

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.

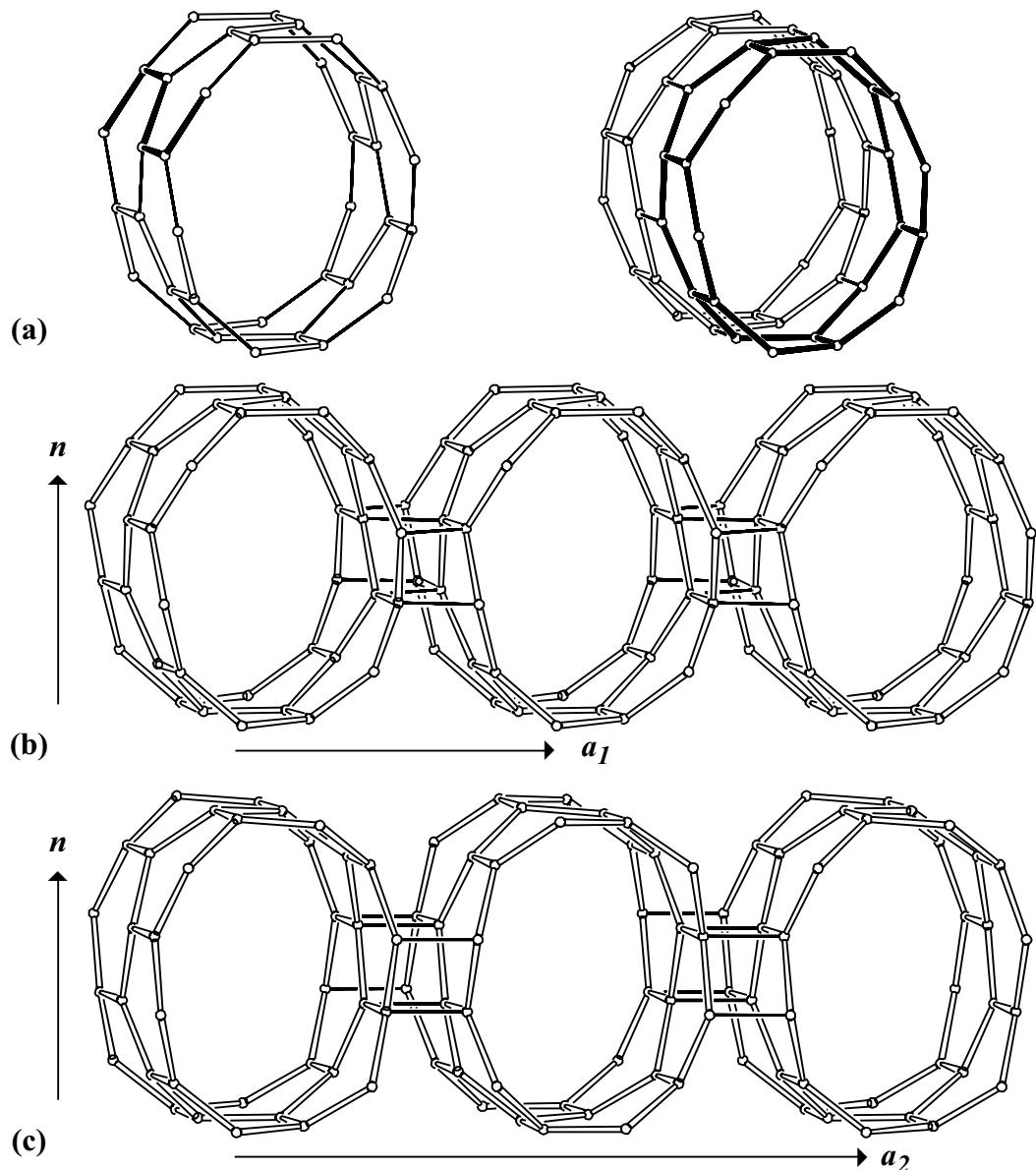


Fig. 1. (a) Tubular pore (top) constructed from crankshaft chains (left) and from 6-ring bands (right) viewed along the pore axis parallel to \mathbf{b} ; (b) PerBU1 viewed perpendicular to the plane normal \mathbf{n} and along the pore axis parallel to \mathbf{b} ; (c) PerBU2 viewed as in (b).

Tubular pores (Fig.1a), related by pure translations along \mathbf{a}_1 , are connected through double crankshaft chains of the narsarsukite type into PerBU1 (Fig.1b). Pores, related by pure transaltions along \mathbf{a}_2 , accompanied by a shift of $\frac{1}{2}\mathbf{b}$ 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 \mathbf{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 \mathbf{n} requires a lateral shift of the PerBU's along \mathbf{a} (and \mathbf{b}). It is convenient to describe the stacking sequence of the PerBU's along \mathbf{n} using the same coordinate system in both PerBU's. Therefore the unit cell length along the \mathbf{a} axis is taken equal to $2 \times |\mathbf{a}_1|$ in PerBU1 and equal to $|\mathbf{a}_2|$ in PerBU2. For both PerBU's the lateral shifts along \mathbf{a} are then given as $\pm\frac{1}{6}\mathbf{a}$. Direct neighbouring PerBUs can be stacked along \mathbf{n} in several ways. The lateral shift of the top layer along \mathbf{a} and \mathbf{b} is:

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

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

As van 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.

