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# Enumeration of four-connected three-dimensional nets. II. Conversion of edges of three-connected 2D nets into zigzag chains

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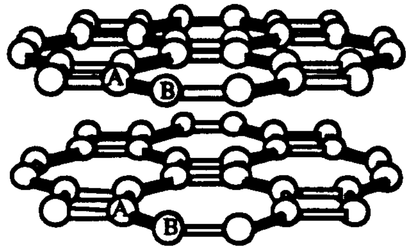
## Abstract

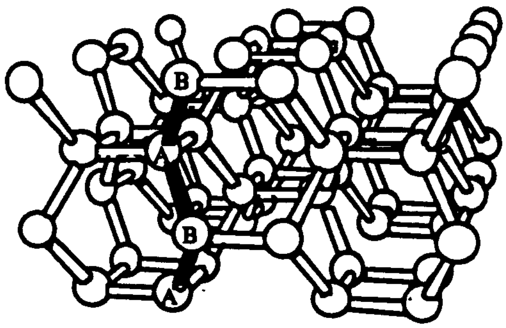
Four-connected three-dimensional (3D) nets were systematically enumerated by converting some horizontal edges of a vertical stack of three-connected two-dimensional (2D) nets into vertical zigzag chains. 77 out of 131 2D nets were selected for enumeration, and different arrangements of zigzag edges and horizontal edges were investigated. This yielded 138 3D nets of which 19 are represented by known structures: cristobalite; tridymite; MAPO-39 (International Zeolite Association Structure Commission code ATN); svyatoslavite; Li-A(BW) (ABW); cancrinite (CAN); AlPO-31 (ATO); MAPO-36 (ATS); $BaFe_2O_4$; 'nepheline hydrate' (JBW); bikitaite (BIK); $KBGe_2O_6$; $CsAlSi_5O_{12}$ (CAS); UiO-6 (OSI); Theta-1 (TON); ZSM-12 (MTW); ZSM-23 (MTT); AlPO-53C; and CIT-5 (CFI).

## 1. Introduction

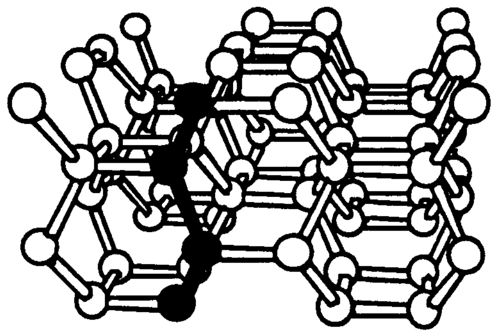
In the first paper of this series, four-connected three-dimensional (3D) nets were obtained by connecting each three-connected vertex of a vertical stack of congruent three-connected two-dimensional (2D) nets by an up or down linkage to generate a crankshaft (*c*) chain [Han & Smith (1999) contains technical details applicable here]. This paper considers zigzag (*z*) chains in which some horizontal edges are broken and refastened. Whereas the *c**-3D nets were restricted by parity of the up–down linkages to 2D nets with only even-numbered rings, all 131 three-connected 2D nets in the catalog of the Consortium for Theoretical Frameworks (Pluth & Smith, 1993) are usable for the *z**-enumeration. Each of the even-numbered 2D nets yielded only one *c**-3D net. In contrast, different arrangements of zigzag (*z*) edges and horizontal (*h*) edges can generate multiple 3D nets from a single parent 2D net. We explored these multiple choices for selected 2D nets, and examined the geometrical and topological properties of the *z**-3D nets. Selected *z**-3D nets were chosen for distance-least-squares (DLS) refinement. An illustrated catalog of nets in known structures and their subunits is being published (Smith, 1999*a*).




(*a*)




(*b*)



(*c*)

Fig. 1. Procedure for generation of tilted edges of a zigzag chain from the horizontal edge linking vertices *A* and *B* in the 2D *fee* net ($48^2$). In (*a*), adjacent horizontal vertices of three-connected 2D nets are labeled *A* and *B*, and all edges are horizontal. Shaded edges become tilted edges. In (*b*), the edges *AB* are converted into tilted edges of a zigzag net in the derived four-connected 3D net. The remaining two edges for each vertex remain horizontal (*h*), but are forced into different heights. (*c*) 3D net after DLS refinement with the *z* chain shaded. This is net 3 in Fig. 2.




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Table 1. *Geometrical properties of regular 3D nets obtained from conversion of edges of a parallel stack of three-connected 2D nets into a zigzag 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) | $\gamma$ (°)† | Space group for alternation | Structure type |
| *hex* | $6^3$ | 1 | $6^6$ | 8 | 227:$Fd3m$ | 7 | 7 | 7 | 90 | 216:$F\bar{4}3m$ | Cristobalite |
| | | 2‡ | | 4 | 194:$P6_3/mmc$ | 5.322 | 5.322 | 8.691 | 120 | 186:$P6_3mc$ | Tridymite |
| *ttw* | $3.12^2$ | 94‡ | $36^5$ | 6 | 194:$P6_3/mmc$ | 9.184 | 9.184 | 5.324 | 120 | i | |
| *fee* | $48^2$ | 93‡ | $4^26^38$ | 16 | 139:$I4/mmm$ | 13.271 | 13.271 | 5.323 | 90 | 87:$I4/m$ | ATN |
| | | 3‡ | $46^5$ | 8 | 139:$I4/mmm$ | 9.085 | 9.085 | 5.323 | 90 | 136:$P4_2/mnm$ | Svyatoslavite |
| | | 370‡ | $(4^26^38)_1(4^26^38)_1$ $(4^26^38)_1(4^26^38)_1$ | 64 | 139:$I4/mmm$ | 26.185 | 26.185 | 5.323 | 90 | 87:$I4/m$ | – |
| | | 4‡ | $4^26^38$ | 8 | 74:$Imam$ | 8.922 | 9.960 | 5.323 | 90 | 62:$Pnam$ | ABW |
| | | 961‡ | $(4^26^38)_1(4^26^38)_1$ $.(4^26^38)_1(4^26^38)_1$ | 32 | 65: | 13.207 | 26.456 | 5.323 | 90 | 55:$Pbam$ | – |
| | | 374‡ | $(4^26^38)_1(4^26^38)_1$ | 16 | 63:$Amam$ | 13.200 | 13.219 | 5.323 | 90 | 62:$Pnam$ | |
| *gml* | 4.6.12 | 95‡ | $4^26^4$ | 12 | 194:$P6_3/mmc$ | 12.683 | 12.683 | 5.323 | 120 | 176:$P6_3/m$ | CAN |
| | | 738‡ | $46^5$ | 36 | 166 : $R\bar{3}m$ | 22.75 | 22.75 | 5.3 | 120 | 148 : $R\bar{3}$ | ATO |
| | | 382‡ | $(4^26^4)_1(4^26^4)_1$ $(4^26^38)_1(4^26^38)_1$ | 48 | 191:$P6/mmm$ | 25.559 | 25.559 | 5.3 | 120 | 175:$P6/m$ | – |
| | | 755 | 12 types | 96 | 65:$Ammm$ | 25 | 42 | 5 | 90 | 12:$A112/m$ | – |
| | | 753‡ | $(4^26^4)_1(4^26^38)_1$ $(4^26^38)_1$ | 24 | 63:$Cmcm$ | 13.339 | 21.890 | 5.323 | 90 | 11:$P112_1/m$ ($b \sim 13$) | ATS |
| | | 384 | $(4^26^4)_1(4^26^4)_1$ $(4^26^38)_1(4^26^38)_1$ $(4^26^38)_1(4^26^38)_1$ | 24 | 59:$Pnmm$ | 12.5 | 21.5 | 5 | 90 | 11:$P112_1/m$ | – |
| | | 754 | $(4^26^4)_1(4^26^4)_1$ $(4^26^4)_1(4^26^4)_1$ $(4^26^38)_1(4^26^38)_1$ | 24 | 59:$Pmnm$ | 13 | 21.5 | 5 | 90 | 11:$P112_1/m$ | – |
| *ffs* | $(4^210)_1(4.10^2)_2$ | 424‡ | $(4^36^3)_1(4^26^38)_1$ $(46^5)_1$ | 24 | 63:$Amam$ | 9.071 | 26.529 | 5.337 | 90 | 36:$A2_1am$ | – |
| *tth* | $(4^212)_1(4.8.12)_2$ | 423‡ | $(4^36^3)_1(4^26^38)_1$ $(46^5)_1$ | 48 | 139:$I4/mmm$ | 22.584 | 22.584 | 5.324 | 90 | 87:$I4/m$ | – |
| *fos* | $(4^212)_1(4.12^2)_1$-*a* | 468‡ | $(4^36^3)_1(4^26^38)_1$ | 16 | 65:$Cmmm$ | 8.382 | 18.420 | 5.324 | 90 | 55:$Pbam$ | – |
| | | 470‡ | $(4^36^3)_1(46^5)_1$ | 16 | 63:$Cmcm$ | 8.826 | 18.421 | 5.324 | 90 | 62:$Pbnm$ | $BaFe_2O_4$ |
| *twy* | $(4^212)_1(4.12^2)_1$-*b* | 718‡ | $(4^36^3)_1(4^26^38]_1$ | 24 | 191:$P6/mmm$ | 17.496 | 17.496 | 5.324 | 120 | 175:$P6/m$ | – |
| *rho* | $(4^216)_1(4.8.16)_1$ | 469‡ | $(4^36^3)_1(46^5)_1$ | 32 | 140:I4/$mcm$ | 19.208 | 19.208 | 5.324 | 90 | 87:$I4/m$ | – |
| | | 467‡ | $(4^36^3)_1(4^26^38)_1$ | 16 | 123:$P4/mmm$ | 13.758 | 13.758 | 5.324 | 90 | 83:$P4/m$ | – |
| *tsv* | $(4^224)_1(4.6.24)_1$ | 719 | $(4^36^3)_1(4^26^4)_1$ | 24 | 191:$P6/mmm$ | 20 | 20 | 5 | 120 | 175:$P6/m$ | – |
| *ltl* | $(468)_1(4.8.12)_1$ | 721‡ | $(4^26^4)_1(4^26^38)_1$ | 24 | 191:$P6/mmm$ | 17.776 | 17.776 | 5.323 | 120 | 175:$P6/m$ | – |
| *fsy* | $(468)_1(6^28)_1$ | 722‡ | $(4^26^38)_1(6^6)_1$ | 16 | 74:$Ibmm$ | 7.994 | 20.425 | 5.323 | 90 | 62:$Pbnm$ | – |
| | | 549‡ | $(46^5)_1(6^6)_1$ | 16 | 65:$Cmmm$ | 8.888 | 18.131 | 5.323 | 90 | 55:$Pbam$ | – |
| | | 7‡ | $(4^26^4)_1(6^58)_1$ | 16 | 63:$Cmcm$ | 9.001 | 17.949 | 5.323 | 90 | 62:$Pbnm$ | – |
| *brw* | $(468)_1(68^2)_1$ | 1246‡ | $(4^26^4)_2(6^6)_1$ | 24 | 69:$Fmmm$ | 14.509 | 15.627 | 5.324 | 90 | 65:$Ammm$ | AlPO-53C |
| | | 723‡ | $(4^26^4)_1(46^5)_1$ $(6^58)_1$ | 24 | 65:$Ammm$ | 8.935 | 27.124 | 5.323 | 90 | 12:$A112/m$ | – |
| | | 96‡ | $(4^26^38)_2(6^6)_1$ | 6 | 51:$Pmcm$ | 7.556 | 8.270 | 5.323 | 90 | 59:$Pmnm$ ($a \sim 14$) | JBW |
| *bor* | $(47^2)_2(7^3)_1$ | 749‡ | $(4^26^37)_1(4^26^37)_1$ $(6^57)_1$ | 12 | 62:$Pnam$ | 10.690 | 10.834 | 5.324 | 90 | *i* | $KBGe_2O_6$ |
| *bik* | $(5^28)_2(58^2)_1$ | 98‡ | $(5^468)_2(56^5)_1$ | 12 | 63:$Cmcm$ | 7.641 | 16.449 | 5.323 | 90 | *i* | BIK |
| | | 242‡ | $(5^468)_1(5^36^3)_1$ $(5^26^38)_1$ | 24 | 63:$Bbmm$ | 14.322 | 17.457 | 5.323 | 90 | *i* | CAS |
| | | 243‡ | $(5^468)_1(5^36^3)_1$ $(5^26^38)_1$ | 12 | 12:$A112/m$ | 9.058 | 14.323 | 5.323 | 105.5 | *i* | – |
| *twl* | $(4^210)_1(4.6.10)_2$ $(6^210)_2$ | 724‡ | $(4^36^3)_1(4^26^4)_1$ $(46^5)_1(6^6)_1$ $(6^58)_1$ | 40 | 63:$Amam$ | 8.727 | 42.819 | 5.327 | 90 | 12:$A112/m$ | – |
| *fsv* | $(4^210)_1(4.6.10)_2$ $(6.10^2)_1$ | 569‡ | $(4^36^3)_1$ $(4^26^4)_1$ $(46^5)_1(6^58)_1$ | 8 | 25:$Pm2m$ | 8.406 | 8.933 | 5.324 | 90 | 6:$P11m$ | – |
| *ttv* | $(4^210)_1(4.8.10)_2$ $(4.8.10)_2$ | 834‡ | $(4^36^3)_1(4^26^38)_1$ $(4^26^38)_1(46^5)_1$ $(46^5)_1$ | 40 | 65:$Ammm$ | 8.961 | 42.425 | 5.324 | 90 | 12:$A112/m$ | – |

