The UTD-1 Family

1. The Periodic Building Units (PerBU1 and **PerBU2)** in the UTD-1 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 T14-ring windows as shown in Figure 1a.

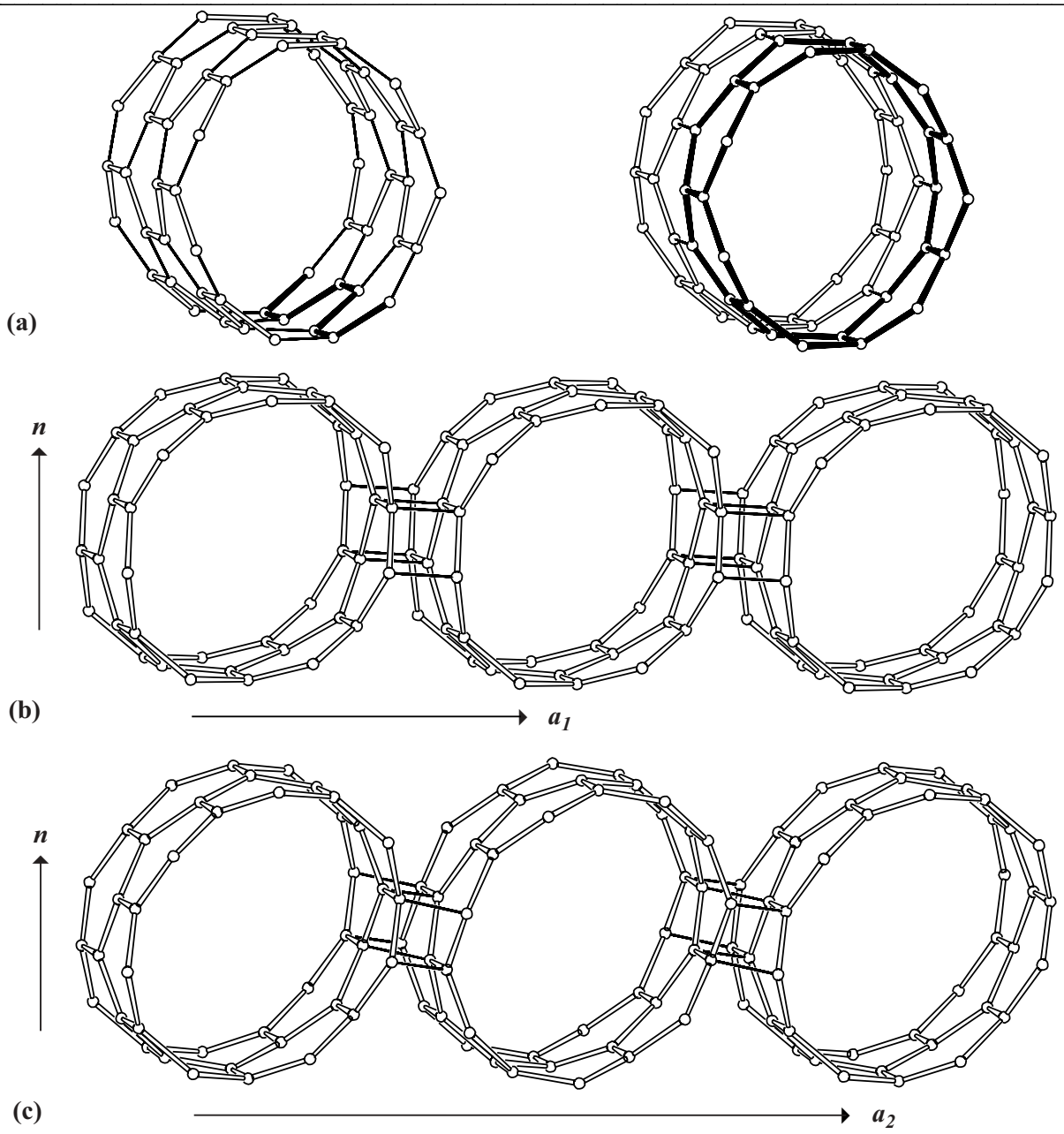

Figure 1: Pore with T14-ring window (a) constructed from seven crankshaft chains (left) or from T6-ring bands each consisting of 28 T atoms (right); PerBU1 (b) and PerBU2 (c) of the UTD-1 family of zeolites seen in perspective view perpendicular to the plane normal ***n*** and along the pore axis ***b***

Tubular pores (Fig.1a), related by pure translations along $\boldsymbol{a}_1$, are connected through double crankshaft chains of the feldspar type into PerBU1 (Fig.1b). Pores, related by pure transaltions along $\boldsymbol{a}_2$ accompanied by a shift of $\frac{1}{2}\boldsymbol{b}$ along the pore axis, are connected through double crankshaft chains of the narsarsukite type into PerBU2 (Fig.1c). [Compare these PerBU's with those in the **ZSM-48** and **SSZ-31** families].

