859	$(4^26^4)_1(46^5)_1$ $(6^6)_1(6^6)_1$	64	72(*Ibam*)	9.5	43	8.5	45(*Iba2*)	
ftu	$(4^214)_2(4^214)_1$ $(4.8.14)_2(4.8.14)_2$	534	$(4^26^4)_2(4^26^4)_1$ $(46^5)_2(46^5)_2$	56	67(*Abmm*)	15	25	8.5	39(*Abm2*)	
xfn	$(4^214)_1(4.6.14)_2$ $(4.6.14)_2(4.6.14)_2$	710	$(4^26^4)_1(46^5)_2$ $(46^5)_2(46^5)_2$	56	74(*Ibmm*)	14	30	8.5	46(*Ibm2*)	

Table 1 (*cont.*)

Three-connected 2D net			Four-connected 3D net							
	Circuit symbol	CTF number	Circuit symbol (Wells)	Z_c	Highest space group	*a* (Å)	*b* (Å)	*c* (Å)	Space group for alternation	Structure type
eop	$(4^214)_2(4.6.14)_2$ $(4.6.14)_2(6^214)_1$	345	$(4^26^4)_2(46^5)_2$ $(46^5)_2(6^6)_1$	56	63(*Ccmm*)	18	21	8.5	36(*Ccm*2$_1$)	
rnn	$(4^216)_1(4.6.16)_1$ $(4.6.16)_1(4.6.16)_1$	717	$(4^26^4)_1(46^5)_1$ $(46^5)_1(46^5)_1$	64	72(*Ibam*)	20	28	8.5	45(*Iba*2)	
uxx	$(46^2)_2(4.6.10)_2$ $(6^210)_2(6^210)_1$	741	$(46^5)_2(46^5)_2$ $(6^6)_2(6^6)_1$	56	63(*Ccmm*)	14	22.5	8.5	36(*Ccm*2$_1$)	
uii	$(46^2)_1(4.6.10)_2$ $(4.10^2)_1(6^210)_1$	736	$(46^5)_2(46^5)_1$ $(46^5)_1(6^6)_1$	40	63(*Cmcm*)	9.5	26	8.5	36(*Cmc*2$_1$)	AFO
uss	$(46^2)_1(4.6.12)_1$ $(4.6.12)_1(6^212)_1$	737	$(46^5)_1(46^5)_1$ $(46^5)_1(6^6)_1$	64	72(*Ibam*)	15	28	8.5	45(*Iba*2)	
bso	$(468)_1(468)_1$ $(48^2)_1(68^2)_1$	813	$(46^5)_1(46^5)_1$ $(46^5)_1(6^6)_1$	64	72(*Ibam*)	9.5	39	8.5	45(*Iba*2)	
tva	$(468)_2(48^2)_1$ $(48^2)_1(68^2)_1$	818	$(46^5)_2(46^5)_1$ $(46^5)_1(6^6)_1$	80	69(*Fmmm*)	15	31.5	8.5	42(*Fmm*2)	
stg	$(468)_2(48^2)_2$ $(48^2)_2(68^2)_1$	711	$(46^5)_2(46^5)_2$ $(46^5)_2(6^6)_1$	56	67(*Abmm*)	9	35	8.5	39(*Abm*2)	
fst	$(468)_1(48^2)_1$ $(6^3)_1(6^28)_1$	712	$(46^5)_1(46^5)_1$ $(6^6)_1(6^6)_1$	32	57(*Pcam*)	9.5	22.5	8.5	29(*Pca*2$_1$)	
fss	$(468)_2(6^3)_2$ $(6^3)_1(6^28)_2$	817	$(46^5)_2(6^6)_2$ $(6^6)_2(6^6)_1$	56	67(*Abmm*)	9	35	8.5	39(*Abm*2)	
knh	$(4^210)_2(468)_2$ $(4.8.10)_2(68^2)_1$ $(8^210)_1$	965	$(4^26^4)_2(46^5)_2$ $(46^5)_2(6^6)_1$ $(6^6)_1$	64	67(*Bmcm*)	15.5	24	8.5	39(*Bma*2)	
eig	$(4^210)_1(4.6.10)_2$ $(6^3)_2(6^3)_1$ $(6^210)_2$	816	$(4^26^4)_2(46^5)_1$ $(6^6)_2(6^6)_2$ $(6^6)_1$	32	51(*Pcmm*)	9	20.5	8.5	26(*Pcm*2$_1$)	
api	$(4^214)_1(46^2)_2$ $(4.6.14)_2(4.6.14)_2$ $(6^214)_2$	73	$(4^26^4)_1(46^5)_2$ $(46^5)_2(46^5)_2$ $(6^6)_2$	72	63(*Ccmm*)	15	33	8.5	36(*Ccm*2$_1$)	AET
rxx	$(46^2)_1(468)_1$ $(4.6.12)_1(4.8.12)_1$ $(6^212)_1$	716	$(46^5)_1(46^5)_1$ $(46^5)_1(46^5)_1$ $(6^6)_1$	80	72(*Ibam*)	18	27	8.5	45(*Iba*2)	
tvt	$(468)_2(468)_2$ $(6^3)_1(6^2$ $8)_2(68^2)_1$	713	$(46^5)_2(46^5)_2$ $(6^6)_2(6^6)_1$ $(6^6)_1$	32	51(*Pcmm*)	9	21	8.5	26(*Pcm*2$_1$)	
fsm	$(468)_2(6^3)_2$ $(6^3)_2(6^3)_1$ $(6^28)_2$	814	$(46^5)_2(6^6)_2$ $(6^6)_2(6^6)_2$ $(6^6)_1$	72	67(*Abmm*)	9	45	8.5	39(*Abm*2)	
kuu	$(4^210)_1(468)_1$ $(4.8.10)_1(4.8.10)_1$ $(4.10^2)_1(6^28)_1$	960	$(4^26^4)_1(46^5)_1$ $(46^5)_1(46^5)_1$ $(46^5)_1(6^6)_1$	48	57(*Pcam*)	10	31	8.5	29(*Pca*2$_1$)	
fui	$(4^210)_1(468)_1$ $(4.6.10)_1(4.8.10)_1$ $(4.8.10)_1(6^28)_1$ $(6^210)_1$	714	$(4^26^4)_1(46^5)_1$ $(46^5)_1(46^5)_1$ $(46^5)_1(6^6)_1$ $(6^6)_1$	56	39(*Ac*2*m*)	9.5	37	8.5	7(*Pc*11) [half-cell]	
oxx	$(46^2)_2(46^2)_1$ $(4.6.10)_2$ $(4.6.12)_2(4.6.12)_2$ $(4.12^2)_1(6^210)_2$ $(6^210)_1$	740	$(46^5)_2(46^5)_2$ $(46^5)_2(46^5)_2$ $(46^5)_1(46^5)_1$ $(6^6)_2(6^6)_1$	104	67(*Bmam*)	25	27	8.5	39(*Bma*2)	
oss	$(46^2)_2(46^2)_1$ $(4.6.12)_2(4.6.12)_2$ $(4.12^2)_1(6^28)_2$ $(6^28)_1(6^28)_1$	739	$(46^5)_2(46^5)_2$ $(46^5)_2(46^5)_1$ $(46^5)_1(6^6)_2$ $(6^6)_1(6^6)_1$	192	69(*Fmmm*)	23	47	8.5	42(*Fmm*2)	
hsc	$(46^2)_1(46^2)_1$ $(46^2)_1(4.6.12)_1$ $(4.6.12)_1(4.6.12)_1$ $(6^212)_1(6^2$ $12)_1(6^212)_1$	815	$(46^5)_1(46^5)_1$ $(46^5)_1(46^5)_1$ $(46^5)_1(46^5)_1$ $(6^6)_1(6^6)_1$ $(6^6)_1$	108	190($P\bar{6}2c$)	27	27	8.5	159(*P*31*c*)	

