

# The ZSM-48 Family

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1. The Periodic Building Units (PerBU1 and PerBU2) in the ZSM-48 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 T6-rings with T10-ring windows as shown in Figure 1a.

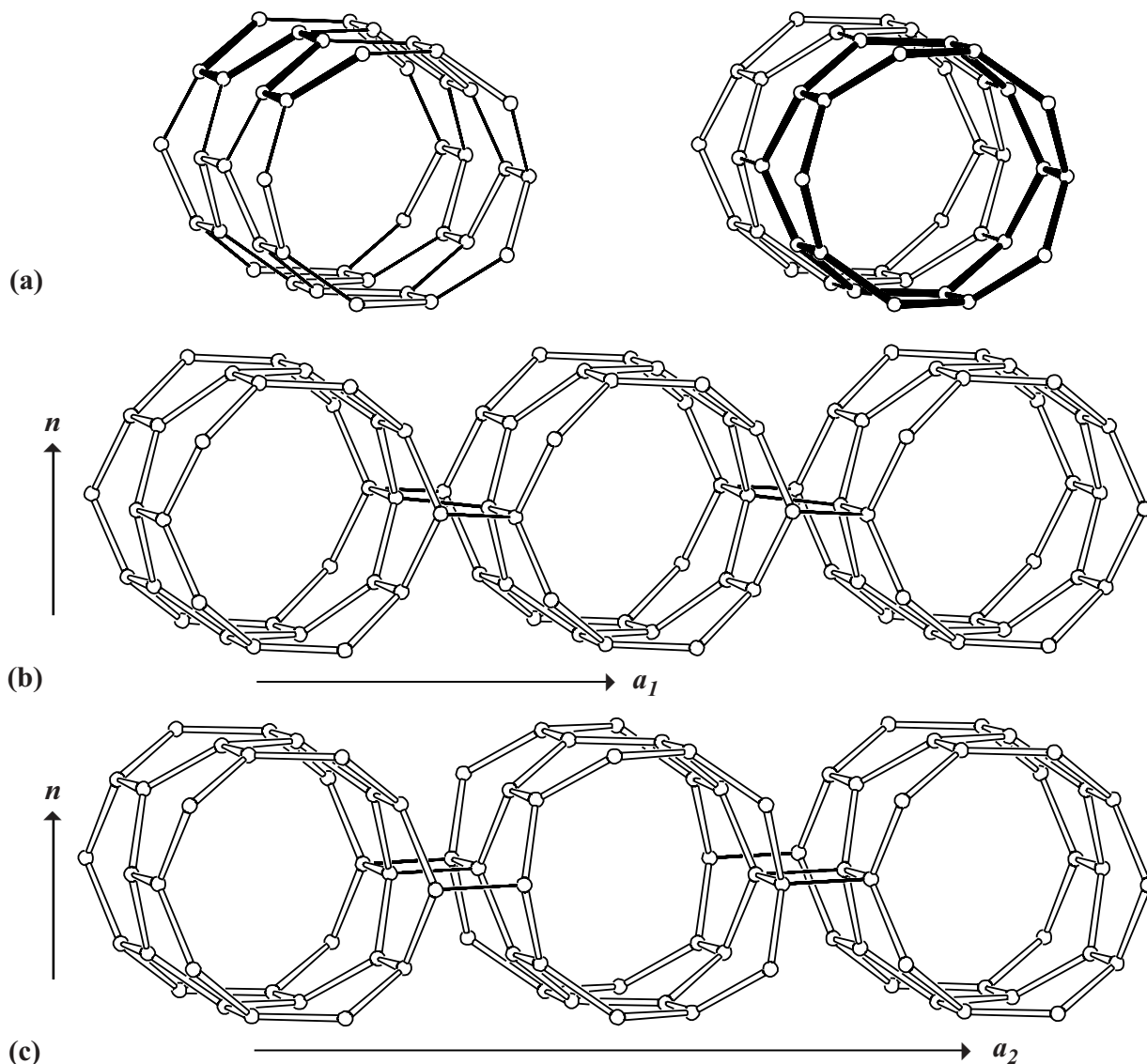


Figure 1: Tubular pore with T10-ring window (a) constructed from five crankshaft chains (left) or from T6-ring bands each consisting of 20 T atoms (right); PerBU1 (b) and PerBU2 (c) of the ZSM-48 family of zeolite frameworks seen in perspective view perpendicular to the plane normal  $n$  and along the pore axis  $b$

Tubular pores (Fig. 1a), related by pure translations along  $a_1$ , are connected through single crankshaft chains into PerBU1 (Fig. 1b). Tubular pores, related by pure translations along  $a_2$  accompanied by a shift of  $\frac{1}{2}b$  along the pore axis, are connected through T4-rings into PerBU2 (Fig. 1c).

[Compare the PerBU's in ZSM-48 with those in the [SSZ-31](#) and [UTD-1](#) families].



**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. Connectivity Pattern of the PerBU's:**

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  $2|a_1|$  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:

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

**(c):**  $-\frac{1}{6}a$  and  $\frac{1}{2}b$ ; denoted as  $(-\frac{1}{6}, \frac{1}{2})$ ;      **(d):**  $\frac{1}{6}a$  and  $\frac{1}{2}b$ ; denoted as  $(\frac{1}{6}, \frac{1}{2})$ .

In Figure 2 the connection modes **(a)** and **(c)** between PerBU1's, and the connection modes **(b)** and **(d)** between PerBU2's are depicted.