2. Type of Faulting: 1-dimensional stacking disorder of the PerBU's along the plane normal $\boldsymbol{n}$.

3. The Layer Symmetry: the plane space group of PerBU1 is P 1 2_1/m (1) and of PerBU2 is C 1 2/m (1).

4. Connectivity Pattern of the PerBU's:

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

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

According to the literature (1,3), UTD-1 materials donot exhibit regions where the PerBU's are stacked using the $(-\frac{1}{6}, 0 \text{ or } \frac{1}{2})$ and the $(+\frac{1}{6}, 0 \text{ or } \frac{1}{2})$ connection modes sequentially. Therefore, only connection modes **(a)** and **(c)** [or, equivalently, **(b)** and **(d)**] need to be considered.

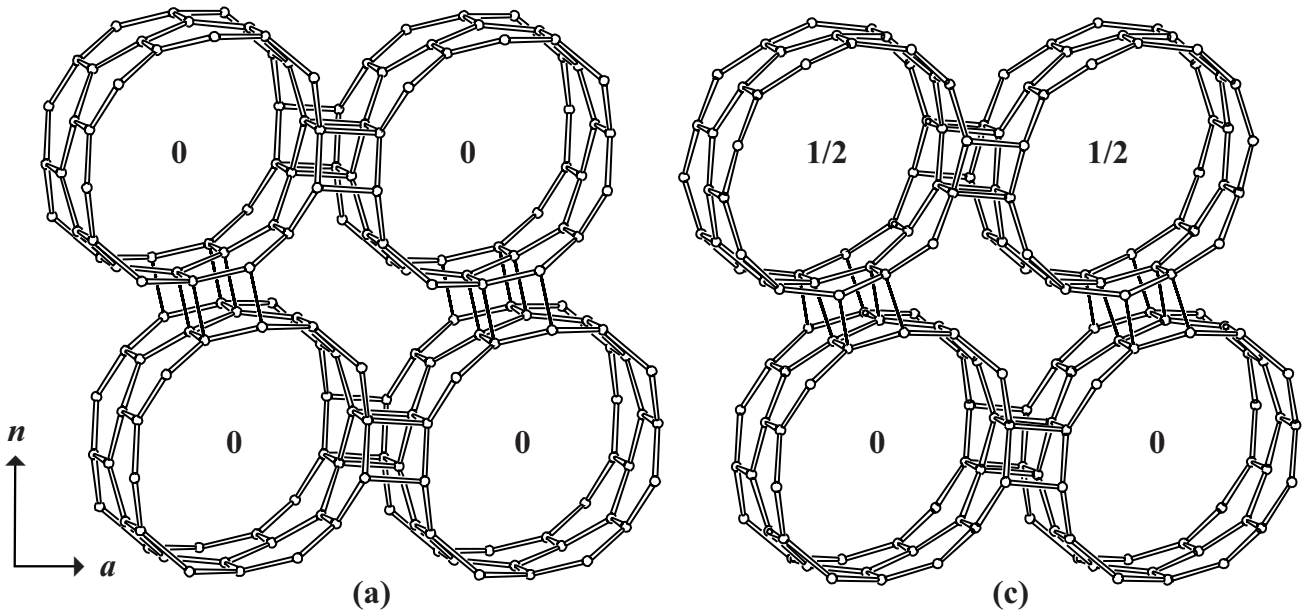

Figure 2: Perspective view along the pore axis $\boldsymbol{b}$ of the connection modes **(a)** and **(c)** between PerBU1's in the UTD-1 family of zeolite frameworks. The PerBU1's are connected through double crankshaft chains of the feldspar- or narsarsukite-type depending on whether the shift along $\boldsymbol{b}$ between direct neighbouring pores is zero or $\frac{1}{2}\boldsymbol{b}$, respectively. The gaps between the pores are filled with T-T dimer units as shown in Figure 3 [Fig. 2 is continued on next page]

