The *STO Family

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.

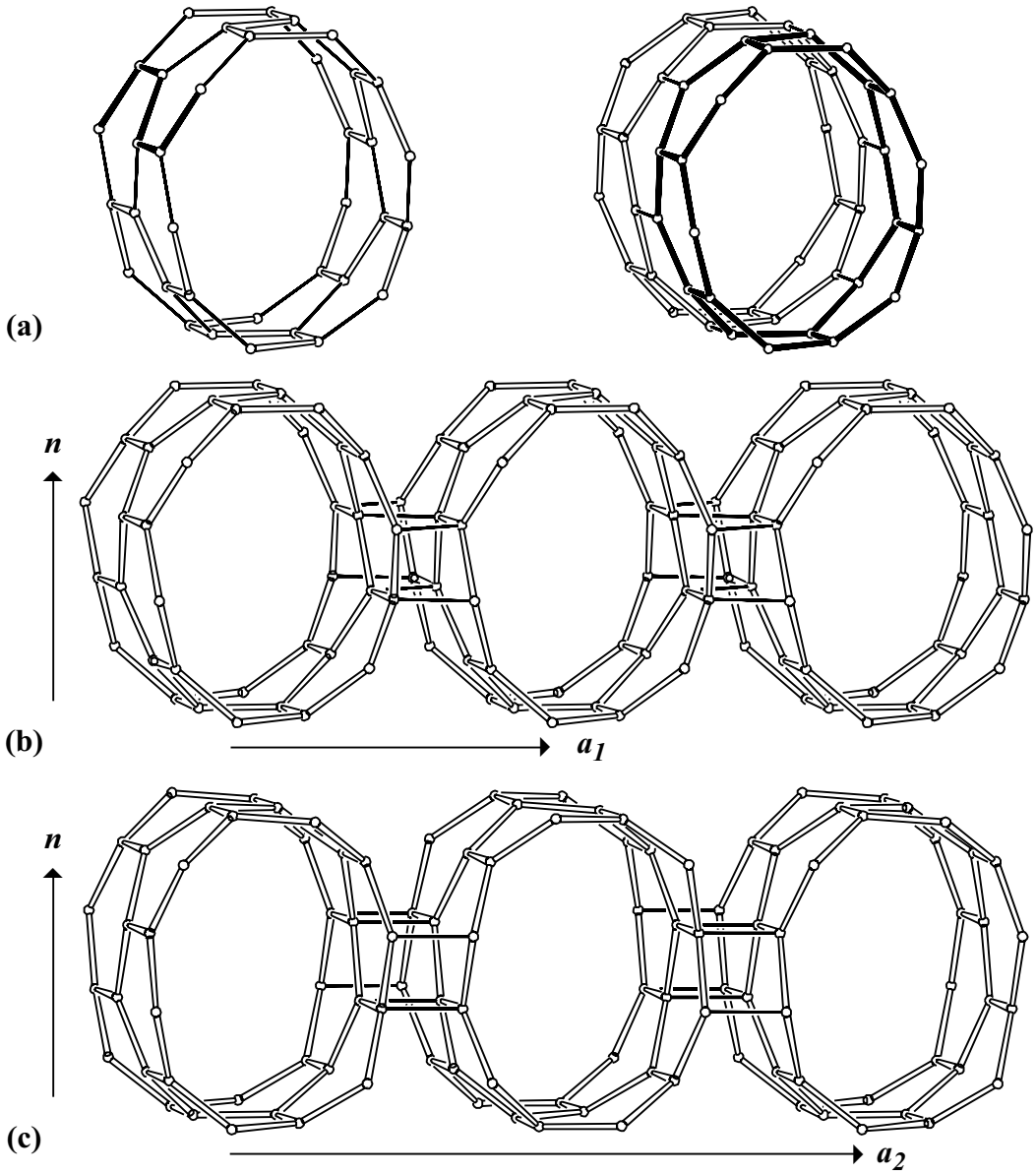

Fig. 1. (a) Tubular pore (top) constructed from crankshaft chains (left) and from 6-ring bands (right) viewed along the pore axis parallel to ***b***; (b) PerBU1 viewed perpendicular to the plane normal ***n*** and along the pore axis parallel to ***b***; (c) PerBU2 viewed as in (b).

Tubular pores (Fig.1a), related by pure translations along $\boldsymbol{a}_1$, are connected through double crankshaft chains of the narsarsukite type into PerBU1 (Fig.1b). Pores, related by pure transaltions along $\boldsymbol{a}_2$ accompanied by a shift of **½*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 $2 \times |\boldsymbol{a}_1|$ in PerBU1 and equal to $|\boldsymbol{a}_2|$ in PerBU2. For both PerBU's the lateral shifts along ***a*** are then given as $\pm^1/_6\,\boldsymbol{a}$. Direct neighbouring PerBUs can be stacked along ***n*** in several ways. The lateral shift of the top layer along ***a*** and ***b*** is:
(1): $-^1/_6\,\boldsymbol{a}$ and zero; denoted as $(-^1/_6, \mathbf{0})$; **(2):** $^1/_6\,\boldsymbol{a}$ and zero; denoted as $(^1/_6, \mathbf{0})$;
(3): $-^1/_6\,\boldsymbol{a}$ and $^1/_2\,\boldsymbol{b}$; denoted as $(-^1/_6, ^1/_2)$; **(4):** $^1/_6\,\boldsymbol{a}$ and $^1/_2\,\boldsymbol{b}$; denoted as $(^1/_6, ^1/_2)$.
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.