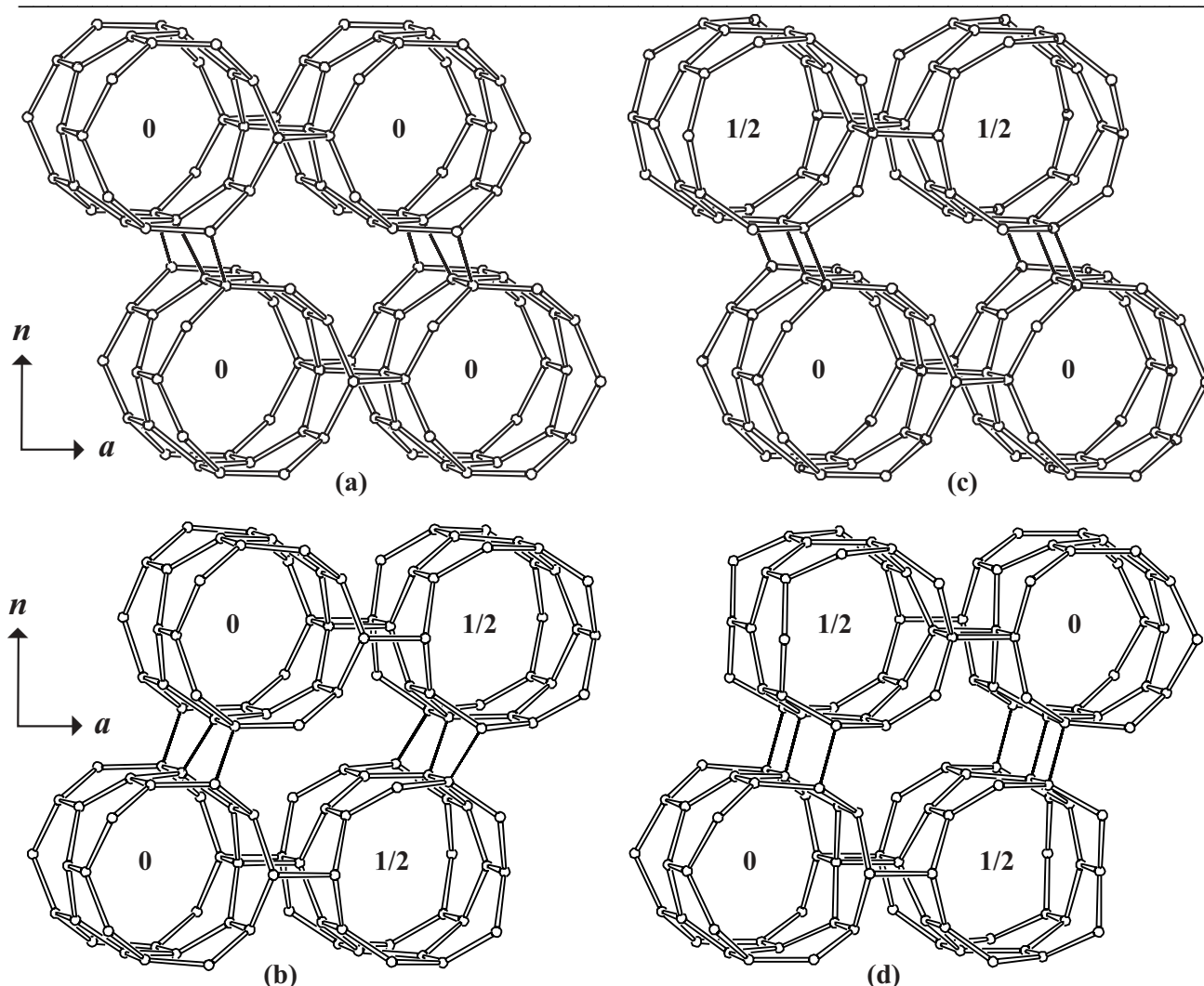


Figure 2: Perspective view along the pore axis  $b$  of the connection modes **(a-d)** in the ZSM-48 family of zeolites. The PerBU's are connected through crankshaft chains or T4-rings depending on whether the shift along  $b$  between direct neighbouring pores is zero or  $\frac{1}{2}b$ , respectively

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 ZSM-48 family of zeolites are shown in Figure 3 and Table 1. The gaps between the pores are filled by T-T dimer units. None of the end-members has been observed as pure single crystal material so far.