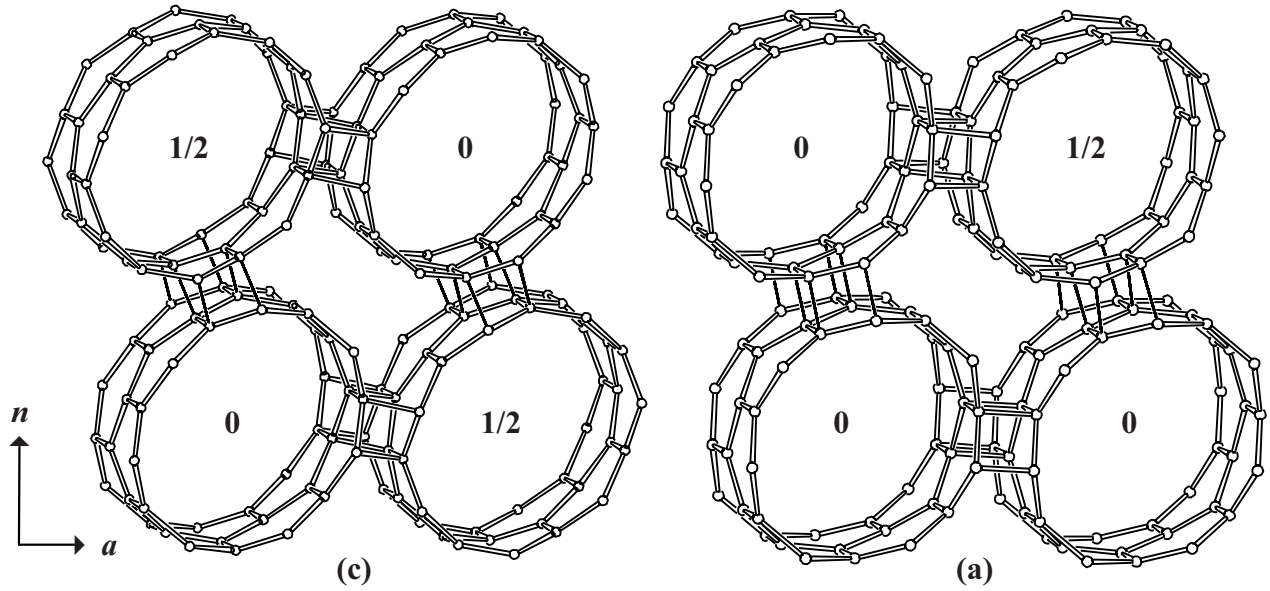

Figure 2 (Continued): Perspective view along the pore axis ***b*** of (left) the connection mode **(c)** between PerBU2's and (right) the connection mode **(a)** between stacking alternately PerBU1 and PerBU2. The PerBU's are connected through double crankshaft chains of the feldspar- or narsarsukite-type depending on whether the shift along ***b*** between direct neighbouring pores is zero or $^1/_2\boldsymbol{b}$, respectively. The gaps between the pores are filled with T-T dimers (See Fig.3)

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 UTD-1 family of zeolites are shown in Figure 3 and Table 1. Only end-member **1** (framework type code: **DON** (2,4)) has been observed as pure single crystal material so far.

