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.

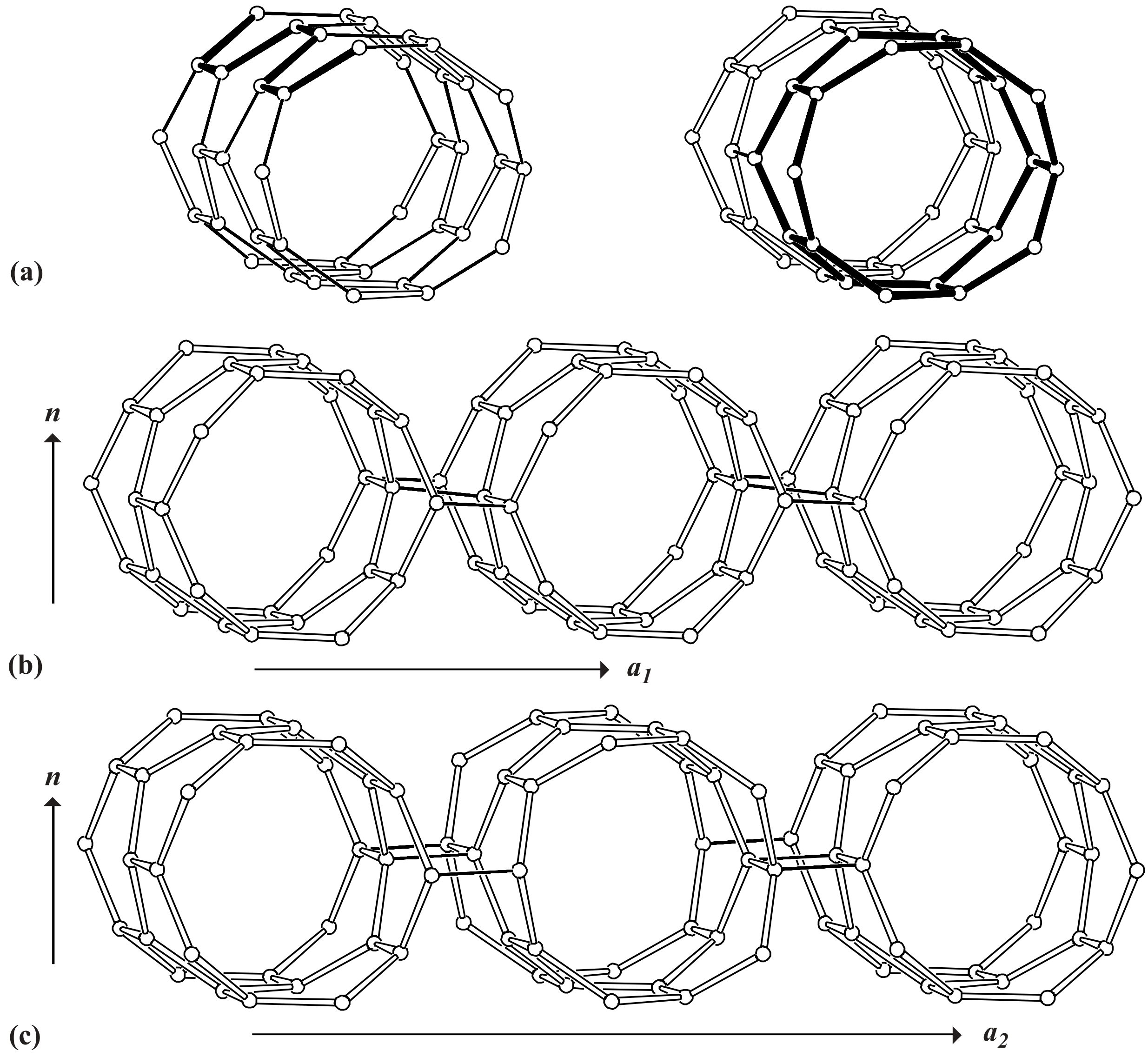


Figure 1: Tubular pore with T10-ring window (a) constructed from five crankshaft chains (left) or from T6-ring bands each consisting of 20 T atoms (right); PerBU1 (b) and PerBU2 (c) of the ZSM-48 family of zeolite frameworks seen in perspective view perpendicular to the plane normal ***n*** and along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

Tubular pores (Fig.1a), related by pure translations along $\boldsymbol{a_1}$, are connected through single crankshaft chains into PerBU1 (Fig.1b). Tubular pores, related by pure transaltions along $\boldsymbol{a_2}$ accompanied by a shift of ½***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 $2|\boldsymbol{a_1}|$ 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:

(a): $-{}^1/_6\,\boldsymbol{a}$ and zero; denoted as $(-{}^1/_6, 0)$; **(b):** ${}^1/_6\,\boldsymbol{a}$ and zero; denoted as $({}^1/_6, 0)$;

(c): $-{}^1/_6\,\boldsymbol{a}$ and ${}^1/_2\,\boldsymbol{b}$; denoted as $(-{}^1/_6, {}^1/_2)$; **(d):** ${}^1/_6\,\boldsymbol{a}$ and ${}^1/_2\,\boldsymbol{b}$; denoted as $({}^1/_6, {}^1/_2)$.

