

# The UTD-1 Family

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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.

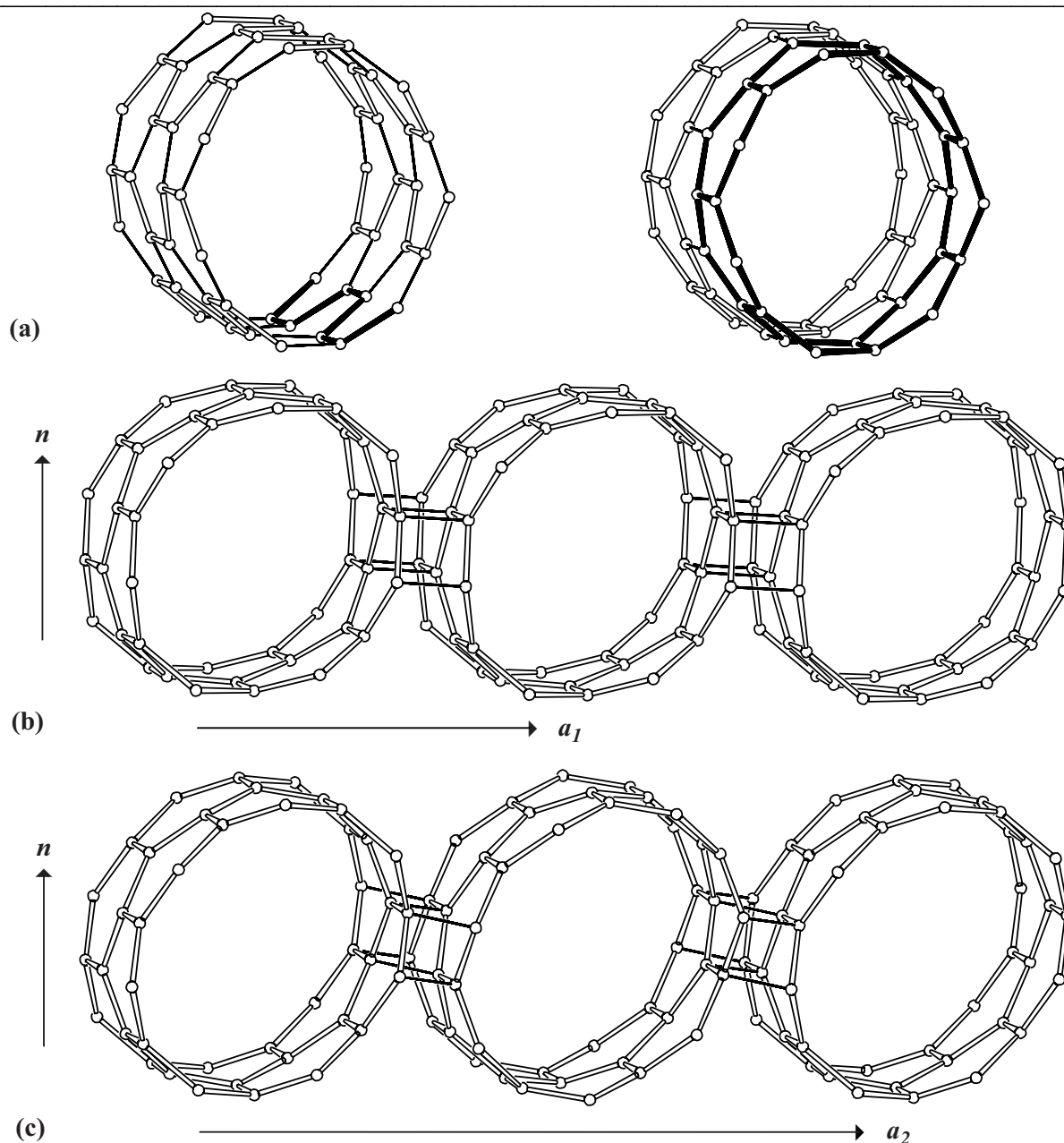


Figure 1: Pore with T14-ring window (a) constructed from seven crankshaft chains (left) or from T6-ring bands each consisting of 28 T atoms (right); PerBU1 (b) and PerBU2 (c) of the UTD-1 family of zeolites seen in perspective view perpendicular to the plane normal  $n$  and along the pore axis  $b$

Tubular pores (Fig. 1a), related by pure translations along  $a_1$ , are connected through double crankshaft chains of the feldspar type into PerBU1 (Fig. 1b). Pores, related by pure translations along  $a_2$  accompanied by a shift of  $\frac{1}{2}b$  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  $n$ .