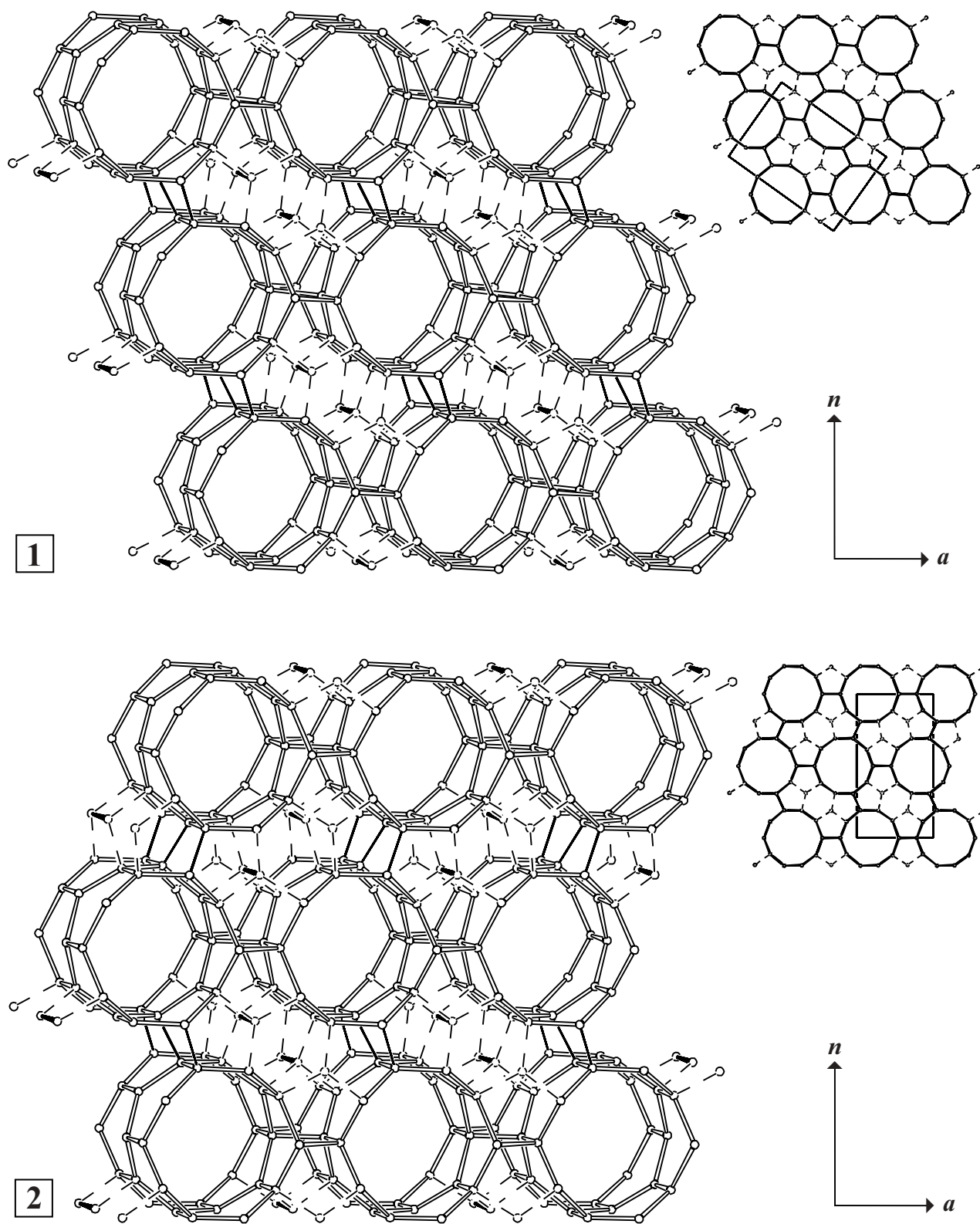


Figure 3: Perspective drawing (left) and parallel projection along the pore axis of the unit cell in standard setting (top right) of the ordered end-members **1** and **2** (cf. Table 1) in the ZSM-48 family. T-T connections to dimer units are striped. (Fig.3 is continued on next page) ▲

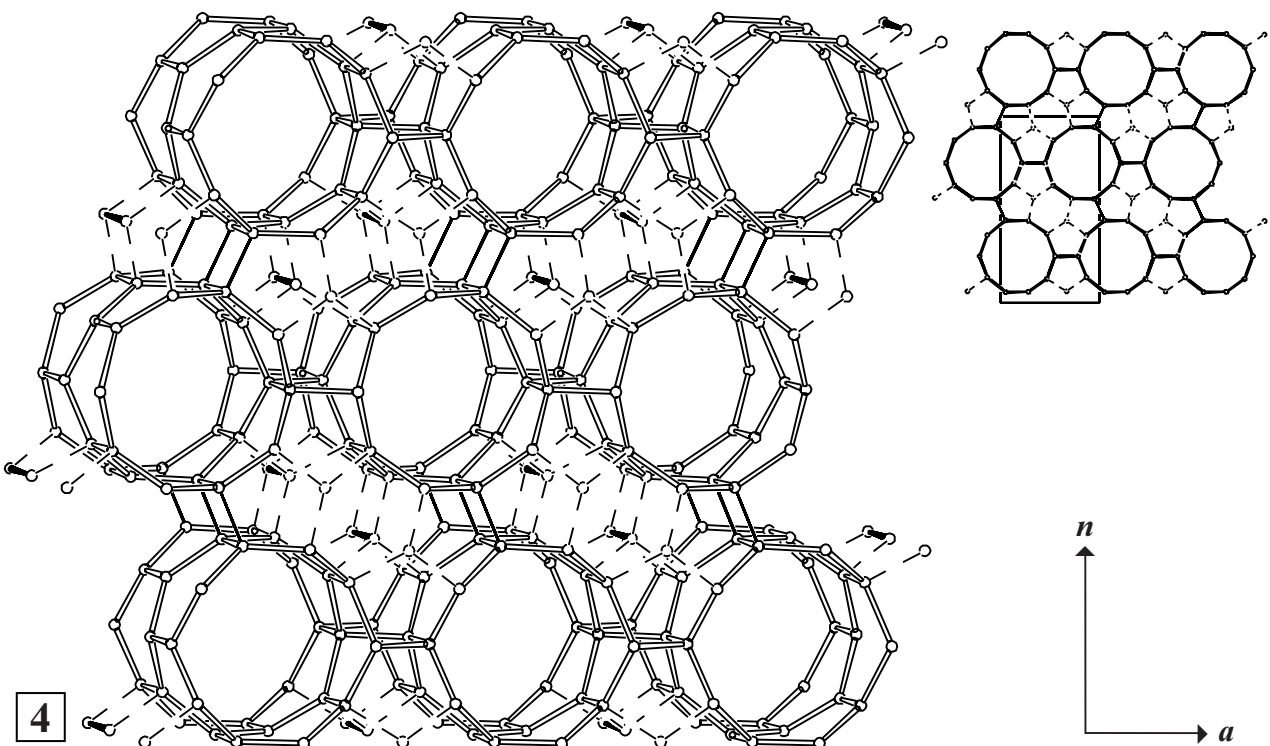
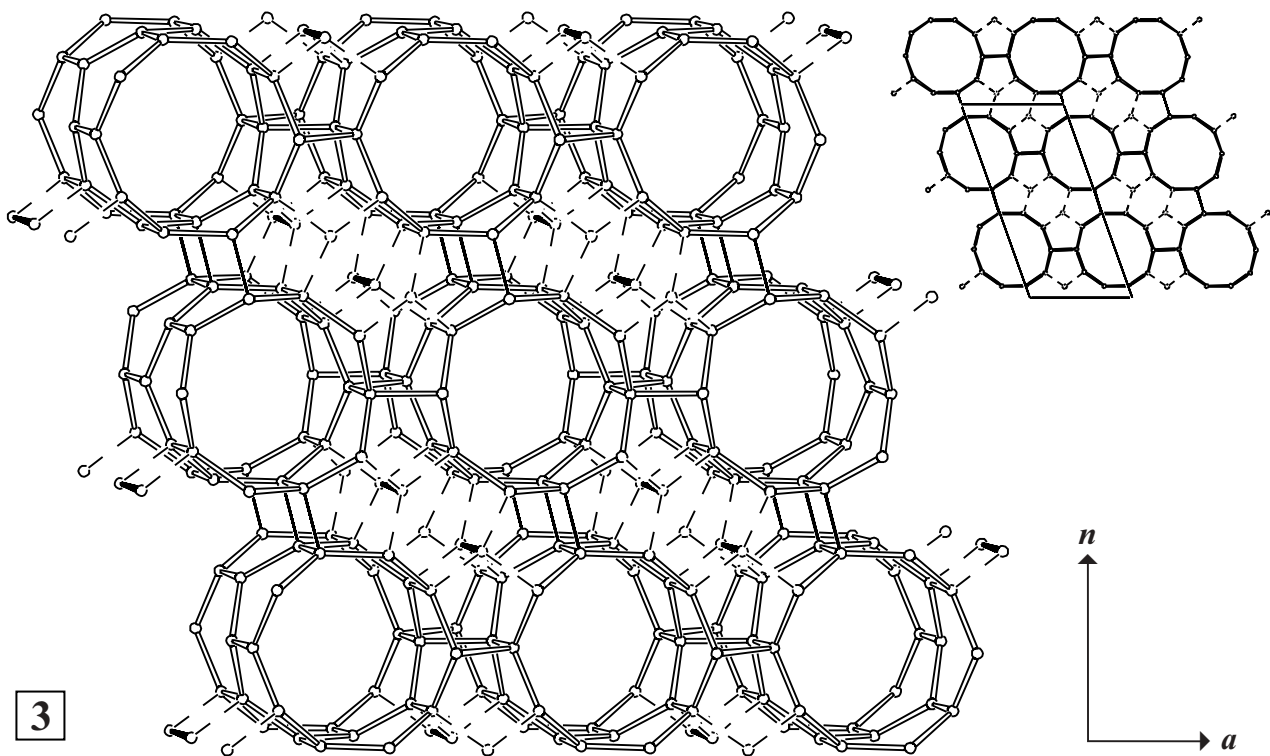