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

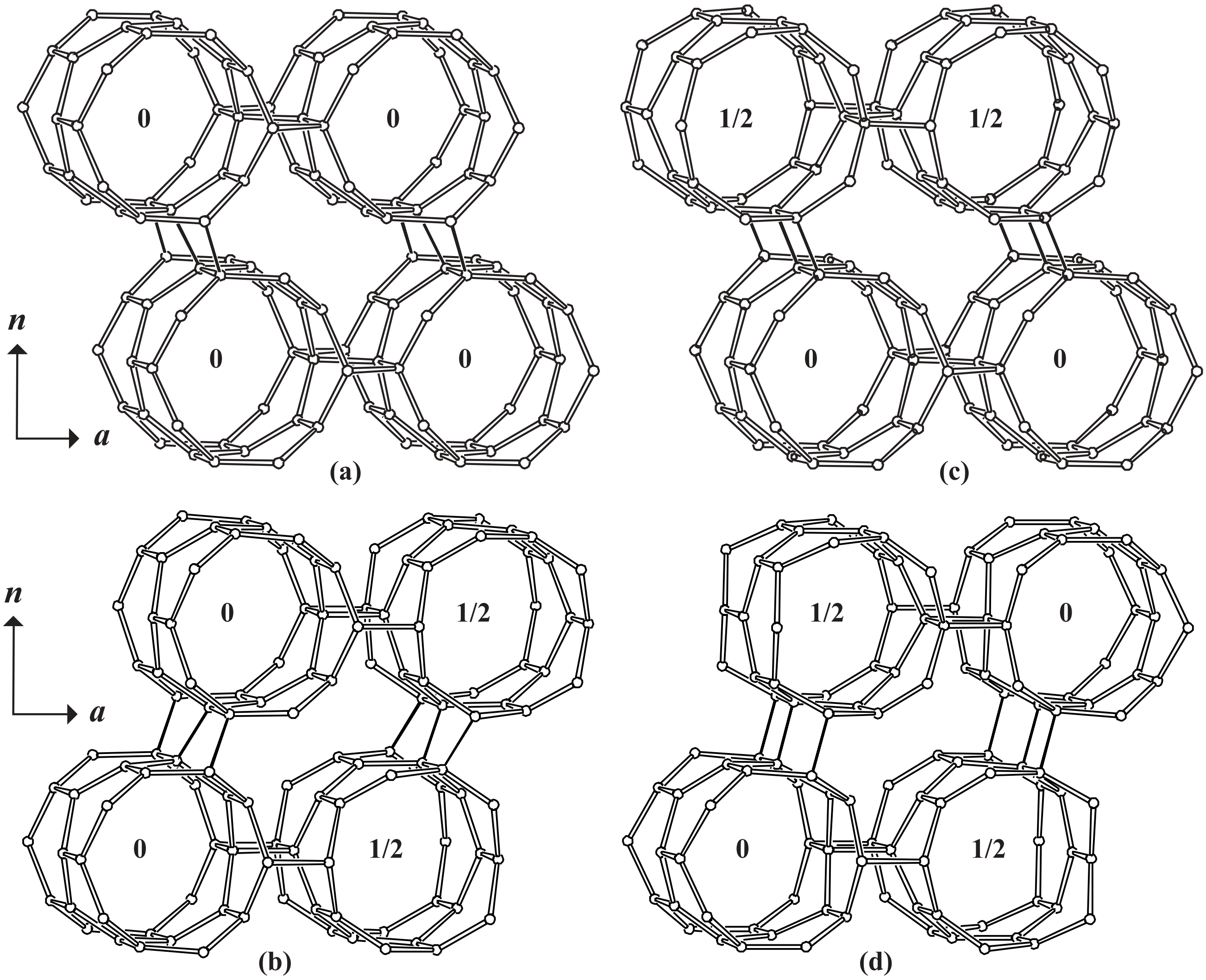


Figure 2: Perspective view along the pore axis ***b*** of the connection modes **(a-d)** in the ZSM-48 family of zeolites. The PerBU's are connected through crankshaft chains or T4-rings depending on whether the shift along ***b*** between direct neighbouring pores is zero or ${}^1/_2\boldsymbol{b}$, 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.