inadequate documentation. The computer outputs for thousands of nets obtained by random-search procedures have not been analyzed systematically for the subunits required for entry into the CTF databases. Currently, the subunits of a 3D net are identified by visual inspection of a model or stereoview, a procedure which commonly requires at least 1 h by a skilled mathematician. To handle the thousands of theoretical nets in the computer databases, computer-compatible search algorithms are desirable.

Because most of the 3D nets in known structures are based on simple subunits and linkages, or a simple combination thereof, theoretical nets with high complexity are not entered into the CTF databases but stored separately.

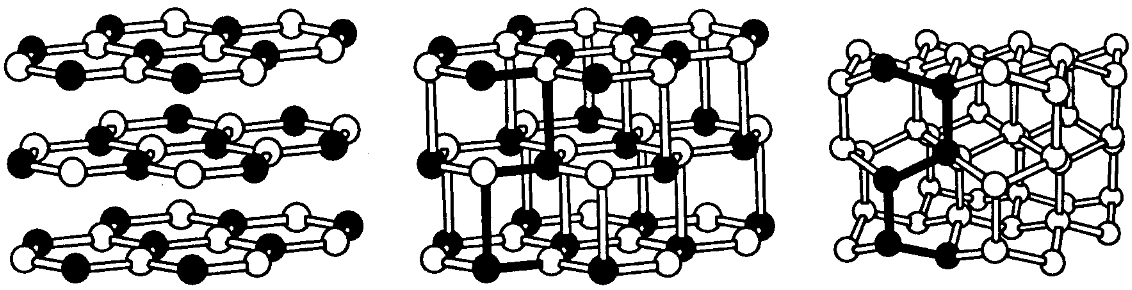
For each 3D net with an idealized geometry, its atomic coordinates can be refined by distance-least-squares (DLS) modeling (Baerlocher *et al.*, 1977). (Coordinates are not available yet for some early nets listed only in the CTF databases.) Because the cell dimensions of isostructural materials depend on the bond distances and angles for individual chemical elements, standard reference values are taken near the middle of the ranges for zeolites and related materials: T(tetrahedral atom)—O = 1.63 Å and O—T—O = 147°. For pure silica variants, reduce the cell edges by ~1.61/1.63 = 0.988. For $Al_{0.5}Si_{0.5}$, increase the edges by ~1.67/1.63 = 1.025. The T—O—T angles in framework structures vary from ~125 to 180°, with median values for individual structures ranging from ~140 to ~155°. New DLS calculations for extreme values of ~137 and 157° may be advisable when search-matching for an unusual chemical composition.

The first step in systematizing the CTF *Catalog of Nets* is enumeration of the combinations of three-connected 2D nets and chains to update the opportunistic pioneering studies begun by Smith and his colleagues two decades ago. Their work includes many 3D frameworks enumerated from simple 2D nets, such as *hex* (6^3), *ttw* (3.12^2), *fee* (48^2), *gml* (4.6.12), *bik* $(5^28)_2(58^2)_1$ and *ael* $(4.6.10)_2(4.6.10)_2(6^210)_1$, with the insertion of simple chains, such as *c* (crankshaft), *z* (zigzag) and *s* (saw), or combination of two types of chains (Smith, 1977, 1978, 1979, 1983; Smith & Bennett, 1984; Smith & Dytrych, 1984, 1986; Bennett & Smith, 1985; Hawthorne & Smith, 1986, 1988).

A three-connected 2D net can be labeled by a three-letter code and a numerical code (columns 1 and 2 of Table 1). The numerical code specifies the connectivity at a vertex [three six-rings for *hex* (6^3); one four-ring and two eight-rings for *fee* (48^2); two types of vertices for *ffs* $(4^210)_1(4.10^2)_2$ with multiplicity as a subscript]. Each three-letter italic code is an arbitrary identification that is searchable uniquely in the computer databases. Some codes refer to a property of a net or a material containing the net: *hex* for the hexagonal net, *fee* for *f*our–*e*ight–*e*ight, *gml* for the mineral gmelinite, *bik* for bikitaite, *ael* for synthetic AlPO-11. The arbitrary single letter for a chain typically refers to a property.