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) | $\gamma$ (°)† | Space group for alternation | Structure type |
| *ooo* | $(4^{2}10)_{2}(4.8.10)_{2}(8^{2}10)_{1}$ | 783‡ | $(4^{3}6^{3})_{2}(4^{2}6^{3}8)_{2}(6^{5}8)_{1}$ | 20 | 65:*Ammm* | 6.950 | 25.966 | 5.324 | 90 | 63:*Amam* ($a \sim 15$) | – |
| *fix* | $(4^{2}12)_{1}(4.6.12)_{1}(6^{2}12)_{1}$ | 550‡ | $(4^{3}6^{3})_{1}(46^{5})_{1}(6^{6})_{1}$ | 24 | 74:*Imcm* | 8.756 | 27.630 | 5.324 | 90 | 62:*Pnam* | – |
| | | 546‡ | $(4^{3}6^{3})_{1}(4^{2}6^{4})_{1}(6^{5}8)_{1}$ | 24 | 71:*Immm* | 8.244 | 27.159 | 5.324 | 90 | 58:*Pnnm* | – |
| *toh* | $(4^{2}12)_{2}(4.6.12)_{2}(6.12^{2})_{1}$ | 785 | $(4^{3}6^{3})_{1}(4^{3}6^{3})_{1}(4^{2}6^{4})_{1}(46^{5})_{1}(6^{5}8)_{1}$ | 40 | 65:*Ammm* | 8.5 | 45 | 5 | 90 | 12:*A*112/*m* | – |
| *vvv* | $(4^{2}12)_{1}(4.8.12)_{1}(4.8.12)_{1}$ | 775‡ | $(4^{3}6^{3})_{1}(4^{2}6^{3}8)_{1}(4^{2}6^{3}8)_{1}$ | 24 | 65:*Ammm* | 8.977 | 27.163 | 5.324 | 90 | 12:*A*12/*ml* | – |
| | | 555‡ | $(4^{3}6^{3})_{1}(46^{5})_{1}(46^{5})_{1}$ | 24 | 65:*Ammm* | 8.982 | 27.383 | 5.324 | 90 | 12:*A*112/*m* | – |
| *uun* | $(4^{2}14)_{2}(4^{2}14)_{1}(4.14^{2})_{2}$ | 835‡ | $(4^{3}6^{3})_{1}(4^{3}6^{3})_{1}(4^{3}6^{3})_{1}(4^{2}6^{3}8)_{1}(46^{5})_{1}$ | 40 | 63:*Amam* | 8.787 | 43.241 | 5.317 | 90 | 36:$A2_1am$ | – |
| *fef* | $(458)_{2}(58^{2})_{2}(58^{2})_{1}$ | 768‡ | $(4^{2}56^{3})_{2}(56^{5})_{2}(56^{5})_{1}$ | 20 | 67:*Abmmm* | 12.936 | 14.438 | 5.323 | 90 | *i* | – |
| | | 769‡ | $(4^{2}56^{3})_{2}(5^{2}6^{3}8)_{2}(56^{5})_{1}$ | 20 | 65:*Ammm* | 7.846 | 25.286 | 5.323 | 90 | *i* | – |
| *bks* | $(4.5.12)_{2}(4.5.12)_{2}(5.12^{2})_{1}$ | 766‡ | $(4^{2}56^{3})_{2}(4^{2}56^{3})_{2}(56^{5})_{1}$ | 20 | 63:*Cmcm* | 11.280 | 19.483 | 5.323 | 90 | *i* | – |
| | | 767‡ | $(4^{2}5^{2}67)_{2}(4^{2}5^{2}67)_{2}(56^{5})_{1}$ | 20 | 63:*Cmcm* | 12.616 | 18.754 | 5.323 | 90 | *i* | – |
| *eus* | $(4.5.18)_{6}(5^{3})_{1}(5^{2}18)_{3}$ | 704 | $(4^{2}5^{2}67)_{2}(4^{2}5^{2}67)_{2}(45^{2}6^{3})_{2}(5^{5}6)_{1}(5^{4}68)_{1}(5^{3}6^{3})_{2}$ | 40 | 71:*Immm* | 17 | 27 | 5 | 90 | *i* | – |
| *krp* | $(46^{2})_{1}(46.12)_{2}(6^{2}12)_{1}$ | 1153 | $(4^{2}6^{4})_{1}(46^{5})_{1}(6^{5}8)_{2}$ | 32 | 139:*I*4/*mmm* | 18 | 18 | 5 | 90 | 71:*Immm* | OSI |
| *fto* | $(468)_{1}(48^{2})_{1}(6^{2}8)_{1}$ | 558‡ | $(4^{2}6^{4})_{1}(4^{2}6^{3}8)_{1}(6^{5}8)_{1}$ | 24 | 63:*Amam* | 8.179 | 27.276 | 5.325 | 90 | 36:$A2_1am$ | – |
| | | 759‡ | $(46^{5})_{1}(46^{5})_{1}(6^{6})_{1}$ | 24 | 63:*Amam* | 8.702 | 27.657 | 5.323 | 90 | 36:$A2_1am$ | – |
| | | 756‡ | $(4^{2}6^{3}8)_{1}(4^{2}6^{3}8)_{1}(6^{6})_{1}$ | 12 | 53:*Pcnm* | 7.608 | 15.971 | 5.323 | 90 | 31:$P2_1nm$ | – |
| *ffv* | $(468)_{2}(48^{2})_{2}(68^{2})_{1}$ | 843‡ | $(4^{2}6^{3}8)_{2}(4^{2}6^{3}8)_{2}(6^{6})_{1}$ | 20 | 74:*Icmm* | 8.628 | 21.834 | 5.321 | 90 | 44:*I*2*mm* | – |
| | | 844‡ | $(4^{2}6^{4})_{1}(4^{2}6^{3}8)_{1}(46^{5})_{1}(46^{5})_{1}(6^{5}8)_{1}$ | 40 | 63:*Amam* | 8.712 | 46.097 | 5.323 | 90 | 36:$A2_1am$ | – |
| *apd* | $(468)_{1}(6^{3})_{1}(6^{2}8)_{1}$ | 760‡ | $(4^{2}6^{4})_{1}(6^{5}8)_{1}(6^{6})_{1}$ | 24 | 74:*Imcm* | 8.342 | 27.145 | 5.324 | 90 | 62:*Pnam* | – |
| | | 762‡ | $(4^{2}6^{3}8)_{1}(6^{6})_{1}(6^{6})_{1}$ | 24 | 74:*Ibmm* | 7.775 | 30.982 | 5.323 | 90 | 62:*Pbnm* | – |
| | | 761‡ | $(46^{5})_{1}(6^{6})_{1}(6^{6})_{1}$ | 24 | 71:*Immm* | 8.805 | 27.262 | 5.323 | 90 | 58:*Pnnm* | – |
| *feo* | $(468)_{2}(6^{3})_{1}(6^{2}8)_{2}$ | 841‡ | $(4^{2}6^{4})_{1}(46^{5})_{1}(6^{6})_{1}(6^{6})_{1}(6^{5}8)_{1}$ | 40 | 65:*Ammm* | 8.383 | 44.423 | 5.324 | 90 | 12:*A*112/*m* | – |
| | | 773‡ | $(4^{2}6^{3}8)_{2}(6^{6})_{2}(6^{6})_{1}$ | 10 | 51:*Pcmm* | 7.856 | 12.854 | 5.323 | 90 | 59:*Pnmm* (double *b*) | – |
| *eui* | $(5^{3})_{1}(5^{2}12)_{3}(5^{2}12)_{3}$ | 852 | $(5^{5}6)_{1}(5^{5}6)_{1}(5^{4}68)_{2}(5_{4}68)_{1}(5^{4}68)_{1}(5^{3}6^{3})_{2}(5^{3}6^{3})_{2}(5^{3}6^{3})_{2}(5^{3}6^{3})_{2}$ | 56 | 63:*Amam* | 13 | 41.5 | 5 | 90 | *i* | – |
| *nos* | $(5^{2}6)_{1}(568)_{2}(58^{2})_{1}$ | 772‡ | $(5^{4}6^{2})_{1}(5^{4}6^{2})_{1}(5^{2}6^{4})_{2}(5^{2}6^{3}8)_{2}(56^{5})_{2}$ | 32 | 65:*Ammm* | 11.583 | 27.098 | 5.323 | 90 | *i* | – |
| | | 322‡ | $(5^{3}6^{3})_{1}(5^{2}6^{4})_{1}(5^{2}6^{3}8)_{1}(5^{2}6^{3}8)_{1}$ | 32 | 65:*Cmmm* | 14.450 | 21.461 | 5.323 | 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) | $\gamma$ (°)† | Space group for alternation | Structure type |
| *vnv* | $(5^27)_1(57^2)_2$ $(57^2)_1$ | 764‡ | $(5^467)_1(5^467)_1$ $(5^26^37)_2(5^26^37)_2$ $(56^5)_2$ | 32 | 63:*Amam* | 11.896 | 27.551 | 5.325 | 90 | *i* | – |
| *urg* | $(56^2)_2(568)_2$ $(58^2)_1$ | 765‡ | $(5^26^4)_2(5^26^38)_2$ $(56^5)_1$ | 20 | 74:*Imcm* | 7.875 | 25.135 | 5.323 | 90 | *i* | – |
| *fsf* | $(4^210)_1(4.6.10)_1$ $(4.10^2)_1(6^210)_1$ | 770‡ | $(4^36^3)_1(4^26^38)_1$ $(46^5)_1(6^6)_1$ | 16 | 51:*Pmam* | 8.694 | 18.440 | 5.323 | 90 | 26:$P2_1am$ | – |
| *ftn* | $(4^210)_1(4.6.10)_2$ $(6^3)_1(6^210)_2$ | 771 | $(4^36^3)_1(4^26^4)_1$ $(46^5)_1(6^6)_1$ $(6^6)_1(6^58)_1$ | 24 | 38:*Am*2*m* | 8.5 | 26.5 | 5 | 90 | 8:*Allm* | – |
| *uiv* | $(4^212)_2(4.5.12)_2$ $(58^2)_1(5.8.12)_2$ | 323 | $(4^36^3)_2(45^26^3)_2$ $(5^26^38)_2(56^5)_1$ | 14 | 51:*Pmcm* | 7.5 | 17 | 5 | 90 | *i* | – |
| *vss* | $(4^212)_1(468)_1$ $(4.6.12)_1(6.8.12)_1$ | 827 | $(4^36^3)_1(4^26^4)_1$ $(4^26^4)_1(6^6)_1$ | 64 | 69:*Fmmm* | 16 | 36 | 5 | 90 | 12:*F*112/*m*→ *C*112/*m* (small cell) | – |
| | | 820 | $(4^36^3)_1(4^26^4)_1$ $(46^5)_1(6^58)_1$ | 16 | 51:*Pmcm* | 8.5 | 17 | 5 | 90 | 11:$P112_1/m$ | – |
| *bsh* | $(4^212)_1(4.6.12)_1$ $(6^3)_1(6^312)_1$ | 861 | $(4^36^3)_1(4^26^4)_1$ $(6^58)_1(6^6)_1$ | 32 | 65:*Cmmm* | 8.5 | 34 | 5 | 90 | 55:*Pbam* | – |
| | | 786 | $(4^36^3)_1(46^5)_1$ $(6^6)_1(6^6)_1$ | 32 | 63:*Cmcm* | 8.5 | 36 | 5 | 90 | 62:*Pbnm* | – |
| *fvo* | $(4^214)_2(4^214)_1$ $(4.6.14)_2(6.14^2)_1$ | 840 | $(4^36^3)_1(4^36^3)_1$ $(4^36^3)_1(4^26^4)_1$ $(46^5)_1(6^58)_1$ | 24 | 38:*Am*2*m* | 8.5 | 26.5 | 5 | 90 | 8:*Allm* | – |
| *mor* | $(458)_1(4.5.12)_1$ $(5^212)_1(5.8.12)_1$ | 792 | $(45^26^3)_1(45^26^3)_1$ $(5^36^3)_1(5^26^38)_1$ | 32 | 65:*Cmmm* | 17 | 19.5 | 5 | 90 | *i* | – |
| | | 793 | $(4^25^267)_1(4^25^267)_1$ $(5^36^3)_1(5^26^38)_1$ | 32 | 65:*Cmmm* | 18 | 19 | 5 | 90 | *i* | – |
| | | 794 | $(4^25^267)_1(4^25^267)_1$ $(5^468)_1(56^5)_1$ | 32 | 63:*Ccmm* | 17.5 | 19 | 5 | 90 | *i* | – |
| *dac* | $(4.5.10)_1(4.5.10)_1$ $(5^210)_1(5.10^2)_1$ | 781 | $(4^25^267)_1(4^25^267)_1$ $(5^36^3)_1(5^26^38)_1$ | 16 | 12:*A*112/*m* | 9 | 19 | 5 | 103 | *i* | – |
| | | 782 | $(4^25^267)_1(4^25^267)_1$ $(5^46^2)_1(56^5)_1$ | 8 | 11:$P112_1/m$ | 9 | 10 | 5 | 105 | *i* | – |
| | | 784 | $(45^26^3)_1(45^26^3)_1$ $(5^36^3)_1(5^26^38)_1$ | 8 | 10:*P*112/*m* | 8.5 | 10 | 5 | 105 | *i* | – |
| *urv* | $(458)_2(48^2)_2$ $(58^2)_2(58^2)_1$ | 863 | $(45^26^3)_2(46^5)_2$ $(56^5)_1(56^48)_2$ | 28 | 63:*Cmcm* | 7.5 | 32.5 | 5 | 90 | *i* | – |
| *dao* | $(4.5.10)_1(4.5.10)_1$ $(5^210)_1(5.10^2)_1$ | 779 | $(4^25^267)_1(4^25^267)_1$ $(5^468)_1(56^5)_1$ | 16 | 59:*Pnmm* | 8.5 | 18.5 | 5 | 90 | *i* | – |
| | | 778 | $(45^26^3)_1(45^26^3)_1$ $(5^36^3)_1(5^26^38)_1$ | 16 | 51:*Pbmm* | 9.5 | 16 | 5 | 90 | *i* | – |
| | | 780 | $(4^25^267)_1(4^25^267)_1$ $(5^36^3)_1(5^26^38)_1$ | 16 | 51:*Pbmm* | 9 | 19 | 5 | 90 | *i* | – |
| *sxn* | $(4.5.10)_1(4.5.10)_1$ $(5^210)_1(5.10^2)_1$ | 791 | $(4^25^267)_1(4^25^267)_1$ $(5^36^3)_1(5^26^38)_1$ | 32 | 63:*Amam* | 17.5 | 19 | 5 | 90 | *i* | – |
| | | 790 | $(4^25^267)_1(4^25^267)_1$ $(5^468)_1(56^5)_1$ | 16 | 57:*Pbcm* | 10 | 16.5 | 5 | 90 | *i* | – |
| | | 789 | $(45^26^3)_1(45^26^3)_1$ $(5^36^3)_1(5^26^38)_1$ | 16 | 51:*Pbmm* | 8.5 | 18.5 | 5 | 90 | *i* | – |
| *fes* | $(4.5.10)_2(56^2)_1$ $(5.6.10)_2(6^210)_1$ | 758 | $(45^26^3)_2(56^5)_1$ $(56^5)_1(6^58)_1$ | 24 | 71:*Immm* | 10 | 24 | 5 | 90 | *i* | – |
| | | 801 | $(4^25^267)_1(4^25^267)_1$ $(5^26^38)_1(56^5)_1$ $(56^5)_1(6^6)_1$ | 24 | 44:*I*2*mm* | 8.5 | 26.5 | 5 | 90 | *i* | – |
| *bab* | $(4.5.12)_2(4.6.12)_2$ $(56^2)_1(5.6.12)_2$ | 800 | $(4^26^38)_2(45^26^3)_2$ $(5^26^4)_2(56^5)_1$ | 28 | 65:*Ammm* | 12.5 | 23.5 | 5 | 90 | *i* | – |
| | | 830 | $(4^25^267)_1(4^25^267)_1$ $(4^26^4)_1(46^5)_1$ $(5^26^4)_1(5^26^38)_1$ $(56^5)_1$ | 56 | 65:*Ammm* | 13.5 | 44 | 5 | 90 | *i* | – |
| *uss* | $(46^2)_1(4.6.12)_1$ $(4.6.12)_1(6^212)_1$ | 864 | $(4^26^4)_1(4^26^38)_1$ $(46^5)_1(6^6)_1$ | 32 | 71:*Immm* | 13.5 | 23 | 5 | 90 | 58:*Pnnm* | – |

