

The *STO Family



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1. The Periodic Building Unit

The two-dimensional PerBUs (PerBU1 and PerBU2) in the *STO family equal the layers shown in Figure 1b and 1c. The layers are built from tubular pores of rolled-up honeycomb-like sheets of fused 6-rings with 12-ring windows as shown in Figure 1a.

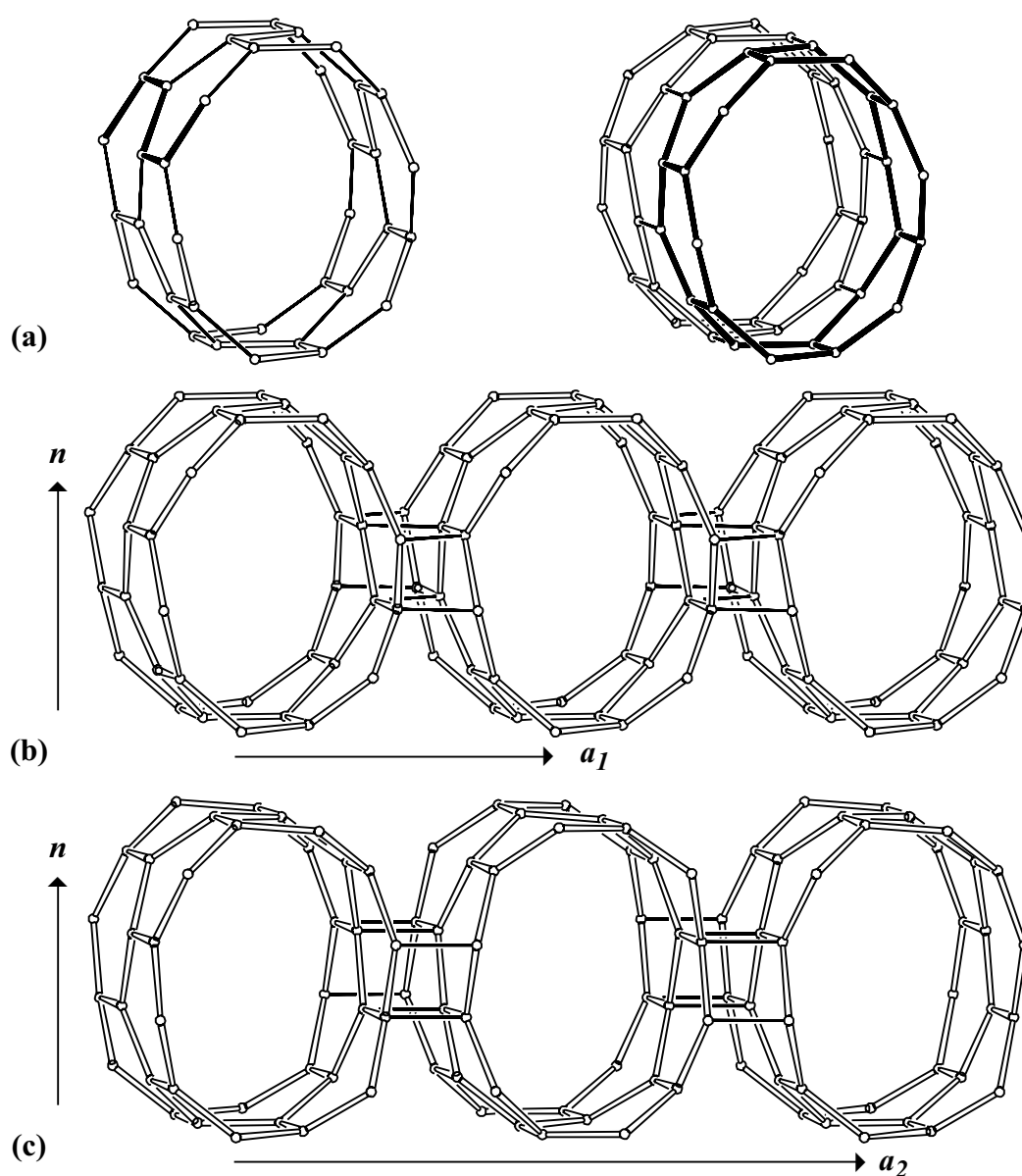


Fig. 1. (a) Tubular pore (top) constructed from crankshaft chains (left) and from 6-ring bands (right) viewed along the pore axis parallel to b ; (b) PerBU1 viewed perpendicular to the plane normal n and along the pore axis parallel to b ; (c) PerBU2 viewed as in (b).



Tubular pores (Fig. 1a), related by pure translations along a_1 , are connected through double crankshaft chains of the narsarsukite type into PerBU1 (Fig. 1b). Pores, related by pure translations along a_2 accompanied by a shift of $\frac{1}{2}b$ along the pore axis, are connected through double crankshaft chains of the feldspar type into PerBU2 (Fig. 1c). [Compare these PerBU's with those in [ZSM-48](#) and [UTD-1](#)].

2. Type of Faulting: 1-dimensional stacking disorder of the PerBU's along the plane normal n . ▲

3. The Layer Symmetry: the plane space group of PerBU1 is $P 2/b 2_1/m (2/m)$ and of PerBU2 is $C 2/m 2/m (2/m)$. ▲

4. Connection Modes

The stacking of PerBU's along n requires a lateral shift of the PerBU's along a (and b). It is convenient to describe the stacking sequence of the PerBU's along n using the same coordinate system in both PerBU's. Therefore the unit cell length along the a axis is taken equal to $2 \times |a_1|$ in PerBU1 and equal to $|a_2|$ in PerBU2. For both PerBU's the lateral shifts along a are then given as $\pm \frac{1}{6}a$. Direct neighbouring PerBUs can be stacked along n in several ways. The lateral shift of the top layer along a and b is:

(1): $-\frac{1}{6}a$ and zero; denoted as $(-\frac{1}{6}, 0)$; (2): $\frac{1}{6}a$ and zero; denoted as $(\frac{1}{6}, 0)$;
 (3): $-\frac{1}{6}a$ and $\frac{1}{2}b$; denoted as $(-\frac{1}{6}, \frac{1}{2})$; (4): $\frac{1}{6}a$ and $\frac{1}{2}b$; denoted as $(\frac{1}{6}, \frac{1}{2})$.