Figure 3 (Continued): Perspective drawing (left) and parallel projection along the pore axis of the unit cell in standard setting (top right) of the ordered end-members **3** and **4** (cf. Table 1) in the ZSM-48 family. T-T connections to dimer units are striped. (Fig.3 is continued on next page) ▲

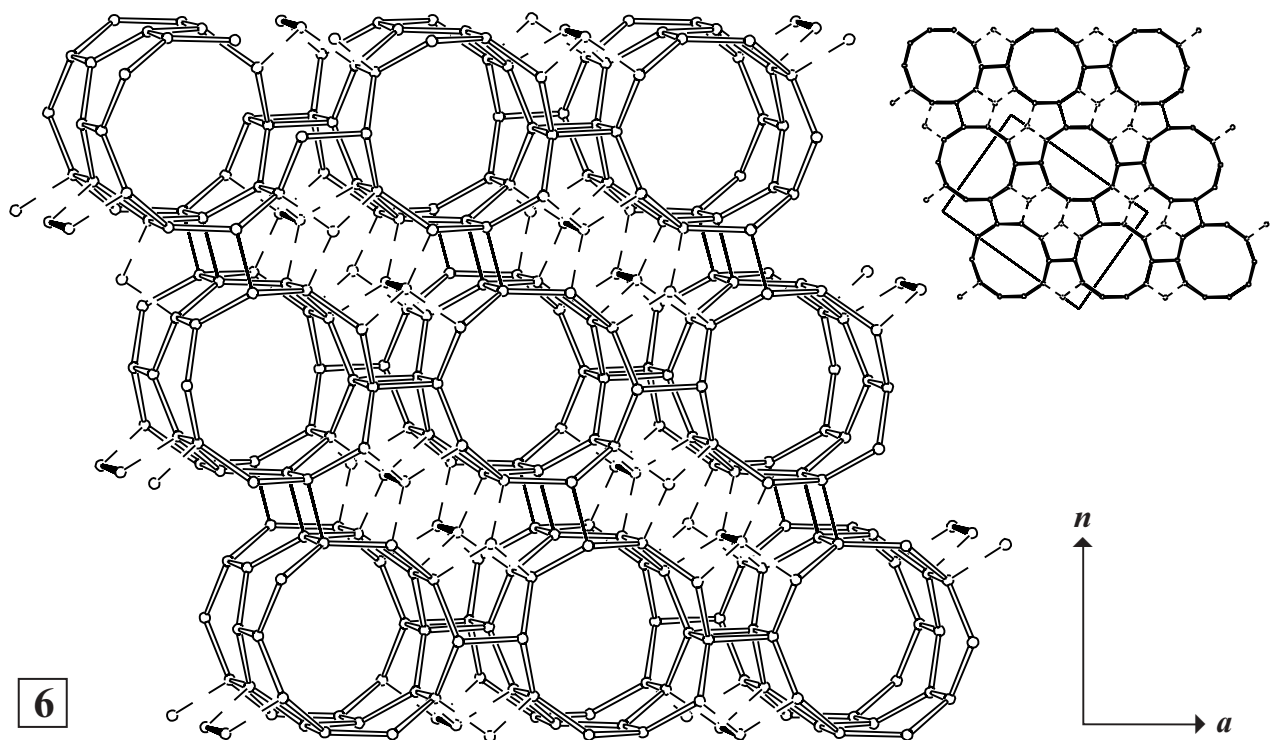
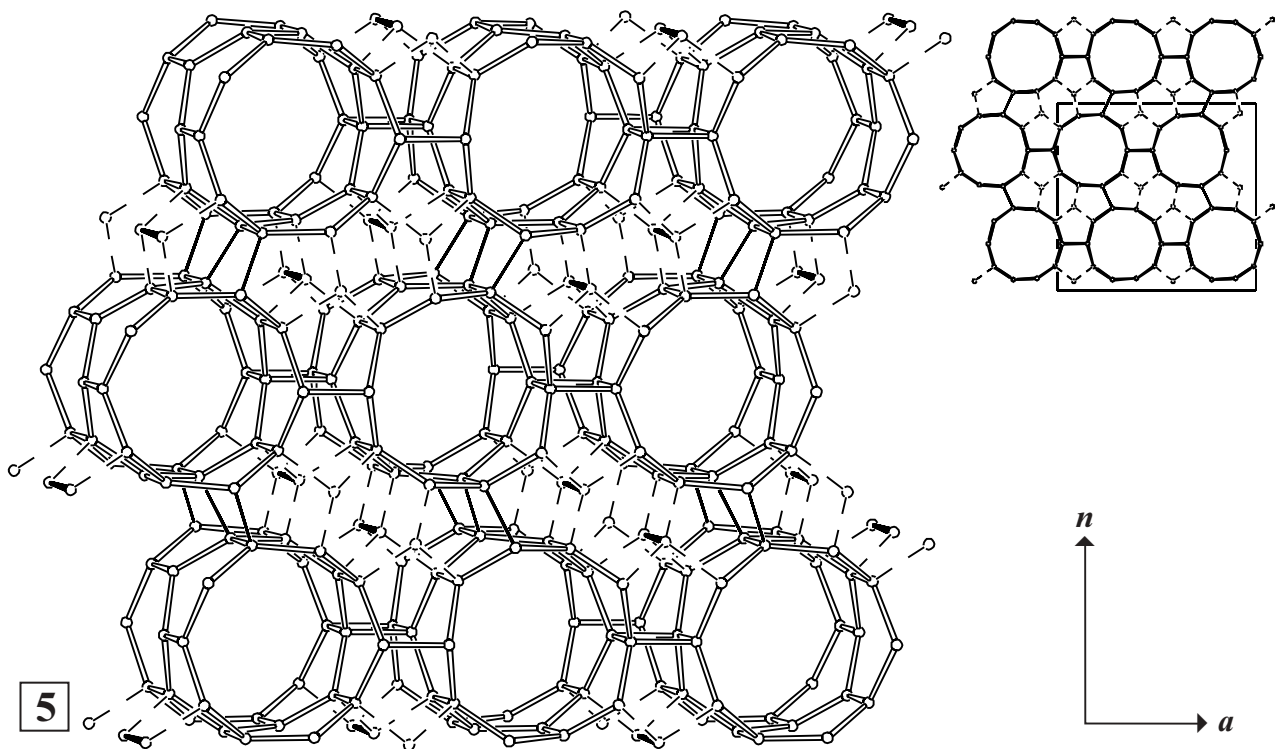