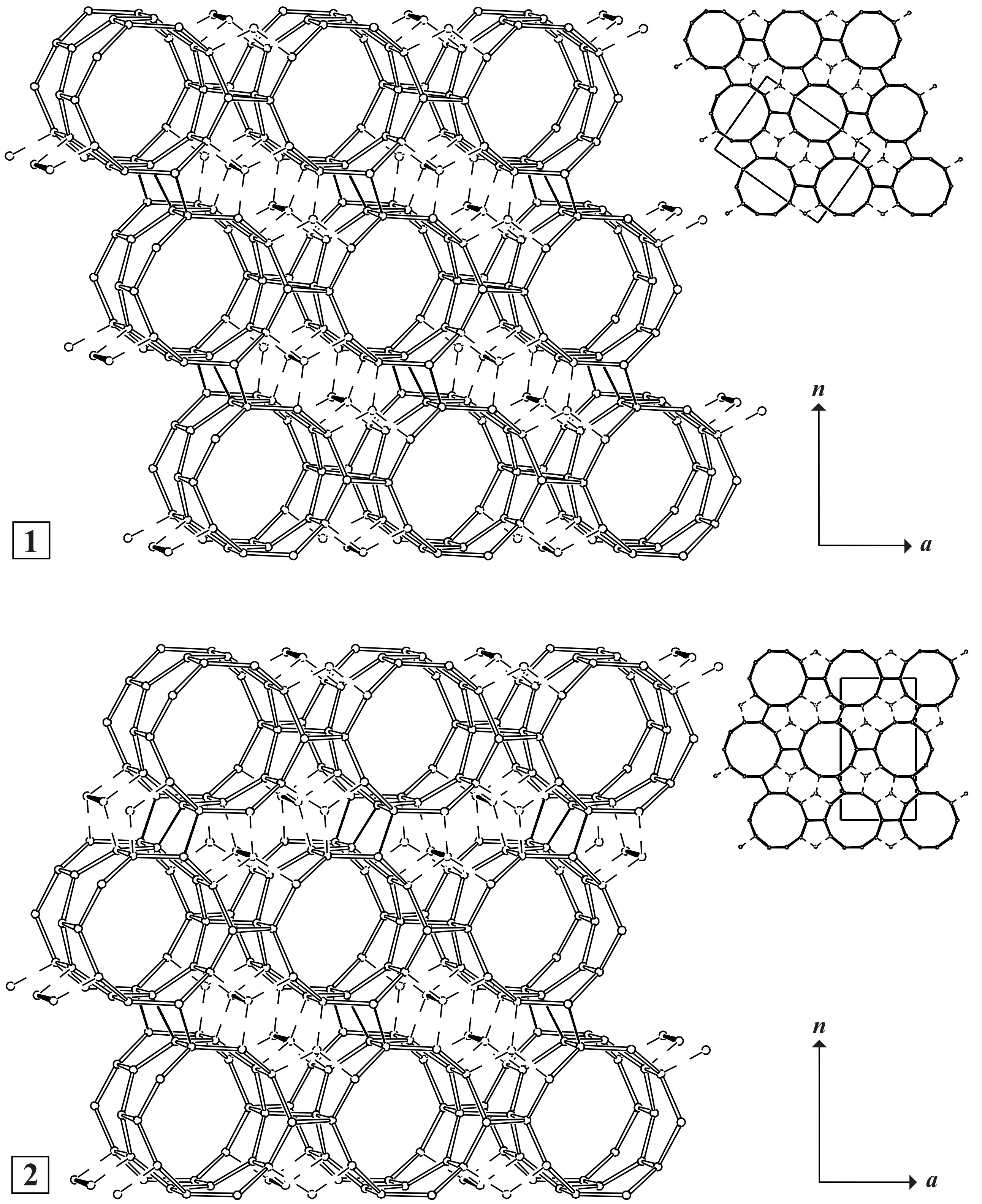
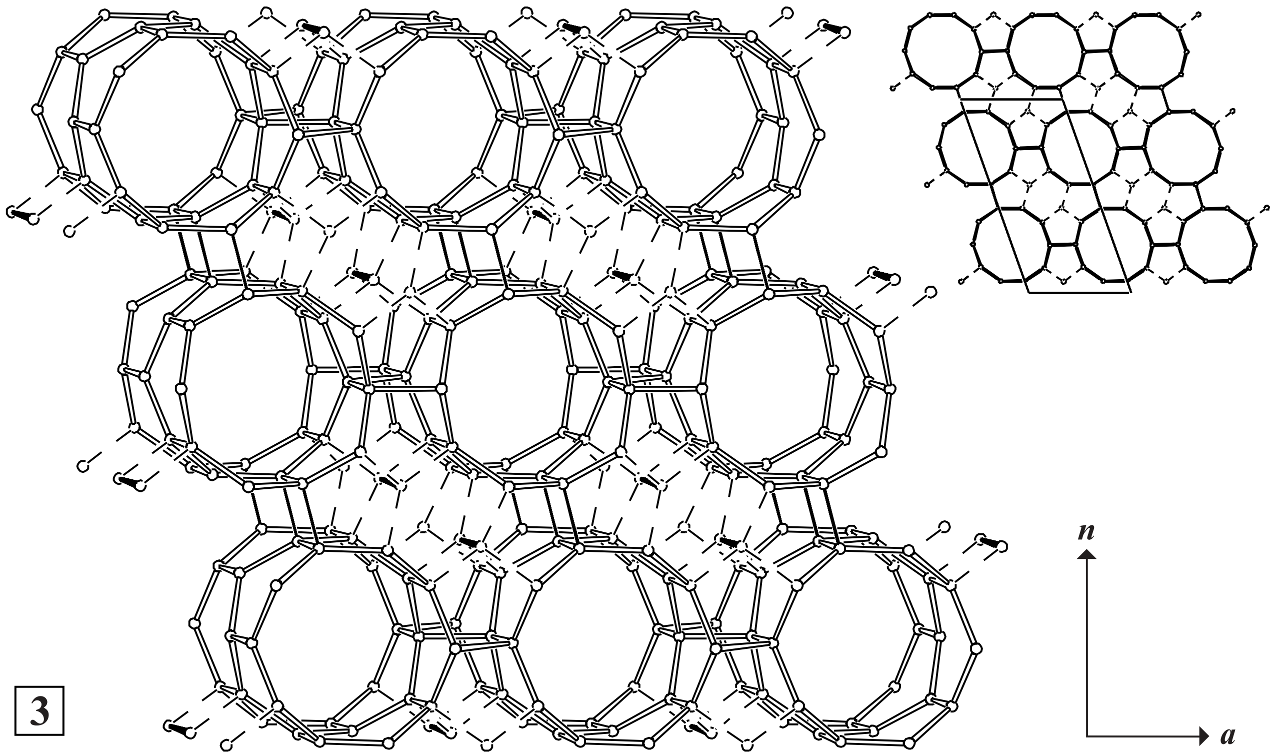


Figure 3: Perspective drawing (left) and parallel projection along the pore axis of the unit cell in standard setting (top right) of the ordered end-members **1** and **2** (cf. Table 1) in the ZSM-48 family. T-T connections to dimer units are striped. (Fig.3 is continued on next page)