As an example, the connection modes (1) and (3) between PerBU1's and the connection modes (2) and (4) between PerBU2's are depicted in Figure 2.

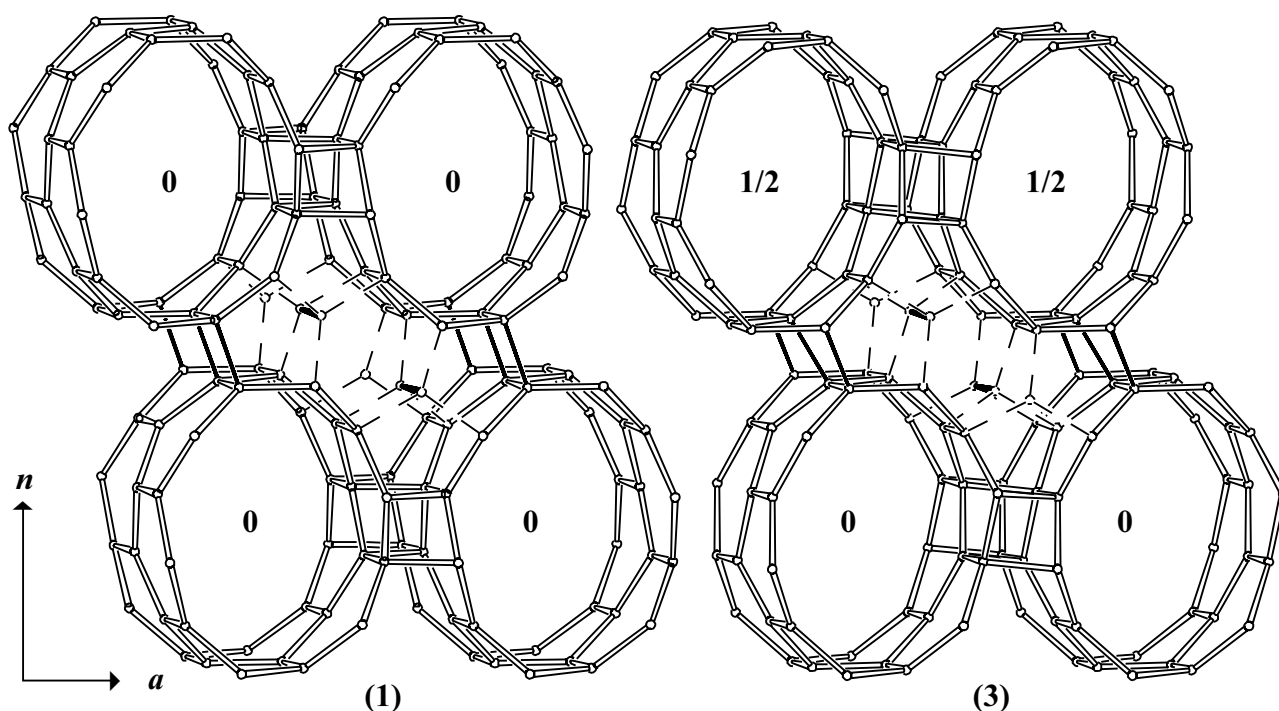


Fig. 2a. Perspective view along the pore axis b of the connection modes (1) and (3) between PerBU1's. The PerBU1's are connected through 4-rings or crankshaft chains depending on whether the shift along b between direct neighbouring pores is zero or $\frac{1}{2}b$, respectively. Connecting T-T modes between PerBUs are drawn as single lines. The connections to the T-T dimers (heavy bold), which fill the space between the tubular pores, are striped. The number in the pore gives the fractional shift of the pore along b . (Figure 2b is on next page).

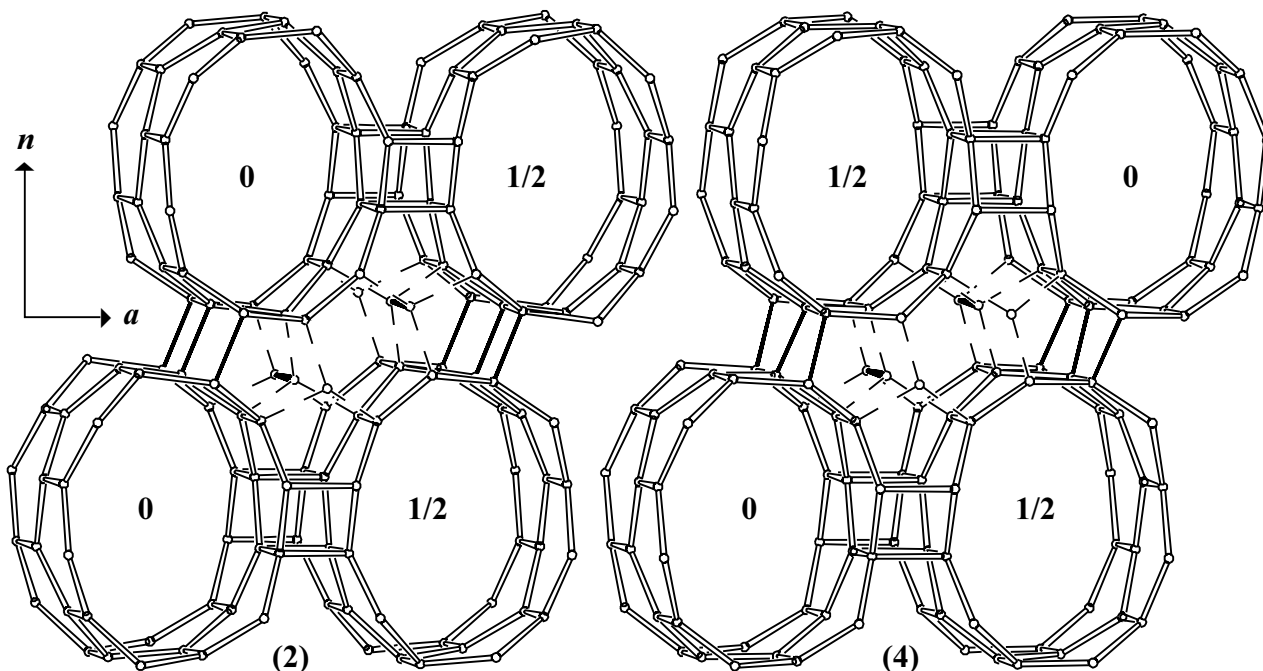


Fig. 2b. Connection modes (2) and (4) between PerBU2s, viewed along b . The PerBU2s are connected as described in Fig. 2a.