This paper lists those four-connected 3D nets obtained from a vertical stack of congruent horizontal (*h*) three-connected 2D nets from the CTF database by conversion of *all* edges into a crankshaft (*c*) chain perpendicular to the 2D net; note the emphasis on *all*. The fourth linkage connects to a vertex from an adjacent 2D net either directly above or below. These fourth linkages must alternate upwards and downwards around each horizontal ring. The regular alternation of up- and down-linkages enforces the generation of only one 3D net from each 2D net. The new edge remains vertical in the distance-least-squares modeling, whereas the original horizontal edges become tilted. The combination of vertical and tilted edges generates a crankshaft geometry for the vertical chain generated from each horizontal edge (Fig. 1). The series of crankshaft nets is specified as *c**-(three-symbol 2D net). Examples for simple 2D nets are given by Smith (1977, 1978).

Allowing some edges to remain unconverted for a particular 2D net would permit an infinity of 3D nets with more complex topology, *e.g.* the infinite (*c*, *h*)**hex* series in which only some edges (*c*) of the *hex* 6^3 2D net become incorporated into a crankshaft net, whereas the other edges (*h*) do not. The surviving *h* edges may become tilted slightly during the DLS modeling, but remain essentially horizontal (Smith, 1977; update in draft).



(*a*) (*b*) (*c*)

Fig. 1. Procedure for generation of crankshaft chains. (*a*) A vertical stack of three-connected 2D *hex* nets (6^3). Dots and circles indicate opposite directions of vertical linkages added later. (*b*) Alternate vertices (dot and circle) from (*a*) are joined by a vertical edge to generate a four-connected 3D net which has 90° angles between the vertical edge and the three horizontal edges. (*c*) 3D net after the *DLS* refinement. The original horizontal edges from the three-connected 2D net are tilted to produce a tetrahedral or near-tetrahedral geometry. This represents the structure of tridymite (net 2).

Subsequent papers in this series cover zigzag and other chains. Because these chains cannot share vertices like the crankshaft chain, some edges of a vertical stack of congruent horizontal 2D nets cannot be cross-linked into a vertical chain. Hence, these series of nets must be specified as (*h*, *z*) *etc*.

2. Procedure

Conversion of *all* edges of a vertical stack of congruent three-connected 2D nets into a *c*-chain requires that each ring in a 2D net is even to generate closure of the up–down vertical cross-linkages between adjacent horizontal nets. Elimination of odd rings leaves 63 of the 131 2D nets in the CTF database (Pluth & Smith, 1993). Six of the 63 2D nets were omitted because either four or five adjacent four-rings share edges and the resultant 3D nets would have geometrical relations rather unlikely for actual crystal structures. Because each resultant 3D net corresponds to only one specific 2D net, 57 3D nets were generated.

Fig. 2 shows the projection of four out of the nine known structures with their International Zeolite Association Structure Commission (IZA-SC) codes AET, AFO, AHT and ATV (Meier *et al.*, 1996), and dots and circles in the projections distinguish between the up- and down-linkages. The other five 3D nets present in known structures were described in the early publications by Smith and co-workers: net 2 (Smith, 1977), net 81 (Smith, 1978), net 520 (Smith & Dytrych, 1984) and net 263 (Bennett & Smith, 1985). Net 39, first proposed by Smith & Rinaldi (1962), occurs in the framework of new compound $Zn_2P_2O_8 \cdot$ organic (Jones *et al.*, 1994). The parent 2D nets for these five 3D nets (*hex* → tridymite; *fee* → $Zn_2P_2O_8 \cdot$ organic; *gml* → AFI; *eoo* → VFI; *ael* → AEL) are illustrated by Pluth & Smith (1993).

Table 1, arranged in order of increasing complexity of the 2D nets, gives the three-letter acronym and circuit symbol of the parent 2D net, the CTF chronological number of the resultant 3D net, together with its circuit symbol (Wells definition; Appendix in Smith, 1978), number of four-connected vertices in the unit cell (Z_c), highest space group and cell dimensions. The space group is also given for the same 3D net assuming an alternation of chemical occupancy of the vertices, as in the $AlPO_4$ molecular sieves. The alternation destroys the horizontal mirror planes that bisect the vertical bonds in the crankshaft chains in the neutral net. The