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) | $\gamma$ (°)† | Space group for alternation | Structure type |
| *uhe* | $(467)_2(478)_2$ $(6^27)_2(78^2)_1$ | 865 | $(4^26^4)_1(4^26^38)_2$ $(6^57)_2(6^57)_1$ | 28 | 63:*Cmcm* | 7.5 | 32 | 5 | 90 | *i* | – |
| *bso* | $(468)_1(468)_1$ $(48^2)_1(68^2)_1$ | 848 | $(4^26^38)_1(4^26^38)_1$ $(4^26^38)_1(6^6)_1$ | 32 | 74:*Ibmm* | 8.5 | 38.5 | 5 | 90 | 62:*Pbnm* | – |
| | | 851 | $(4^26^4)_1(4^26^38)_1$ $(46^5)_1(6^58)_1$ | 32 | 65:*Cmmm* | 8.5 | 34 | 5 | 90 | 55:*Pbam* | – |
| | | 787 | $(4^26^4)_1(46^5)_1$ $(46^5)_1(6^58)_1$ | 32 | 63:*Cmcm* | 8.5 | 36 | 5 | 90 | 62:*Pbnm* | – |
| *tva* | $(468)_2(48^2)_1$ $(48^2)_1(68^2)_1$ | 866 | $(4^26^4)_2(46^5)_1$ $(46^5)_1(6^6)_1$ | 20 | 65:*Bmmm* | 13 | 14.5 | 5 | 90 | 71:*Immm* ($b \sim 29$) | – |
| *stg* | $(468)_2(48^2)_2$ $(48^2)_2(68^2)_1$ | 803 | $(4^26^4)_2(4^26^4)_2$ $(4^26^38)_2(6^6)_1$ | 28 | 65:*Ammm* | 16.5 | 18.5 | 5 | 90 | 63:*Amam* ($a \sim 33$) | – |
| | | 802 | $(4^26^38)_2(4^26^38)_2$ $(4^26^38)_2(6^6)_1$ | 14 | 51:*Pcmm* | 7.5 | 17 | 5 | 90 | 59:*Pnmm* ($b \sim 34$) | – |
| *fst* | $(468)_1(48^2)_1$ $(6^3)_1(6^28)_1$ | 807 | $(46^5)_1(46^5)_1$ $(6^6)_1(6^6)_1$ | 16 | 59:*Pmnm* | 8.5 | 17 | 5 | 90 | 31:$P2_1nm$ | – |
| | | 806 | $(4^26^38)_1(4^26^38)_1$ $(6^6)_1(6^6)_1$ | 16 | 53:*Pcnm* | 7.5 | 19 | 5 | 90 | 31:$P2_1nm$ | – |
| | | 805 | $(4^26^4)_1(4^26^38)_1$ $(6^58)_1(6^6)_1$ | 16 | 51:*Pmam* | 8.5 | 17 | 5 | 90 | 26:$P2_1am$ | – |
| *rxt* | $(468)_2(568)_2$ $(568)_2(58^2)_1$ | 796 | $(4^26^4)_2(5^26^38)_2$ $(5^26^38)_2(56^5)_1$ | 14 | 51:*Pmcm* | 7.5 | 19 | 5 | 90 | *i* | – |
| *fss* | $(468)_2(6^3)_2$ $(6^3)_1(6^28)_2$ | 867 | $(4^26^38)_2(6^6)_2(6^6)_2$ $(6^6)_1$ | 14 | 51:*Pcmm* | 7.5 | 17 | 5 | 90 | 59:*Pnmm* ($b \sim 34$) | – |
| *uhi* | $(478)_2(478)_2$ $(478)_2(78^2)_1$ | 868 | $(4^26^37)_2(4^26^38)_2$ $(4^26^38)_2(6^57)_1$ | 14 | 51:*Pmcm* | 8.5 | 16 | 5 | 90 | *i* | – |
| *fer* | $(5^26)_1(5^210)_2$ $(5^210)_1(5.6.10)_2$ | 804 | $(5^46^2)_1(5^468)_1$ $(5^36^3)_2(5^46^2)_2$ | 24 | 65:*Cmmm* | 13.5 | 17 | 5 | 90 | *i* | – |
| | | 606‡ | $(5^46^2)_1(5^468)_1$ $(5^468)_2(56^5)_2$ | 24 | 63:*Cmcm* | 14.294 | 18.089 | 5.323 | 90 | *i* | TON |
| *een* | $(5^27)_1(57^2)_1$ $(57^2)_1(57^2)_1$ | 823 | $(5^467)_1(5^26^37)_1$ $(5^26^37)_1(56^5)_1$ | 16 | 62:*Pbnm* | 8.5 | 17.5 | 5 | 90 | *i* | – |
| | | 821 | $(5^36^3)_1(5^26^37)_1$ $(5^26^37)_1(5^26^37)_1$ | 16 | 55:*Pbam* | 9.5 | 15 | 5 | 90 | *i* | – |
| *biz* | $(5^28)_2(5^28)_1$ $(5^28)_1(5^28)_2$ | 244 | $(5^468)_2(5^468)_1$ $(5^468)_1(56^5)$ | 12 | 59:*Pnmm* | 8.5 | 13 | 5 | 90 | *i* | – |
| | | 245 | $(5^468)_1(5^468)_1$ $(5^36^3)_2(5^26^38)_2$ | 12 | 51:*Pbmm* | 8.5 | 13 | 5 | 90 | *i* | – |
| *fex* | $(5^28)_1(56^2)_1$ $(568)_2(6^28)_1$ | 824 | $(5^468)_1(5^468)_1$ $(5^26^4)_2(5^26^38)_2$ $(56^5)_2(6^6)_2$ | 10 | 25:*P2mm* | 8 | 10 | 5 | 90 | *i* | – |
| *exn* | $(56^2)_1(567)_2(57^2)_2$ $(6^27)_1$ | 832 | $(5^26^4)_2(5^26^37)_2$ $(56^5)_1(6^57)_1$ | 24 | 74:*Imcm* | 10 | 23.5 | 5 | 90 | *i* | – |
| | | 833 | $(5^26^4)_1(5^26^37)_1$ $(5^26^37)_1(5^26^37)_1$ $(56^5)_1(6^6)_1$ | 24 | 44:*I2mm* | 9 | 26.5 | 5 | 90 | *i* | – |
| *exe* | $(56^2)_1(567)_2(57^2)_2$ $(6^27)_1$ | 825 | $(5^26^4)_2(5^26^37)_2$ $(56^5)_1(6^57)_1$ | 24 | 63:*Amam* | 9.5 | 23 | 5 | 90 | *i* | – |
| | | 826 | $(5^26^4)_1(5^26^37)_1$ $(5^26^37)_1(5^26^37)_1$ $(56^5)_1(6^6)_1$ | 12 | 31:$P2_1nm$ | 9 | 13 | 5 | 90 | *i* | – |
| *eig* | $(4^210)_1(4.6.10)_2$ $(6^3)_2(6^3)_1$ $(6^210)_2$ | 869 | $(4^36^3)_1(4^26^4)_1$ $(46^5)_1(6^6)_1$ $(6^6)_1(6^6)_1$ $(6^6)_1(6^58)_1$ | 16 | 25:*Pm2m* | 8.5 | 17.5 | 5 | 90 | 6:*P11m* | – |
| *eug* | $(4.5.14)_2(5^3)_1$ $(5^214)_2(5^214)_2$ $(5^214)_1$ | 870 | $(45^26^3)_2(5^56)_1$ $(5^468)_2(5^468)_1$ $(5^36^3)_2$ | 32 | 71:*Immm* | 13.5 | 25.5 | 5 | 90 | *i* | – |
| | | 1247 | $(4^256^3)_2(5^56)_1$ $(5^468)_1(5^36^3)_2$ $(5^36^3)_2$ | 32 | 74:*Imam* | 13.5 | 25.5 | 5 | 90 | *i* | CFI |
| *tvt* | $(468)_2(468)_2$ $(6^3)_1(6^28)_2$ $(68^2)_1$ | 828 | $(4^26^38)_2(4^26^38)_2$ $(6^6)_2(6^6)_1$ $(6^6)_1$ | 16 | 51:*Pcmm* | 7.5 | 19 | 5 | 90 | 25:*P2mm* | – |