**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  $n$  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  $(\frac{1}{6}, \frac{1}{2})$ .

According to the literature (1,3), UTD-1 materials do not exhibit regions where the PerBU's are stacked using the  $(-\frac{1}{6}, 0$  or  $\frac{1}{2})$  and the  $(+\frac{1}{6}, 0$  or  $\frac{1}{2})$  connection modes sequentially. Therefore, only connection modes (a) and (c) [or, equivalently, (b) and (d)] need to be considered.

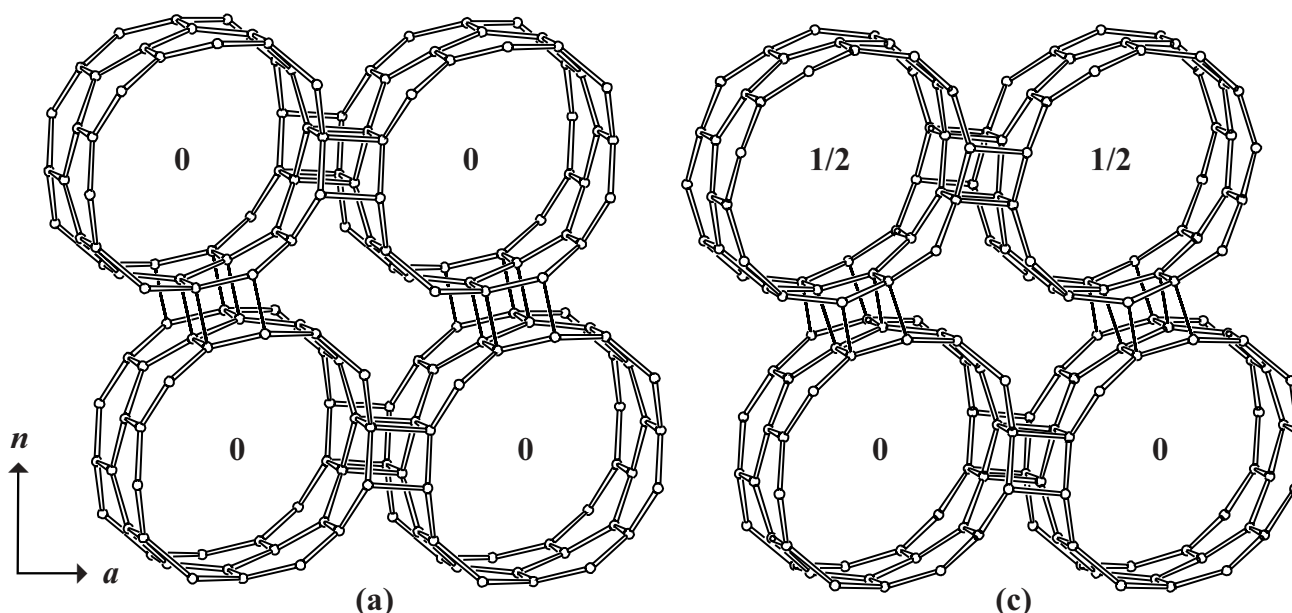


Figure 2: Perspective view along the pore axis  $b$  of the connection modes (a) and (c) between PerBU1's in the UTD-1 family of zeolite frameworks. The PerBU1's are connected through double crankshaft chains of the feldspar- or narsarsukite-type depending on whether the shift along  $b$  between direct neighbouring pores is zero or  $\frac{1}{2}b$ , 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]