Figure 3 (Continued): Perspective drawing (left) and parallel projection along the pore axis of the unit cell in standard setting (top right) of the ordered end-members **5** and **6** (cf. Table 1) in the ZSM-48 family. T-T connections to dimer units are striped. (Fig.3 is continued on next page) ▲

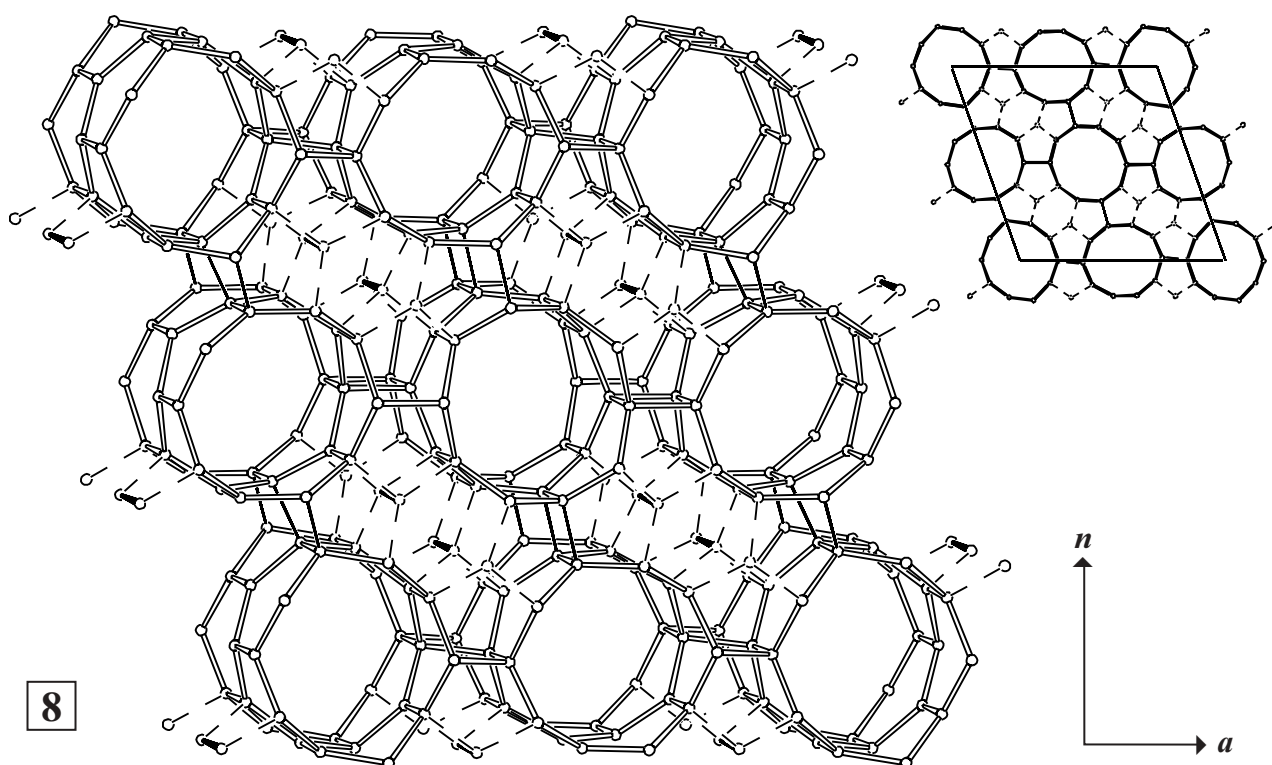
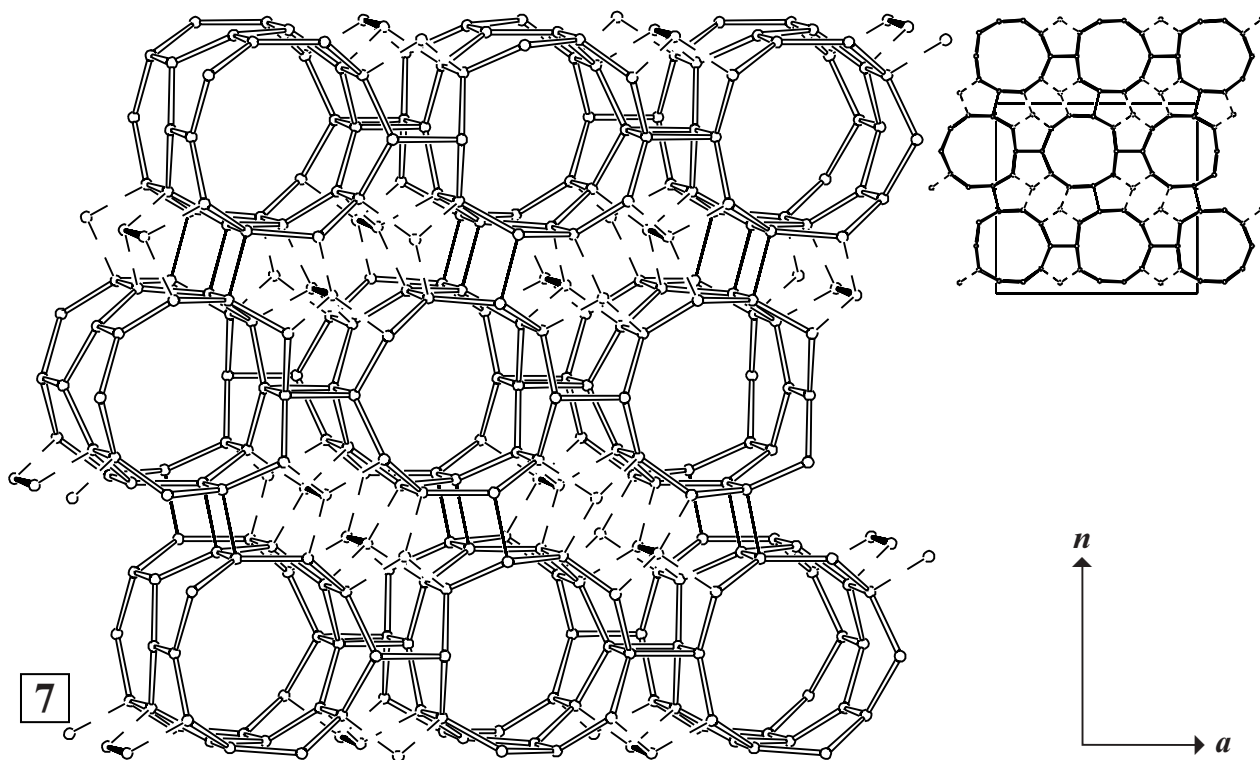