Once the distribution of the lateral shifts between the PerBU's along n is known, the three-dimensional structure is defined. ▲

5. The Simplest Ordered End-Members in the *STO family of zeolites are shown in Figure 3 and listed Table 1. None of the end-members has been observed as pure single crystal material so far.

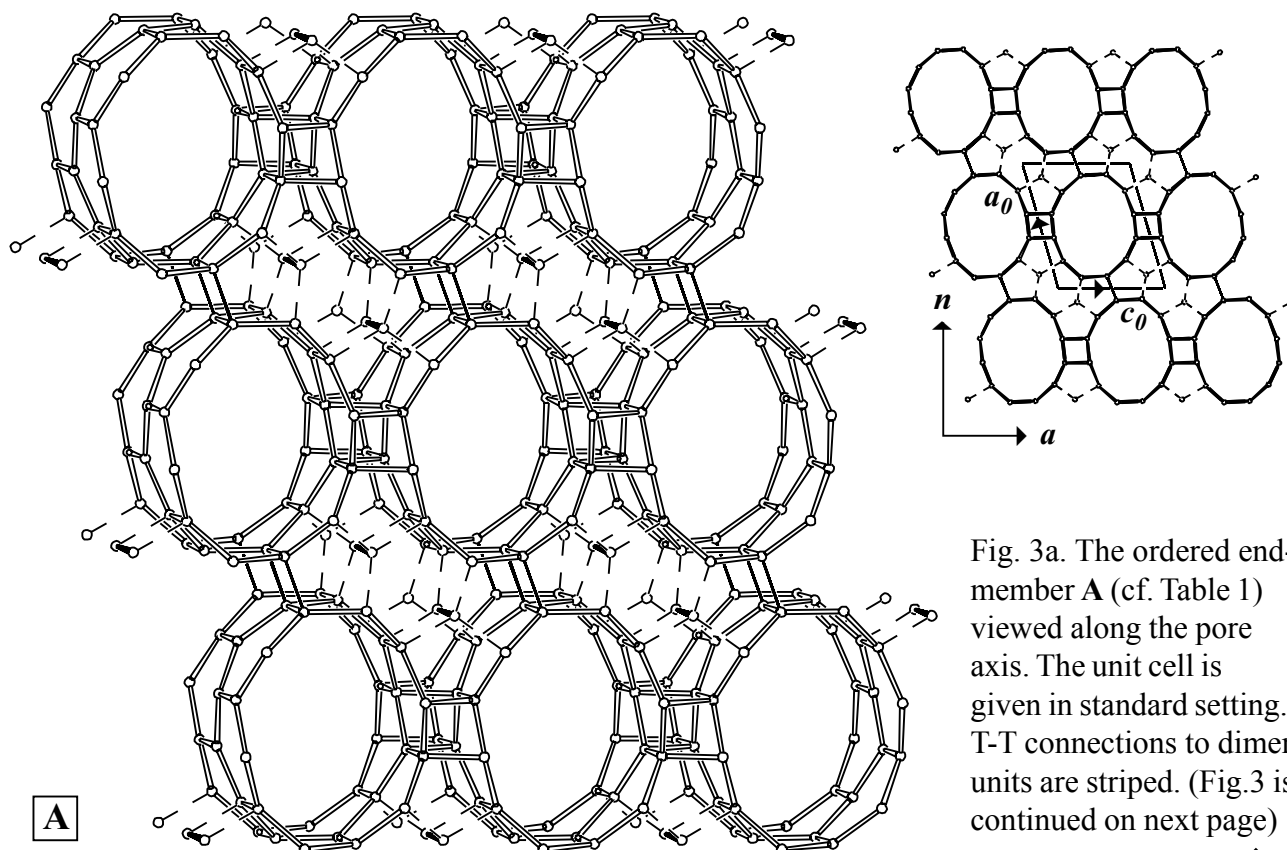


Fig. 3a. The ordered end-member A (cf. Table 1) viewed along the pore axis. The unit cell is given in standard setting. T-T connections to dimer units are striped. (Fig.3 is continued on next page) ▲