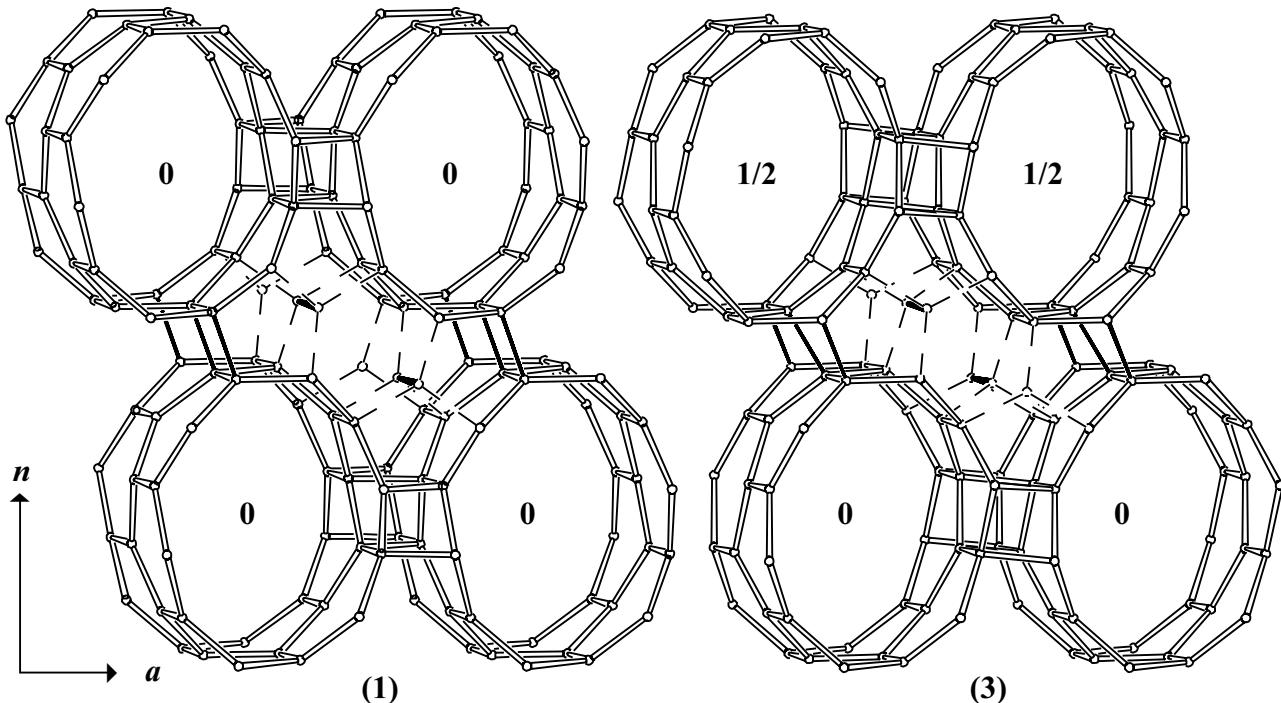


Fig. 2a. Perspective view along the pore axis \mathbf{b} of the connection modes (1) and (3) between PerBU1's. The PerBU1's are connected through 4-rings or crankshaft chains depending on whether the shift along \mathbf{b} between direct neighbouring pores is zero or $\frac{1}{2}\mathbf{b}$, respectively. 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 \mathbf{b} . (Figure 2b is on next page).

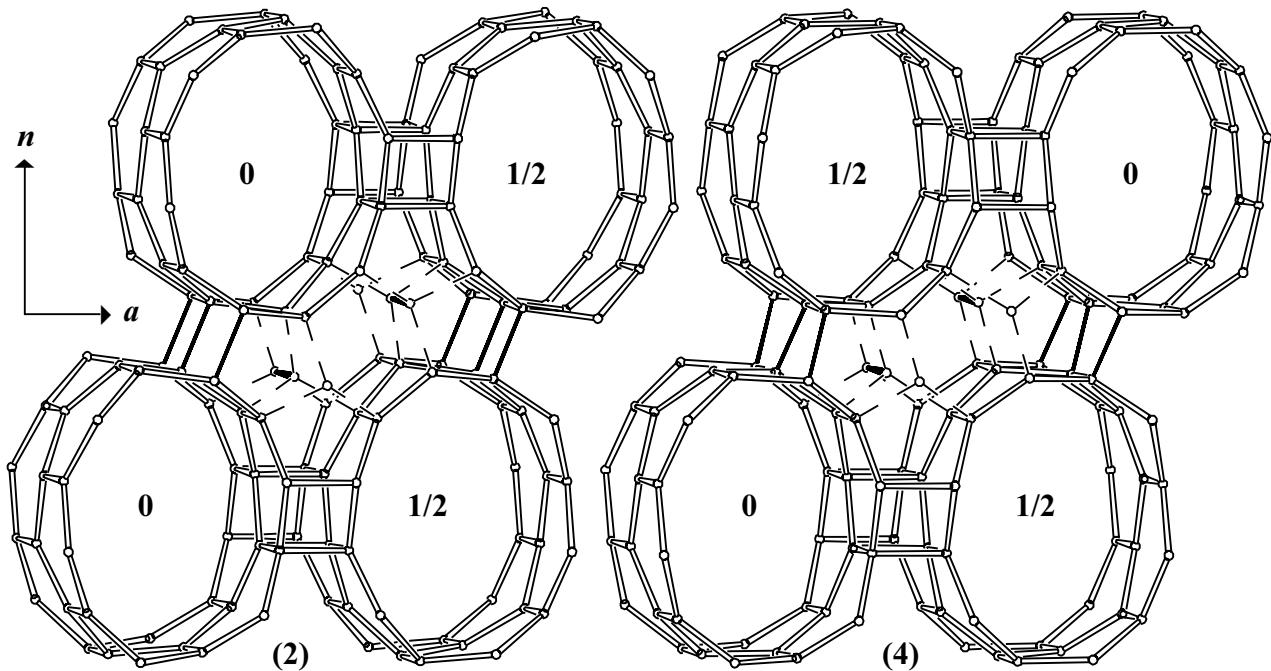


Fig. 2b. Connection modes (2) and (4) between PerBU2s, viewed along \mathbf{b} . The PerBU2s are connected as described in Fig. 2a.

Once the distribution of the lateral shifts between the PerBU's along \mathbf{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.