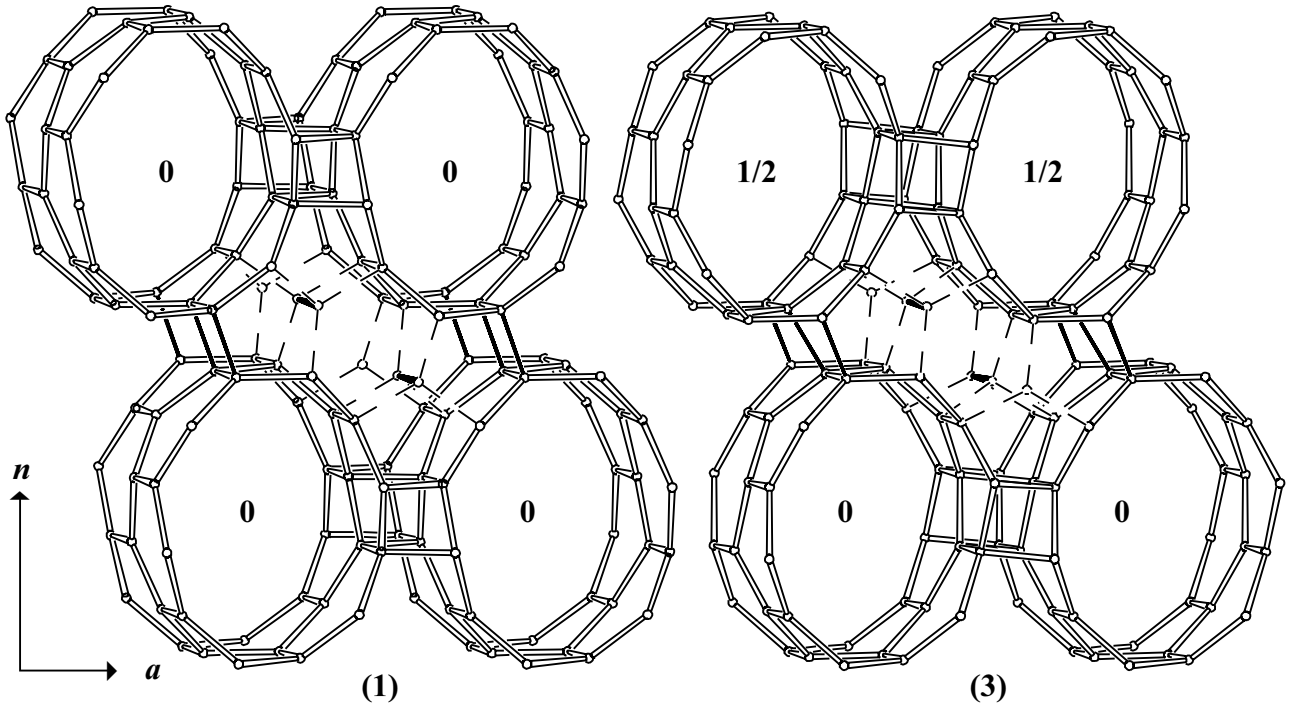

Fig. 2a. Perspective view along the pore axis ***b*** of the connection modes **(1)** and **(3)** between PerBU1s. The PerBU1's are connected through 4-rings or crankshaft chains depending on whether the shift along ***b*** between direct neighbouring pores is zero or $^1/_2\,\boldsymbol{b}$, respectively. 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).

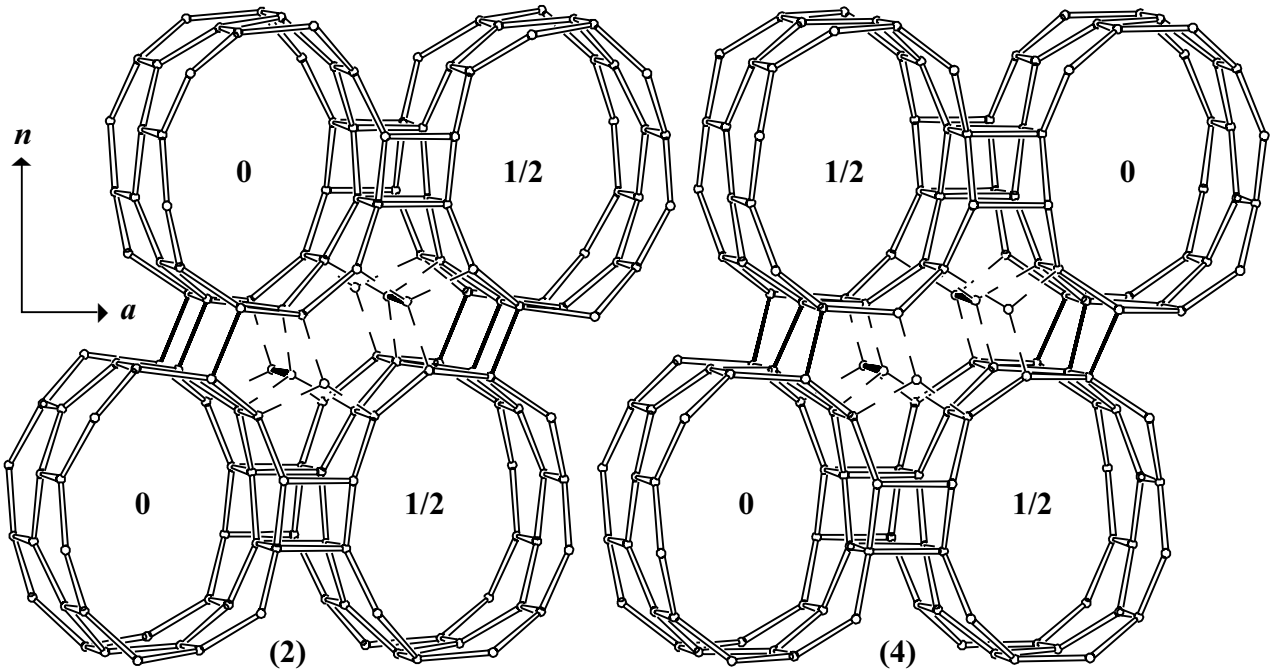

Fig. 2b. Connection modes **(2)** and **(4)** between PerBU2s, viewed along ***b***. The PerBU2s are connected as described in Fig. 2a.