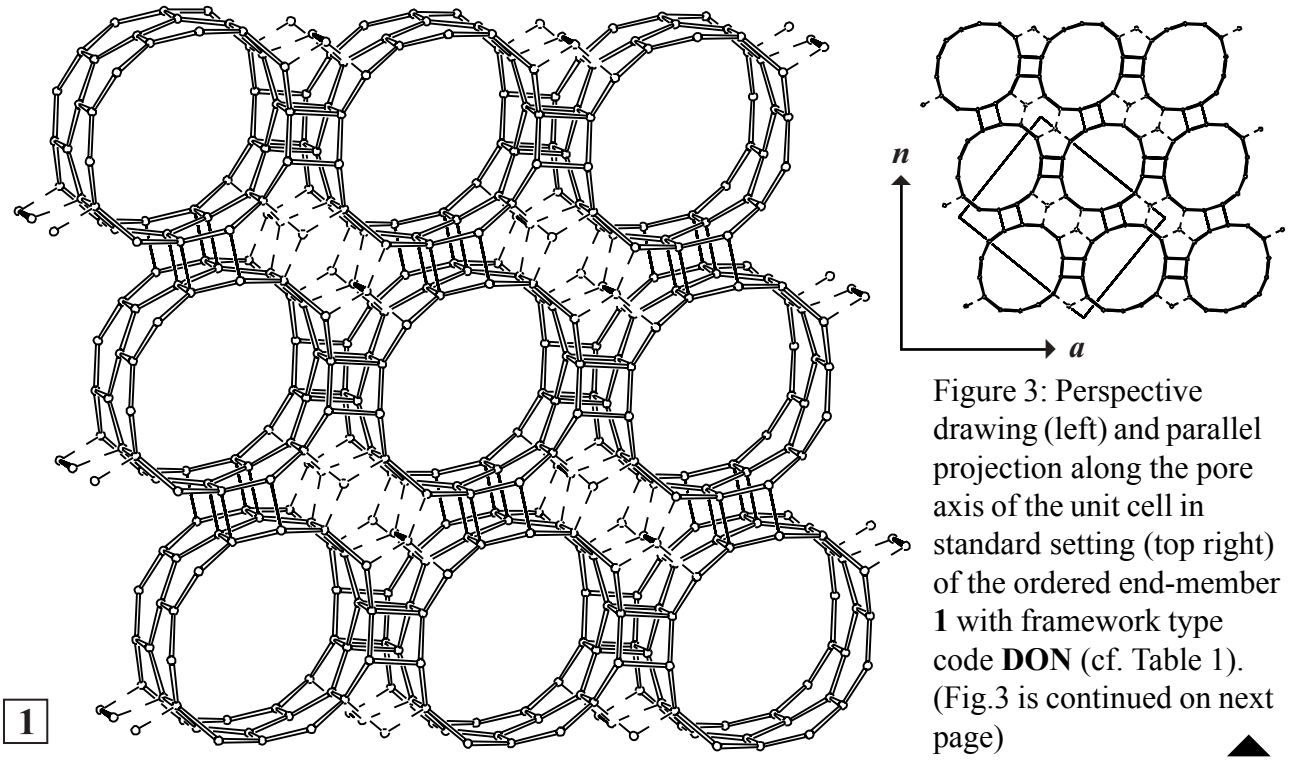

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Figure 3: Perspective drawing (left) and parallel projection along the pore axis of the unit cell in standard setting (top right) of the ordered end-member **1** with framework type code **DON** (cf. Table 1). (Fig.3 is continued on next page)