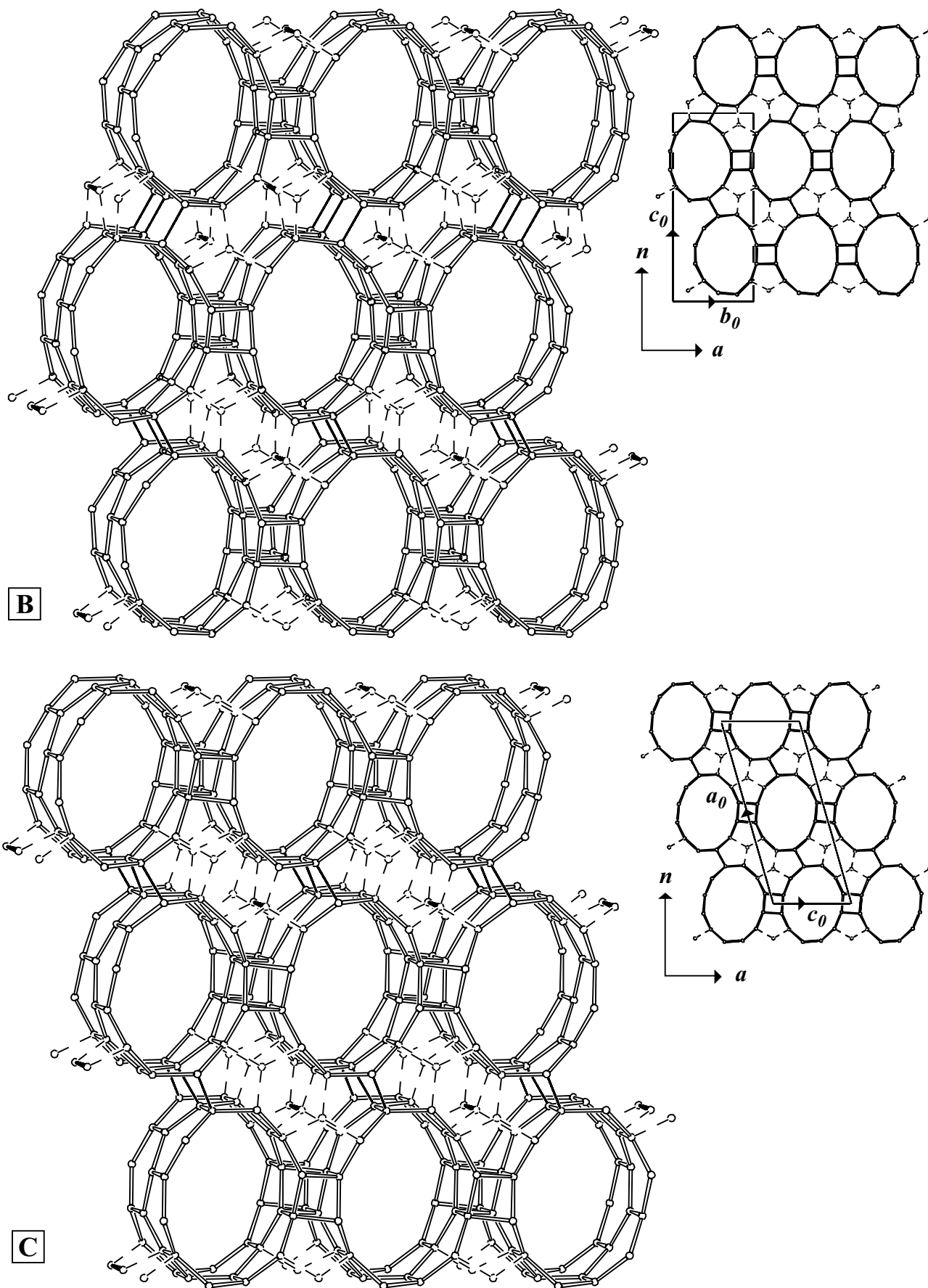


Fig. 3b. The ordered end-members **B** and **C** (cf. Table 1) viewed along the pore axis. The unit cells are given in standard setting. T-T connections to dimer units are striped. (Fig.3 is continued on next page)



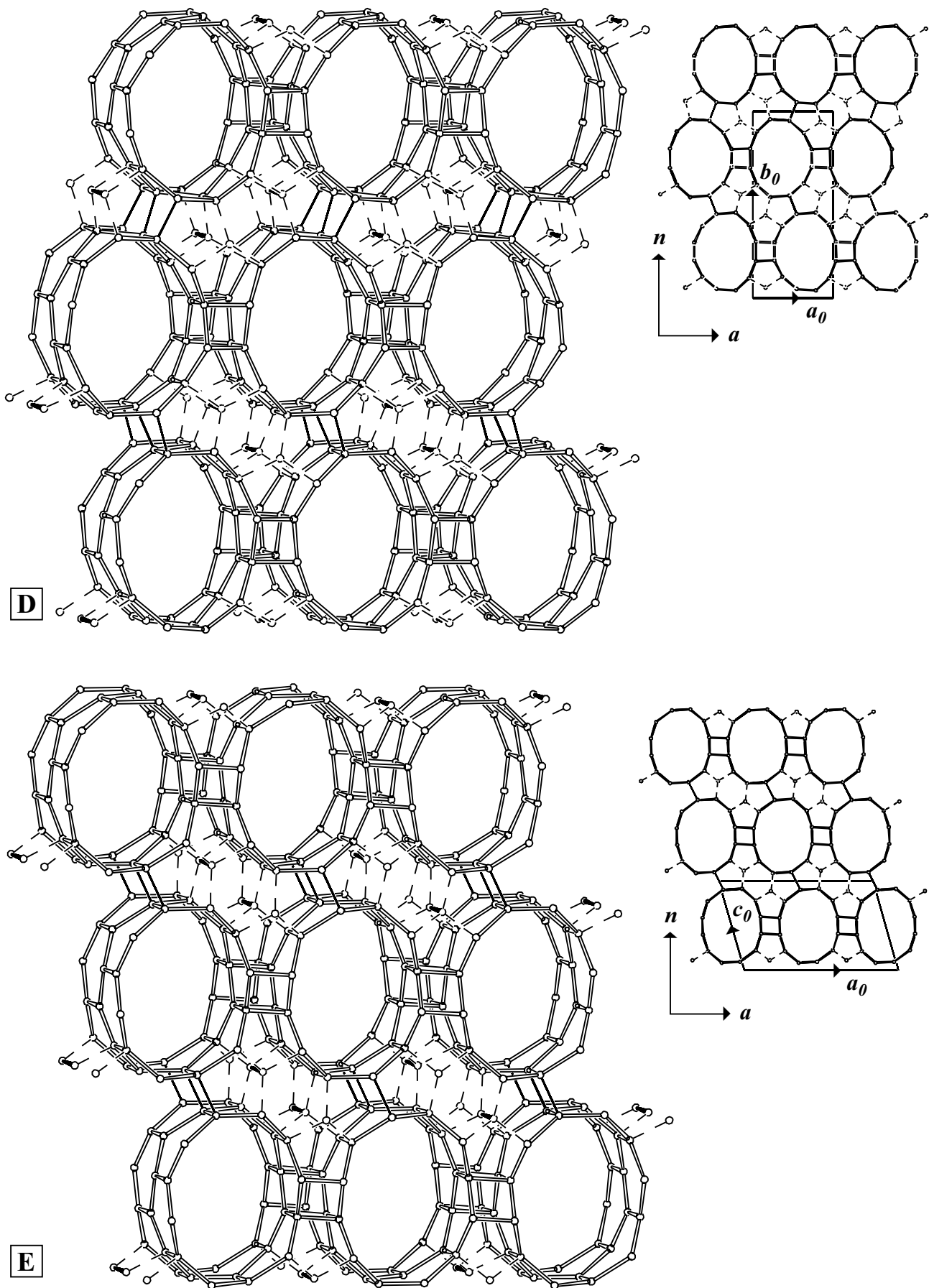


Fig. 3c. The ordered end-members **D** and **E** (cf. Table 1) viewed along the pore axis. The unit cells are given in standard setting. T-T connections to dimer units are striped. (Fig.3 is continued on next page)