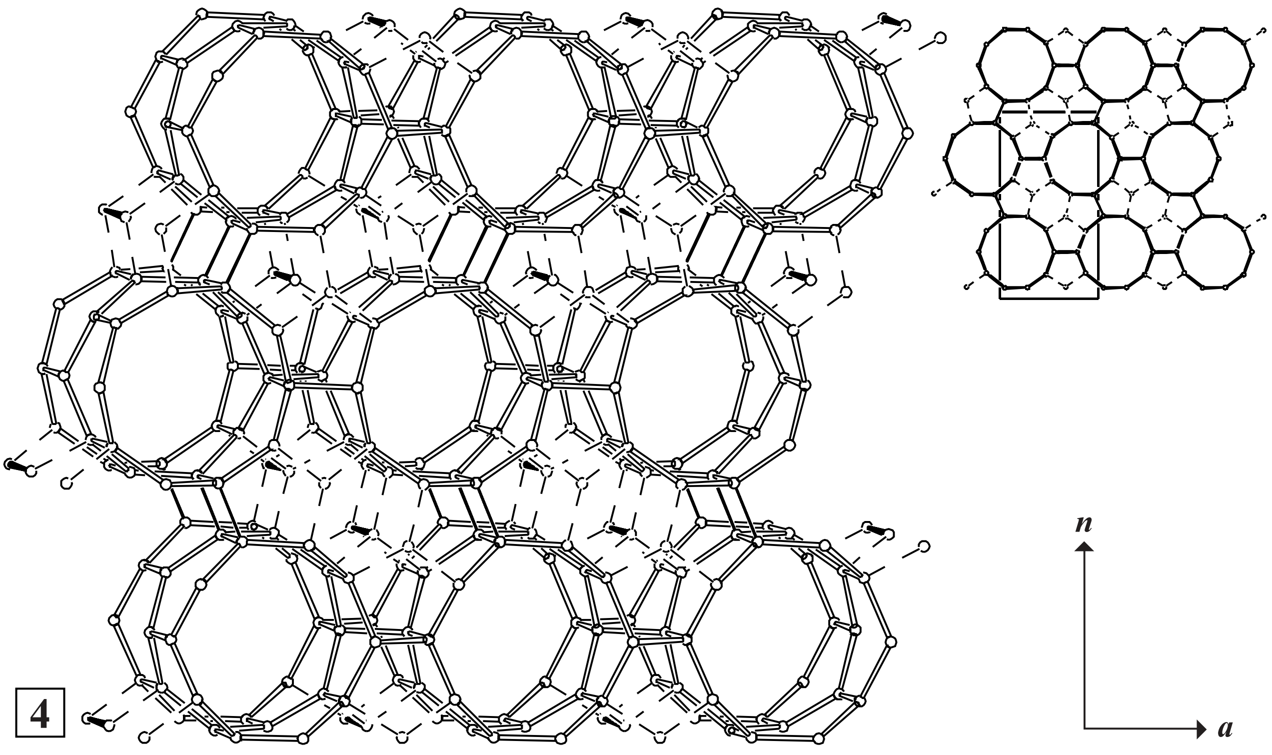
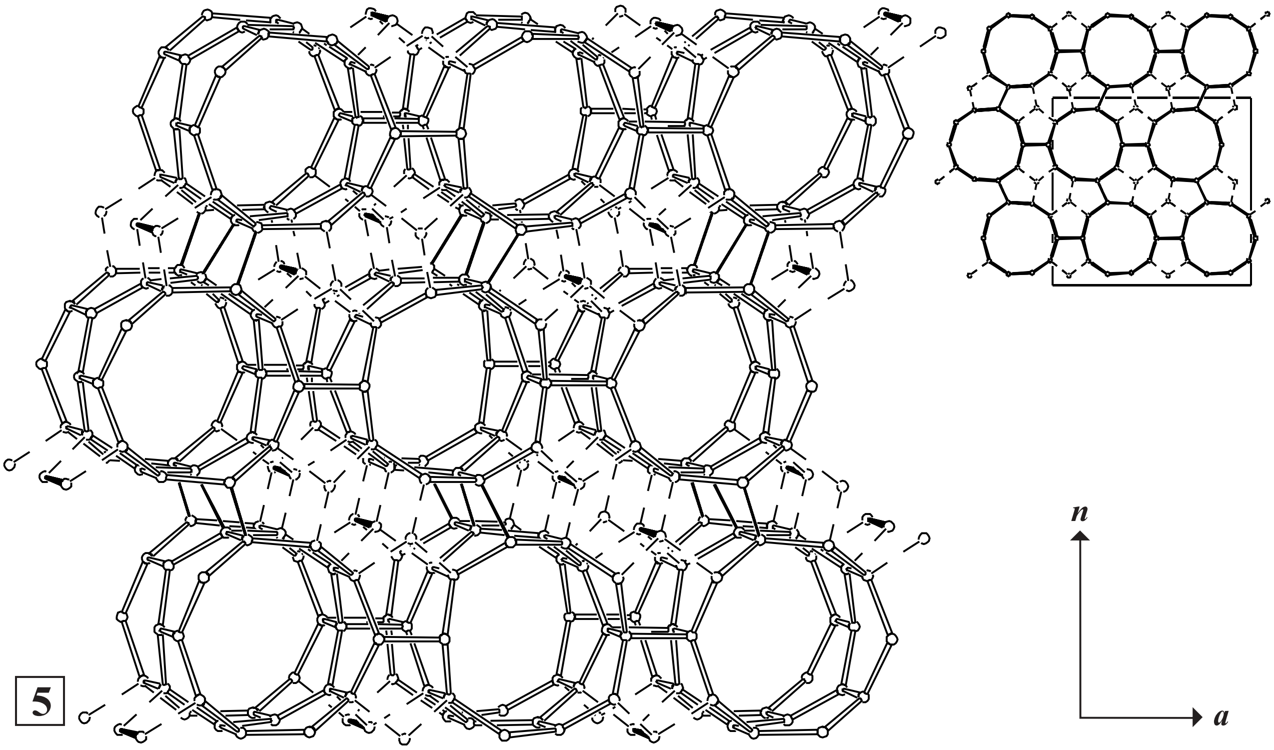


Figure 3 (Continued): Perspective drawing (left) and parallel projection along the pore axis of the unit cell in standard setting (top right) of the ordered end-members **3** and **4** (cf. Table 1) in the ZSM-48 family. T-T connections to dimer units are striped. (Fig.3 is continued on next page)