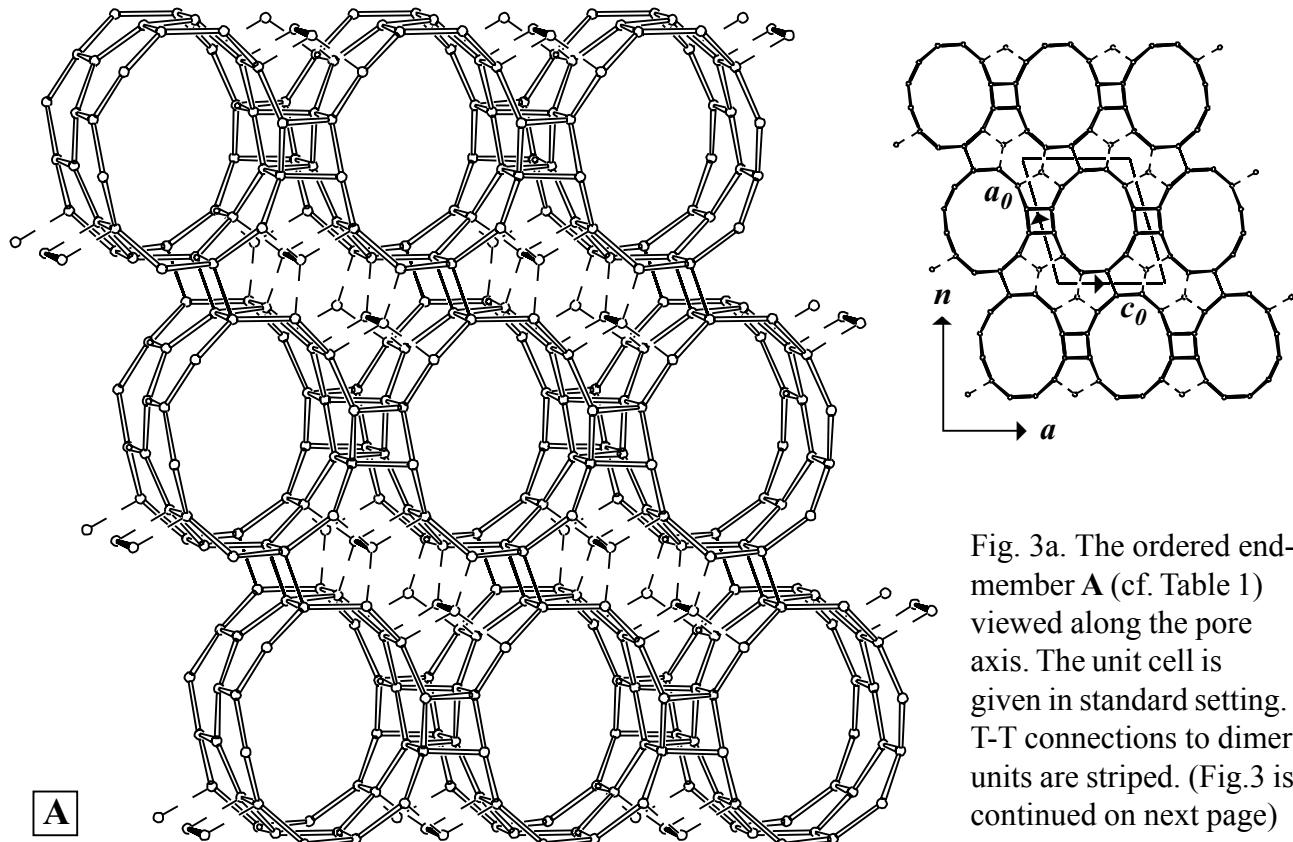


Fig. 3a. The ordered end-member A (cf. Table 1) viewed along the pore axis. The unit cell is given in standard setting. T-T connections to dimer units are striped. (Fig. 3 is continued on next page) ▲