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.

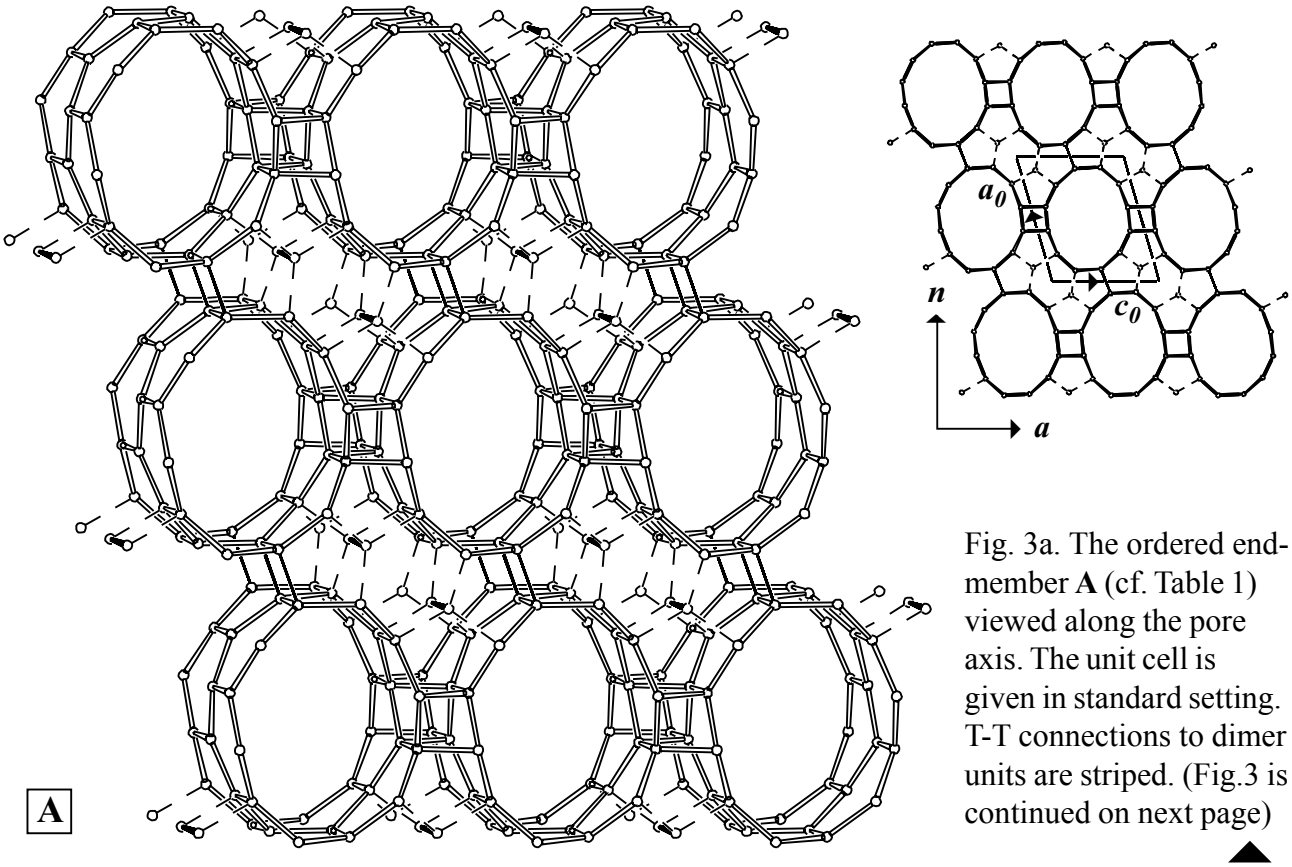

Fig. 3a. The ordered end-member **A** (cf. Table 1) viewed along the pore axis. The unit cell is given in standard setting. T-T connections to dimer units are striped. (Fig.3 is continued on next page)