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) | $\gamma$ (°)† | Space group for alternation | Structure type |
| | | 829 | 2 each of $(4^{2}6^{4})_{1}$<br>$(46^{5})_{1}(6^{6})_{1}$<br>$(6^{5}8)_{1}$ | 16 | 25:*Pm*2*m* | 8.5 | 17 | 5 | 90 | 6:*P*11*m* | – |
| *fsm* | $(468)_{2}(6^{3})_{2}$<br>$(6^{3})_{2}(6^{3})_{1}$<br>$(6^{2}8)_{2}$ | 850 | $(4^{2}6^{4})_{1}(46^{5})_{1}$<br>$(6^{6})_{1}(6^{6})_{1}$<br>$(6^{6})_{1}(6^{6})_{1}$<br>$(6^{6})_{1}(6^{6})_{1}$<br>$(6^{5}8)_{1}$ | 72 | 65:*Ammm* | 8.5 | 77 | 5 | 90 | 12:*A*112/*m* | – |
| | | 849 | $(4^{2}6^{3}8)_{2}(6^{6})_{2}$<br>$(6^{6})_{2}(6^{6})_{2}(6^{6})_{1}$ | 18 | 51:*Pcmm* | 8.5 | 22 | 5 | 90 | 59:*Pnmm*<br>($b \sim 44$) | – |
| *svn* | $(47^{2})_{2}(478)_{2}$<br>$(5^{2}8)_{2}(58^{2})_{1}$<br>$(78^{2})_{1}$ | 831 | $(4^{2}6^{3}7)_{2}(4^{2}6^{3}8)_{2}$<br>$(5^{4}68)_{2}(56^{5})_{1}$<br>$(6^{5}7)_{1}$ | 32 | 63:*Amam* | 8 | 39 | 5 | 90 | *i* | – |
| *fev* | $(4.5.10)_{1}(4.5.10)_{1}$<br>$(56^{2})_{1}(5.6.10)_{1}$<br>$(5.6.10)_{1}(6^{2}10)_{1}$ | 799 | $(4^{2}5^{2}67)_{1}(4^{2}5^{2}67)_{1}$<br>$(5^{2}6^{4})_{1}(56^{5})_{1}$<br>$(5^{2}6^{3}8)_{1}(6^{6})_{1}$ | 24 | 57:*Pcam* | 15 | 16 | 5 | 90 | *i* | – |
| *nee* | $(468)_{2}(5^{2}8)_{2}$<br>$(5^{2}8)_{2}(58^{2})_{1}$<br>$(58^{2})_{1}(68^{2})_{1}$ | 872 | $(4^{2}6^{3}8)_{2}(5^{4}68)_{2}$<br>$(5^{4}68)_{2}(56^{5})_{1}$<br>$(56^{5})_{1}(6^{6})_{1}$ | 18 | 51:*Pmcm* | 7.5 | 23 | 5 | 90 | *i* | – |
| *eon* | $(4.6.10)_{2}(5^{2}6)_{1}$<br>$(5^{2}10)_{1}(568)_{2}$<br>$(568)_{2}(5.6.10)_{2}$ | 795 | $(4^{2}6^{4})_{2}(5^{4}6^{2})_{1}$<br>$(5^{4}68)_{1}(5^{2}6^{3}8)_{2}$<br>$(5^{2}6^{3}8)_{2}(56^{5})_{2}$ | 20 | 51:*Pmcm* | 11 | 17.5 | 5 | 90 | *i* | – |
| *mfv* | $(4.5.10)_{2}(56^{2})_{1}$<br>$(5.6.10)_{2}(6^{3})_{2}$<br>$(6^{3})_{1}(6^{3})_{1}$<br>$(6^{2}10)_{1}$ | 776 | $(45^{2}6^{3})_{2}(5^{2}6^{4})_{2}$<br>$(56^{5})_{1}(6^{6})_{2}$<br>$(6^{6})_{1}(6^{6})_{1}$<br>$(6^{5}8)_{1}$ | 40 | 65:*Ammm* | 10 | 38 | 5 | 90 | *i* | – |
| | | 836 | 10 types | 20 | 25:*P*2*mm* | 8.5 | 21.5 | 5 | 90 | *i* | – |
| *bta* | $(4.5.12)_{1}(4.5.12)_{1}$<br>$(5^{2}6)_{1}(5^{2}12)_{1}$<br>$(5^{2}12)_{1}(5.6.12)_{1}$<br>$(5.6.12)_{1}$ | 777 | $(45^{2}6^{3})_{1}(45^{2}6^{3})_{1}$<br>$(5^{4}68)_{1}(5^{3}6^{3})_{1}$<br>$(5^{3}6^{3})_{1}(5^{2}6^{4})_{1}$<br>$(5^{2}6_{3}8)_{1}$ | 28 | 59:*Pnmm* | 12 | 24 | 5 | 90 | *i* | – |
| *btb* | $(4.5.12)_{1}(4.5.12)_{1}$<br>$(5^{2}6)_{1}(5^{2}12)_{1}$<br>$(5^{2}12)_{1}(5.6.12)_{1}$<br>$(5.6.12)_{1}$ | 605‡ | $(45^{2}6^{3})_{1}(45^{2}6^{3})_{1}$<br>$(5^{4}68)_{1}(5^{3}6^{3})_{1}$<br>$(5^{3}6^{3})_{1}(5^{2}6^{4})_{1}$<br>$(5^{2}6^{3}8)_{1}$ | 28 | 12:*A*112/*m* | 12.682 | 25.362 | 5.323 | 107.6 | *i* | MTW |
| *mtt* | $(5^{2}6)_{2}(5^{2}10)_{2}(5^{2}10)_{2}$<br>$(5^{2}10)_{1}(5^{2}10)_{1}$<br>$(5.6.10)_{2}(5.6.10)_{2}$ | 604‡ | $(5^{4}6^{2})_{2}(5^{4}68)_{2}$<br>$(5^{4}68)_{2}(5^{4}68)_{1}$<br>$(5^{4}68)_{1}(56^{5})_{2}$<br>$(56^{5})_{2}$ | 24 | 59:*Pnmm* | 11.534 | 22.317 | 5.323 | 90 | *i* | MTT |
| *sft* | $(5^{2}8)_{2}(5^{2}8)_{2}$<br>$(5^{2}8)_{2}(5^{2}8)_{1}$<br>$(5^{2}8)_{1}(5^{2}8)_{2}$<br>$(5^{2}8)_{2}$ | 797 | $(5^{4}68)_{2}(5^{4}68)_{2}$<br>$(5^{4}68)_{2}(5^{4}68)_{1}$<br>$(5^{4}68)_{1}(56^{5})_{2}$<br>$(56^{5})_{1}$ | 24 | 59:*Pnmm* | 8.5 | 27 | 5 | 90 | *i* | – |
| *mln* | $(458)_{1}(4.5.12)_{1}$<br>$(468)_{1}(468)_{1}$<br>$(4.6.12)_{1}(568)_{1})$<br>$(5.6.12)_{1}(58^{2})_{1}$<br>$(6^{2}8)_{1}(6^{2}8)_{1}$ | 839 | $(4^{2}6^{3}8)_{1}(4^{2}6^{3}8)_{1}$<br>$(4^{2}6^{3}8)_{1}(45^{2}6^{3})_{1}$<br>$(45^{2}6^{3})_{1}(5^{2}6^{4})_{1}$<br>$(5^{2}6^{3}8)_{1}(56^{5})_{1}$<br>$(6^{6})_{1}(6^{6})_{1}$ | 80 | 65:*Ammm* | 19.5 | 38 | 5 | 90 | *i* | – |
| | | 838 | $(4^{2}5^{2}67)_{1}(4^{2}5^{2}67)_{1}$<br>$(4^{2}6^{4})_{1}(4^{2}6^{4})_{1}$<br>$(4^{2}6^{4})_{1}(5^{2}6^{3}8)_{1}$<br>$(5^{2}6^{3}8)_{1}(56^{5})_{1}$<br>$(6^{5}8)_{1}(6^{5}8)_{1}$ | 40 | 51:*Pcmm* | 17.5 | 21.5 | 5 | 90 | *i* | – |

‡ 3D nets refined by *DLS* program. † $\alpha = 90°$, $\beta = 90°$.

## 2. Enumeration

The zigzag chain is the *zweier* single chain of Liebau (1985) with a repeat distance near 5 Å for silicates. Smith (1979) converted some horizontal (*h*) edges of a congruent stack of simple three-connected 2D nets into vertical zigzag chains of four-connected $(h,z)^*$-3D nets. We extend this enumeration to those three-connected 2D nets of special interest to synthesis chemists.

Consider a horizontal (*h*) edge between two vertices *A* and *B* of a representative three-connected 2D net *fee*