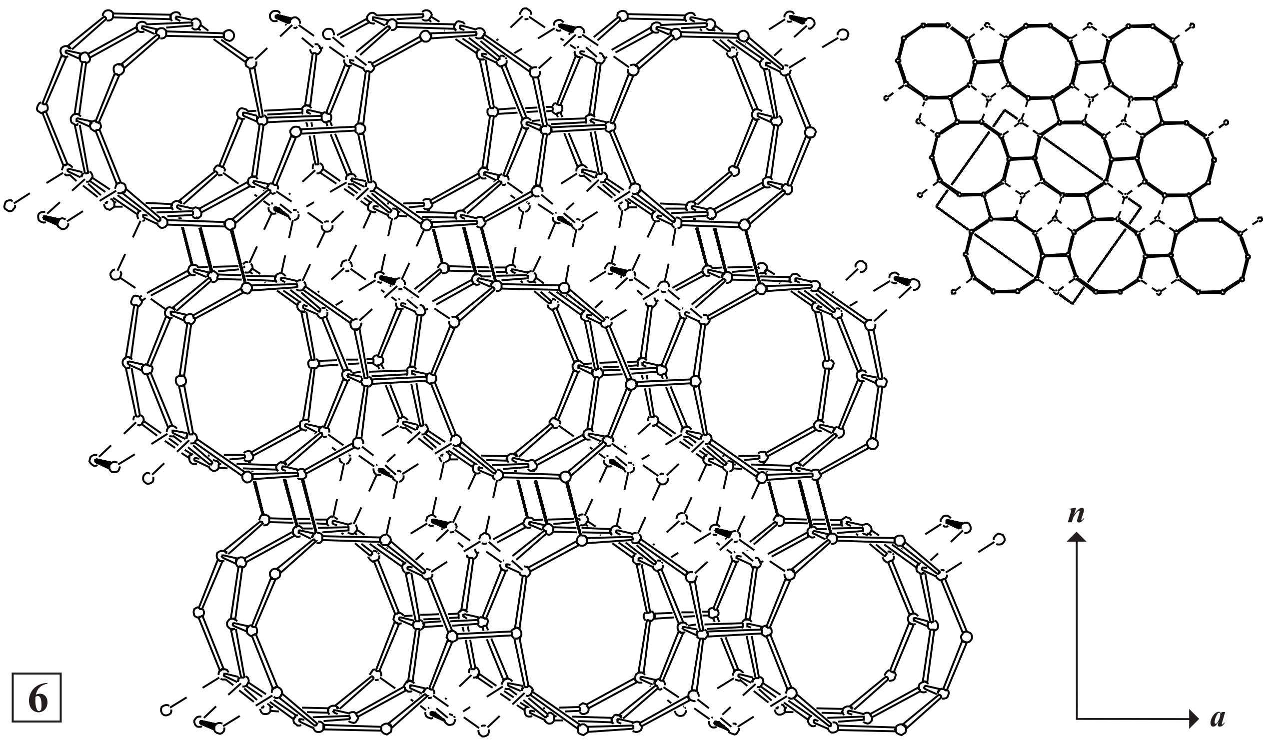
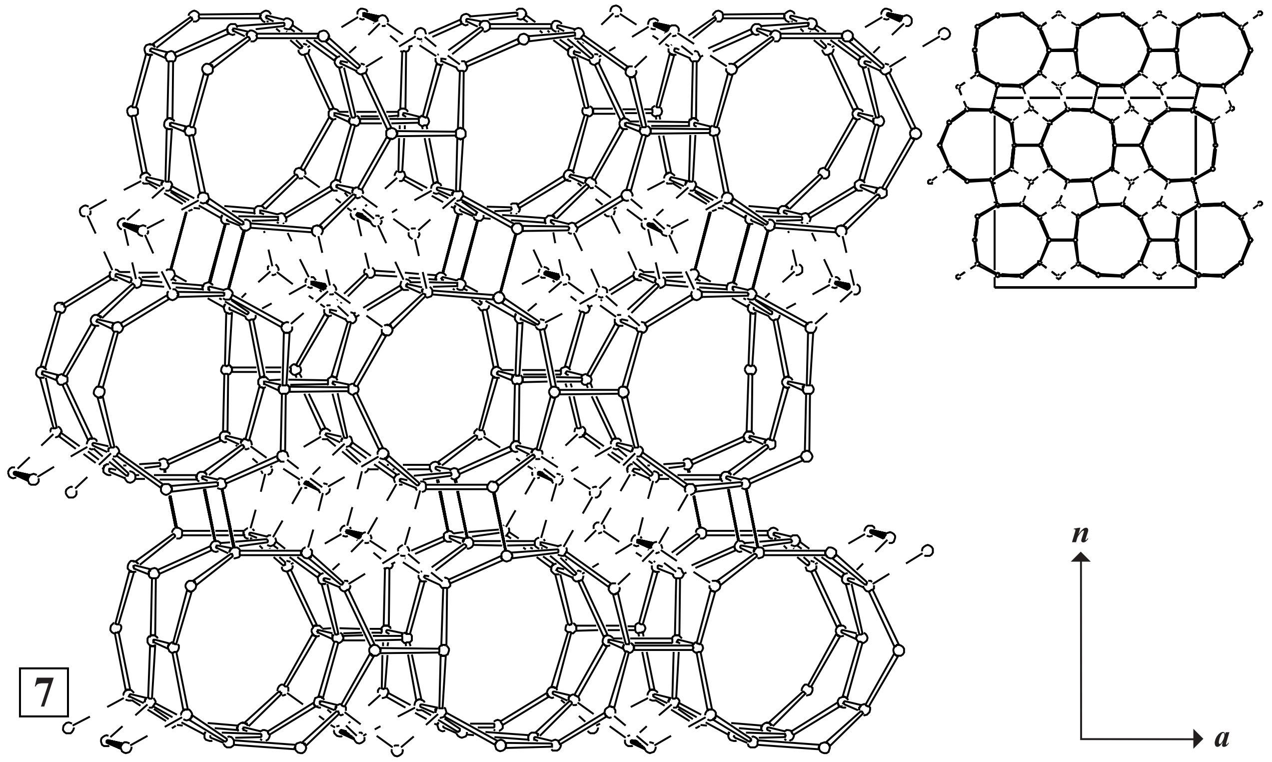


Figure 3 (Continued): Perspective drawing (left) and parallel projection along the pore axis of the unit cell in standard setting (top right) of the ordered end-members **5** and **6** (cf. Table 1) in the ZSM-48 family. T-T connections to dimer units are striped. (Fig.3 is continued on next page)