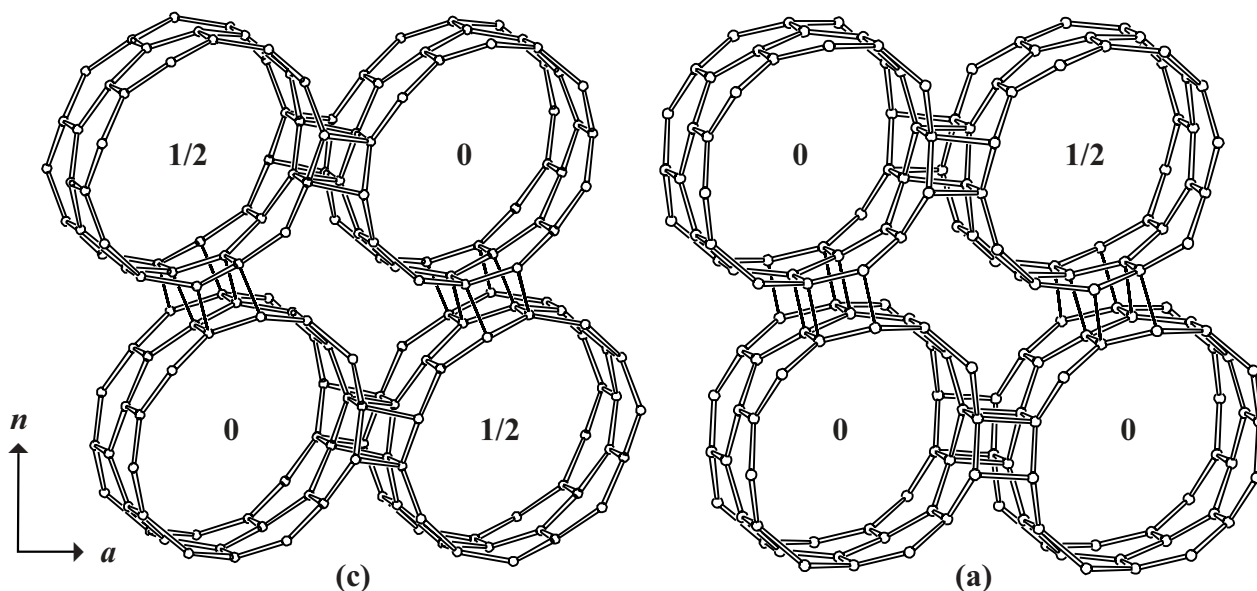


Figure 2 (Continued): Perspective view along the pore axis  $b$  of (left) the connection mode (c) between PerBU2's and (right) the connection mode (a) between stacking alternately PerBU1 and PerBU2. The PerBU's are connected through double crankshaft chains of the feldspar- or narsarsukite-type depending on whether the shift along  $b$  between direct neighbouring pores is zero or  $1/2b$ , 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.