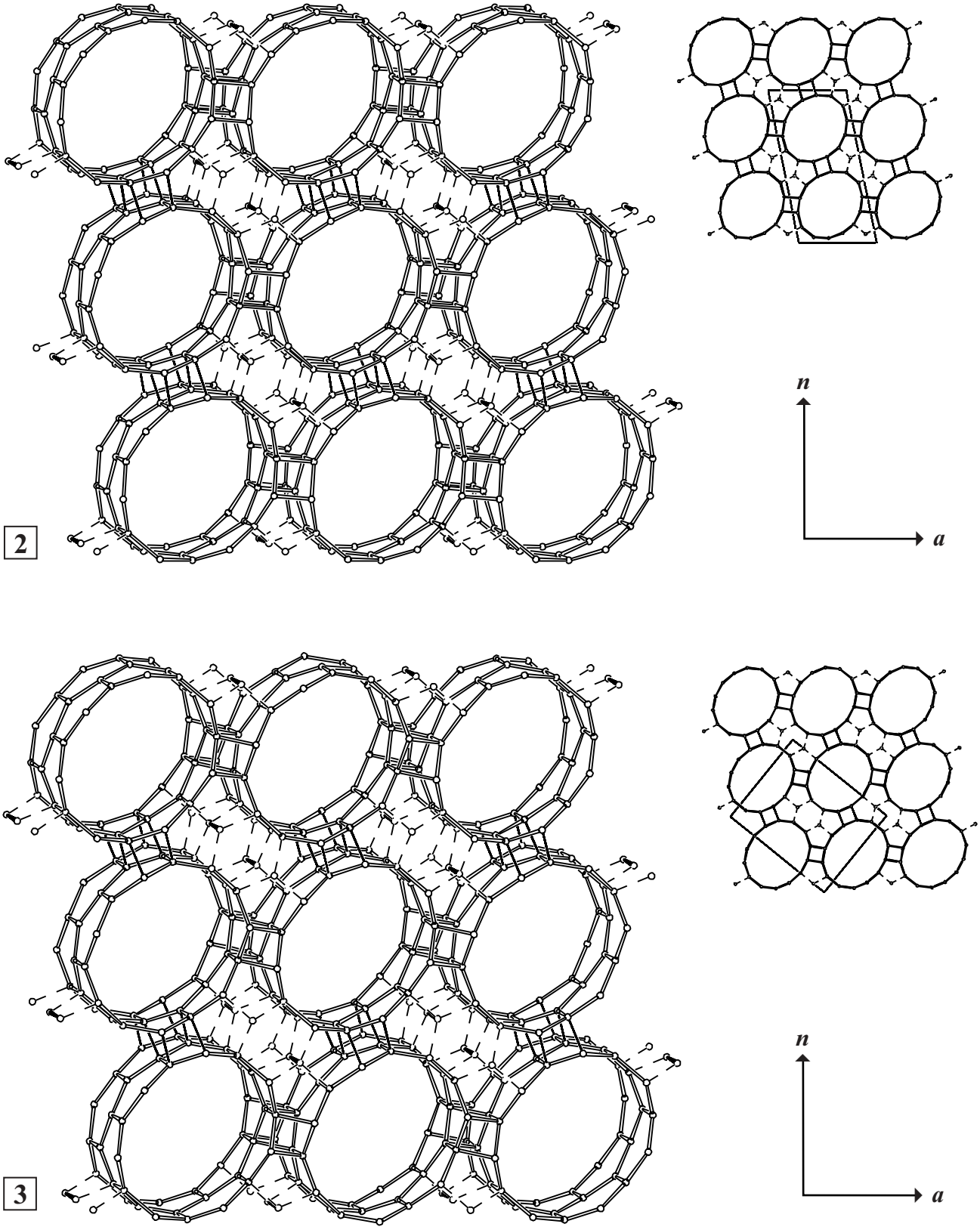

Figure 3 (Continued): Perspective drawing (left) and parallel projection along the pore axis of the unit cell in standard setting (top right) of the ordered end-members **2** and **3** (cf. Table 1) in the UTD-1 family. T-T connections to dimer units are striped. (Fig.3 is continued on next page)