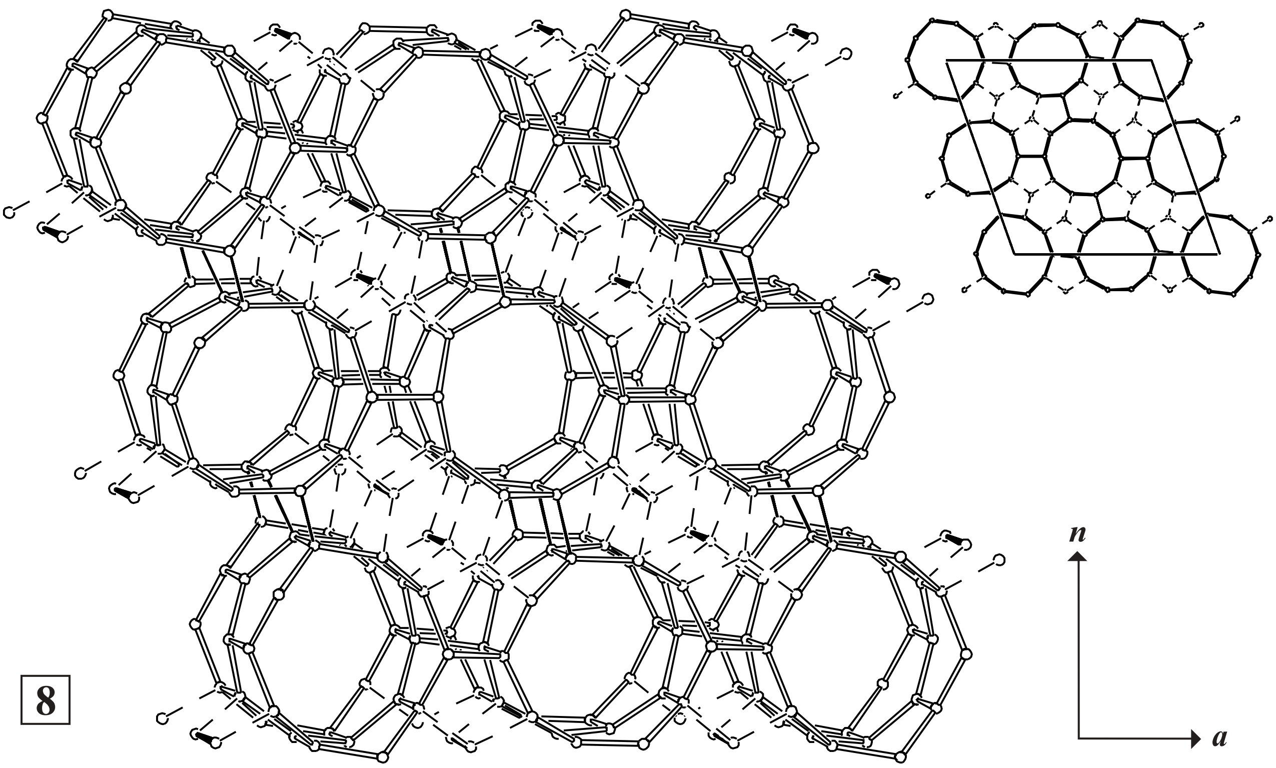


Figure 3 (Continued): Perspective drawing (left) and parallel projection along the pore axis of the unit cell in standard setting (top right) of the ordered end-members **7** and **8** (cf. Table 1) in the ZSM-48 family. T-T connections to dimer units are striped. (Fig.3 is continued on next page)

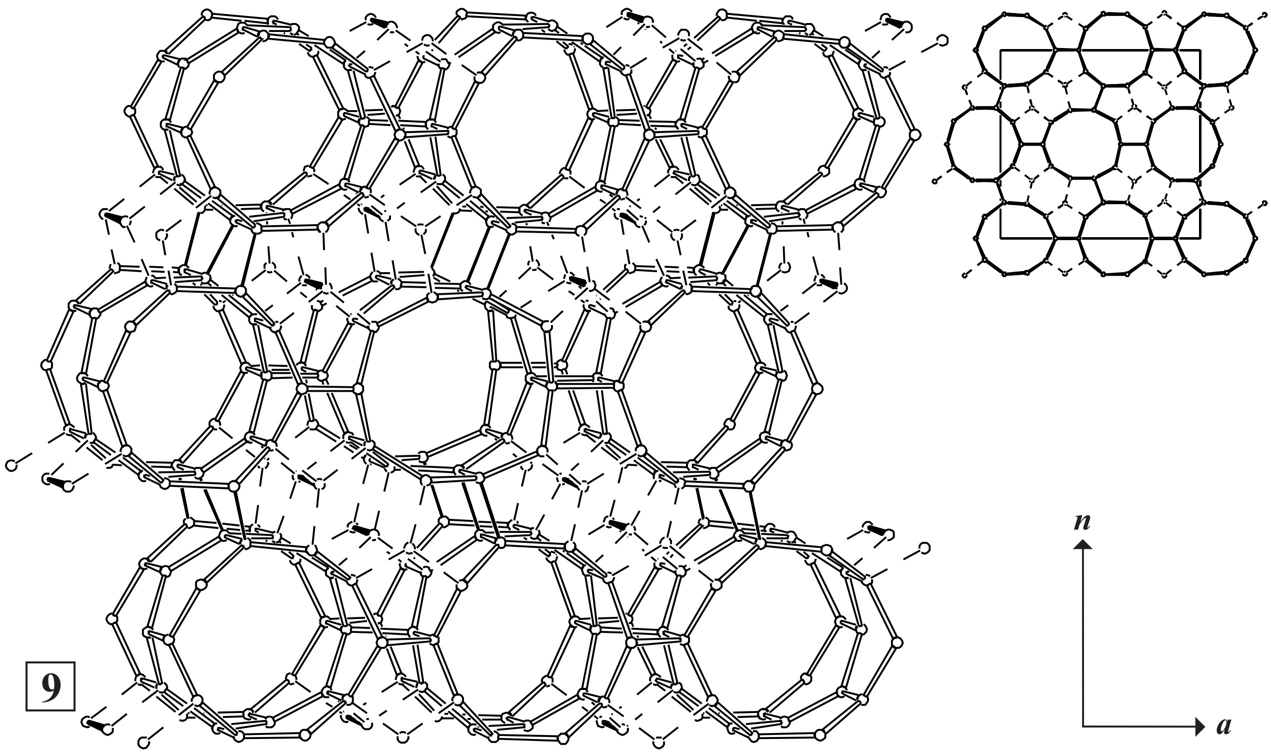


Figure 3 (Final page): Perspective drawing (left) and parallel projection along the pore axis of the unit cell in standard setting of the ordered end-member **9** (cf. Table 1) in the ZSM-48 family. T-T connections to dimer units are striped.