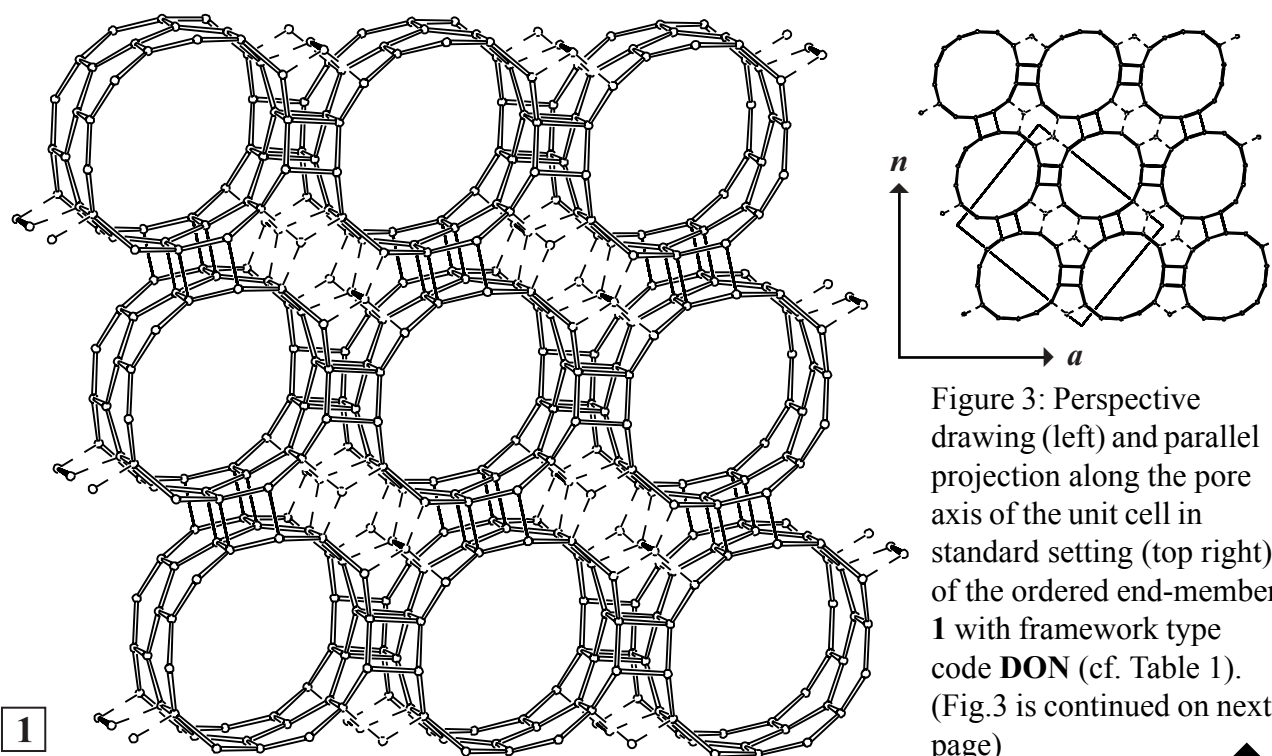


Figure 3: Perspective drawing (left) and parallel projection along the pore axis of the unit cell in standard setting (top right) of the ordered end-member **1** with framework type code **DON** (cf. Table 1). (Fig.3 is continued on next page) ▲