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 zigzag 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 |
|---|---|---|---|---|---|---|
| 1 | *hex*-cccccc-rotated | 6 | fhe,kch,kga,kub,ton,z | *hex*,*cri''* | hes,lai | Near-compact: hes cages *via* crown-6 |
| 2 | *hex*-cccccc | 6 | afv,c,kbg,keg,lao,z | *hex* (2 types) | afi,kah,kyw | Near-compact: afi cages *via* crown- & rocker-6 |
| 94 | | 3,6,12 | cnc,z,zqa | *hex*,*ttw* | stp | 1D-channel-doublecrown-12 |
| 93 | | 4,6,8 | ati,atn,zz | *fee*,*kyn''* | kaa,kom,ocn | 1D: ocn cages *via* circular-8; 1D:atn-tube *via* rocker 8 |
| 3 | *hex*-ccsccs | 4,6,8 | atn,c,kay,kaz,thr,z | *fee*,*hex* | kaa,kom,lau | 1D-atn channel-rocker-8; lau cages *via* rocker-6 |
| 370 | | 4,6,8 | ati,atn,klg,sao,zz | *fee* | ocn,vvs | 1D-straight-channel of ocn cages sharing circular-8; 1D-zigzag-channel-chair-8 with sidepockets |
| 4 | *hex*-cssccss; (*c*,*h*)**fsy* | 4,6,8 | c,kcb,kea,kei,ken, kew,sao,zz | *fee*,*hex* | kdq,vvs | 1D-channel-chair-8; linked *via* near-circular-6 |
| 961 | | 4,6,8 | ati,atn,klg,zz | *fee* | kaa,ocn | 1D-channel-planar-circular-8; 1D channel-sofa-8 |
| 374 | | 4,6,8 | klg,zz | *fee* | – | 1D-channel-ovate-non-planar-8 with sidepockets |
| 95 | | 4,6,12 | cnc,voi,zz | *gml*,*kuz''*,*kyd''* | can,kok | 1D-cnc-tube with double-crown-12; can cages *via* 6 |
| 738 | | 4,6,12 | cnc,kay,z,zhp | *gml*,*hex* | kab,kah,kok,lau,zlv | 1D-channel-elliptical-crown-12 |
| 382 | | 4,6,12 | eng,nao,voi,zhz,zz | *gml* | can,eni,kah,oth | 1D-channel-eni cages *via* circular-12; 1D-channel-elliptical-nonplanar-12 |
| 755 | | 4,6,12 | eng,nao,voi,zhz,zz | *gml* | can,eni,oth | 1D-channel-circular-12 & 1D-channel-nonplanar-asymmetric crown-12 |
| 753 | | 4,6,12 | kcn,nao,zz | *gml*,*kuz''* | kah,koh,oth | 1D-channel *via* nonplanar-12; alternating sidepockets |
| 384 | | 4,6,12 | nao,zz | *gml* | kah,oth | 1D-channel-nearcircular-lounger-12 |
| 754 | | 4,6,12 | nao,voi,zz | *gml* | can,oth | 1D-channel *via* nonplanar-12; annular sidepockets on one side |
| 424 | *hex*-ccssss, cssccs | 4,6,10 | c,z,zz | *ffs*,*hex* (2 types) | baf | 1D-channel-very nonplanar-10 with sidepockets |
| 423 | | 4,6,8,12 | ati,atn,cnc,z,zz | *tth* | baf,kaa,ocn | 1D-channel-doublecrown-12; 1D-circular-8 *via* ocn cages; 1D-channel-rocker-8 |
| 468 | *hex*: csscss, ssssss | 4,6,12 | c,oxv,zhz,zz | *fos*,*hex* | hpr | 1D-channel-elliptical-nonplanar-12 |
| 470 | *hex*: ccssss-*ortho* | 4,6,12 | c,cnc,z,zz | *fos*,*hex* | baf | 1D-channel-very distorted-12; baf cages *via* nearplanar & rocker-6 |
| 718 | | 4,6,12 | cnc,eng,oxv,zz | *twy* | eni,hpr | 1D-channel-circular-12; 1D-channel-doublecrown-12 |
| 469 | | 4,6,8,16 | atn,oiv,z,zz | *hex*,*rho* | baf | 1D-channel-doublecrown-16; 1D-channel- doublecrown-8 |
| 467 | | 4,6,8,16 | ati,oiv,oxv,zz | *rho* | hpr,ocn | 1D-channel-square-doublecrown-16 |
| 719 | | 4,6,24 | oxv,voi,von,zz | *tsv* | can,hpr | 1D-channel-doublecrown-24 |
| 721 | | 4,6,8,12 | atn,eng,voi,zz | *ltl* | can,eni,kaa | 1D-channel-circular-12 *via* eni cages; 1D-channel-very distorted-8 |
| 722 | | 4,6,8 | ksf,p,sao,ton,z,zz | *fsy*,*hex* | hes,kdq,lai,vvs | 1D-channel-elliptical-nonplanar-8 |
| 549 | *hex*: cccccc, ccsccs | 4,6,8 | afv,atn,c,kay,lao,thr,z | *fsy*,*hex* (2 types) | afi,kaa,kah,lau | 1D-channel-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 |
|---|---|---|---|---|---|---|
| 7 | *hex*: ccccss | 4,6,8 | c,mao,nao,z,zz | *fsy*,*hex* (2 types) | kah,oth | 1D-channel-distorted-8; separated by oth cages in vertical direction |
| 1246 | | 4,6,8 | atn,z,zz | *brw* | kaa,kom,xib | 1D-channel-circular-6 |
| 723 | *hex*: ccccss, ccsccs | 4,6,8 | atn,c,kay,mao,nao, thr,z,zz | *brw*,*hex* (2 types) | kah,lau,oth | 1D-channel-chair-8; 1D-channel-rocker-8 |
| 96 | | 4,6,8 | fhe,kei,kua,kub,s,sao, ton,z,zz | *brw*,*hex* | hes,kdq,lai,vvs | 1D-channel-chair-8 |
| 749 | | 4,6,7 | kci,kft,z,zz | *bor*,*kuz″* | kdp | Compact: nonplanar-7,6,6 |
| 98 | (*c*,*s*)**hex* | 5,6,8 | c,hhz,mao,s,scs,z | *bik*,*hex* | pes | 1D-channel-elliptical-sofa-8 with annular sidepockets |
| 242 | | 5,6,8 | hhz,kce,kcg,kcl,z | *bik*,*hex* | eun,kum,pes | 1D-channel-chaiselongue-8 with sidepockets |
| 243 | | 5,6,8 | hhz,mao,z | *bik*,*hex* | eun,pes | 1D-channel-elliptical-nonplanar-8 |
| 724 | *hex*: cccccc, ccccss,cccsss | 4,6,10 | afv,c,lao,nao,z,zz | *hex* (2 types), *twl* | afi,baf,oth | 1D-channel-elliptical-nonplanar-10 |
| 569 | *hex*: ccccss, ccssss | 4,6,10 | c,nao,z,zz | *fsv*,*hex* (2 types) | baf,kah,oth | 1D-channel-elliptical-nonplanar-10 |
| 834 | *hex*: ccsccs, ccssss,csscss | 4,6,8,10 | atn,c,kay,sao,thr,z,zz | *hex* (2 types), *ttv* | baf,lau | 1D-channel-elliptical-nonplanar-10; 1D-channel-rocker-8 |
| 783 | (*h*,*s*)**hex* | 4,6,8,10 | oxv,s,sao,tao,z,zz | *hex*,*ooo* | hpr,kdq,vvs | 1D-channel-elliptical-bifurcated-10 & sofa-8 |
| 550 | *hex*: cccccc, ccssss | 4,6,12 | afv,c,cnc,lao,z,zz | *fix*,*hex* (2 types) | afi,baf,kah | 1D-channel-elliptical-nonplanar-12 |
| 546 | *hex*: ccccss, ssssss | 4,6,12 | c,nao,oxv,z,zz | *fix*,*hex* (2 types) | hpr,kah,oth | 1D-channel-elliptical-nonplanar-12 |
| 785 | *hex*: ccccss, ccssss,ssssss | 4,6,12 | c,cnc,nao,oxv,z,zz,zzi | *hex* (2 types), *toh* | baf,hpr,kah,oth | 1D-channel-elliptical-nonplanar-12; 1D-channel-elliptical-very nonplanar-12 |
| 775 | *hex*: csscss, ssssss | 4,6,8,12 | c,sao,zz | *hex*,*vvv* | hpr,vvs | 1D-channel-elliptical-rocker-12; 1D-channel-chair-8 |
| 555 | *hex*: ccsccs, ccssss | 4,6,8,12 | atn,c,cnc,kay,thr,z,zz | *hex* (2 types), *vvv* | baf,lau | 1D channel-nonplanar-elliptical-12; 1D-channel-rocker-8 |
| 835 | *hex*: ccssss, csscss,ssssss | 4,6,14 | c,oxv,z,zz | *hex* (2 types), *uun* | baf,hpr | 1D-channel-elliptical-nonplanar-14 |
| 768 | | 4,5,6,8 | atn (2 types), z,zz | *fef* | hsp,kaa | 1D-channels-twisted-rocker-8 (2 types) |
| 769 | (*c*,*z*)**hex* | 4,5,6,8 | atn,c,hhz,kcf,mao,s,z | *fef*,*hex* (2 types) | kaa,kah,mtw,pes | 1D-channels-chair & rocker-8 |
| 766 | | 4,5,6,12 | cnc,z,zz | *bks* | hvx | 1D-channel-elliptical-doublecrown-12 |
| 767 | | 4,5,6,12 | hhz,kcn,z,zz | *bks* | pes | 1D-channel-elliptical-nonplanar-12 |
| 704 | | 4,5,6,18 | kcf,z,zz | *eus* | mtw,pes | 1D-channel-nearcircular-planar-18 except for four z |
| 115 | 3(*h*,*z*)**krp* | 4,6,12 | kay,nao,osi,z,zz | *krp* | kah,lau,oth | 1D-channel-nonplanar-12 with 4 zigs |
| 558 | *hex*: ccccss, csscss | 4,6,8 | c,nao,wao,z,zz | *fto*,*hex* (2 types) | kah,oth | 1D-channel-chair-8 |
| 759 | *hex*: cccccc, ccsccs | 4,6,8 | afv,atn,c,kay,lao,thr,z | *fto*,*hex* | afi,kaa,kah,lau | 1D-channel-rocker-8 |
| 756 | *n***hex* | 4,6,8 | n,sao,ton,z,zz | *fto*,*hex* | hes,lai | 1D-channel-chair-8 with sidepockets |
| 843 | (*d*,*h*)**hex* | 4,6,8 | d,sao,ton,z,zz | *ffv*,*hex* | lai,vvs | 1D-channel-sofa-8 |
| 844 | *hex*: ccccss, ccsccs,csscss | 4,6,8 | atn,c,kay,nao,thr,wao, z,zz | *ffv*,*hex* (2 types) | kah,lau,oth | 1D-channel-chair-8; 1D-channel-rocker-8 |
| 760 | *hex*: cccccc, ccccss | 4,6,8 | afv,c,lao,mao,nao,z,zz | *apd*,*hex* | afi,kah,oth | 1D-channel-chair-8 |
| 762 | *l***hex* | 4,6,8 | fhe,l,sao,ton,z,zz | *apd*,*hex* | hes,vvs | 1D-channel-nonplanar-8 |
| 761 | *hex*: cccccc, ccsccs | 4,6,8 | afv,atn,c,kay,lao,thr,z | *apd*,*hex* (2 types) | afi,kaa,kah,lau | 1D-channel-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 |
|---|---|---|---|---|---|---|
| 841 | *hex*: cccccc, ccccss,ccsccs | 4,6,8 | afv,atn,c,kay,lao,mao, thr,z,zz | *feo*,*hex* (2 types) | afi,kab,kah,oth | 1D-channel-chair-8 |
| 773 | *f*hex* | 4,6,8 | f,fhh,sao,ton,z,zz | *feo*,*hex* | hes,lai,vvs | 1D-channel-elliptical-chair-8 |
| 852 | | 5,6,12 | hhz,z | *eui*,*hex* | eun,pes,xia | 1D-channel-nonplanar-12 |
| 772 | | 5,6,8 | atn,hhz,kck,mao,ton,z | *hex*,*nos* | hes,kah,lai,pes,son | 1D-channels-chair & rocker-8 |
| 322 | | 5,6,8 | atn,hhz,lao,z,zqc | *nos* | afi,eun,kaa,kah, pes,sop | 1D-channel *via* sop cages-elliptical-8; 1D channel-rocker-8 |
| 764 | | 5,6,7 | hhz,hzh,z,zhh | *hex*,*vnv* | pes,zsv,zzh (and other complex units) | 1D-channels-nonplanar-7 |
| 765 | (*c*,*s*)**hex* | 5,6,8 | afv,c,hhz,lao,mao,s,z | *hex*,*urg* | afi,kah,pes | 1D-channel-mao tube |
| 770 | *hex*: cccccc, ccssss,cssscs | 4,6,10 | afv,c,lao,z,zz | *fsf*,*hex* (2 types) | afi,baf,kah,xio | 1D-channel-elliptical-nonplanar-10 |
| 771 | *hex*: cccccc, ccccss,ccssss | 4,6,8 | afv,c,lao,nao,z,zz | *ftn*,*hex* (2 types) | afi,baf,kah,oth,xio | 1D-channel-elliptical-nonplanar-10 |
| 323 | (*c*,*s*)**hex* | 4,5,6,8,12 | c,cnc,hhz,mao,s,z,zz | *hex* (2 types), *uiv* | kac,kah,pes | 1D-channel-elliptical-nonplanar-12; 1D-channel-chair-8 |
| 827 | | 4,6,8,12 | atn,cnc,oxv,z,zqb,zz | *vss* | hpr,xib | 1D-channel-elliptical-doublecrown-12; 1D-channel-elliptical-rocker-8 |
| 820 | *hex*: ccccss, ccssss | 4,6,8,12 | c,cnc,mao,nao,z,zz | *hex* (2 types), *vss* | baf,kah,oth | 1D-channel-elliptical-nonplanar-12; 1D-channel-chair-8 |
| 861 | *hex*: cccccc, ccccss,ssssss | 4,6,12 | c,lao,nao,oxv,z,zz,zzi | *bsh*,*hex* (2 types) | afi,hpr,kah,oth | 1D-channel-zzi-tube *via* elliptical-nonplanar-12 |
| 786 | *hex*: cccccc, ccssss | 4,6,12 | afv,c,cnc,lao,z,zz | *bsh*,*hex* (2 types) | afi,baf,kah,xio | 1D-channel-elliptical-nonplanar-12 |
| 840 | *hex*: ccccss, ccssss,ssssss | 4,6,14 | c,nao,oxv,z,zz | *fvo*,*hex* (2 types) | baf,hpr,kah,oth | 1D-channel-elliptical-nonplanar-14 |
| 792 | (*h*,*p*)**hex* | 4,5,6,8,12 | atn,hhz,kcf,p,z,zzi | *hex*,*mor* | kaa,kah,eun,mtw, pes | 1D-channel-rocker-12 (zzi tube with sidepockets); 1D-channel-rocker-8 |
| 793 | | 4,5,6,8,12 | hhz,z,zhz,zqd,zz | *hex*,*mor* | eun,kah,pes,xic | 1D-channel-hammock-12 (zhz tube with sidepockets); 1D-channel-elliptical-8 *via* xic cages |
| 794 | | 4,5,6,8,12 | hhz,sao,xao,z,zz | *hex*,*mor* | kah,pes,vvs | 1D-channels-sofa-12 & sofa-8 |
| 781 | | 4,5,6,10 | hhz,z,zz | *dac*,*hex* | eun,kah,pes | 1D-channel-distorted-sofa-10 |
| 782 | (4-repeat,*h*,*h*′) **hex* | 4,5,6,10 | hhz,z,zz | *dac*,*hex* | kah,pes | 1D-channel-distorted-sofa-10 |
| 784 | (4-repeat,*h*,*h*′) **hex* | 4,5,6,10 | hhz,kcf,tao,z | *dac*,*hex* | eun,kah,mtw,pes | 1D-channel-offset-rocker-10 |
| 863 | (*c*,*h*,*s*)**hex* | 4,5,6,8 | atn,c,hhz,mao,s,z | *hex* (2 types), *urv* | kaa,kah,pes | 1D-channels-sofa & rocker-8 |
| 779 | | 4,5,6,10 | hhz,z,zz | *dao*,*hex* | kah,pes | 1D-channel-sofa-10 |
| 778 | (*h*′,*z*′,4)**hex* | 4,5,6,10 | hhz,kcf,tao,z | *dao*,*hex* | eun,kah,mtw,pes | 1D-channel-rocker-10 |
| 780 | | 4,5,6,10 | hhz,z,zz | *dao*,*hex* | eun,kah,pes | 1D-channel-sofa-10 |
| 791 | | 4,5,6,10 | hhz,z,zz | *hex*,*sxn* | eun,kah,pes | 1D-channel-chaiselongue-10 |
| 790 | | 4,5,6,10 | hhz,z,zz | *hex*,*sxn* | kah,pes | 1D-channel-sofa-10 |
| 789 | | 4,5,6,10 | hhz,kcf,z | *hex*,*sxn* | eun,kah,pes | 1D-channel-ovate-nonplanar-10 |
| 758 | (*h*′,*z*′,4)**hex* | 4,5,6,10 | hhz,kcf,tao,ton,z | *fes*,*hex* | kah,hes,lai,mtw,pes | 1D-channel-rocker-10 |
| 801 | | 4,5,6,10 | hhz,lao,z,zz | *fes*,*hex* | afi,kah,pes | 1D-channel-sofa-10 |
| 800 | (*f*,*h*′,)**hex* | 4,5,6,12 | f,hhz,kcf,ton,z,zhz,zz | *bab*,*hex* | hes,kah,lai,pes | 1D-channel-nearcircular-rocker-12 |
| 830 | | 4,5,6,12 | hhz,lao,nao,xao,z, zhz,zz | *bab*,*hex* | afi,kah,oth,pes | 1D-channels-boat & sofa-12 |
| 864 | | 4,6,12 | kay,nao,ton,z,zhz,zz | *hex*,*uss* | hes,kab,kah,lai,oth | 1D-channel-elliptical-nonplanar-12 |
| 865 | (*c*,*h*,*s*)**hex* | 4,6,7,8 | c,hzh,nao,s,sao,z,zz | *hex*,*uhe* | ccs,kah,oth,vvs,zsv | 1D-channels-sofa-8 & chair-7 |
| 848 | (*h*,*x*)**hex* | 4,6,8 | hhx,sao,ton,x,z,zz | *bso*,*hex* | hes,lai,vvs | 1D-channel-sofa-8 |
| 851 | *hex*: ccccss, ccsccs,cssscs | 4,6,8 | atn,c,nao,thr,wao,z,zz | *bso*,*hex* (2 types) | kah,lau,oth | 1D-channel-chair-8; 1D-channel-rocker-8 |
| 787 | *hex*: ccccss, ccsccs | 4,6,8 | atn,c,kay,mao,nao, thr,z,zz | *bso*,*hex* (2 types) | kah,lau,oth | 1D-channel-chair-8; 1D-channel-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 |
|---|---|---|---|---|---|---|
| 866 | | 4,6,8 | atn,kay,z,zqb,zz | *tva* | kaa,lau,xib | 1D-channel-rocker-8 |
| 803 | | 4,6,8 | ati,atn,z,zqb,zz | *stg* | kaa,ocn,xib | 1D-channel-circular-8 *via* ocn cages; 1D-channel-rocker-8 |
| 802 | (*h*,*v*)**hex* | 4,6,8 | ksr,sao,ton,v,z,zz | *hex*,*stg* | hes,lai,vvs | 1D-channel-sofa-8 |
| 807 | *hex*: cccccc, ccsccs | 4,6,8 | afv,atn,c,kay,lao,thr,z | *fst*,*hex* (2 types) | afi,kaa,kah,lau | 1D-channel-rocker-8 |
| 806 | (*e*,*h*)**hex* | 4,6,8 | e,kta,sao,ton,z,zz | *fst*,*hex* | hes,lai,vvs | 1D-channel-sofa-8 |
| 805 | *hex*: cccccc, cccccss,cssscss | 4,6,8 | afv,c,lao,nao,wao,z,zz | *fst*,*hex* (2 types) | afi,kah,oth | 1D-channel-chair-8 |
| 796 | (*c*,*h*,*s*)**hex* | 4,5,6,8 | c,hhz,mao,nao,s,z,zz | *hes* (2 types), *rxt* | kah,oth,pes | 1D-channels-sofa & chair-8 |
| 867 | (*h*,*w*)**hex* | 4,6,8 | ktc,sao,ton,w,z,zz | *fss*,*hex* | hes,lai,vvs | 1D-channel-sofa-8 |
| 868 | (*c*,*h*,*s*)**hex* | 4,6,7,8 | c,s,sao,vao,z,zz | *hex*,*uhi* | vvs,zfs,zsv | 1D-channels-chair-8 & -7 |
| 804 | | 5,6,10 | hhz,kck,tao,z | *fer*,*hex* | eun,kah,pes,son | 1D-channel-hammock-10 |
| 606 | | 5,6,10 | hhz,kcg,kcj,tno,ton,z | *fer*,*hex* | hes,kdx,lai,pes | 1D-channel-chair-10 |
| 823 | | 5,6,7 | hhz,hzh,z | *een*,*hex* | kah,pes,zsv | 1D-channel-chair-7 |
| 821 | (*c*,*h*,*z*′)**hex* | 5,6,7 | c,hhz,hzh,z | *een*,*hex* | eun,kah,pes,zsv | 1D-channel-chair-7 |
| 244 | | 5,6,8 | hhz,z,zao | *biz*,*hex* | kah,pes | 1D-channel-near elliptical-nonplanar-8 |
| 245 | | 5,6,8 | hhz,sss,z,zao | *biz*,*hex* | eun,pes | 1D-channel-near elliptical-nonplanar-8 |
| 824 | | 5,6,8 | hhz,lao,z,zao | *fex*,*hex* | afi,kah,pes | 1D-channel-distorted-8 |
| 832 | (*c*,*h*′,*z*′)**hex* | 5,6,7 | c,hhz,hzh,ton,z | *exn*,*hex* | eun,hes,kah,lai, pes,zsv | 1D-channel-chair-7 |
| 833 | | 5,6,7 | hhz,hzh,lao,z | *exn*,*hex* | afi,kah,pes | 1D-channel-chair-7 |
| 825 | (*c*,*h*′,*z*′)**hex* | 5,6,7 | c,hhz,hzh,ton,z | *exe*,*hex* | hes,kah,lai,pes,zsv | 1D-channel-chair-7 |
| 826 | | 5,6,7 | hhz,hzh,lao,z | *exe*,*hex* | afi,kah,pes,zsv | 1D-channel-hzh tube *via* chair-7 |
| 869 | *hex*: cccccc, ccccss,ccssss | 4,6,10 | c,lao,nao,z,zz | *eig*,*hex* (2 types) | afi,baf,kah,oth | 1D-channel-elliptical-nonplanar-10 |
| 870 | | 4,5,6,14 | hhz,kcf,z | *eug*,*hex* | eun,kah,mtw,pes | 1D-channel-elliptical-rocker-14 |
| 1247 | | 4,5,6,14 | hhz,hsr,hst,hsu,z,zz | *eug*,*hex* | eun,hsp,pes | 1D-channel-irregular-nonplanar-14 |
| 828 | (*g*,*h*′)**hex* | 4,6,8 | g,ksk,sao,ton,z,zz | *hex*,*tvt* | hes,lai,vvs | 1D-channel-elliptical-sofa-10 |
| 829 | *hex*: cccccc, ccccss,ccsccs | 4,6,8 | atn,c,kay,lao,mao, nao,z,zz | *hex*,*tvt* | afi,kaa,kab,kah, lau,oth | 1D-channel-elliptical-nonplanar-8; 1D-channel-rocker-8 |
| 850 | *hex*: cccccc, ccccss,ccsccs | 4,6,8 | afv,atn,c,kay,lao,mao, nao,thr,z,zz | *fsm*,*hex* (2 types) | afi,kah,lau,oth | 1D-channel-chair-8 |
| 849 | (*h*,*i*)**hex* | 4,6,8 | hhi,i,sao,ton,z,zz | *fsm*,*hex* | hes,lai,vvs | 1D-channel-sofa-8 |
| 831 | (*c*,*h*′,*s*,4)**hex* | 4,5,6,7,8 | c,hhz,s,vao,wao,z,zz | *hex*,*svn* | kah,pes,zsv | 1D-channel-sofa-8; 1D-channel-chair-7 |
| 799 | | 4,5,6,10 | hhz,ton,z,zz | *fev*,*hex* | hes,kah,lai,pes | 1D-channel-nearelliptical-nonplanar-10 |
| 872 | (*c*,*h*,*s*)**hex* | 4,5,6,8 | c,hhz,mao,s,ton,wao,z,zz | *hex*,*nee* | hes,kah,pes | 1D-channel-sofa-8 |
| 795 | | 4,5,6,8,10 | hhz,mao,nao,tno,ton,z,zz | *eon*,*hex* | hes,kah,lai,oth,pes | 1D-channel-chair-10; 1D-channel-elliptical-chair-8 |
| 776 | (*h*′,*z*′,4)**hex* | 4,5,6,10 | hhz,kcf,tao,ton,z | *hex*,*mfv* | hes,kah,lai,mtw,pes | 1D-channel-elliptical-rocker-10 |
| 836 | | 4,5,6,10 | hhz,lao,z,zz | *hex*,*mfv* | afi,kah,pes | 1D-channel-nearelliptical-nonplanar-10 |
| 777 | *f***hex* | 4,5,6,12 | f,hhz,kcf,ton,z,zzi | *bta*,*hex* | eun,hes,kah,lai, mtw,pes | 1D-channel-rocker-12 |
| 605 | (*f*,*h*′,4)**hex* | 4,5,6,8,12 | f,hhz,kce,kcf,kcg,kfq, kug,ton,z,zzi | *btb*,*hex* | eun,hes,lai,mtw,pes | 1D-channel-rocker-12 |
| 604 | | 5,6,10 | hhz,kcg,kcj,kcm,ton,z | *hex*,*mtt* | hes,kdx,lai,pes | 1D-channel-chaiselongue-10 |
| 797 | | 5,6,8 | hhz,mao,z | *hex*,*sft* | kah,pes | 1D-channel-sofa-8 |
| 839 | (*h*,*p*)**hex* | 4,5,6,8,12 | atn,hhz,kcf,p,ton,wao, z,zhz,zz | *hex*,*mln* | hes,kah,lai,mtw,pes | 1D-channels-rocker-12 & sofa-8 |
| 838 | | 4,5,6,8,12 | hhz,mao,nao,sao,xao, z,zz | *hex*,*mln* | kah,oth,pes | 1D-channels-sofa-12 & chair-8 |