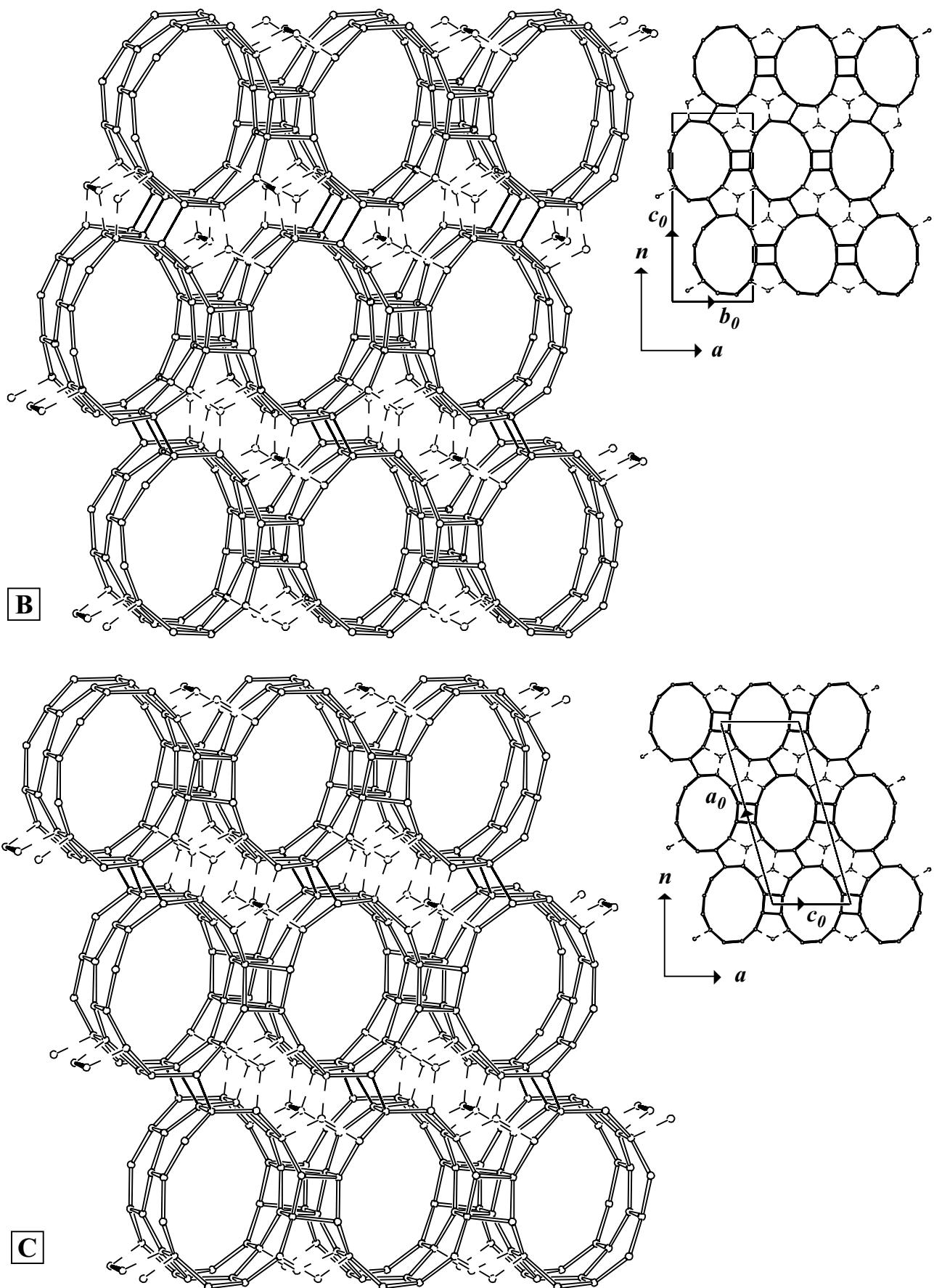


Fig. 3b. The ordered end-members **B** and **C** (cf. Table 1) viewed along the pore axis. The unit cells are given in standard