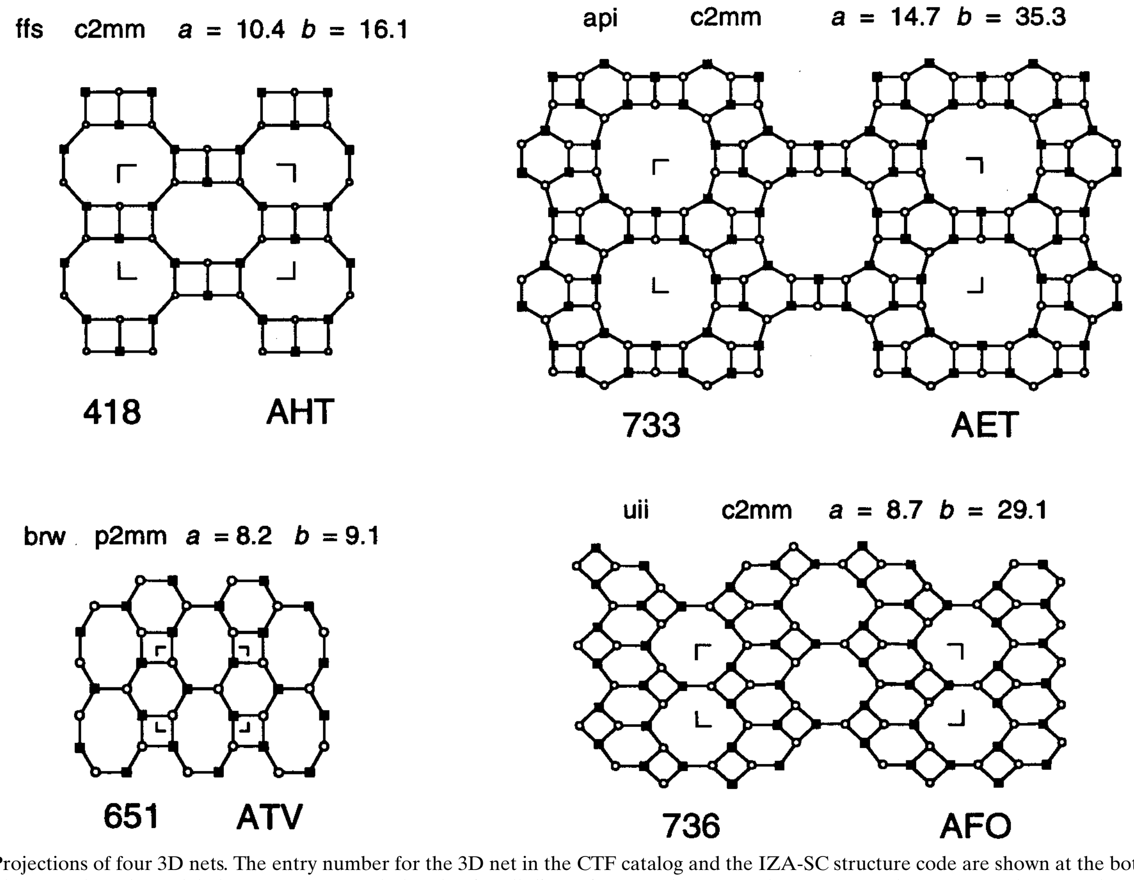


Fig. 2. Projections of four 3D nets. The entry number for the 3D net in the CTF catalog and the IZA-SC structure code are shown at the bottom, and the CTF three-letter label, space-group symbol and unit-cell dimensions for the parent three-connected 2D net are shown at the top.

Table 2. *Alternative topological description, subunits and pore space of regular 3D nets obtained by conversion of each edge of a parallel stack of three-connected nets into a crankshaft chain*

CTF no.	Rings providing access to pores	1D subunits including chains, columns and tubes	2D three-connected nets	3D polyhedra and cages (*sensu lato*)	Pores, channels and access
2	6	afv, c, kbg, keg, lao, z	*hex* (two types)	afi, kah, kyw	afi cages *via* crown- and rocker-6
39	4, 6, 8	bhs, c, ecc, kbg, kbn, keg	*fee*, *hex*	bog, kah, loh, lov, oop	1D-channel-circular-crown-8
81	4, 6, 12	afv, ave, bhs, c, kbg, kbn, keg	*gml*, *hex*	afi, apf, bog, kah, kyw, loh, lov	1D-channel-circular-crown-12
418	4, 6, 10	ape, bhs, c, kbg, kbn, keg, ktv, vfi	*ffs*, *hex* (two types)	bog, kah, ktw, loh, lov, odp	1D-channel-elliptical-crown-10
417	4, 6, 8, 12	ave, bhs, c, ecc, kbg, kbn, keg, ktv, vfi	*hex*, *tth*	apf, bog, kah, ktw, loh, lov, oop	1D-channel-square-crown-12; 1D-channel-circular-crown-8
456	4, 6, 12	ave, bhs, c, kbg, keg, vfi	*fos*, *hex* (two types)	apf, bog, kah, loh, lov	1D-channel-elliptical-crown-12
854	4, 6, 12	ave, bhs, c, kbg, keg, vfi	*hex*, *twy*	apf, bog, kah, loh, lov	1D-channel-triangular-crown-12
455	4, 6, 8, 16	bhs, c, ecc, kbg, keg, oii, vfi	*hex*, *rho*	bog, kah, loh, lov, oin, oop	1D-channel-square-crown-16; 1D-channel-circular-crown-8
520	4, 6, 18	afv, bhs, c, kbg, keg, ktv, vfi, yee	*eoo*, *hex*	afi, bog, kah, ktw, kup, kyw, loh, lov	1D-channel-nearcircular-crown-18
531	4, 6, 24	afv, bhs, c, ctf, kbg, keg, vfi	*hex*, *tsv*	afi, bog, kah, jtf, kyw, loh, lov	1D-channel-circular-crown-24
656	4, 6, 8, 12	afv, ave, bhs, c, ecc, kbg, kbn, keg	*hex*, *ltl*	afi, apf, bog, kah, kyw, loh, lov, oop	1D-channel-circular-crown-12; 1D-channel-elliptical-crown-8
657	4, 6, 8	afv, bhs, c, ecc, kbg, kbn, keg	*fsy*, *hex* (two types)	afi, bog, kah, kyw, loh, lov, oop	1D-channel-elliptical-crown-8
651	4, 6, 8	afv, bhs, c, ecc, kbg, kbn, keg	*brw*, *hex* (two types)	afi, bog, kah, kyw, loh, lov, oop	1D-channel-elliptical-crown-8