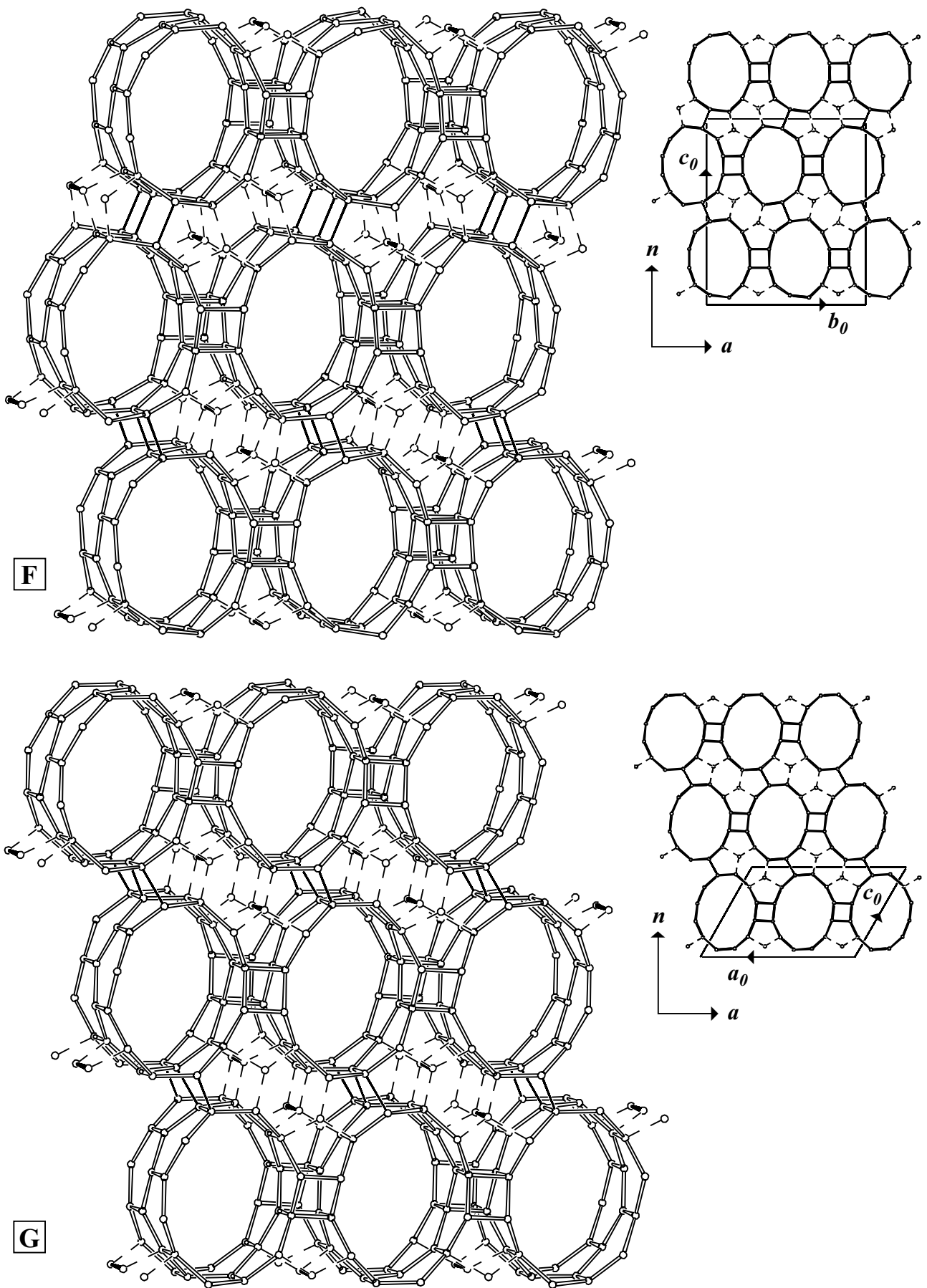


Fig. 3d. The ordered end-members F and G (cf. Table 1) viewed along the pore axis. The unit cells are given in standard setting. T-T connections to dimer units are striped. (Fig.3 is continued on next page)