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 ($\boldsymbol{a_0}$, $\boldsymbol{b_0}$ and $\boldsymbol{c_0}$) of the space group is used

End-Member	***Lateral shifts (along n) in fractions of (a, and b)*** [1]			***space group***	$\boldsymbol{a_0}$	$\boldsymbol{b_0}$ **(Å)**	$\boldsymbol{c_0}$	***ß*** **(º)**
				PerBU1				
1 [2]	$(-^1/_6, 0)$;	$(-^1/_6, 0)$;	$(-^1/_6, 0)$;......	Cmcm	14.24	20.14	8.4	-
2	$(-^1/_6, 0)$;	$(+^1/_6, 0)$;	$(-^1/_6, 0)$;......	Pmmm	8.4	23.26	12.33	-
3	$(-^1/_6, ^1/_2)$;	$(-^1/_6, ^1/_2)$;	$(-^1/_6, ^1/_2)$;.....	C2/m	24.66	8.4	12.33	109.47
4	$(-^1/_6, ^1/_2)$;	$(+^1/_6, ^1/_2)$;	$(-^1/_6, ^1/_2)$;.....	Pmma	8.4	23.26	12.33	-
				PerBU2				
3 [3]	$(-^1/_6, 0)$;	$(-^1/_6, 0)$;	$(-^1/_6, 0)$;......	C2/m	24.66	8.4	12.33	109.47
5	$(-^1/_6, 0)$;	$(+^1/_6, 0)$;	$(-^1/_6, 0)$;......	Cmcm	8.4	24.66	23.26	-
6 [4]	$(-^1/_6, ^1/_2)$;	$(-^1/_6, ^1/_2)$;	$(-^1/_6, ^1/_2)$;.....	Imma	8.4	14.24	20.14	-
7	$(-^1/_6, ^1/_2)$;	$(+^1/_6, ^1/_2)$;	$(-^1/_6, ^1/_2)$;.....	Cmcm	8.4	24.66	23.26	-
				PerBU1 and PerBU2				
8	$(-^1/_6, 0)$;	$(-^1/_6, 0)$;	$(-^1/_6, 0)$;......	$P2_1/m$	24.66	8.4	24.66	109.47
9	$(-^1/_6, 0)$;	$(+^1/_6, 0)$;	$(-^1/_6, 0)$;......	Pmm2	8.4	23.26	24.66	-

[1] $\boldsymbol{a}$ = 24.66 Å (See Fig.1 and Section **4**); the pore axis $\boldsymbol{b}$ = 8.4 Å; $\boldsymbol{n}$ is parallel to $\boldsymbol{a}$ x $\boldsymbol{b}$.

[2] End-member **1** equals polytype 48A from Ref. 5.

[3] This end-member, built from PerBU2, is identical to end-member **3** built from PerBU1.

[4] 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)].