701	4, 6, 8	bhs, c, ecc, kbg, keg, ktv, vfi	*eee*, *hex* (two types)	bog, kah, ktw, loh, lov, oop	1D-channel-nearcircular-crown-8; 1D-channel-elliptical-crown-8
702	4, 6, 10	afv, ape, bhs, c, kbg, keg, ktv, vfi	*hex* (two types), *twl*	afi, bog, kah, ktw, kyw, loh, lov, odp	1D-channel-elliptical-crown-10
703	4, 6, 10	afv, ape, bhs, c, kbg, keg, ktv, vfi	*fsv*, *hex* (two types)	afi, bog, kah, ktw, kyw, loh, lov, odp	1D-channel-elliptical-crown-10
532	4, 6, 8, 10	ape, bhs, c, ecc, kbg, keg, ktv, vfi	*hex* (two types), *ttv*	bog, kah, ktw, loh, lov, odp, oop	1D-channel-elliptical-crown-10; 1D-channel-circular-crown-8
855	4, 6, 8, 10	ape, bhs, c, ecc, kbg, keg, vfi	*hex* (two types), *ooo*	bog, kah, loh, lov, odp, oop	1D-channel-elliptical-crown-10; 1D-channel-circular-crown-8
715	4, 6, 12	afv, ave, bhs, c, kbg, keg, ktv, vfi	*hex*, *ree*	afi, apf, bog, kah, ktw, kyw, loh, lov	1D-channels-circular- and elliptical-crown-12
856	4, 6, 12	afv, ave, bhs, c, kbg, keg, vfi	*fix*, *hex* (two types)	afi, apf, bog, kah, kyw, loh, lov	1D-channel-elliptical-crown-12
857	4, 6, 12	afv, ave, bhs, c, kbg, keg, vfi	*hex* (two types), *toh*	afi, apf, bog, kah, kyw, loh, lov	1D-channel-elliptical-crown-12
533	4, 6, 8, 12	afv, ave, bhs, c, ecc, kbg, kbn, keg, vfi	*hex* (two types), *vvv*	afi, apf, bog, kah, loh, lov, oop	1D-channel-elliptical-crown-12; 1D-channel-nearcircular-crown-8
343	4, 6, 12	afv, ave, bhs, c, kbg, kbn, keg	*hex*, *krp*	afi, apf, bog, kah, kyw, loh, lov	1D-channel-nearcircular-crown-12
344	4, 6, 8	afv, bhs, c, ecc, kbg, kbn, keg	*hex*, *wek*	afi, bog, kah, kyw, loh, lov, oop	1D-channel-elliptical-crown-8
705	4, 6, 8	afv, bhs, c, ecc, kbg, kbn, keg	*fto*, *hex* (two types)	afi, bog, kah, kyw, loh, lov, oop	1D-channel-elliptical-crown-8
842	4, 6, 8	afv, bhs, c, ecc, kbg, kbn, keg	*ffv*, *hex* (two types)	afi, bog, kah, kyw, loh, lov, oop	1D-channel-nearcircular-crown-8
706	4, 6, 8	afv, bhs, c, ecc, kbg, kbn, keg	*apd*, *hex* (two types)	afi, bog, kah, kyw, loh, lov, oop	1D-channel-elliptical-crown-8
707	4, 6, 8	afv, bhs, c, ecc, kbg, kbn, keg	*feo*, *hex* (two types)	afi, bog, kah, kyw, loh, lov, oop	1D-channel-elliptical-crown-8
263	4, 6, 10	afv, ape, bhs, c, kbg, kbn, keg	*ael*, *hex* (two types)	afi, bog, kah, kyw, loh, lov, odp	1D-channel-elliptical-crown-10
535	4, 6, 10, 12	afv, ape, ave, bhs, c, kbg, keg, ktv, vfi	*ftf*, *hex* (two types)	afi, apf, bog, kah, ktw, loh, lov, odp	1D-channel-elliptical-crown-12; 1D-channel-elliptical-crown-10