Figure 3 (Continued): Perspective drawing (left) and parallel projection along the pore axis of the unit cell in standard setting (top right) of the ordered end-members **7** and **8** (cf. Table 1) in the ZSM-48 family. T-T connections to dimer units are striped. (Fig.3 is continued on next page) ▲

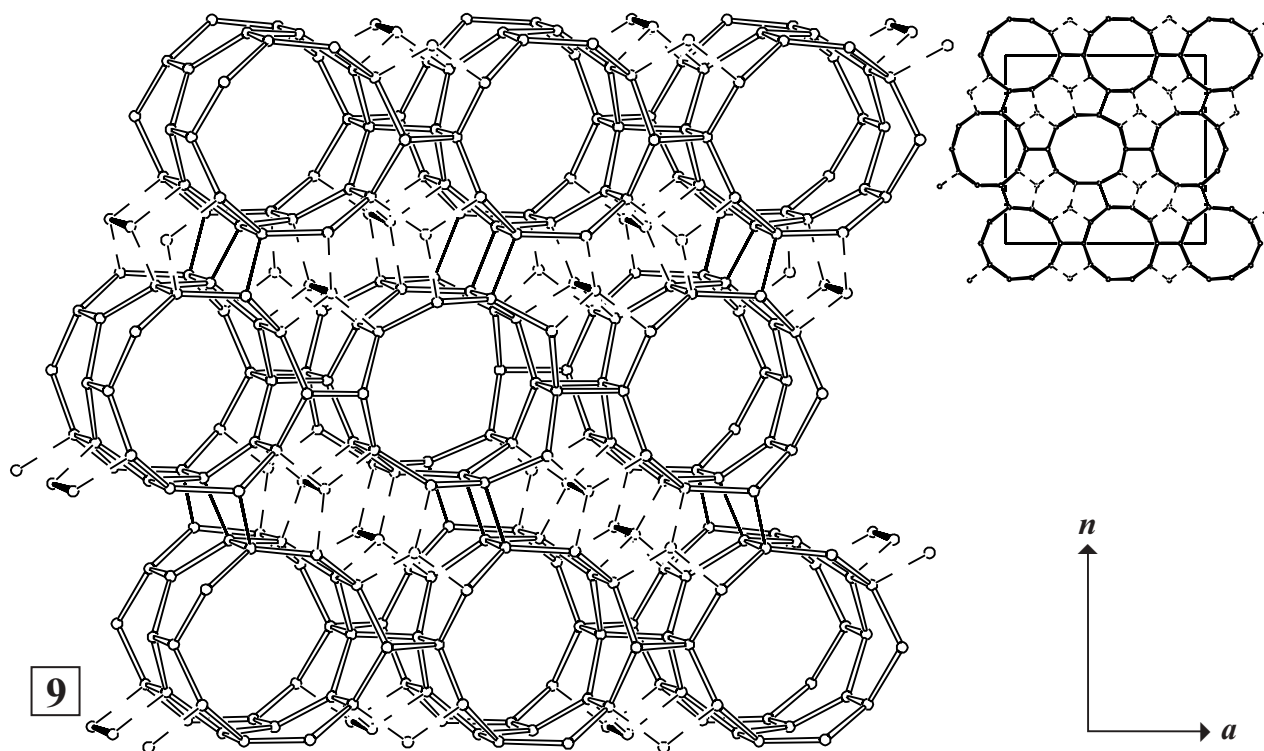


Figure 3 (Final page): Perspective drawing (left) and parallel projection along the pore axis of the unit cell in standard setting of the ordered end-member **9** (cf. Table 1) in the ZSM-48 family. T-T connections to dimer units are striped.