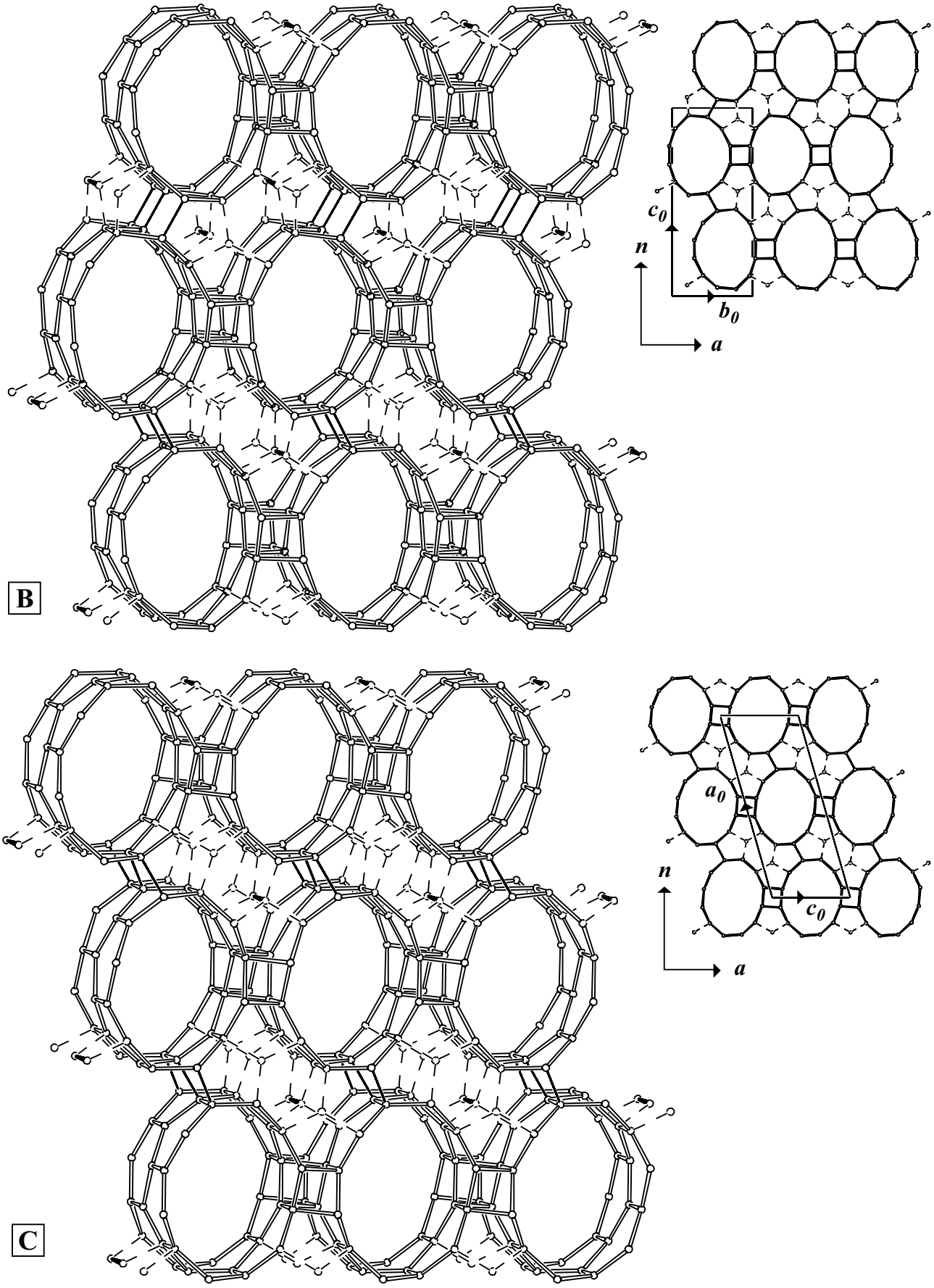

Fig. 3b. The ordered end-members **B** and **C** (cf. Table 1) viewed along the pore axis. The unit cells are given in standard setting. T-T connections to dimer units are striped.

(Fig.3 is continued on next page)