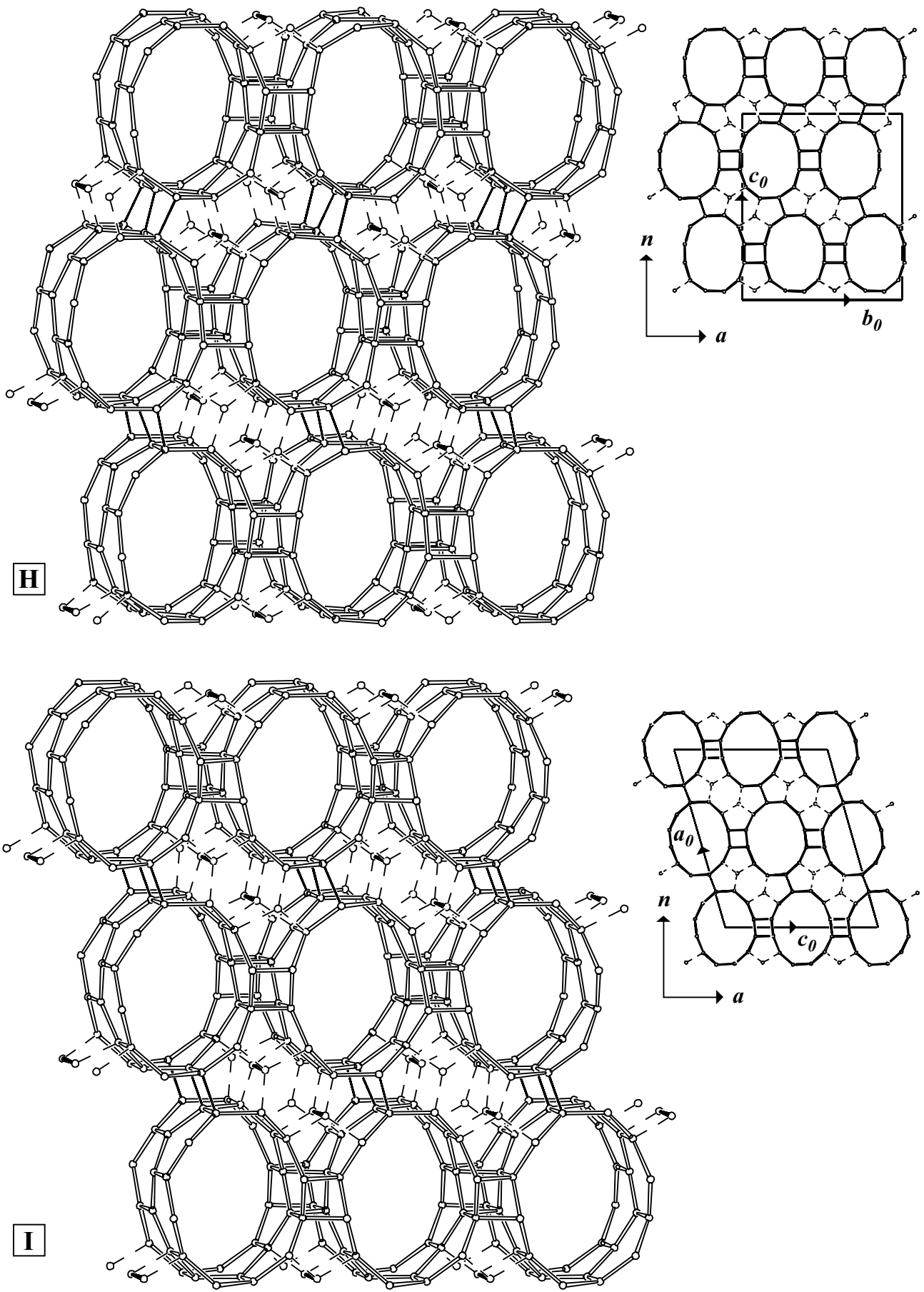


Fig. 3e. The ordered end-members **H** and **I** (cf. Table 1) viewed along the pore axis. The unit cells are given in standard setting. T-T connections to dimer units are striped. (Fig.3 is continued on next page)



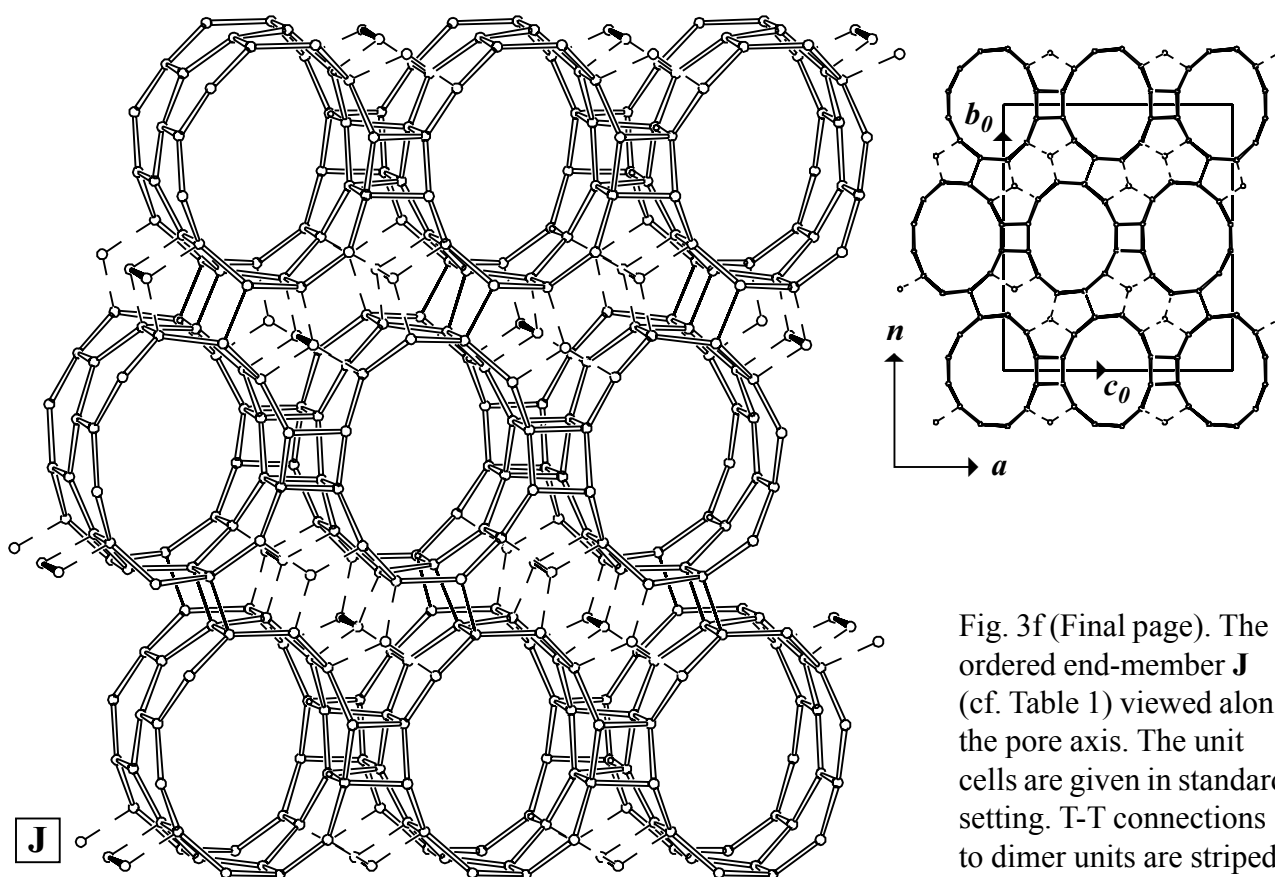


Fig. 3f (Final page). The ordered end-member **J** (cf. Table 1) viewed along the pore axis. The unit cells are given in standard setting. T-T connections to dimer units are striped.