Table 1: Stacking sequences of the PerBU's for the simplest ordered end-members in the ZSM-48 family. The end-member number refers to the framework plots **1-9** on this and 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) <sup>1</sup></i>			<i>space group</i>	$a_0$	$b_0$ (Å)	$c_0$	$\beta$ (°)
PerBU1								
<b>1</b> <sup>2</sup>	$(-1/6, 0)$ ;	$(-1/6, 0)$ ;	$(-1/6, 0)$ ;	Cmcm	14.24	20.14	8.4	-
<b>2</b>	$(-1/6, 0)$ ;	$(+1/6, 0)$ ;	$(-1/6, 0)$ ;	Pmmm	8.4	23.26	12.33	-
<b>3</b>	$(-1/6, 1/2)$ ;	$(-1/6, 1/2)$ ;	$(-1/6, 1/2)$ ;	C2/m	24.66	8.4	12.33	109.47
<b>4</b>	$(-1/6, 1/2)$ ;	$(+1/6, 1/2)$ ;	$(-1/6, 1/2)$ ;	Pmma	8.4	23.26	12.33	-
PerBU2								
<b>3</b> <sup>3</sup>	$(-1/6, 0)$ ;	$(-1/6, 0)$ ;	$(-1/6, 0)$ ;	C2/m	24.66	8.4	12.33	109.47
<b>5</b>	$(-1/6, 0)$ ;	$(+1/6, 0)$ ;	$(-1/6, 0)$ ;	Cmcm	8.4	24.66	23.26	-
<b>6</b> <sup>4</sup>	$(-1/6, 1/2)$ ;	$(-1/6, 1/2)$ ;	$(-1/6, 1/2)$ ;	Imma	8.4	14.24	20.14	-
<b>7</b>	$(-1/6, 1/2)$ ;	$(+1/6, 1/2)$ ;	$(-1/6, 1/2)$ ;	Cmcm	8.4	24.66	23.26	-
PerBU1 and PerBU2								
<b>8</b>	$(-1/6, 0)$ ;	$(-1/6, 0)$ ;	$(-1/6, 0)$ ;	P2 <sub>1</sub> /m	24.66	8.4	24.66	109.47
<b>9</b>	$(-1/6, 0)$ ;	$(+1/6, 0)$ ;	$(-1/6, 0)$ ;	Pmm2	8.4	23.26	24.66	-

<sup>1</sup>  $a = 24.66$  Å (See Fig.1 and Section 4); the pore axis  $b = 8.4$  Å;  $n$  is parallel to  $a \times b$ .

<sup>2</sup> End-member **1** equals polytype 48A from Ref. 5.

<sup>3</sup> This end-member, built from PerBU2, is identical to end-member **3** built from PerBU1.

<sup>4</sup> End-member **6** equals polytype 48B from Ref. 5. ▲

## 6. Disordered Materials Synthesized and Characterized to Date:

ZSM-48 (1,2,3,4,5,6); EU-2 (7); ZBM-30 (8); EU-11 (9). ▲

## 7. Supplementary Information

### 7.1 Comparison with the SSZ-31 family:

The Periodic Building Units (PerBU1 and PerBU2) in the SSZ-31 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 T6-rings with T12-ring windows. [Compare these PerBU's (with T12-ring windows) with the PerBU's in ZSM-48 (with T10-ring windows) and in UTD-1 (with T14-ring windows)].

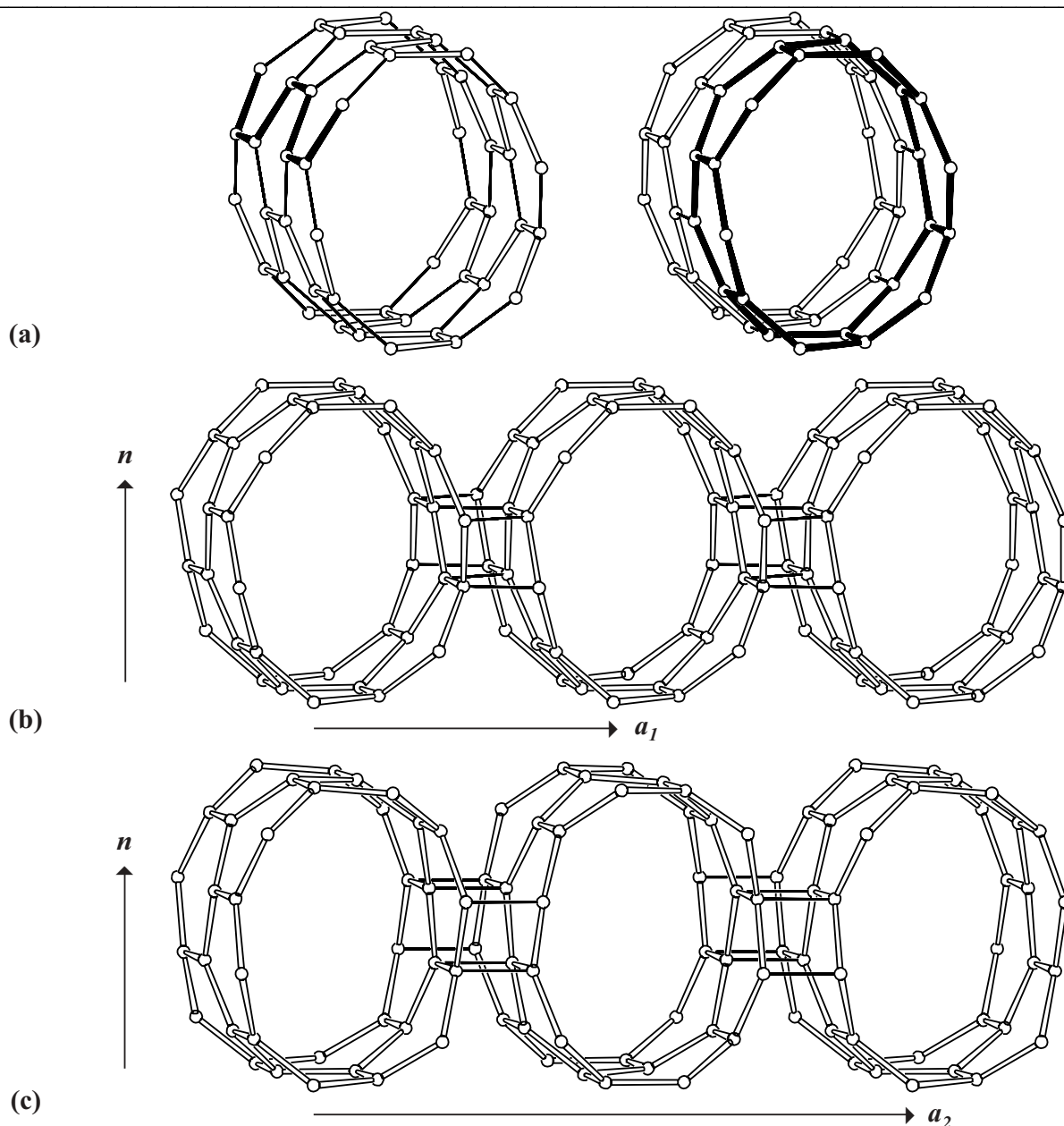


Figure 4: Tubular pore with T12-ring window (a) constructed from six crankshaft chains (left) or from T6-ring bands each consisting of 24 T atoms (right); PerBU1 (b) and PerBU2 (c) of the SSZ-31 family of zeolite frameworks seen in perspective view perpendicular to the plane normal  $n$  and along the pore axis  $b$  ▲

For more details: see the description of the [SSZ-31](#) 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 T6-rings with T14-ring windows. [Compare these PerBU's (with T14-ring windows) with the PerBU's in ZSM-48 (with T10-ring windows) and in SSZ-31 (with T12-ring windows)].