($48^2$) (Fig. 1*a*). Each heavy-line edge of the 2D net is converted into a tilted edge in the enumeration, while each open-line edge remains horizontal. Conversion of a heavy-line edge into a zigzag chain generates two tilted edges at each of the two vertices *A* and *B* (Fig. 1*b*). Each vertex retains the other two *h* edges to become four-connected. The sequence of zig and zag is repeated indefinitely to generate a *z* chain. Fig. 1(*c*) shows the 3D net (CTF catalogue number 3) after DLS refinement. The adjacent horizontal edges cannot be converted into a zigzag chain for an enumeration restricted to four-connected 3D nets, and the $z$ edges must be separated by the $h$ edges. A framework silicate with adjacent tetrahedral atoms at ~3.1 Å has a $z$-repeat near 5 Å, with a height increment of 2.5 Å between adjacent zigzag left ($A$) and right ($B$). Closure of each ring of the parent 2D net requires that an even number of horizontal branches be converted into zigzag chains.

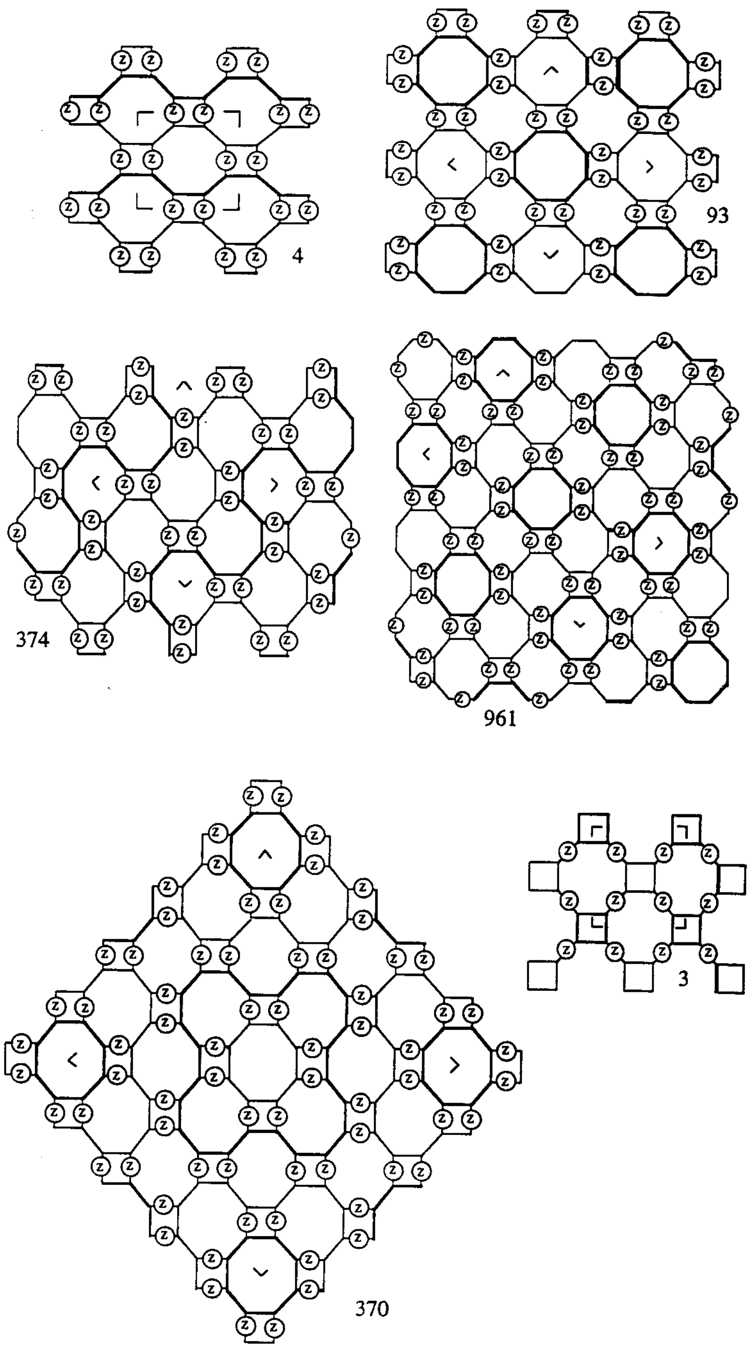


Fig. 2. Six 3D nets derived from the 2D *fee* net ($48^2$). Projections of the four-connected 3D nets display different arrangements of $h$ (unlabeled) and $z$ (labeled) edges. The $h$ edges have two different heights indicated by thick and thin lines. The geometrical projection of $z$ edges should be shorter than for the $h$ edges to attain tetrahedral or near-tetrahedral geometry.

Tilting of the *unconverted* horizontal edges would permit conversion of a horizontal ring into a spiral. Thus conversion of a horizontal 12-ring into six *z*, each alternating with a quasi-horizontal edge, generates a small set of 3D nets with helical channels spanned by a non-planar 12-ring window. Enumeration of such 3D nets, using different sequences of tilts, was performed for the 4.6.12 *gml* 2D net (Smith *et al.*, in preparation), and is underway for other selected 2D nets. They are important for chemists attempting to synthesize chiral materials.

Returning to the simpler (*h,z*)*-3D nets, one 2D net can yield several 3D nets with different arrangements of *h* and *z* edges; for example, two 3D (*h,z*)*-nets from the 2D *hex* ($6^3$) net (Smith, 1979). The surviving horizontal edges can form a *closed ring* (*e.g.* Fig. 2, nets 3, 93, 370 and 961; catalog number in the CTF databases) or an *infinite chain* (in 2D; *band* in 3D) along certain directions of the unit cell (Fig. 2, nets 4 and 374).

The six 3D nets in Fig. 2 were derived from the 2D net *fee* ($48^2$) by Smith (1979) and Hawthorne & Smith (1988). Horizontal four- and eight-rings occur in nets 3 and 93. Infinite crankshafts of *h* edges lie at two levels running east–west in net 4. In net 374, pairs of *z* edges across the four-rings alternate in orientation to generate serrated chains at two levels. In net 370, *h* edges form an eight-ring surrounded by a 24-ring at a different height to form a 'square' subfragment of the net. Eight-rings can be combined with infinite chains in 2D to produce another type of 3D net; the simplest (961) has eight-rings alternating with serrated chains. The *hex* ($6^3$) net yields only two 3D (*h,z*)*-nets (Smith, 1979).