setting. T-T connections to dimer units are striped.
 (Fig.3 is continued on next page)



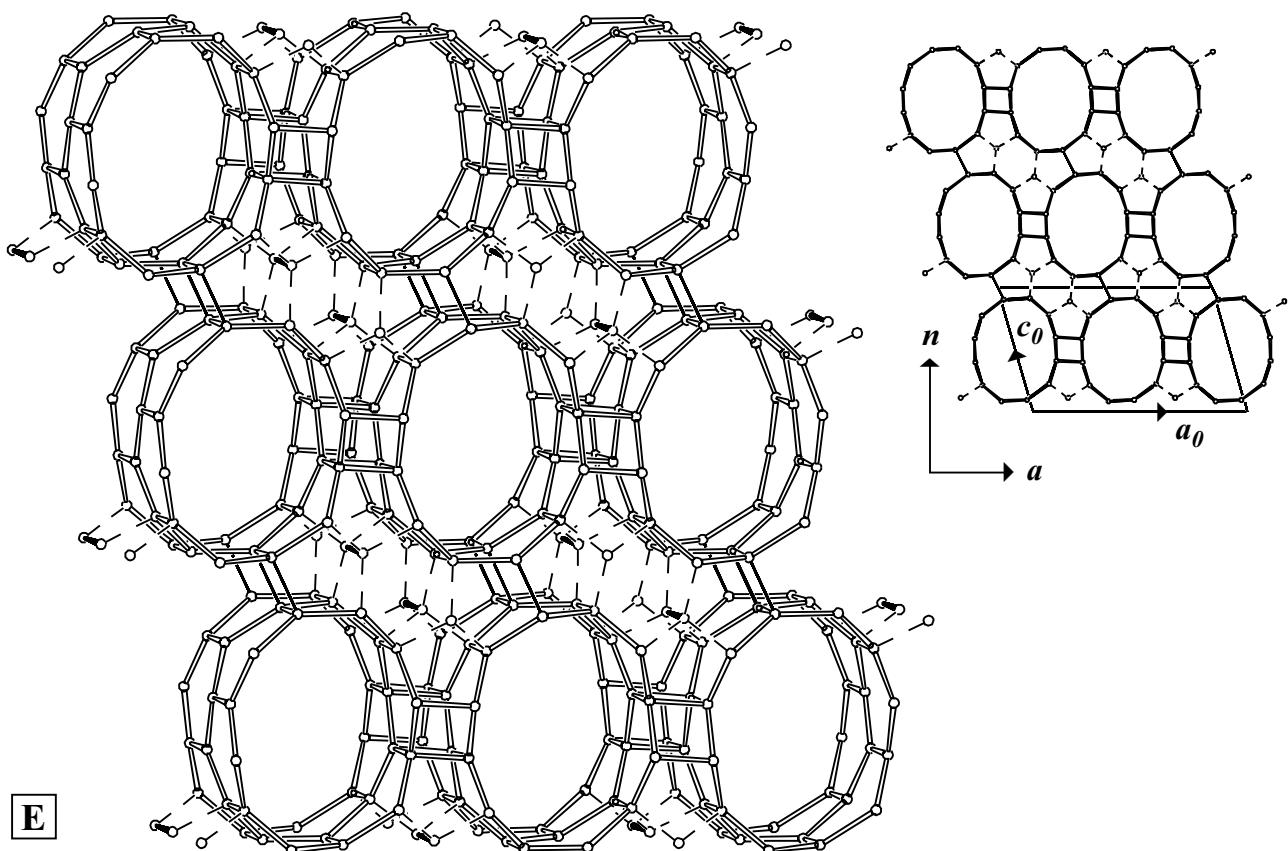
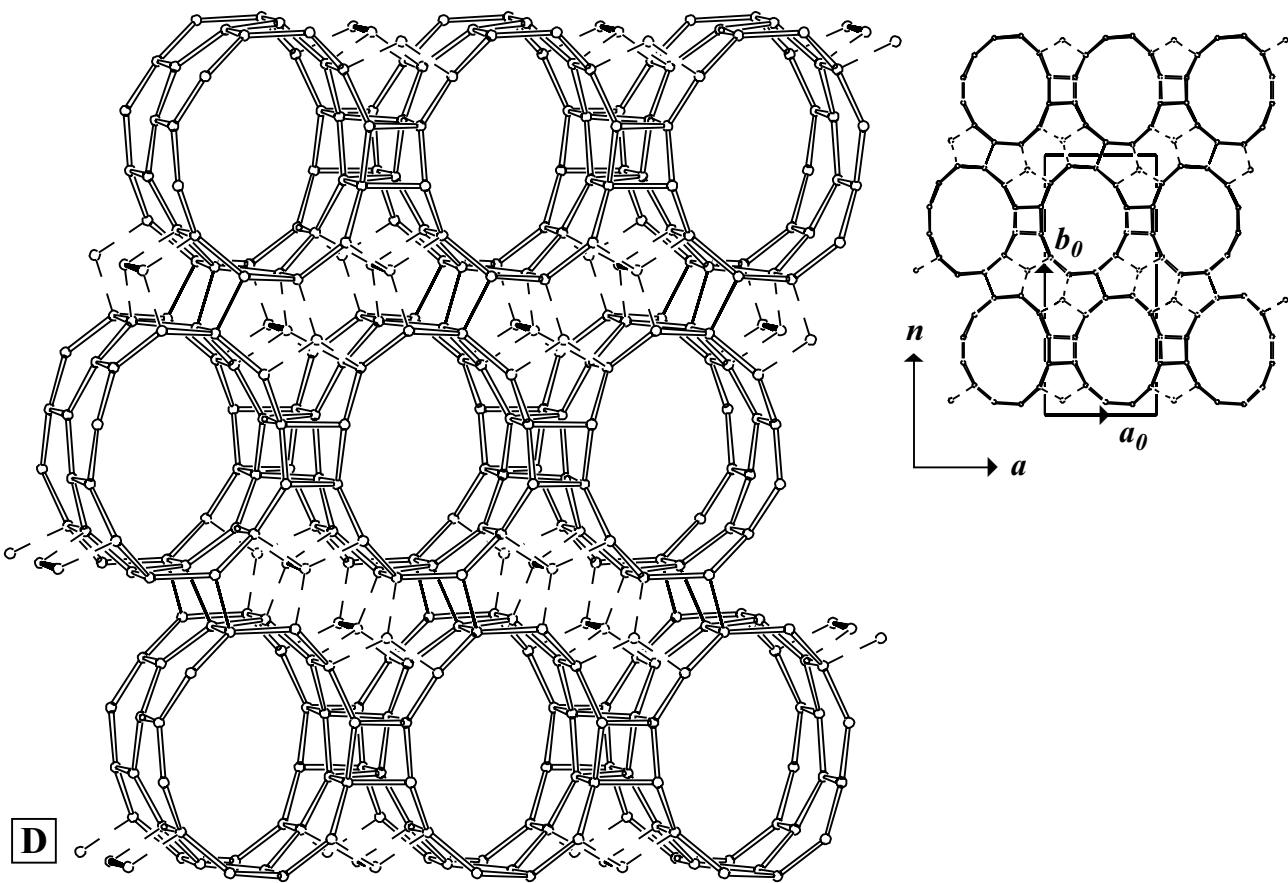