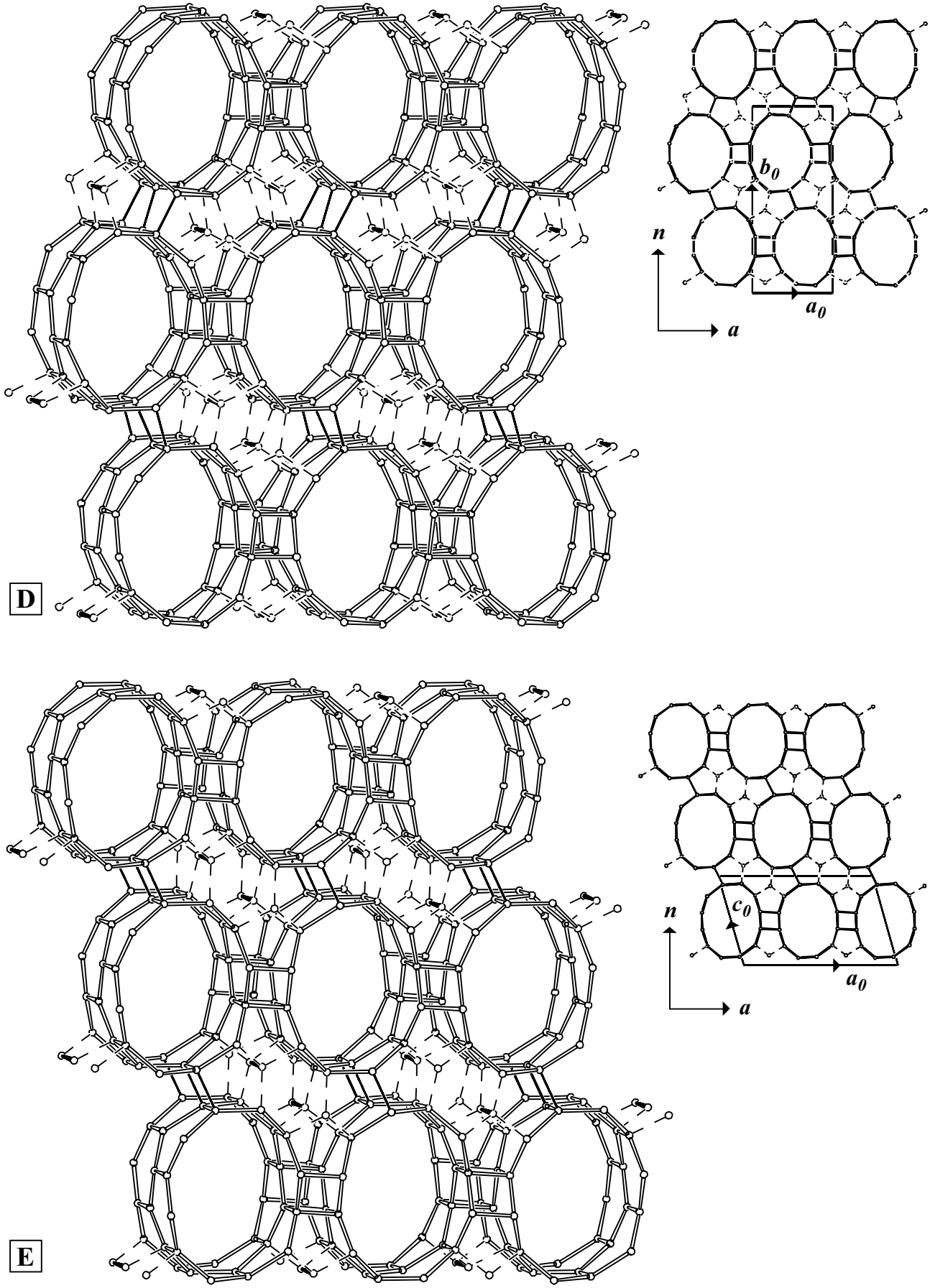

Fig. 3c. The ordered end-members **D** and **E** (cf. Table 1) viewed along the pore axis. The unit cells are given in standard setting. T-T connections to dimer units are striped.

(Fig.3 is continued on next page)

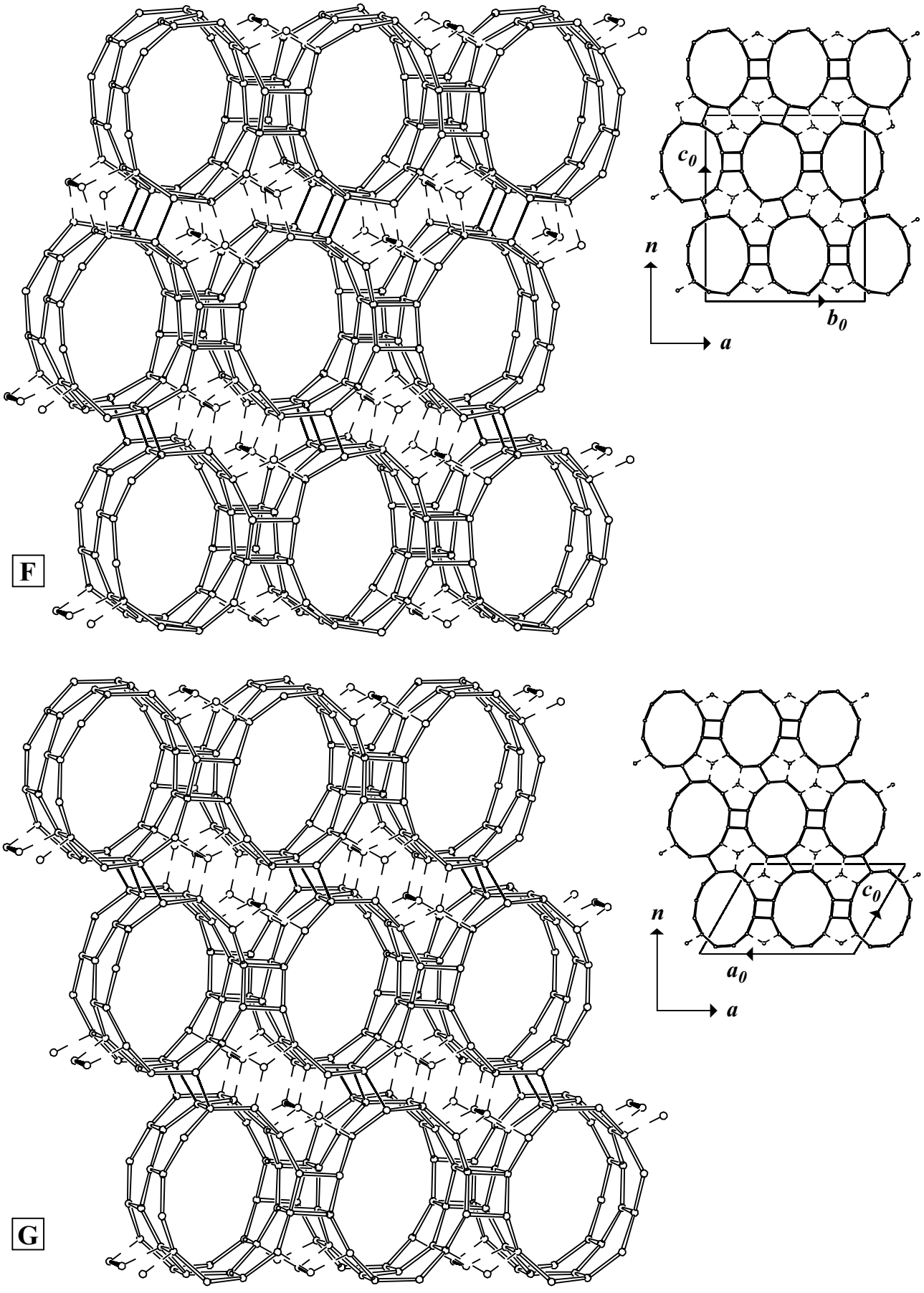

Fig. 3d. The ordered end-members **F** and **G** (cf. Table 1) viewed along the pore axis. The unit cells are given in standard setting. T-T connections to dimer units are striped.