For the 2D net *gml* (4.6.12), 3D net 95 (found in cancrinite) was described by Smith (1979), and nets 382,

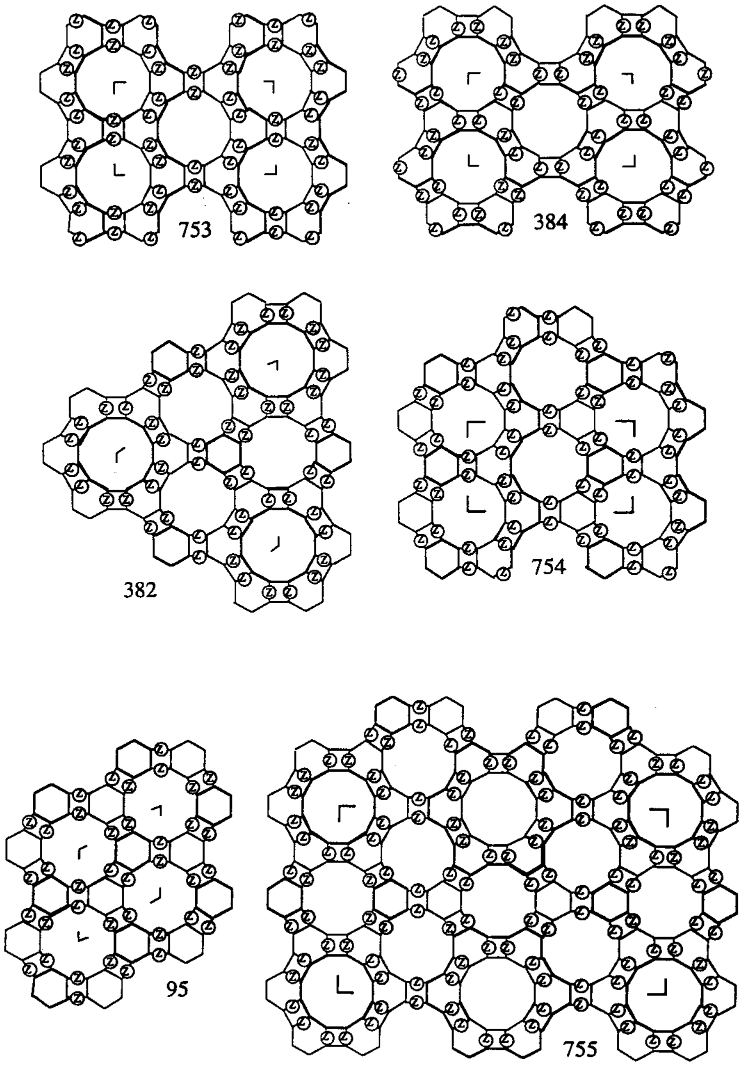


Fig. 3. Six 3D nets with different assignments of *z* and *h* edges on the *gml* net (4.6.12).

384 and 753 were generated by Hawthorne & Smith (1988). Two more nets (754 and 755) are added here (Fig. 3). Net 753 with horizontal chains running north–south occurs in the aluminophosphate $AlPO_4$-36 (Smith *et al.*, 1993). In net 382, a 12-ring is surrounded by a gear-shaped 24-membered horizontal circuit to form a nested unit which is joined *via* a six-ring through zigzag chains; the *a* axis of the unit cell is twice as large as that of net 95. In net 384, serrated chains run east–west. In net 754, serrated chains alternate with six-rings, which themselves alternate at two levels. Net 755 is an orthorhombic relative of net 382.

For the 2D nets with five-rings, *bik* $(5^28)_2(58^2)_1$ provides an instructive triple set of 3D nets (Fig. 4). Net 98 is represented by bikitaite (Smith, 1979). Nets 242, represented by the framework structure of $CsAlSi_5O_{16}$ (Araki, 1980), and 243 were derived by Smith & Bennett (1984). A common feature of these three nets is that horizontal edges do not form closed rings. The chains differ: three-repeat saw (*s*) lying north–south on the page in net 98; 12-repeat serrated east–west in net 242, and six-repeat serrated southwest–northeast in net 243.

Sometimes it is not obvious how to arrange *h* and *z* in a 2D net, especially for those with odd-number rings. For example, a zigzag 3D net was overlooked initially from the 2D net *bor* $(47^2)_2(7^3)_1$, but it turned up later as net 749 (Fig. 5) in the framework structure of $KBGe_2O_6$ (Klaska *et al.*, 1986). Also in Fig. 5, net 1153 represents the structure of a new aluminophosphate UiO-6 derived from the 2D net $(46^2)_1(4.6.12)_2(6^{12}12)_1$ (Akporiaye *et al.*, 1996). Distortion of the 2D *krp* net allows a neat transformation of some edges into a *z* chain to form the 3D net.

Net 1246 (Fig. 5) has just been found in the crystal structure of AlPO-53C, the dehydration product of as-synthesized AlPO-53. Details of this crystal structure are being submitted to the IZA-SC with suggested code AFC, and are given by Smith (1999*a*).

Originally, 3D net 870 was generated from the 2D net *eug* $(4.5.14)_2(5^3)_1(5^214)_2(5^214)_2(5^214)_1$. The new structure of CIT-5 (CFI) (Wagner *et al.*, 1997) turned out to be another 3D *z**-net from the *eug* 2D net with a different arrangment of the *h* and *z* edges (Fig. 6). In net 870, the *h* edges form squares while in net 1247 they form pentagons.

Table 1 lists the 3D (*h*,*z*)-3D nets, of which 20 occur in known structures. 77 out of the 131 three-connected 2D nets yielded 138 3D nets. The remaining 2D nets have parity or incompatibility problems. Most of the nets occurring in known structures have simple 2D nets. However, nets 604 and 605 in the ZSM-23 (Rohrman *et al.*, 1985) and ZSM-12 (Lapierre *et al.*, 1985) structures (Fig. 7) have complex 2D nets with seven circuit symbols each. Each 3D net with only even-number rings permits alternation of two types of atoms on the *T* vertices; the lowering of the space-group symmetry is given in Table 1. Unlike the all-crankshaft nets, the mirror plane perpendicular to the zigzag chain is retained for atomic alternation. Table 2 lists alternative topological

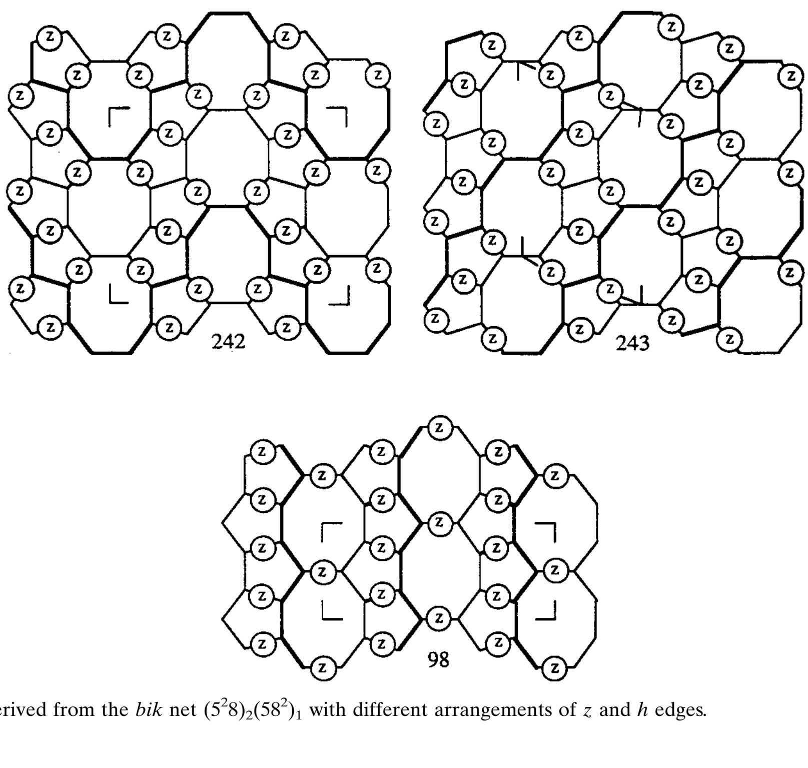


Fig. 4. Three 3D nets derived from the *bik* net $(5^28)_2(58^2)_1$ with different arrangements of *z* and *h* edges.

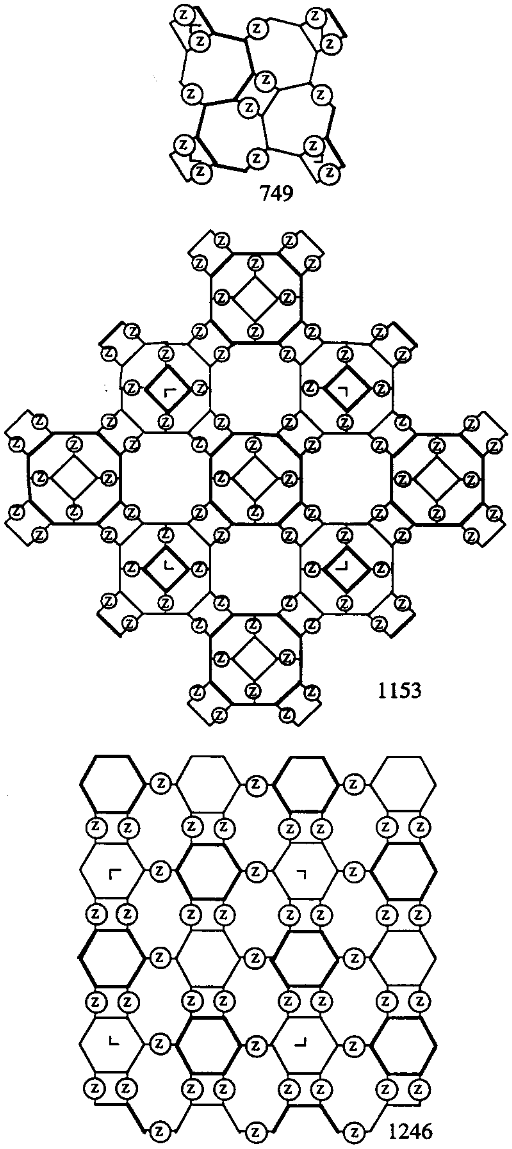


Fig. 5. Projection of nets 749, 1153 and 1246 down the *z* chain.

descriptions, subunits and pore space of 3D zigzag nets using the conventions of Han & Smith (1999).

### 3. DLS refinement

59 nets with higher symmetry and smaller unit cell were selected for DLS refinement (Baerlocher *et al.*, 1977), including most known structures (Table 3†). For cristobalite, the geometry is constrained by the space-group symmetry with angle $T—O—T$ at 180°,

† Table 3 has been deposited and is available from the IUCr electronic archives (Reference: BR0076). Services for accessing these data are described at the back of the journal.

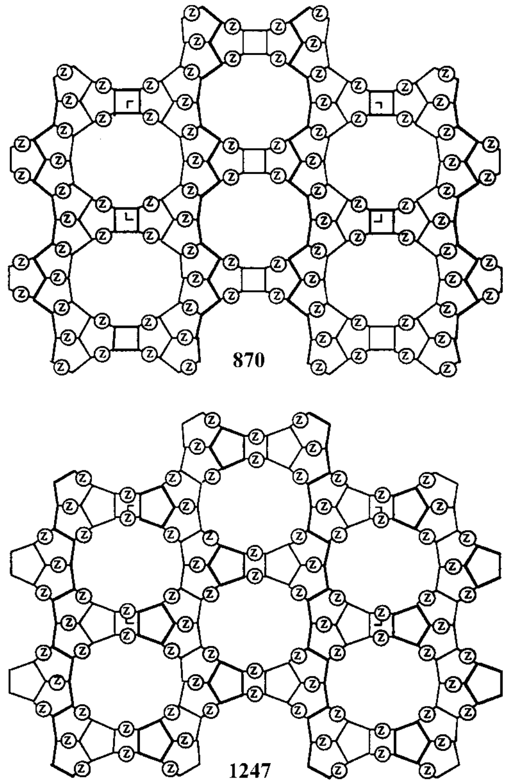


Fig. 6. Projection of nets 870 and 1247 derived from the 2D net *eug* $(4.5.14)_2(5^3)_1(5^214)_2(5^214)_2(5^214)_1$.

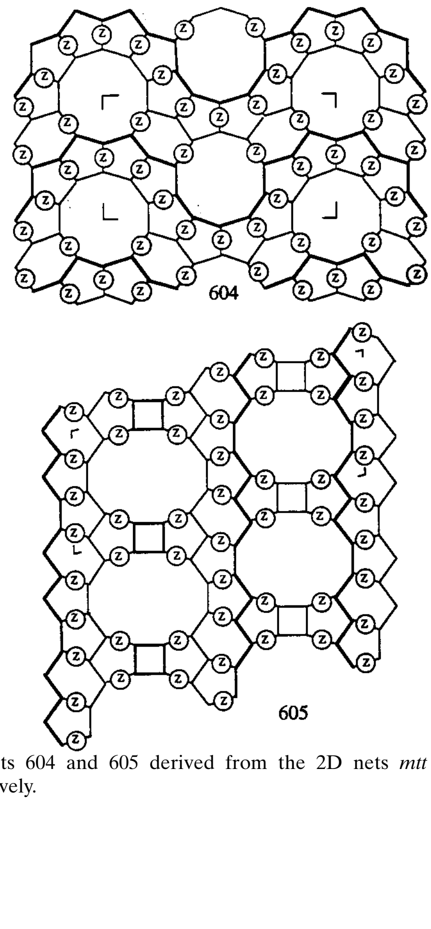


Fig. 7. Nets 604 and 605 derived from the 2D nets *mtt* and *btb*, respectively.

precluding a simple DLS refinement. Most of the DLS refinements yielded satisfactory results with the $R$ factor between 0.001 and 0.002. Several 3D nets have a higher $R$ factor because of their lower flexibility. In particular, the location of the $T$ vertices on the horizontal mirror plane limits their freedom to adjust to constraints in the horizontal direction. The near-constancy of the $c$ repeat at ~5.3 Å for most 3D nets is useful in searching for potential new members in unknown structures.