Table 2 (*cont.*)

CTF no.	Rings providing access to pores	1D subunits including chains, columns and tubes	2D three-connected nets	3D polyhedra and cages (*sensu lato*)	Pores, channels and access
708	4, 6, 10	afv, ape, bhs, c, kbg, keg, ktv, vfi	*fsf*, *hex* (two types)	afi, bog, kah, ktw, kyw, loh, lov, odp	1D-channel-elliptical-crown-10
709	4, 6, 10	afv, ape, bhs, c, kbg, keg, ktv, vfi	*ftn*, *hex* (two types)	afi, bog, kah, ktw, kyw, loh, lov, odp	1D-channel-elliptical-crown-10
858	4, 6, 8, 12	afv, ave, bhs, c, ecc, kbg, kbn, keg, vfi	*hex* (two types), *vss*	afi, apf, bog, kah, kyw, loh, lov, oop	1D-channel-elliptical-crown-12; 1D-channel-elliptical-crown-8
859	4, 6, 12	afv, ave, bhs, c, kbg, keg, vfi	*bsh*, *hex* (two types)	afi, apf, bog, kah, kyw, loh, lov	1D-channel-elliptical-crown-12
534	4, 6, 8, 14	bhs, c, ecc, kbg, keg, ktv, vfi, vtn	*ftu*, *hex* (two types)	bog, etn, kah, ktw, loh, lov, oop	1D-channel-rectangular-crown-14; 1D-circular-crown-8
710	4, 6, 14	afv, bhs, c, kbg, kbn, keg, ktv, vfi, vtn	*hex* (two types), *xfn*	afi, bog, etn, kah, ktw, kyw, loh, lov	1D-channel-elliptical-crown-14
345	4, 6, 14	afv, bhs, c, kbg, keg, ktv, vfi, vtn	*eop*, *hex*	afi, bog, etn, kah, ktw, kyw, loh, lov	1D-channel-elliptical-crown-8
717	4, 6, 16	afv, bhs, c, kbg, kbn, keg, ktv, oii, vfi	*hex* (two types), *rnn*	afi, bog, kah, ktw, kyw, loh, lov, oin	1D-channel-elliptical-crown-16
741	4, 6, 10	afv, ape, bhs, c, kbg, kbn, keg	*hex* (two types), *uxx*	afi, bog, kah, kyw, loh, lov, odp	1D-channel-elliptical-crown-10
736	4, 6, 10	afv, ape, bhs, c, kbg, kbn, keg	*hex* (two types), *uii*	afi, bog, kah, kyw, loh, lov, odp	1D-channel-elliptical-crown-10
737	4, 6, 12	afv, ave, bhs, c, kbg, kbn, keg	*hex* (two types), *uss*	afi, apf, bog, kah, kyw, loh, lov	1D-channel-elliptical-crown-12
813	4, 6, 8	afv, bhs, c, ecc, kbg, kbn, keg	*bso*, *hex* (two types)	afi, bog, kah, kyw, loh, lov, oop	1D-channel-nearcircular-crown-8 (two types)
818	4, 6, 8	afv, bhs, c, ecc, kbg, kbn, keg	*hex* (two types), *tva*	afi, bog, kah, kyw, loh, lov, oop	1D-channel-circular-crown-8
711	4, 6, 8	afv, bhs, c, ecc, kbg, kbn, keg	*hex* (two types), *stg*	afi, bog, kah, kyw, loh, lov, oop	1D-channel-near circular-crown-8 (two types)
712	4, 6, 8	afv, bhs, c, ecc, kbg, kbn, keg	*fst*, *hex* (two types)	afi, bog, kah, kyw, loh, lov, oop	1D-channel-nearcircular-crown-8
817	4, 6, 8	afv, bhs, c, ecc, kbg, kbn, keg	*fss*, *hex* (two types)	afi, bog, kah, kyw, loh, lov, oop	1D-channel-elliptical-crown-8
965	4, 6, 8, 10	afv, ape, bhs, c, ecc, kbg, kbn, keg, vfi	*hex*, *knh*	afi, bog, kah, kyw, loh, lov, odp, oop	1D-channels-elliptical-crown-10 & -8
816	4, 6, 10	afv, ape, bhs, c, kbg, keg, ktv, vfi	*eig*, *hex* (two types)	afi, bog, kah, ktw, kyw, loh, lov, odp	1D-channel-elliptical-crown-10
733	4, 6, 14	afv, bhs, c, kbg, kbn, keg, ktv, vfi, vtn	*api*, *hex* (two types)	afi, bog, etn, kah, ktw, kyw, loh, lov	1D-channel-elliptical-crown-14
716	4, 6, 8, 12	afv, ave, bhs, c, ecc, kbg, kbn, keg	*hex* (two types), *rxx*	afi, apf, bog, kah, kyw, loh, lov, oop	1D-channel-nearcircular-crown-12; 1D-channel-elliptical-crown-8
713	4, 6, 8	afv, bhs, c, ecc, kbg, kbn, keg	*hex* (two types), *tvt*	afi, bog, kah, kyw, loh, lov, oop	1D-channel-elliptical-crown-8
814	4, 6, 8	afv, bhs, c, ecc, kbg, kbn, keg	*fsm*, *hex* (two types)	afi, bog, kah, kyw, loh, lov, oop	1D-channel-elliptical-crown-8
960	4, 6, 8, 10	afv, ape, bhs, c, ecc, kbg, kbn, keg, ktv, vfi	*kuu*, *hex*	afi, bog, kah, ktw, kyw, loh, lov, odp, oop	1D-channel-elliptical-crown-10 & -8
714	4, 6, 8, 10	afv, ape, bhs, c, ecc, kbg, kbn, keg, ktv, vfi	*fui*, *hex* (two types)	afi, bog, kah, ktw, kyw, loh, lov, odp, oop	1D-channel-elliptical-crown-10; 1D-channel-elliptical-crown-8
740	4, 6, 10, 12	afv, ape, ave, bhs, c, kbg, kbn, keg	*hex* (two types), *oxx*	afi, apf, bog, kah, kyw, loh, lov, odp	1D-channel-elliptical-crown-12; 1D-channel-nearcircular-crown-10
739	4, 6, 8, 12	afv, ave, bhs, c, ecc, kbg, kbn, keg	*hex* (two types), *oss*	afi, apf, bog, kah, kyw, loh, lov, oop	1D-channel-elliptical-crown-12 and -8
815	4, 6, 12	afv, ave, bhs, c, kbg, kbn, keg	*hex* (two types), *hsc*	afi, apf, bog, kah, kyw, loh, lov	1D-channel-triangular-crown-12

final column of Table 1 indicates the structure type of nine known phases.

Table 2 gives the topological properties of the 3D nets. Access to the pores is specified by the order of the rings which act as windows. Subunits in the CTF databases are listed in Table 2 by alphabetical codes which are keyed to the drawings of the 1D subunits (Fig. 3; chains, columns and tubes) and 3D polyhedra and cages (Fig. 4). In addition to being the parent 2D net of the tridymite 3D net, the *hex* net is also present in a vertical plane of every 3D net simply because of the strict up-and-down alternation. The final column of Table 2 specifies the nature of the pores and channels.

3. Solution of unknown structures

The simplest way to use theoretical nets in the solution of unknown structures is to compare cell dimensions and space-group symmetry, bearing in mind the likelihood of geometrical distortion caused by specifics of chemical bonding. Ideally, a single crystal is available from which the cell geometry and symmetry can be obtained rigorously by X-ray or electron diffraction techniques. As a practical matter, it is desirable to heat the sample to check whether there is a structural transition to a high-temperature phase of higher symmetry. Also it may be desirable to exchange ions of high ionic potential with weaker ions incapable of making significant distortion of the framework.

Structure determinations of fine-grained zeolites often depend on model building and interpretation of powder diffraction data [see the review by McCusker (1994)]. Sometimes an unknown structure can be solved by successively matching its experimental powder pattern with the calculated powder patterns of theoretical nets. Atomic coordinates and other structural parameters after refinement then provide a quantitative criterion of the significance of the match.

4. DLS refinement and significance of the cell geometry and symmetry

In performing distance-least-squares refinement of a hypothetical TO_2 crystal structure corresponding to a theoretical net, the initial x and y coordinates of atoms for each 3D net were determined from drawings of the 2D nets, and the z coordinates were determined from examination of a plastic star-tube 3D model. 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 five-figure numbers merely result from assuming T—O—T = 147°). Using the *DLS* program (Baerlocher *et al.*, 1977), unit-cell parameters and atomic coordinates for each 3D net were refined (Table 3†). Values for net 815 are omitted because the highly distorted structure led to a high residual and structurally meaningless coordinates.

† Table 3 has been deposited and is available from the IUCr electronic archives (Reference: BR0075). Services for accessing these data are described at the back of the journal.

The powder-diffraction patterns of the hypothetical structures were calculated from the refined coordinates using the *POWD* program (Smith & Smith, 1986). The calculated powder patterns for nets in known structures agree reasonably with those of simulated powder patterns from known structures by von Ballmoos & Higgins (1990), taking into account slightly different control parameters.