(Fig.3 is continued on next page)

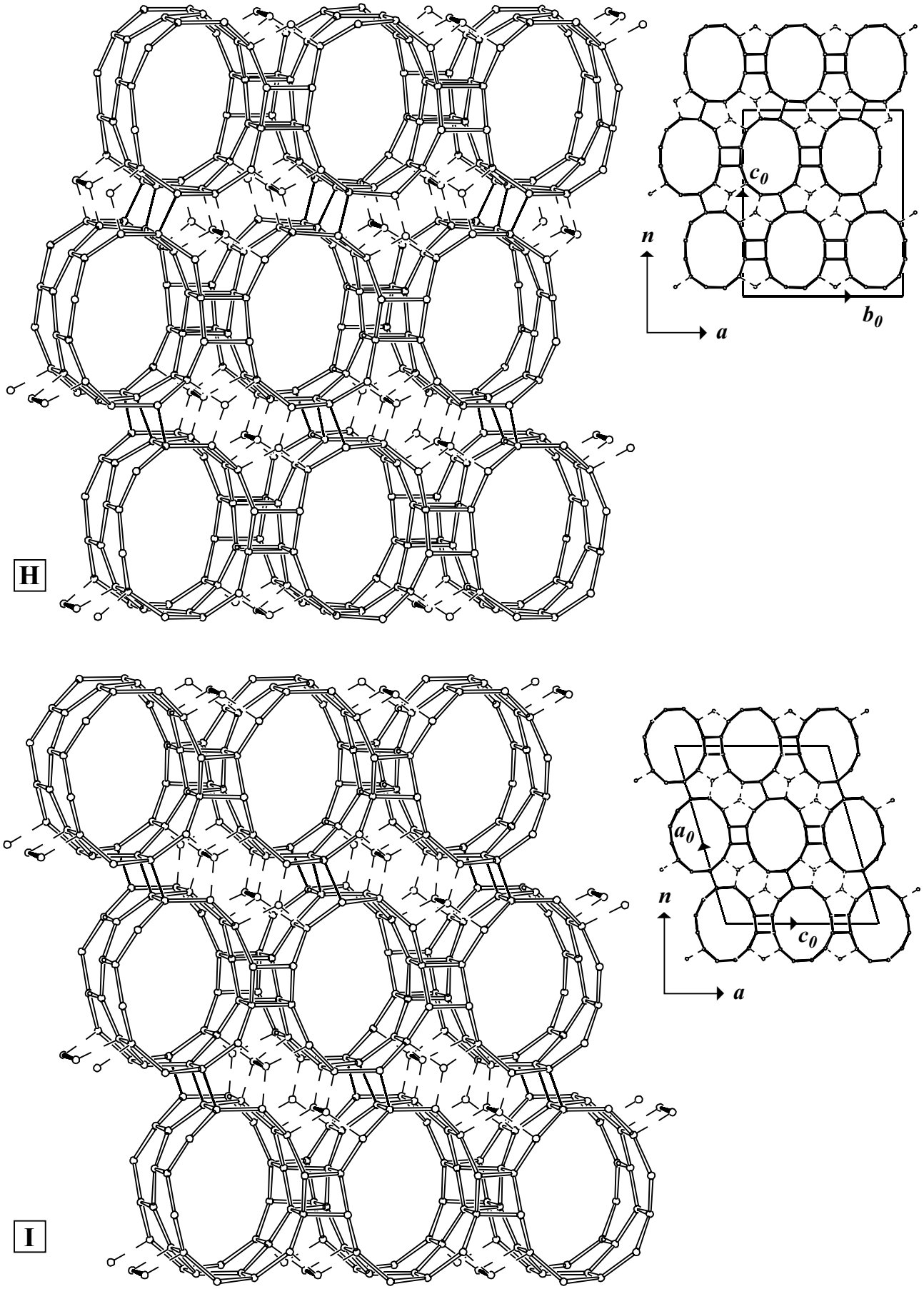

Fig. 3e. The ordered end-members **H** and **I** (cf. Table 1) viewed along the pore axis. The unit cells are given in standard setting. T-T connections to dimer units are striped.

(Fig.3 is continued on next page)