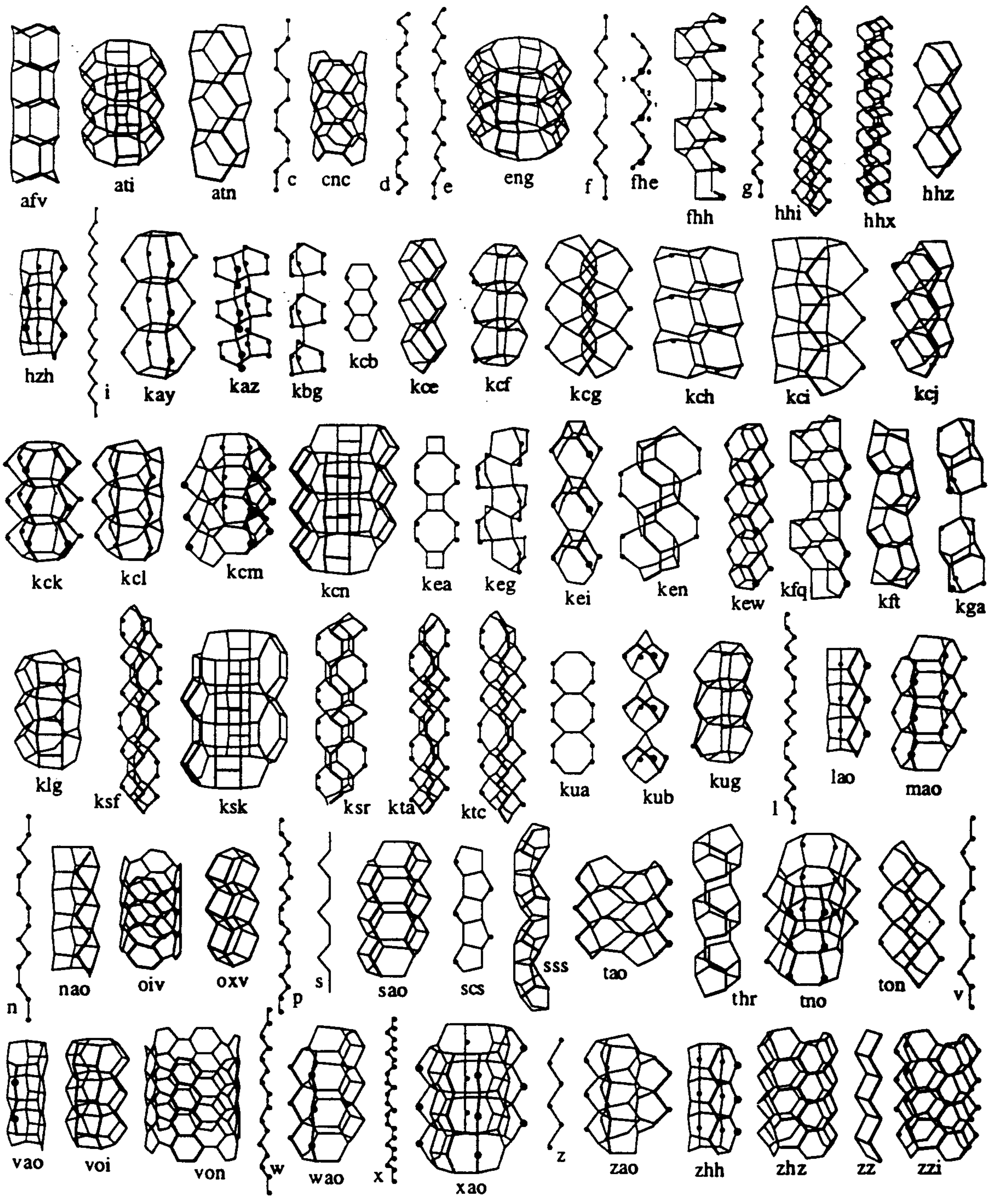


Fig. 8. 1D subunits with CTF three-letter codes arranged alphabetically. Four units are not shown: *zqa*, *zqb*, *zqc* and *zqd*.

## 4. Topology

### 4.1. *1D subunits*

Many one-dimensional (1D) subunits exist in these 3D nets, including chains, tubes and columns entered into the CTF database (Andries & Smith, 1993*b*). Obviously each net has either zigzag chains (*z*) or double zigzag chains (*zz*), or both. Fig. 8 shows the 1D subunits in Table 2 except *zqa*, *zqb*, *zqc* and *zqd*. Some common ones are now described. The *hhz* and *ton* units combine a five- and six-ring with zigzag chains, respectively. The *nao* unit is the combination of a six-ring with both *z* and *zz* chains. The *atn* unit combines an eight-ring with zigzag chains, and the *mao* unit uses a different configuration. The *sao* unit is formed by an eight-ring coupled with *z* and *zz* chains. The *cnc* unit is the combination of a 12-ring with *z* chains. The *afv* and *thr* units are tubes formed by a six-ring and crankshaft chains with different up–down sequence.

In addition to the *z* and *c* chains, the following chains (Fig. 8) are present in the alternative descriptions (see §4.2) given in column 2 of Table 2: *d*, *e*, *f*, *g*, *i*, *l*, *n*, *p*, *s*, *v*, *w*, *x*.

### 4.2. *2D subunits*

The combination of a horizontal three-connected 2D net with a perpendicular *z* chain may generate another 2D net in a vertical plane (Table 2, column 5). The new net may be three-connected or four-connected (denoted by double-prime).

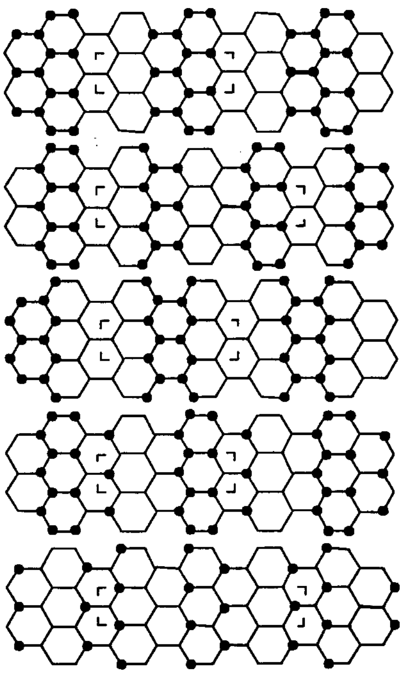


Fig. 9. Simple ways of adding a vertical linkage to each vertex of the *hex* net ($6^3$) to give a four-connected 3D net where one, two and three sequences are allowed. Presence and absence of dots show opposite directions of vertical linkages. For nets 468 and 771, the multiplicities of the three types of vertices are equal. The unit cell is marked by corner symbols.

For many 3D nets in this enumeration, zigzag chains connected by *h* edges generate six-rings which link up to give a 2D *hex* net ($6^3$) in a vertical plane (common in column 5). Perpendicular to this vertical *hex* net there may be one or more simple chains to give an alternate topological description of the 3D net (Table 2, column 2). For example, net 98 was originally generated from the 2D net *bik* with the *z* chain, and it can also be described as (*c,s*)**hex* (Table 2, column 2). Here, a stretched three-repeat saw chain (*s*) is coupled with a compressed four-repeat crankshaft chain.

38 3D nets are members of the up–down-*hex* group for which the simpler members were described by Smith (1977), and further ones will be given by Smith (1999*b*). Five examples are shown in Fig. 9. Following Smith's nomenclature, two adjacent vertices of a horizontal hexagon may point either in the same (s) or changed directions (c). Smith allowed only one kind of sequence around the six-ring to generate eight simple 3D nets from the *hex* net. Mixing of sequences allows an infinity of 3D nets. Net 470 has only one sequence, ccssss. Nets 427 and 468 have two sequences: (ccssss)$_2$(csscss)$_1$ and (csscss)$_1$(ssssss)$_1$, respectively, and nets 770 and 771 have three: (cccccc)$_1$(ccssss)$_2$(csscss)$_1$ and (cccccc)$_1$(ccccss)$_1$-(ccssss)$_1$.

### 4.3. *Polyhedral subunits*

39 polyhedral subunits (Andries & Smith, 1993*a*) were identified among the 138 3D zigzag nets (Fig. 10). Some polyhedral subunits occur in more than ten 3D nets and many are related to the hexagonal prism, *hpr* ($4^6 6^2$): *baf* ($4^2 4^2 6^2 6^1$-*a*), 1-open hexagonal prism; *lau* ($4^2 6^4$-*a*), 1,4-open hexagonal prism, which is equivalent to the 1,2,3,4-stellated cube; *oth* ($4^2 6^2 6^2$), 1,3-open hexagonal prism; *afi* ($6^3 6^2$), 1,3,5-open hexagonal prism; *kaa* ($6^2 8^2$), 1,2,4,5-open hexagonal prism; *mtw* ($4^2 5^4 6^2$), 1,4-stellated hexagonal prism. The penta-edge-stellated tetrahedron, *pes* ($5^2 6^4$), may also be described as the combination of a five-ring with zigzag chains, and *eun* ($5^4 6^2$-*a*) is two *pes* sharing a six-ring. Two hexa-edge-stellated tetrahedra *hes* ($6^4$) share a six-ring to give *lai* ($6^6$). The *kah* unit ($6^3$) is two vertices joined by three handles.

### 4.4. *Channel system*

Each 3D net has a 1D channel system whose aperture is reduced over that for the undistorted parent 2D net. Conversion of a horizontal edge into a tilted edge of a zigzag chain shortens the horizontal projection by about 30%. In the vertical sections of the 3D nets, no rings are larger than six.

### 5. Conclusions

We obtained 138 3D nets, of which 20 occur in known structures, by enumerating a selection of the infinite combinations of 2D nets with zigzag chains. Although most of the 3D nets in known structures are based on simple 2D nets, such as *fee* ($48^2$) and *gml* (4.6.12), 3D nets 604 and 605 contain complex 2D nets. Hence the simpler nets are not always the preferred candidates for natural and synthetic materials. We hope that further theoretical nets will turn up in new microporous materials. The detailed topological description and atomic coordinates of the 59 chosen theoretical nets provide the basis for characterization and matching.

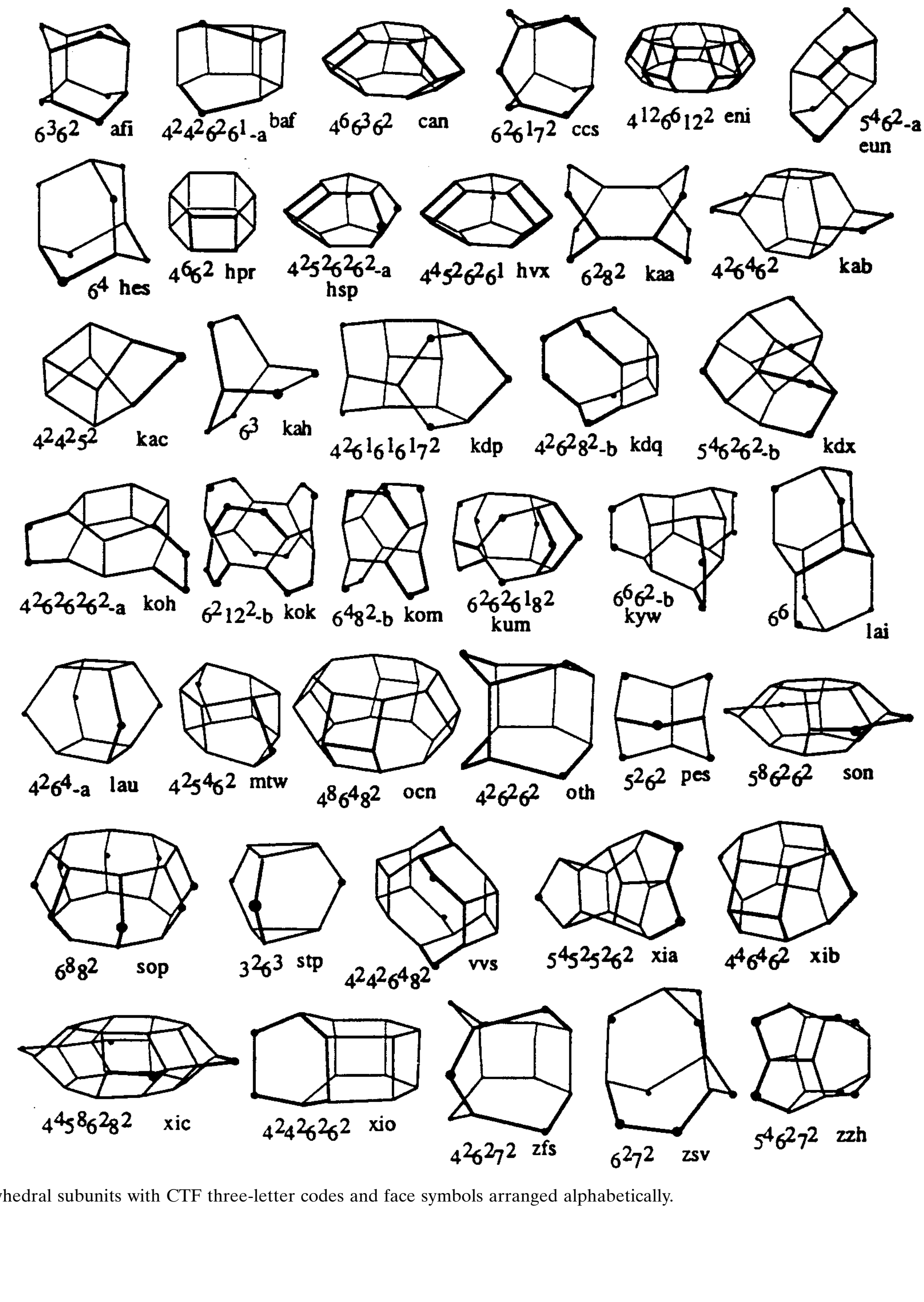


Fig. 10. Polyhedral subunits with CTF three-letter codes and face symbols arranged alphabetically.

See acknowledgements in Han & Smith (1999). We especially thank Koen Andries who drew most of the subunits in the CTF databases.

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