Fig. 3c. The ordered end-members **D** and **E** (cf. Table 1) viewed along the pore axis. The unit cells are given in standard setting. T-T connections to dimer units are striped.
(Fig.3 is continued on next page)



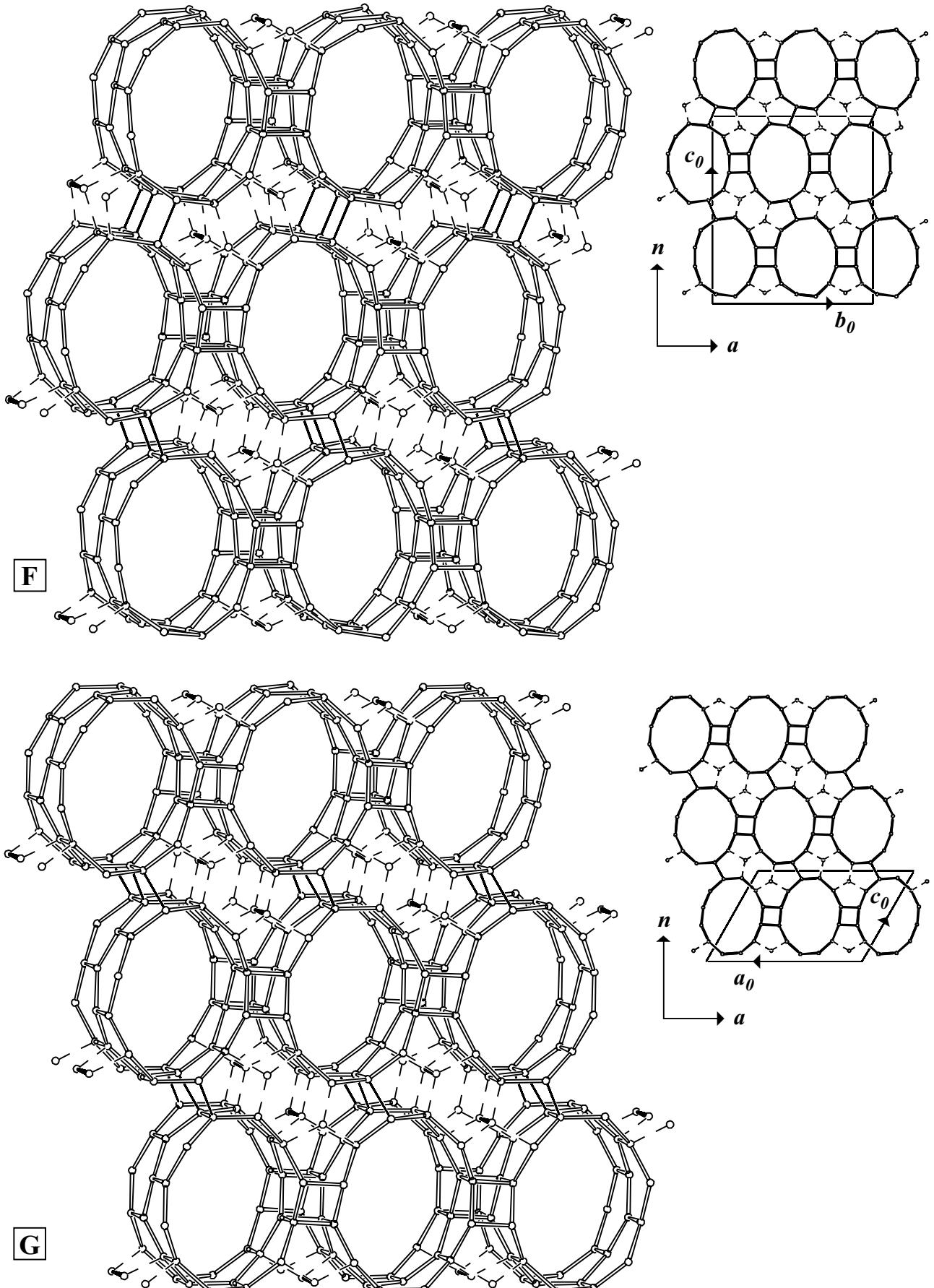


Fig. 3d. The ordered end-members **F** and **G** (cf. Table 1) viewed along the pore axis. The unit cells are given in standard setting. T-T connections to dimer units are striped.
(Fig.3 is continued on next page)

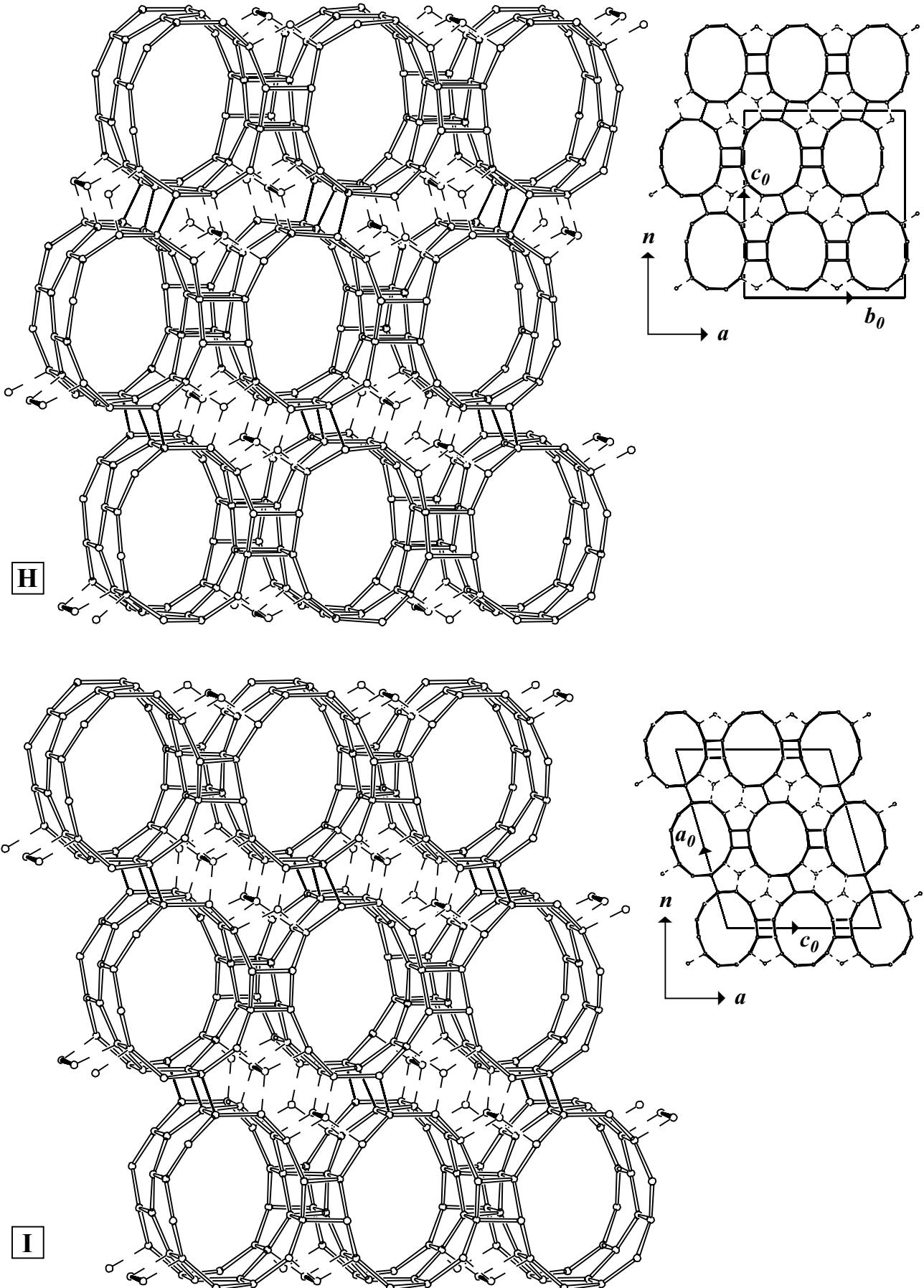


Fig. 3e. The ordered end-members **H** and **I** (cf. Table 1) viewed along the pore axis. The unit cells are given in standard setting. T-T connections to dimer units are striped.
(Fig.3 is continued on next page)