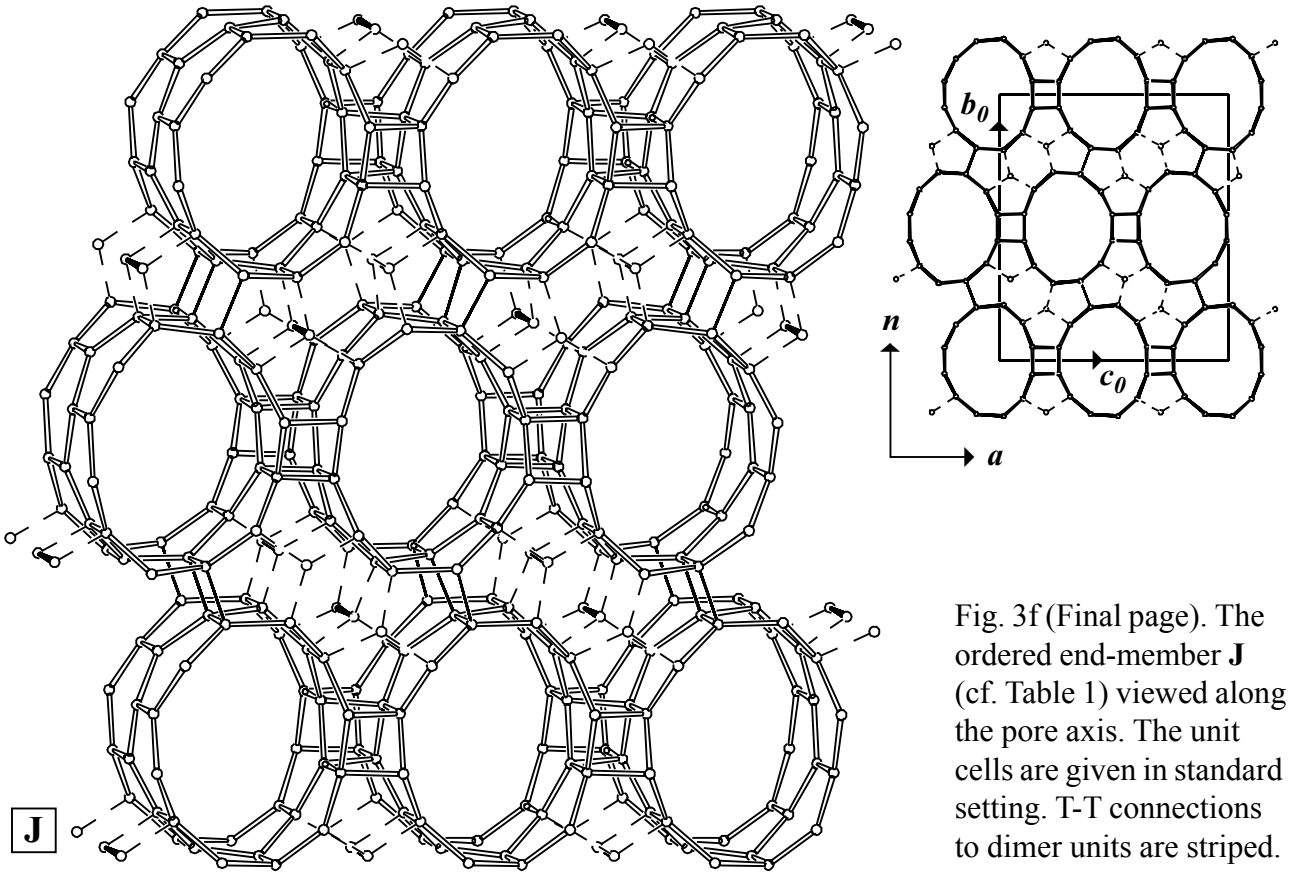

Fig. 3f (Final page). The ordered end-member **J** (cf. Table 1) viewed along the pore axis. The unit cells are given in standard setting. T-T connections to dimer units are striped.

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	ß (°)
				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 Å (See Fig.1 and Section **4**); the pore axis ***b*** = 8.4 Å; ***n*** is parallel to ***a*** x ***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].