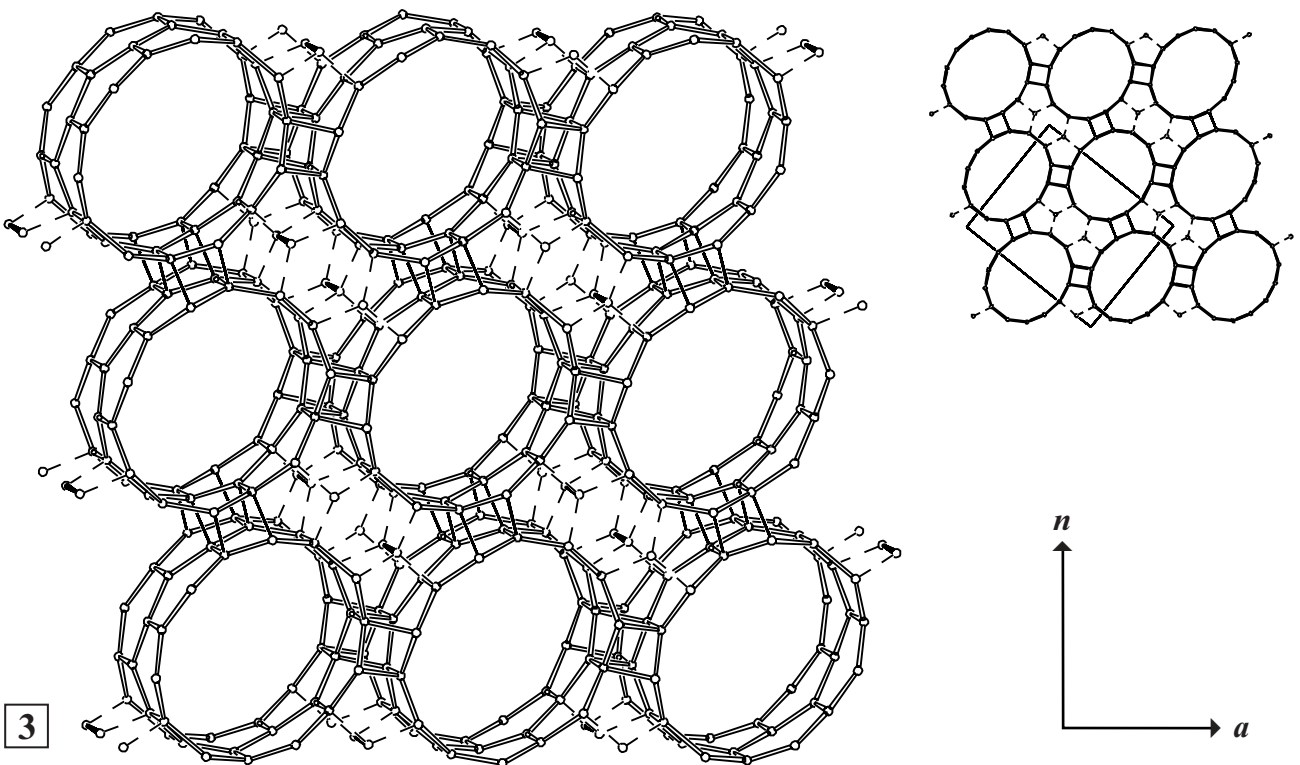
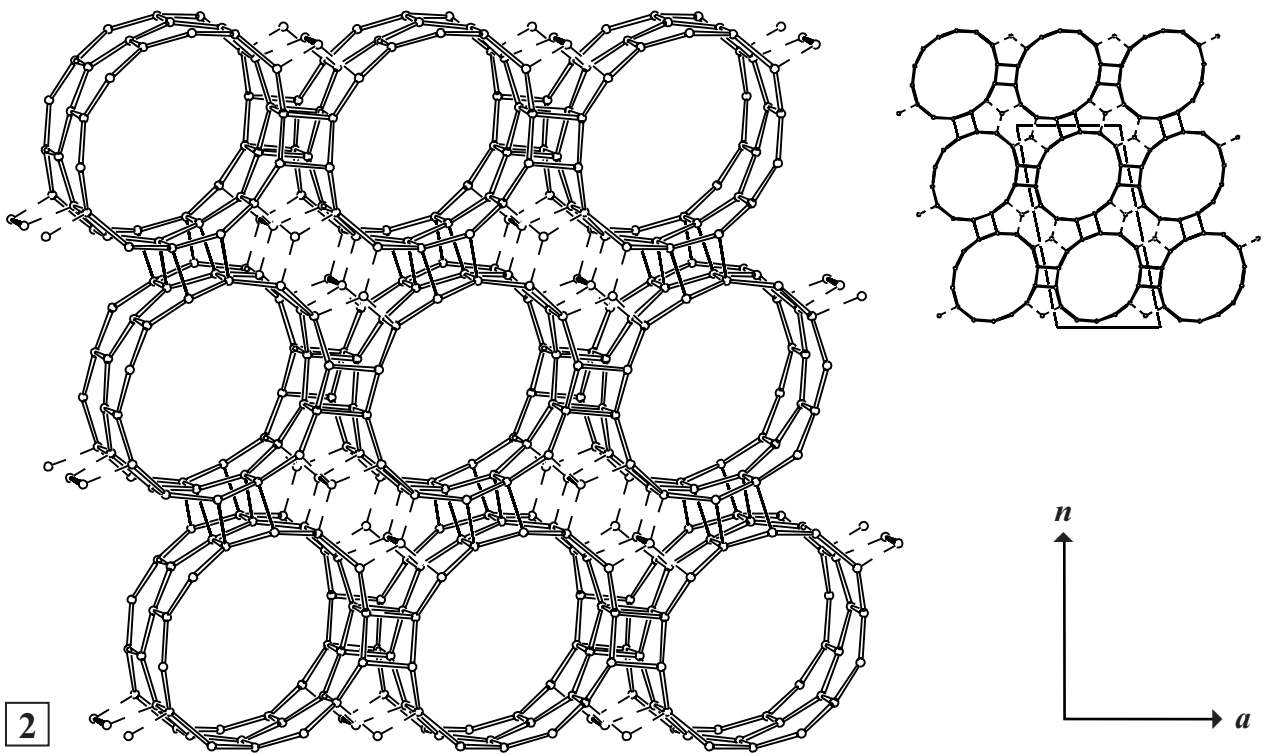


Figure 3 (Continued): Perspective drawing (left) and parallel projection along the pore axis of the unit cell in standard setting (top right) of the ordered end-members **2** and **3** (cf. Table 1) in the UTD-1 family. T-T connections to dimer units are striped. (Fig.3 is continued on next page) ▲