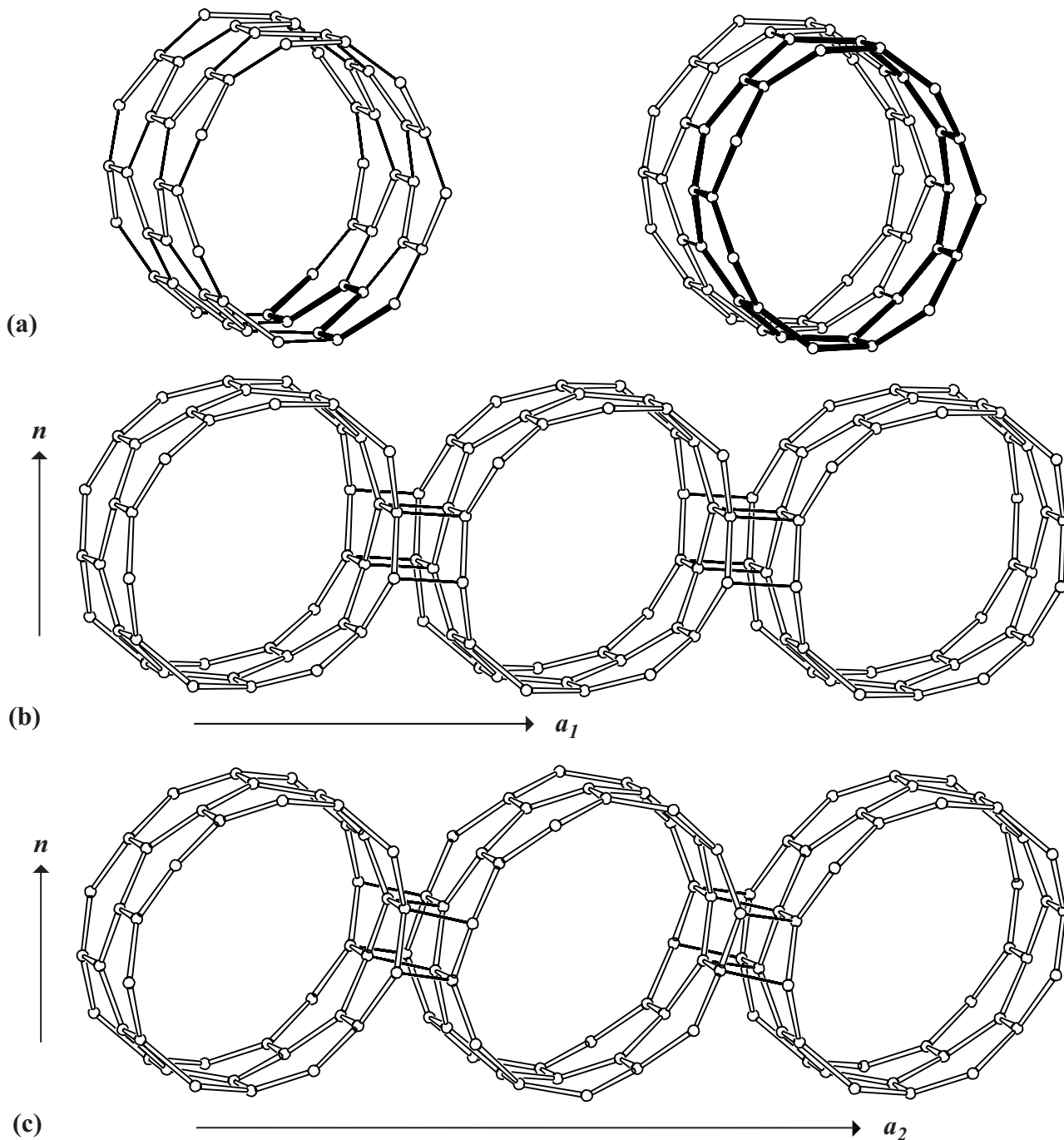


Figure 5: Tubular pore with T14-ring window (a) constructed from seven crankshaft chains (left) or from T6-ring bands each consisting of 28 T atoms (right); PerBU1 (b) and PerBU2 (c) of the UTD-1 family of zeolite frameworks seen in perspective view perpendicular to the plane normal  $n$  and along the pore axis  $b$

## 8. References

- (1) J.L. Schlenker, F.G. Dwyer, E.E. Jenkins, W.J. Rohrbaugh and G.T. Kokotailo, *Nature* **294**, 340 (1981).
- (2) P. Chu, US Patent 4,397,827(1981).
- (3) L.D. Rollmann and E.W. Valyocsik, US Patent 4,423,021(1983).
- (4) P. Chu, US Patent 4,448,675(1984).
- (5) J.L. Schlenker, W.J. Rohrbaugh, P. Chu, E.W. Valyocsik and G.T. Kokotailo, *Zeolites* **11**, 355 (1985).
- (6) R.F. Lobo and H. van Koningsveld, *J. Am. Chem. Soc.* **124**, 13222 (2002).
- (7) J.L. Casci, B.M. Lowe and T.V. Whittam, UK Patent Appl. GB 2077709A (Imperial Chemical Industries, Limited), (1981).
- (8) L. Marosci, M. Schwartzmann and J. Stabenow, *J. Eur. Pat. Appl. No. EP A 0046504* (BASF Aktiengesellschaft), (1982).