Cell dimensions were originally measured with a ruler from a model built from plastic stars and 3.1 cm tubes. Changes up to 10% resulted from the *DLS* calculations, partly because the angles in the star-tube models differ considerably from the target values in the *DLS* program. Hence, 10% might be a reasonable tolerance when attempting to match cell dimensions for an unknown structure with *DLS* values for hypothetical nets.

The actual symmetry of a framework structure is commonly lower than the topologic symmetry of its four-connected net because of some chemical perturbation (*e.g.* alternation of T atoms), crinkling of the framework or both. However, it must be a possible subgroup of the highest space group of the theoretical net.

5. Topology

To satisfy the strict alternation of up–down sequence in the enumeration, only the 2D nets with even-numbered rings were used. Because the combination of those 2D nets with the crankshaft chain produce only six-rings in the third direction, odd-numbered rings are absent.

5.1. *1D and 2D subunits*

Besides the crankshaft chain there are 16 other 1D subunits, including *afv*, *bhs*, *ecc*, *ape*, *ave* and *vfi* (Fig. 3). Each 1D subunit is generated by converting each edge of a ring from a 2D net into a crankshaft chain. Some chains are highlighted with thick lines in Fig. 3, using figures from Andries & Smith (1993*b*) as a basis. Each 3D net has two types of three-connected 2D net. One is the horizontal parent 2D net perpendicular to the crankshaft chain. The other is the 2D *hex* net, parallel to the chain, whose six-rings are the consequence of the combination of the 2D net with the crankshaft chain. Some 3D nets contain two types of *hex* net along directions perpendicular to the 2D net.

5.2. *Polyhedral subunits*

Fig. 4 shows 13 polyhedral subunits copied from Andries & Smith (1993*a*); only *jtf* is not drawn. Six units occur frequently. The *bog* unit, 4^26^4-*b*, a 1,3-handle cube (Andries & Smith, 1994) in which the 1 and 3 edges are replaced by handles, occurs in the mineral boggsite (Pluth & Smith, 1990). The *loh* unit, $4^26^26^1$, is a 1-open, 3-handle cube. The *lov* unit, 4^26^2, a 1,3-open cube, is a subunit of both the *bog* and *loh* units, and occurs in $AlPO_4$-11, $AlPO_4$-8, $AlPO_4$-5, BOG, VPI-5, lovdarite, laumontite, feldspar and banalsite. The *afi* unit, 6^36^2, is a 1,3,5-open hexagonal prism. The *oop* unit, 6^48^2, is a

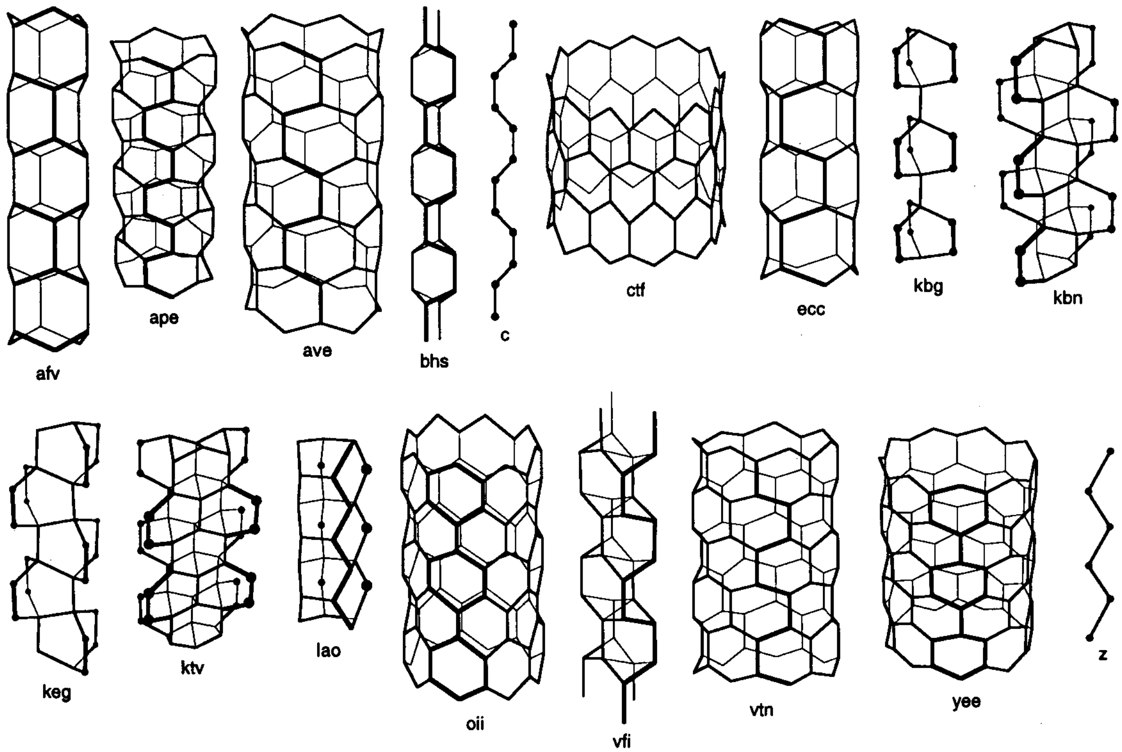


Fig. 3. 1D subunits with CTF label. Each unit is infinite in the vertical direction.