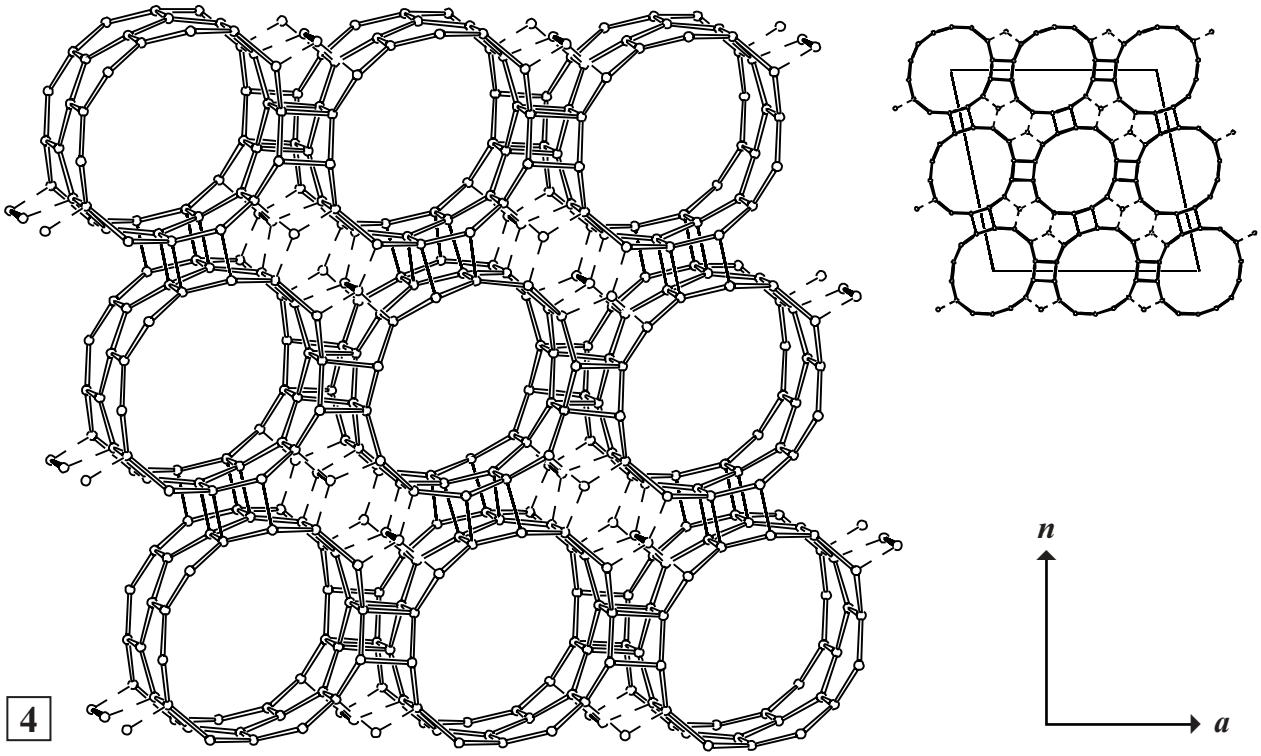

Figure 3 (Final page): Perspective drawing (left) and parallel projection along the pore axis of the unit cell in standard setting (top right) of the ordered end-member **4** (cf. Table 1) in the UTD-1 family. T-T connections to dimer units are striped

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Table 1: Stacking sequences of the PerBU's for the simplest ordered end-members in the UTD-1 family of zeolite frameworks. The end-member number refers to the framework plots **1-4** on this and 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 (º)
				PerBU1				
1 [2]	(-1/6, 0);	(-1/6, 0);	(-1/6, 0);.....	Cmcm	18.89	23.37	8.41	-
2 [3]	(-1/6, 1/2);	(-1/6, 1/2);	(-1/6, 1/2);.....	C2/m	29.87	8.41	14.94	101.3
				PerBU2				
3 [4]	(-1/6, 1/2);	(-1/6, 1/2);	(-1/6, 1/2);.....	Imma	18.94	8.41	23.10	-
				PerBU1 and PerBU2				
4 [5]	(-1/6, 0);	(-1/6, 0);	(-1/6, 0);.....	$P2_1/m$	29.87	8.41	29.87	101.3

[1] ***a*** = 29.87 Å (See Fig.1 and Section **4**); the pore axis ***b*** = 8.41 Å; ***n*** is parallel to ***a*** x ***b***.
[2] End-member **1** equals polytype **C** with framework type code **DON** (1,2).
[3] End-member **2** equals polytype **E** (3).
[4] End-member **3** equals polytype **A** (1).
[5] End-member **4** equals polytype **F** (3).

6. Disordered Materials Synthesized and Characterized to Date:

UTD-1 (1), UTD-1F (2)

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 T6-rings with T10-ring windows. [Compare these PerBU's (with T10-ring windows) with the PerBU's in SSZ-31 (with T12-ring windows) and in UTD-1 (with T14-ring windows)].