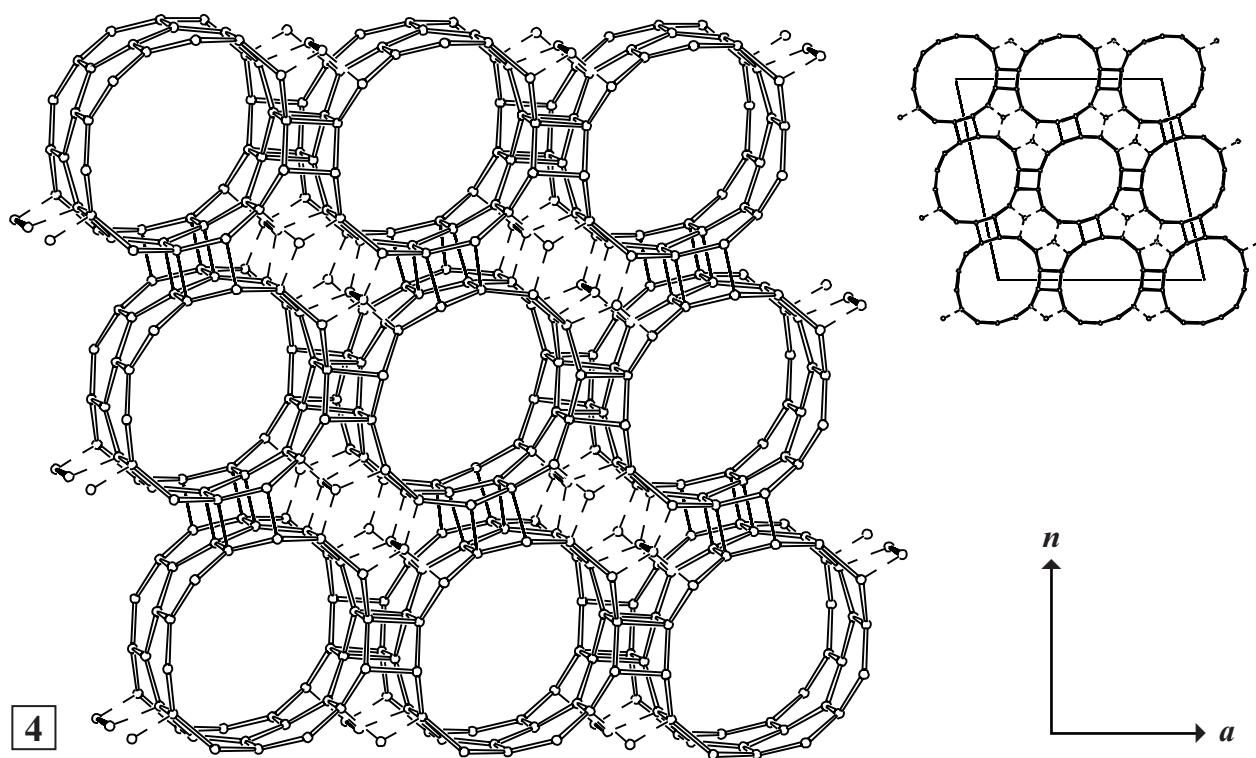


Figure 3 (Final page): Perspective drawing (left) and parallel projection along the pore axis of the unit cell in standard setting (top right) of the ordered end-member **4** (cf. Table 1) in the UTD-1 family. T-T connections to dimer units are striped

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

<i>End-Member</i>	<i>Lateral shifts (along <math>n</math>) in fractions of (<math>a</math>, and <math>b</math>)<sup>1</sup></i>	<i>space group</i>	$a_0$	$b_0$ (Å)	$c_0$	$\beta$ (°)
PerBU1						
<b>1</b> <sup>2</sup>	$(-1/6, 0); (-1/6, 0); (-1/6, 0); \dots$	Cmcm	18.89	23.37	8.41	-
<b>2</b> <sup>3</sup>	$(-1/6, 1/2); (-1/6, 1/2); (-1/6, 1/2); \dots$	C2/m	29.87	8.41	14.94	101.3
PerBU2						
<b>3</b> <sup>4</sup>	$(-1/6, 1/2); (-1/6, 1/2); (-1/6, 1/2); \dots$	Imma	18.94	8.41	23.10	-
PerBU1 and PerBU2						
<b>4</b> <sup>5</sup>	$(-1/6, 0); (-1/6, 0); (-1/6, 0); \dots$	P2 <sub>1</sub> /m	29.87	8.41	29.87	101.3

<sup>1</sup>  $a = 29.87$  Å (See Fig.1 and Section 4); the pore axis  $b = 8.41$  Å;  $n$  is parallel to  $a \times b$ .

<sup>2</sup> End-member **1** equals polytype **C** with framework type code **DON** (1,2).

<sup>3</sup> End-member **2** equals polytype **E** (3).