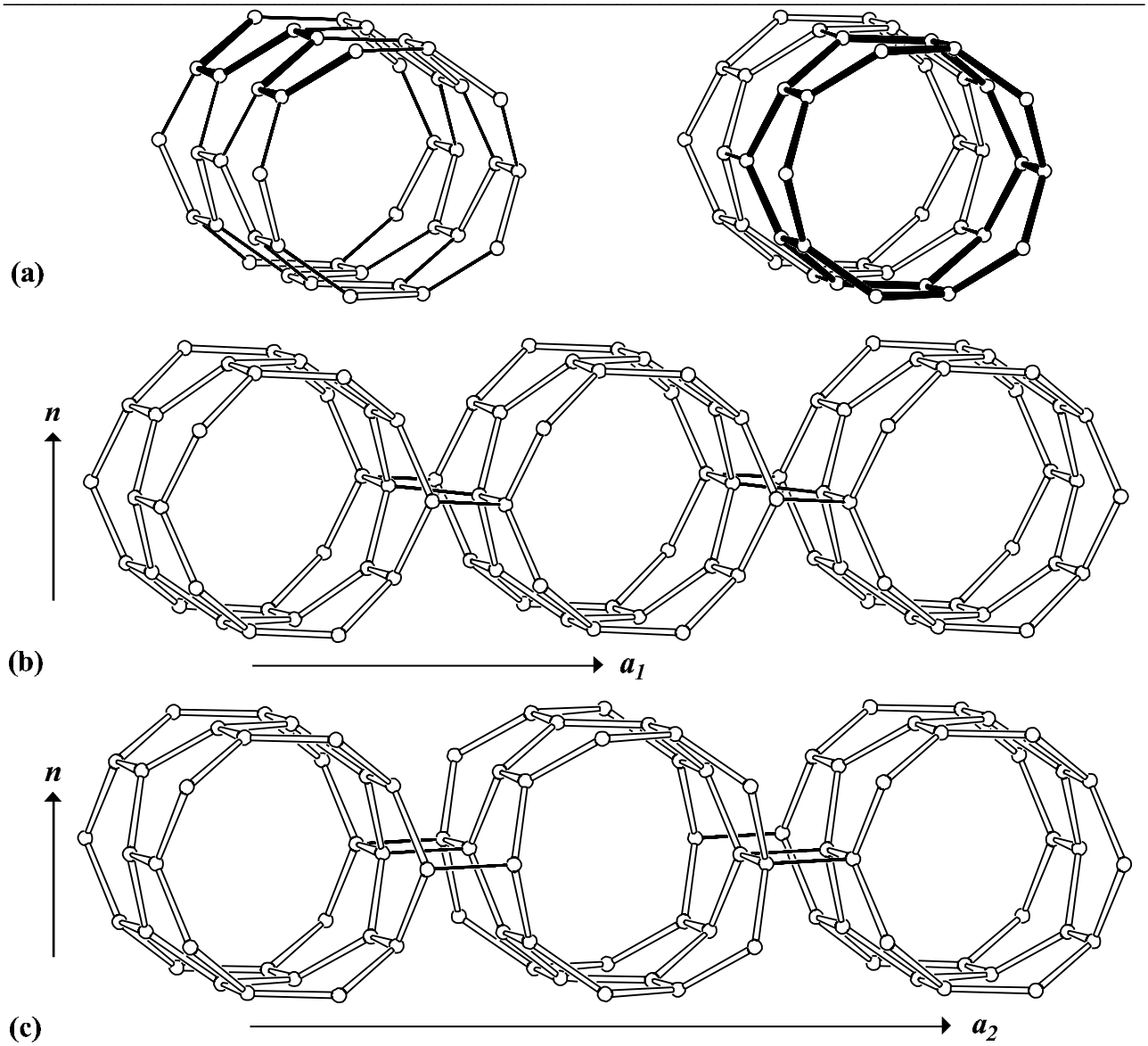

Fig. 4. Tubular pore with 10-ring window (a) constructed from five crankshaft chains (left) or from 6-ring bands each consisting of 20 T atoms (right); PerBU1 (b) and PerBU2 (c) of the ZSM-48 family of zeolite frameworks seen in perspective view perpendicular to the plane normal ***n*** and along the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

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].

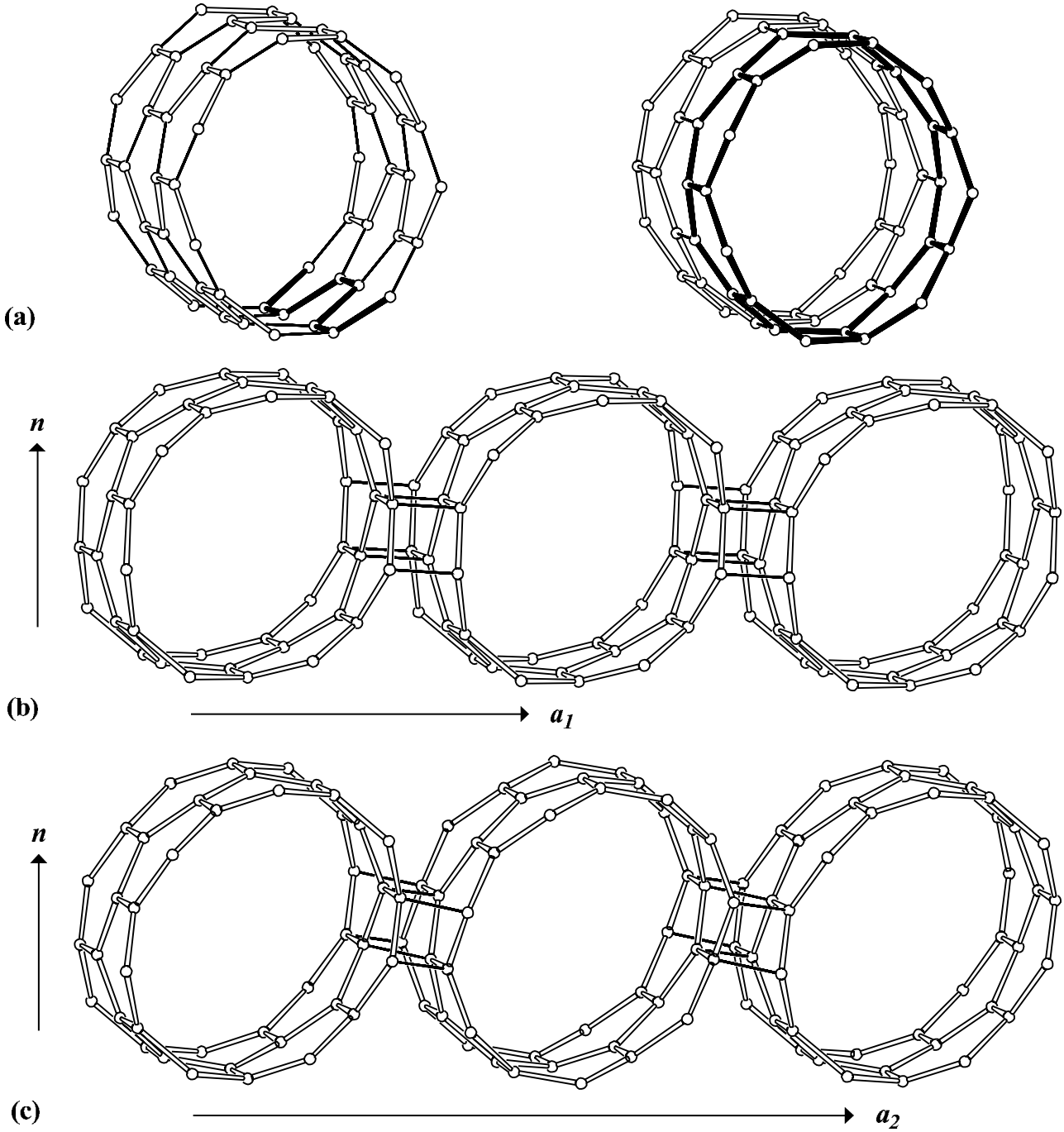

Fig. 5. Tubular pore with 14-ring window constructed from seven crankshaft chains (left) or from 6-ring bands each consisting of 28 T atoms (right); PerBU1 (b) and PerBU2 (c) of the UTD-1 family of zeolite frameworks seen in perspective view perpendicular to the plane normal ***n*** and along the pore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

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

8. References

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[2] S.I. Zones, Y. Nakagawa, L.T. Yuen and T.V. Harris, J. Am. Chem. Soc., 118 (1996) 7558.
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[4] H. van Koningsveld and R.F. Lobo, J. Phys. Chem. B, 107 (2003) 10983.
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