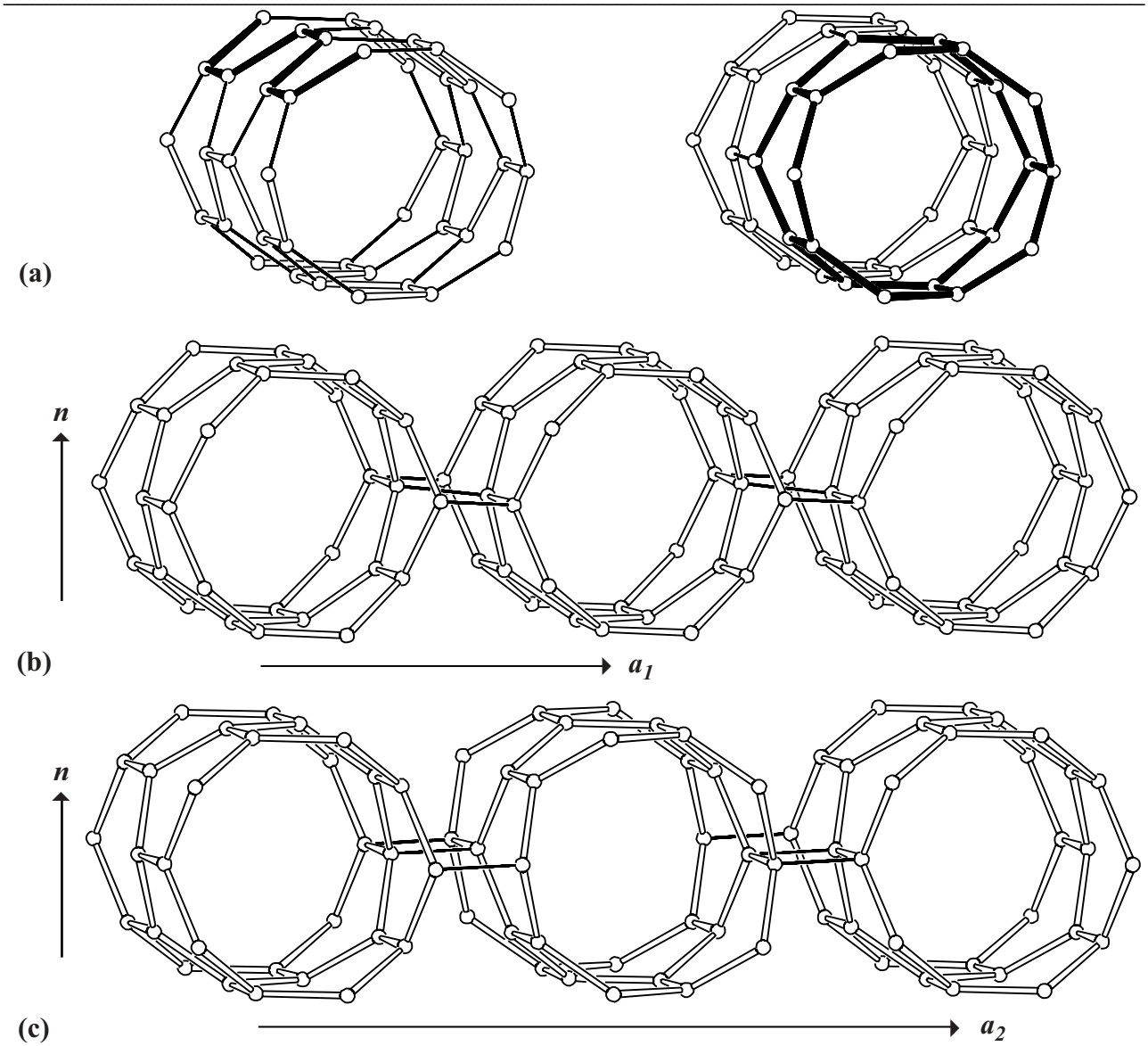

Figure 4: Tubular pore with T10-ring window (a) constructed from five crankshaft chains (left) or from T6-ring bands each consisting of 20 T atoms (right); PerBU1 (b) and PerBU2 (c) of the ZSM-48 family of zeolite frameworks seen in perspective view perpendicular to the plane normal ***n*** and along the pore axis ***b***

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

7.2 *Comparison with the SSZ-31 family:*

The Periodic Building Units (PerBU1 and PerBU2) in the SSZ-31 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 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)].