Table 1. Stacking sequences of the PerBU's for the simplest ordered end-members in the *STO family of zeolite frameworks. The end-member number refers to the framework plots A-J on previous pages. The standard setting (a_0 , b_0 and c_0) of the space group is used.

End-Member	Lateral shifts (along n) in fractions of (a , and b) ¹			space group	a_0	b_0 (Å)	c_0	β (°)
PerBU1								
A	$(-1/6, 0)$	$(-1/6, 0)$	$(-1/6, 0); \dots$	P2/m	14.97	8.4	12.35	106.0
B	$(-1/6, 0)$	$(+1/6, 0)$	$(-1/6, 0); \dots$	Pmna	8.4	12.35	28.78	-
C	$(-1/6, 1/2)$	$(-1/6, 1/2)$	$(-1/6, 1/2); \dots$	C2/m	29.94	8.4	12.35	106.0
D	$(-1/6, 1/2)$	$(+1/6, 1/2)$	$(-1/6, 1/2); \dots$	Pbcm	12.35	28.78	8.4	-
PerBU2								
E	$(-1/6, 0)$	$(-1/6, 0)$	$(-1/6, 0); \dots$	C2/m	24.70	8.4	14.97	106.0
F	$(-1/6, 0)$	$(+1/6, 0)$	$(-1/6, 0); \dots$	Cmca	8.4	24.70	28.78	-
G	$(-1/6, 1/2)$	$(-1/6, 1/2)$	$(-1/6, 1/2); \dots$	C2/m	24.70	8.4	16.58	119.8
H	$(-1/6, 1/2)$	$(+1/6, 1/2)$	$(-1/6, 1/2); \dots$	Cmca	8.4	24.70	28.78	-
PerBU1 and PerBU2								
I ²	$(-1/6, 0)$	$(-1/6, 0)$	$(-1/6, 0); \dots$	P2/m	29.94	8.4	24.70	106.0
J	$(-1/6, 0)$	$(+1/6, 0)$	$(-1/6, 0); \dots$	Pma2	8.4	28.78	24.70	-

¹ $a = 24.70$ Å (See Fig.1 and Section 4); the pore axis $b = 8.4$ Å; n is parallel to $a \times b$.

² This is the end-member with framework type code *STO.



6. Disordered Materials Synthesized and Characterized to Date

SSZ-31 (1,2,3,4); NCL-1 (5). ▲

7. Supplementary Information ▲

7.1 Comparison with the ZSM-48 family:

The Periodic Building Units (PerBU1 and PerBU2) in the ZSM-48 family equal the layers shown in Figure 4b and 4c. The layers are built from tubular pores (Fig. 4a) of rolled-up honeycomb-like sheets of fused 6-rings with 10-ring windows. [Compare these PerBU's (with 10-ring windows) with the PerBU's in the *STO (with 12-ring windows) and UTD-1 (with 14-ring windows) families].