<sup>4</sup> End-member **3** equals polytype **A** (1).

<sup>5</sup> 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)].

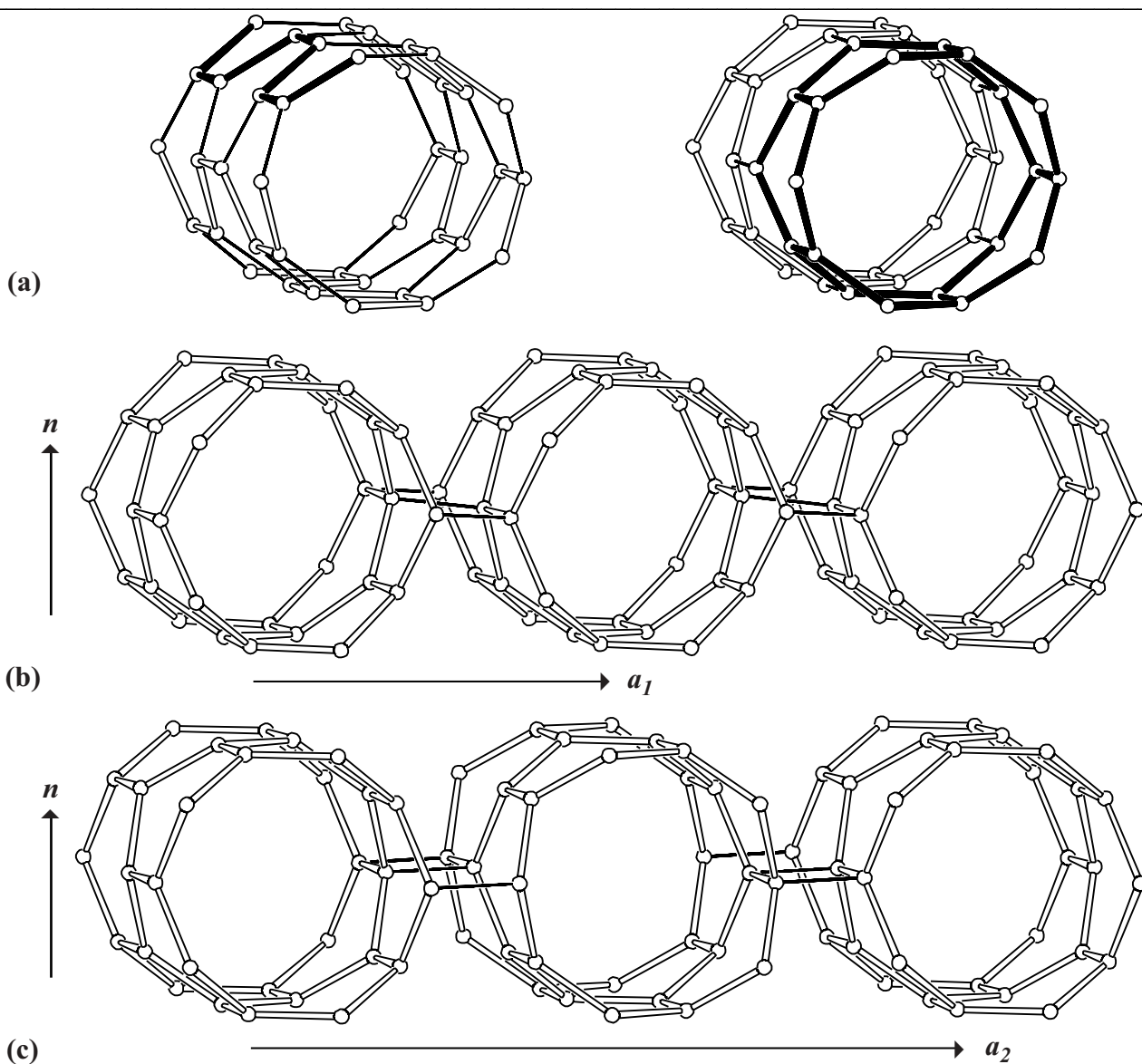


Figure 4: Tubular pore with T10-ring window (a) constructed from five crankshaft chains (left) or from T6-ring bands each consisting of 20 T atoms (right); PerBU1 (b) and PerBU2 (c) of the ZSM-48 family of zeolite frameworks seen in perspective view perpendicular to the plane normal  $n$  and along the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