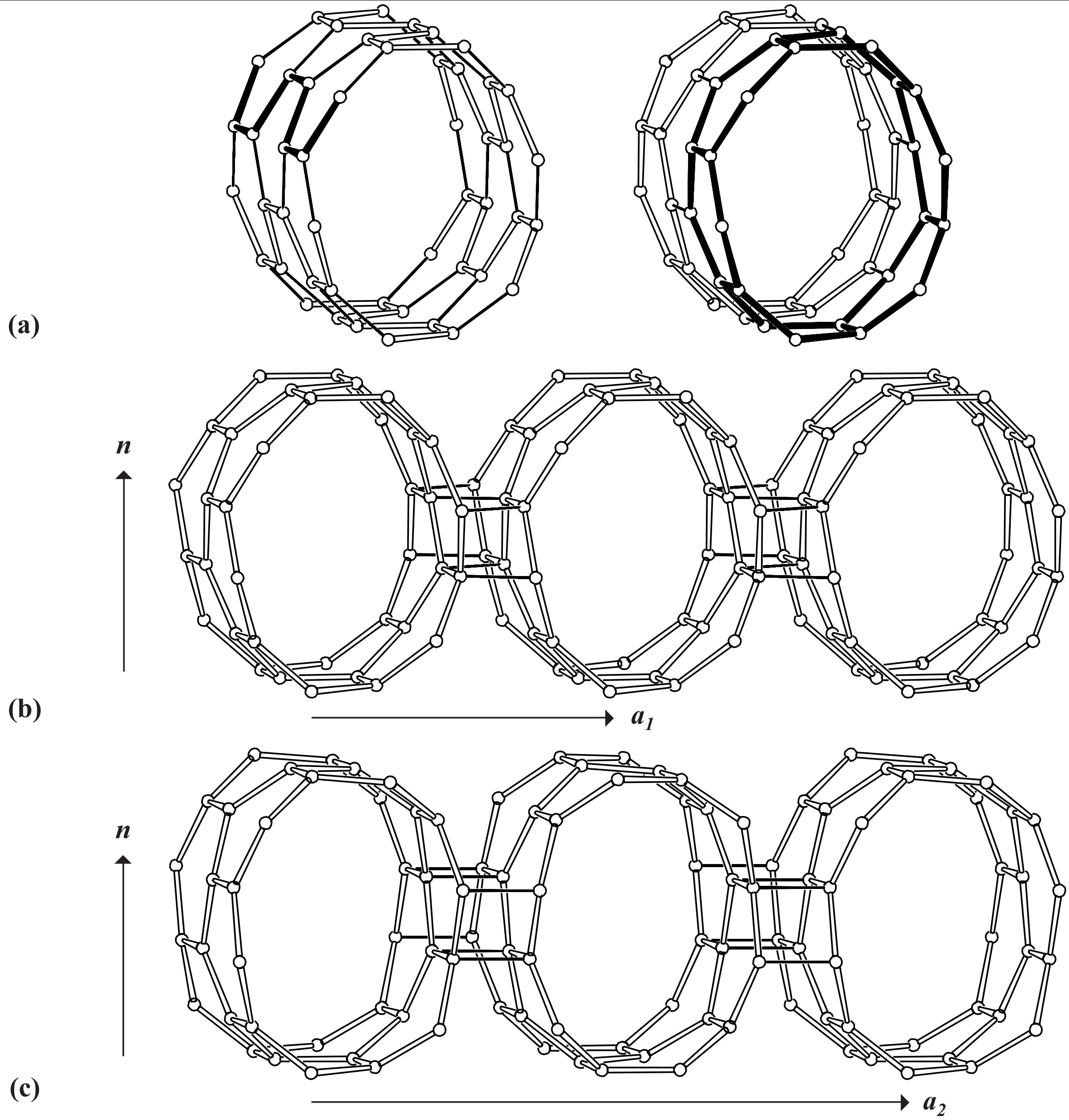


Figure 4: Tubular pore with T12-ring window (a) constructed from six crankshaft chains (left) or from T6-ring bands each consisting of 24 T atoms (right); PerBU1 (b) and PerBU2 (c) of the SSZ-31 family of zeolite frameworks seen in perspective view perpendicular to the plane normal ***n*** and along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

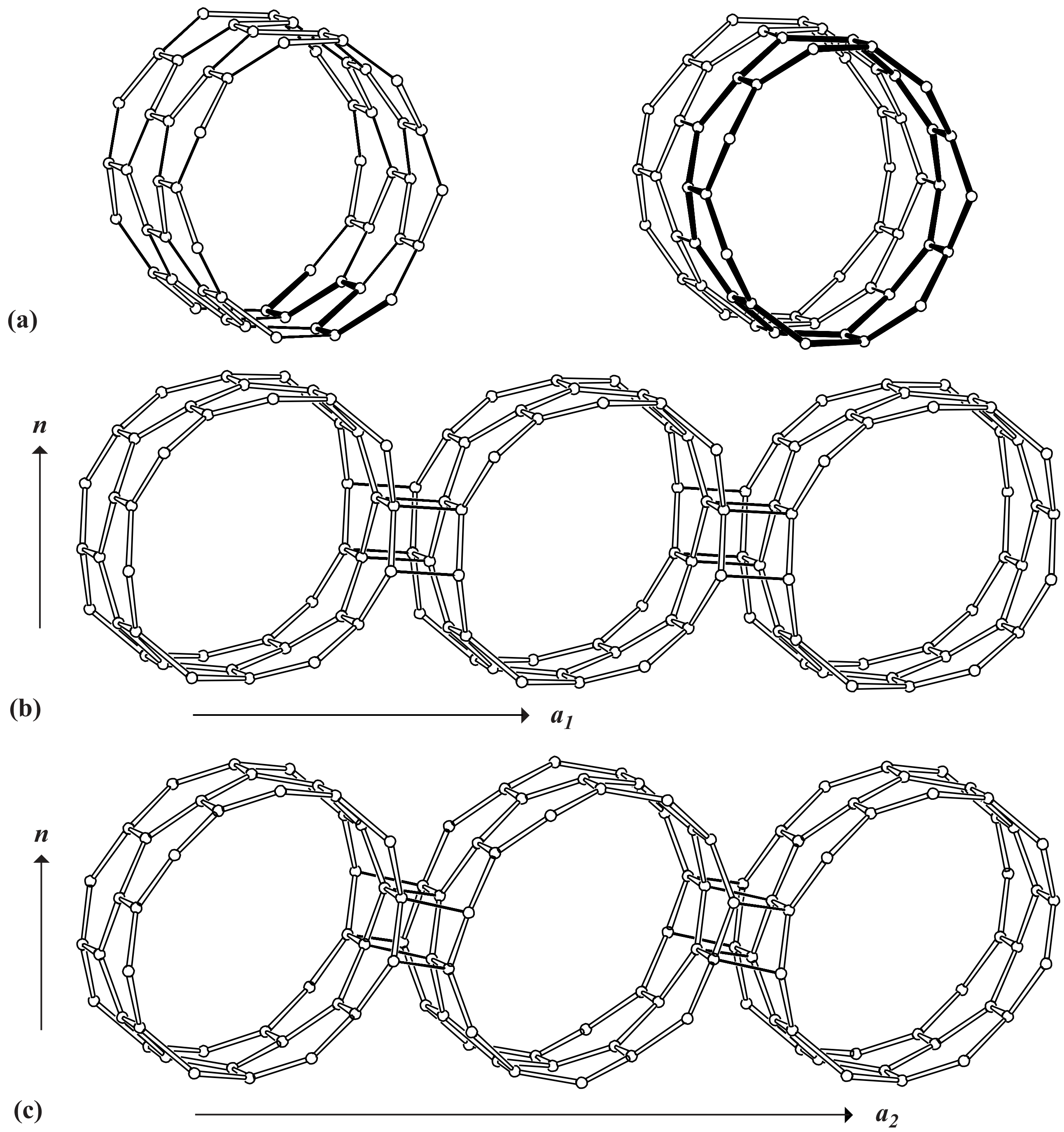


Figure 5: Tubular pore with T14-ring window (a) constructed from seven crankshaft chains (left) or from T6-ring bands each consisting of 28 T atoms (right); PerBU1 (b) and PerBU2 (c) of the UTD-1 family of zeolite frameworks seen in perspective view perpendicular to the plane normal ***n*** and along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

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

8. References

(1) J.L. Schlenker, F.G. Dwyer, E.E. Jenkins, W.J. Rohrbaugh and G.T. Kokotailo, Nature **294**, 340 (1981).

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(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).

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