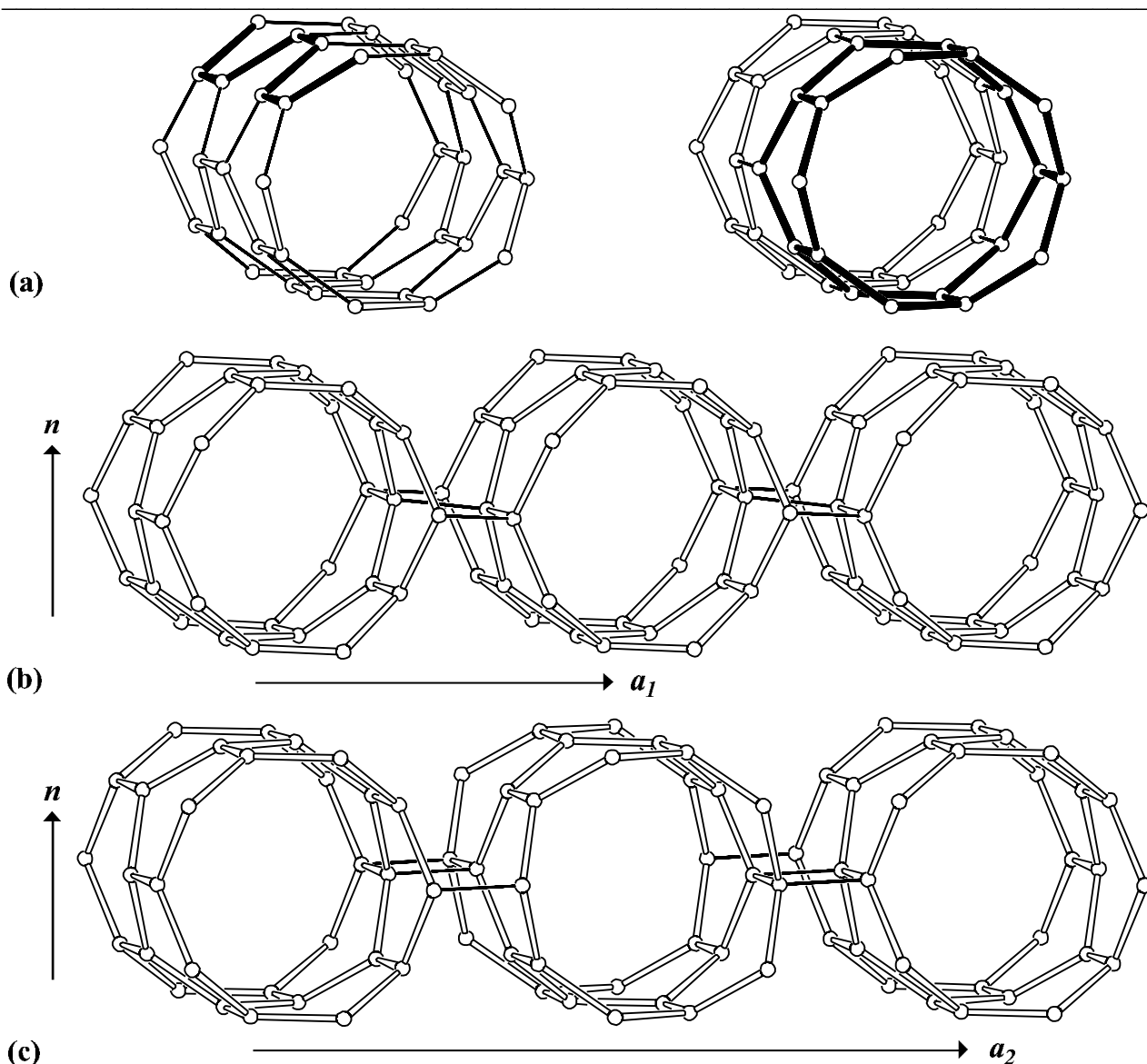


Fig. 4. Tubular pore with 10-ring window (a) constructed from five crankshaft chains (left) or from 6-ring bands each consisting of 20 T atoms (right); PerBU1 (b) and PerBU2 (c) of the ZSM-48 family of zeolite frameworks seen in perspective view perpendicular to the plane normal n and along the pore axis b .

7.2 Comparison with the UTD-1 family:

The Periodic Building Units (PerBU1 and PerBU2) in the UTD-1 family equal the layers shown in Figure 5b and 5c. The layers are built from tubular pores (Fig. 5a) of rolled-up honeycomb-like sheets of fused 6-rings with 14-ring windows. [Compare these PerBU's (with 14-ring windows) with the PerBU's in the ZSM-48 (with 10-ring windows and SSZ-31 (with 12-ring windows) families].

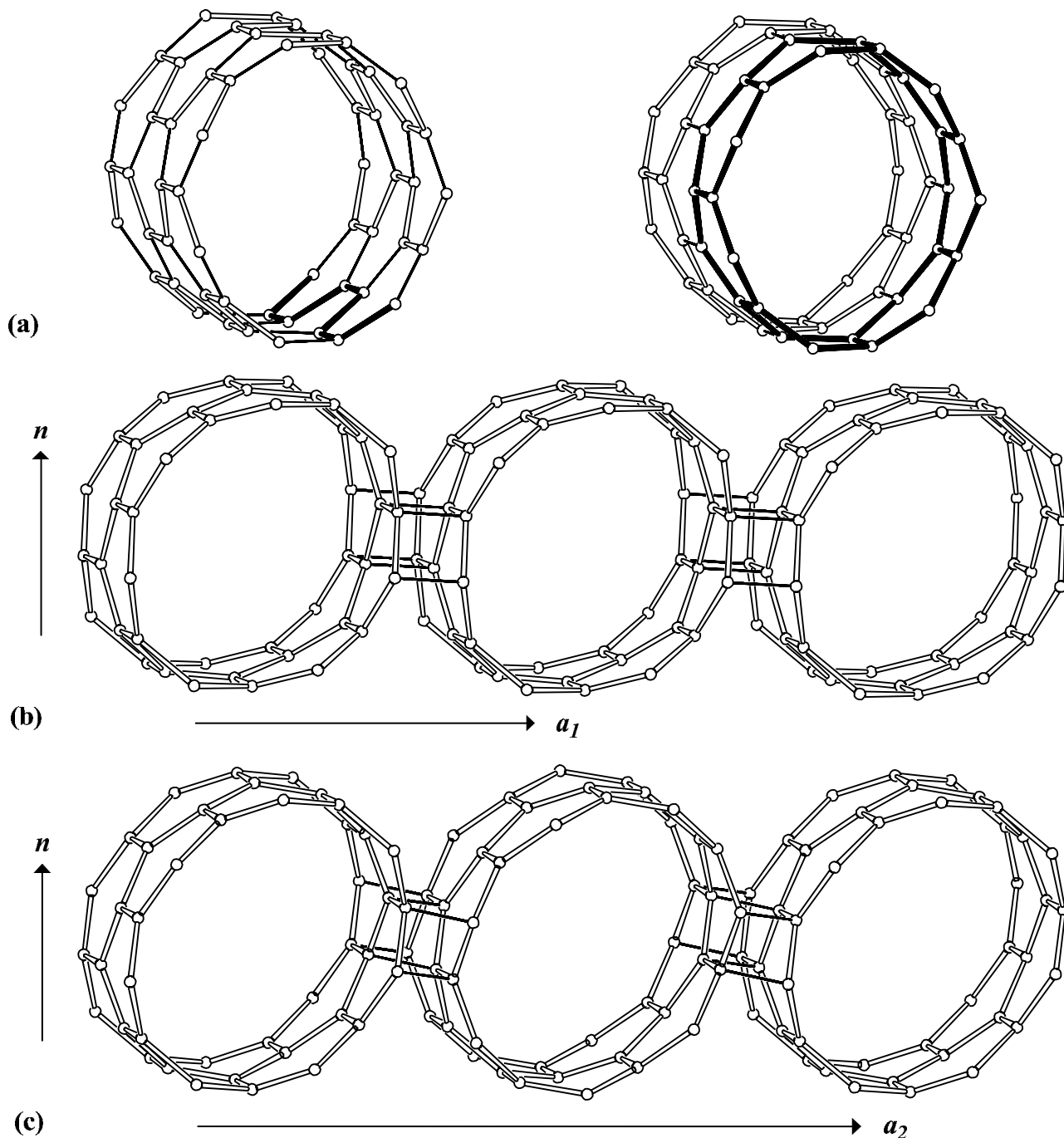


Fig. 5. Tubular pore with 14-ring window constructed from seven crankshaft chains (left) or from 6-ring bands each consisting of 28 T atoms (right); PerBU1 (b) and PerBU2 (c) of the UTD-1 family of zeolite frameworks seen in perspective view perpendicular to the plane normal n and along the pore axis b .

8. References

- [1] S.I. Zones, T.V. Harris, A. Rainis and D.S. Santilli, US Patent 5,106,801(1992).
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- [3] R.F. Lobo, M. Tsapatsis, C.C. Freyhardt, I. Chan, C-Y. Chen, S.I. Zones and M.E. Davis, J. Am. Chem. Soc., 119 (1997) 3732.
- [4] H. van Koningsveld and R.F. Lobo, J. Phys. Chem. B, 107 (2003) 10983.
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