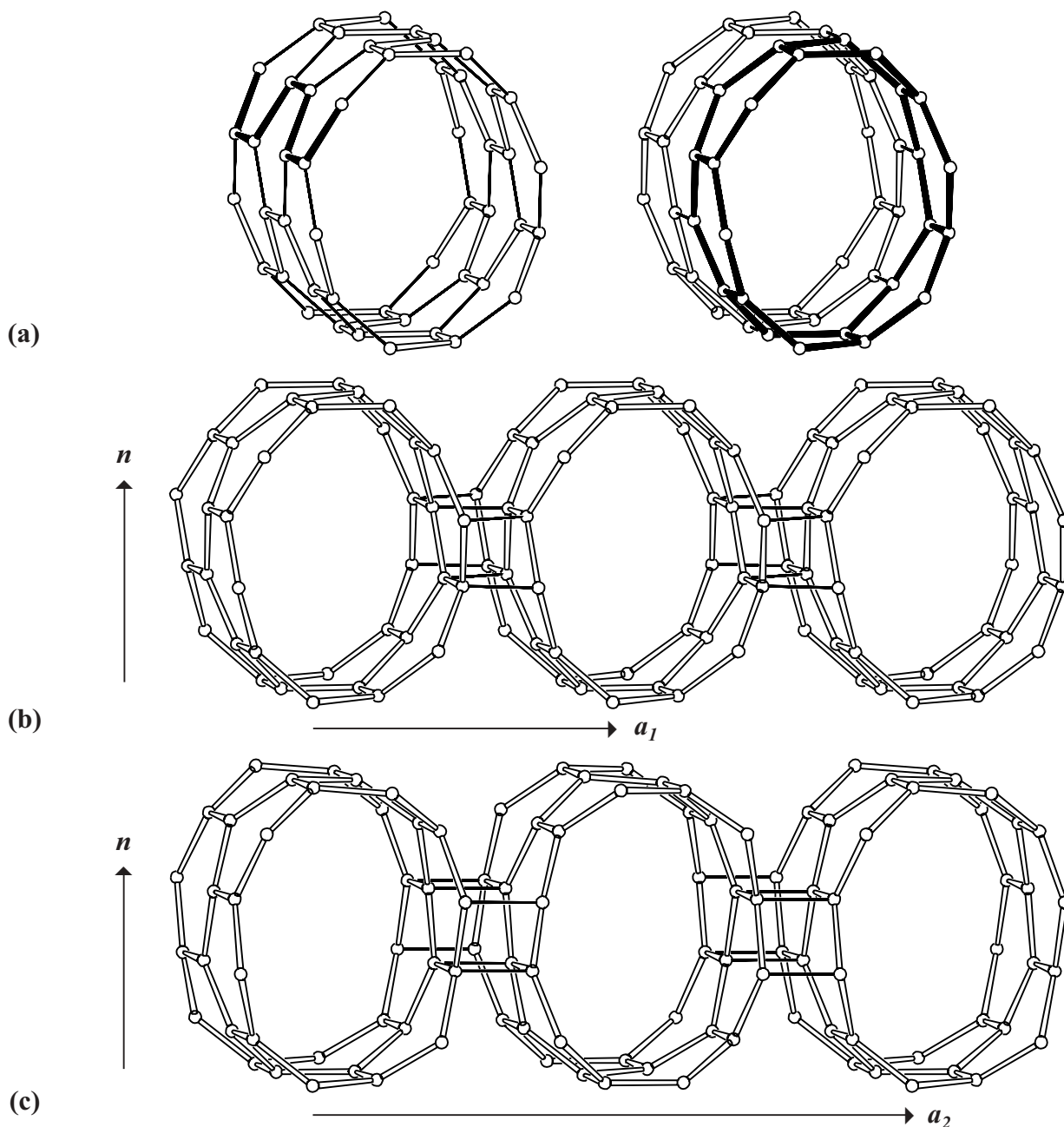


Figure 5: Tubular pore with T12-ring window constructed from six crankshaft chains (left) or from T6-ring bands each consisting of 24 T atoms (right); PerBU1 (b) and PerBU2 (c) of the SSZ-31 family of zeolite frameworks seen in perspective view perpendicular to the plane normal  $n$  and along the pore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

## 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. Croyghton, *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.