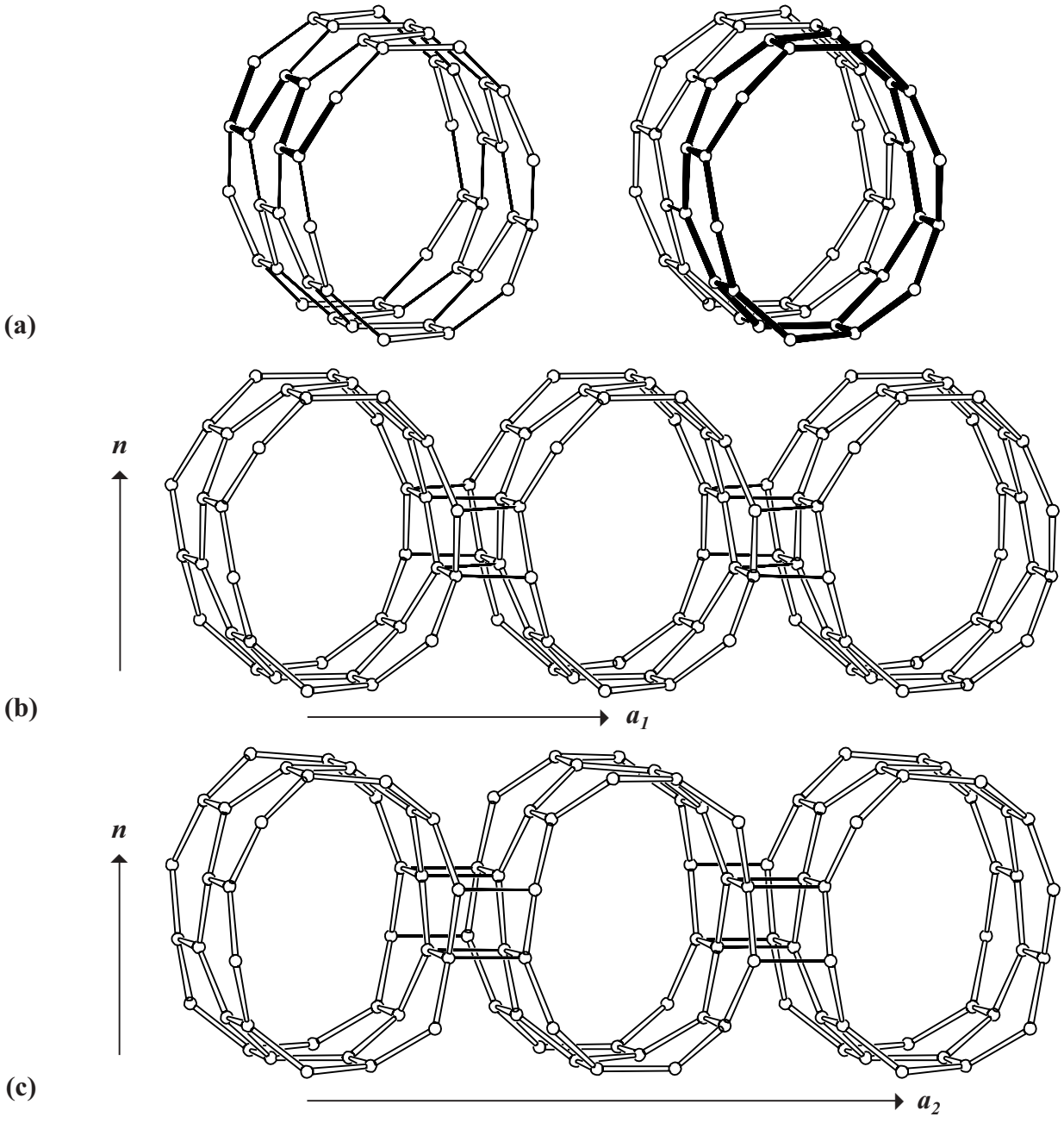

Figure 5: Tubular pore with T12-ring window constructed from six crankshaft chains (left) or from T6-ring bands each consisting of 24 T atoms (right); PerBU1 (b) and PerBU2 (c) of the SSZ-31 family of zeolite frameworks seen in perspective view perpendicular to the plane normal ***n*** and along the pore axis ***b***

For more details: see the description of the **SSZ-31** family in this 'Catalog'.

8. References

(1) R.F. Lobo, M. Tsapatsis, C.C. Freyhardt, S. Khodabandeh, P. Wagner, C-Y. Chen, K.J. Balkus, S.I. Zones and M.E. Davis, J. Am. Chem. Soc. **119**, 8474 (1997).

(2) T. Wessels, Ch. Baerlocher, L.B. McCusker and E.J. Creyghton, J. Am. Chem. Soc. **121**, 6242 (1999).

(3) H. van Koningsveld, R.F. Lobo and M.M. Martinez-Inesta, Accepted for publication at the IUCr Congress (2004), Cape Town, South Africa.

(4) Atlas of Zeolite Framework Types, p.116. Ch. Baerlocher, W.M. Meier and D.H. Olson, eds.. Fifth Rev. Ed., 2001, Elsevier. Amsterdam, London, New York.