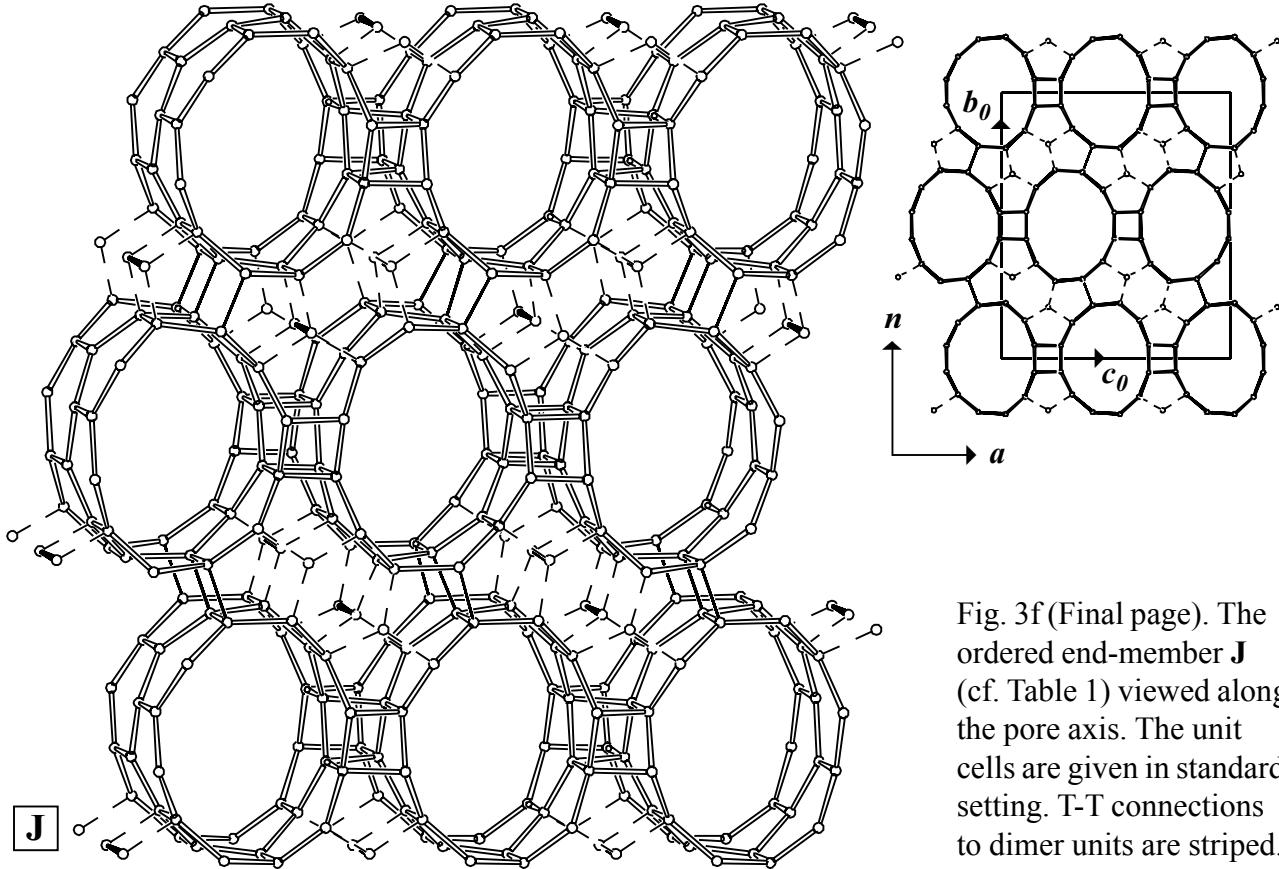


Fig. 3f (Final page). The ordered end-member **J** (cf. Table 1) viewed along the pore axis. The unit cells are given in standard setting. T-T connections to dimer units are striped.

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.

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

¹ $a = 24.70 \text{ \AA}$ (See Fig.1 and Section 4); the pore axis $b = 8.4 \text{ \AA}$; 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].