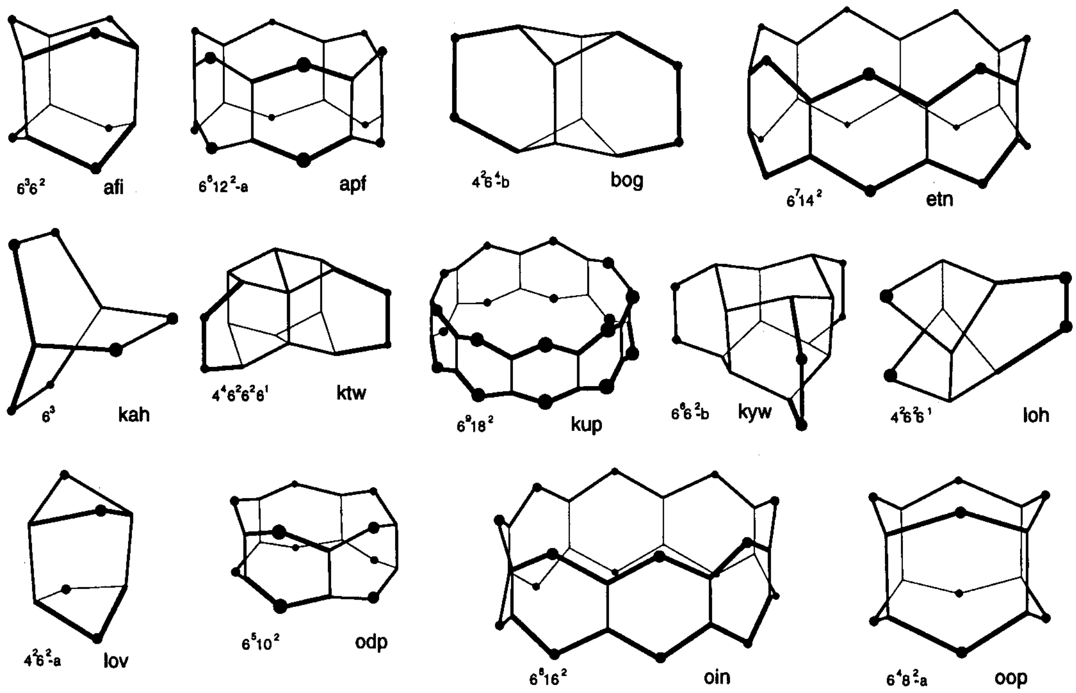


Fig. 4. Polyhedral units with CTF label and face symbol (*e.g. ktw* has four symmetrically equivalent four-rings, two types of pairs of six-rings, and a single six-ring at the back). [*jtf* is given by Smith (1999).]

1,3,5,7-open octagonal prism. The *kah* unit, 6^3, consists of two vertices joined by three handles.

5.3. *Channel system*

All the 3D nets have a 1D channel system because each ring of the parent 2D net combines with the crankshaft chain to generate a channel wall of six-rings parallel to the crankshaft. The large 10, 12, 14, 16 and 18 rings span wide channels of potential significance for molecular sieves.

6. Conclusions

Systematic conversion of all edges of three-connected 2D nets into a crankshaft chain generated 57 3D nets, some of which have large 1D cylindrical channels. The alternation of up and down linkages in these all-crankshaft nets allows considerable geometrical flexibility compared to many other types of frameworks to be presented in later papers. This may be one reason why crankshaft chains are common in known framework structures. Any unknown phase with one cell constant between 8 and 10 Å is worth consideration as a potential member of the all-crankshaft group.

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 Andries and Joseph J. Pluth generated the original graphics of most subunits in the CTF databases. Koen Andries and James W. Richardson Jr assisted with the *DLS* and *POWD* programs. The detailed advice of the Associate Editor was invaluable in clarifying mathematical matters that had become too facile to us.

References

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

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

Andries, K. J. & Smith, J. V. (1994). *Proc. R. Soc. London Ser. A*, **444**, 217–238.

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.

Ballmoos, R. von & Higgins, J. B. (1990). *Collection of Simulated XRD Powder Patterns for Zeolites.* Guildford: Butterworths.

Bennett, J. M. & Smith, J. V. (1985). *Z. Kristallogr.* **171**, 65–68.

Hawthorne, F. C. & Smith, J. V. (1986). *Z. Kristallogr.* **175**, 15–30.

Hawthorne, F. C. & Smith, J. V. (1988). *Z. Kristallogr.* **183**, 213–231.

Jones, R. H., Chen, J., Sankar, G. & Thomas, J. M. (1994). *Zeolites and Related Microporous Materials: State of the Art*, edited by J. Weitkamp, H. G. Pfeifer & W. Holderich, pp. 2229–2236. Amsterdam: Elsevier.

McCusker, L. B. (1994). *Stud. Surf. Sci Catal.* **84**, 341–355.

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

O'Keeffe, M. & Hyde, B. G. (1996). *Crystal Structures. I. Patterns and Symmetry.* Washington, DC: Mineralogical Society of America.

Pluth, J. J. & Smith, J. V. (1990). *Am. Mineral.* **75**, 501–507.

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

Smith, D. K. & Smith, K. L. (1986). *POWD. A Fortran-77 Program for Calculating X-ray Powder Diffraction Patterns.* Pennsylvania State University, University Park, Pennsylvania, USA.

Smith, J. V. (1977). *Am. Mineral.* **62**, 703–709.

Smith, J. V. (1978). *Am. Mineral.* **63**, 960–969.

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

Smith, J. V. (1983). *Z. Kristallogr.* **165**, 191–198.

Smith, J. V. (1988). *Chem. Rev.* **88**, 149–182.

Smith, J. V. (1989). *Zeolites: Facts, Figures, Future*, edited by P. A. Jacobs & R. van Santen, pp. 29–47. Amsterdam: Elsevier.

Smith, J. V. (1999). *Tetrahedral Frameworks of Zeolites and Other Microporous Materials*, in Landolt-Börnstein, Vol. III/14*a*, *Zeolites*, edited by W. H. Baur & R. Fischer. Berlin: Springer-Verlag. In the press.

Smith, J. V. & Andries, K. J. (1993). Am. Crystallogr. Assoc. Meet., Albuquerque, Abstract PA26.

Smith, J. V. & Bennett, J. M. (1984). *Proc. Am. Mineral.* **69**, 104–111.

Smith, J. V. & Dytrych, W. J. (1984). *Nature (London)*, **309**, 607–608.

Smith, J. V. & Dytrych, W. J. (1986). *Z. Kristallogr.* **175**, 31–36.

Smith, J. V. & Rinaldi, F. (1962). *Mineral. Mag.* **33**, 202–212.