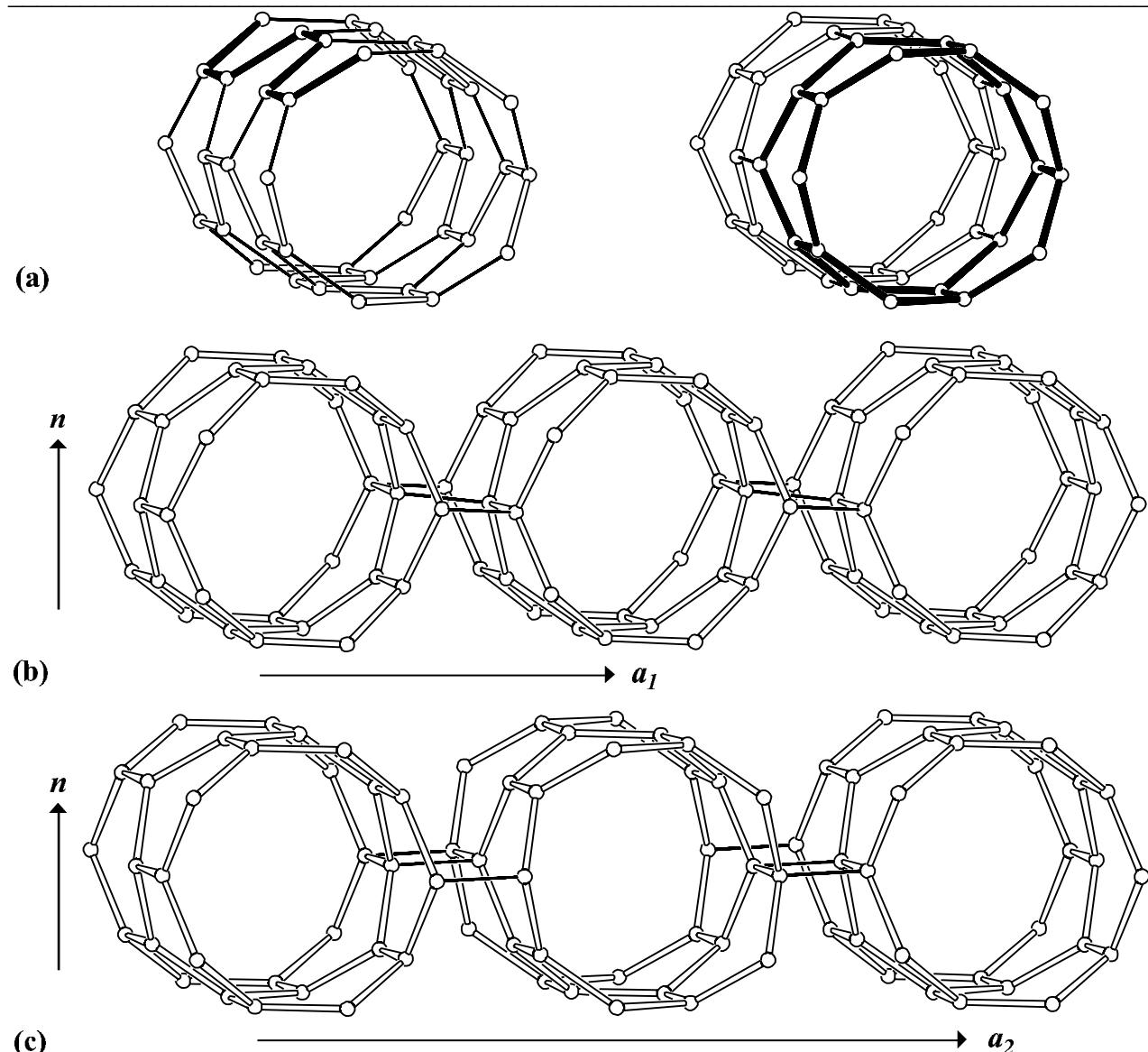


Fig. 4. Tubular pore with 10-ring window (a) constructed from five crankshaft chains (left) or from 6-ring bands each consisting of 20 T atoms (right); PerBU1 (b) and PerBU2 (c) of the ZSM-48 family of zeolite frameworks seen in perspective view perpendicular to the plane normal \mathbf{n} and along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

For more details: see the description of the **ZSM-48** family in this ‘Catalog’.



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].

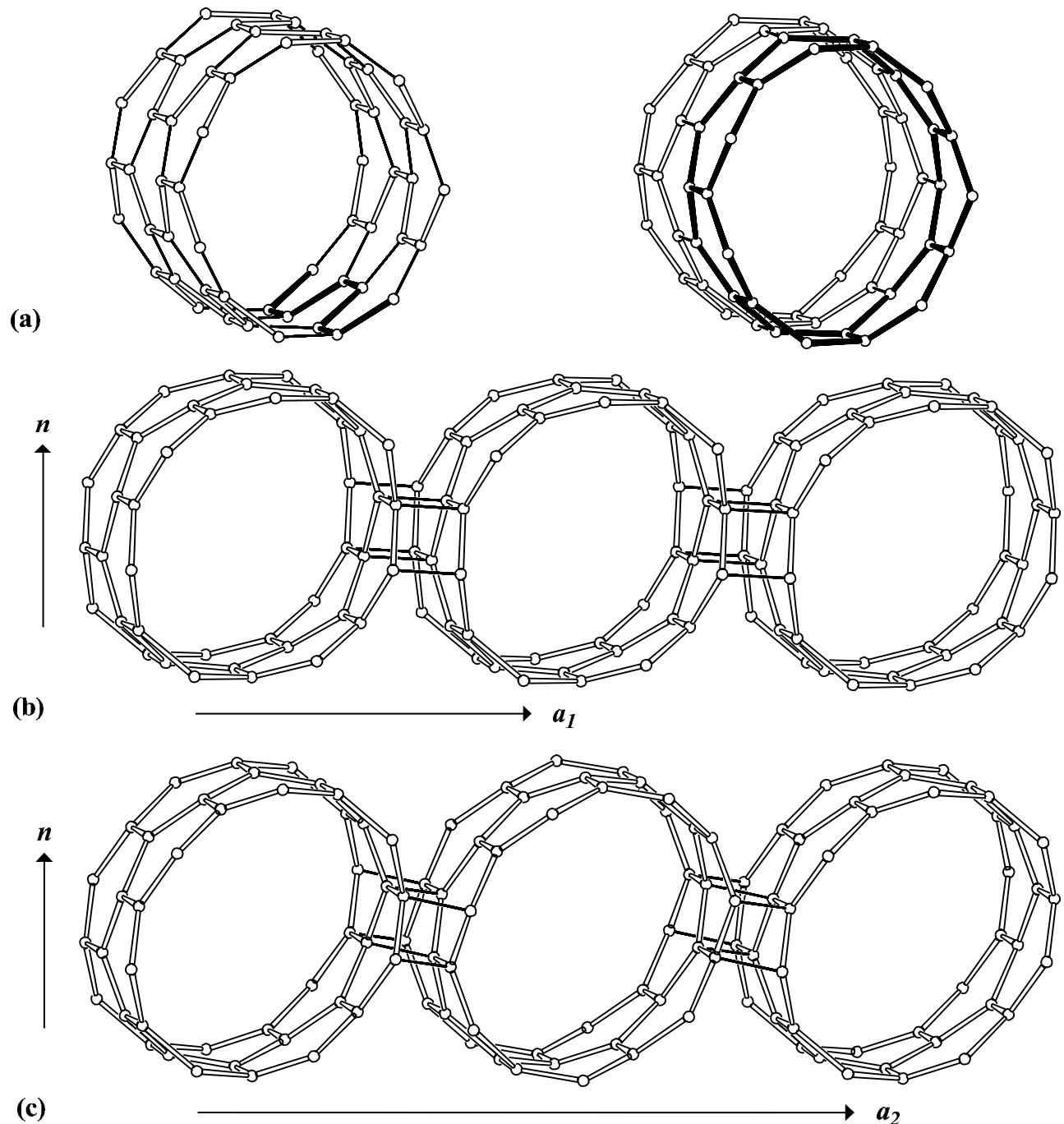


Fig. 5. Tubular pore with 14-ring window constructed from seven crankshaft chains (left) or from 6-ring bands each consisting of 28 T atoms (right); PerBU1 (b) and PerBU2 (c) of the UTD-1 family of zeolite frameworks seen in perspective view perpendicular to the plane normal n and along the pore axis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

For more details: see the description of the **UTD-1** family in this ‘Catalog’.



8. References

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