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 \( a_1 \), are connected through double crankshaft chains of the narsarsukite 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 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 \( P 2_1/b 2_1/m (2/m) \) 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 \( 2 \times |a_j| \) 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 PerBU’s can be stacked along \( n \) in several ways. The lateral shift of the top layer along \( a \) and \( b \) is:

- **(1):** \(-\frac{1}{6} a \) and zero; denoted as \((-\frac{1}{6}, 0)\);
- **(2):** \(\frac{1}{6} a \) and zero; denoted as \((\frac{1}{6}, 0)\);
- **(3):** \(-\frac{1}{6} a \) and \(\frac{1}{2} b \); denoted as \((-\frac{1}{6}, \frac{1}{2})\);
- **(4):** \(\frac{1}{6} a \) and \(\frac{1}{2} b \); denoted as \((\frac{1}{6}, \frac{1}{2})\).

As an 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.

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Fig. 2a. Perspective view along the pore axis \( b \) of the connection modes (1) and (3) between PerBU1’s. 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 \( \frac{1}{2} b \), respectively. Connecting T-T modes between PerBU’s 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).
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. 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 $\textbf{H}$ and $\textbf{I}$ (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 \((a_0, b_0 \text{ and } c_0)\) of the space group is used.

<table>
<thead>
<tr>
<th>End-Member</th>
<th>Lateral shifts (along (n) in fractions of ((a, \text{ and } b))</th>
<th>space group</th>
<th>(a_0) (Å)</th>
<th>(b_0)</th>
<th>(c_0) (Å)</th>
<th>(\beta) (°)</th>
</tr>
</thead>
<tbody>
<tr>
<td>PerBU1</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>((-1/6, 0); (-1/6, 0); (-1/6, 0);)\ldots</td>
<td>P2/m</td>
<td>14.97</td>
<td>8.4</td>
<td>12.35</td>
<td>106.0</td>
</tr>
<tr>
<td>B</td>
<td>((-1/6, 0); (+1/6, 0); (-1/6, 0);)\ldots</td>
<td>Pnma</td>
<td>8.4</td>
<td>12.35</td>
<td>28.78</td>
<td>-</td>
</tr>
<tr>
<td>C</td>
<td>((-1/6, 1/2); (-1/6, 1/2); (-1/6, 1/2);)\ldots</td>
<td>C2/m</td>
<td>29.94</td>
<td>8.4</td>
<td>12.35</td>
<td>106.0</td>
</tr>
<tr>
<td>D</td>
<td>((-1/6, 1/2); (+1/6, 1/2); (-1/6, 1/2);)\ldots</td>
<td>Pbcm</td>
<td>12.35</td>
<td>28.78</td>
<td>8.4</td>
<td>-</td>
</tr>
<tr>
<td>PerBU2</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>E</td>
<td>((-1/6, 0); (-1/6, 0); (-1/6, 0);)\ldots</td>
<td>C2/m</td>
<td>24.70</td>
<td>8.4</td>
<td>14.97</td>
<td>106.0</td>
</tr>
<tr>
<td>F</td>
<td>((-1/6, 0); (+1/6, 0); (-1/6, 0);)\ldots</td>
<td>Cmca</td>
<td>8.4</td>
<td>24.70</td>
<td>28.78</td>
<td>-</td>
</tr>
<tr>
<td>G</td>
<td>((-1/6, 1/2); (-1/6, 1/2); (-1/6, 1/2);)\ldots</td>
<td>C2/m</td>
<td>24.70</td>
<td>8.4</td>
<td>16.58</td>
<td>119.8</td>
</tr>
<tr>
<td>H</td>
<td>((-1/6, 1/2); (+1/6, 1/2); (-1/6, 1/2);)\ldots</td>
<td>Cmca</td>
<td>8.4</td>
<td>24.70</td>
<td>28.78</td>
<td>-</td>
</tr>
<tr>
<td>PerBU1 and PerBU2</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>I(^2)</td>
<td>((-1/6, 0); (-1/6, 0); (-1/6, 0);)\ldots</td>
<td>P2/m</td>
<td>29.94</td>
<td>8.4</td>
<td>24.70</td>
<td>106.0</td>
</tr>
<tr>
<td>J</td>
<td>((-1/6, 0); (+1/6, 0); (-1/6, 0);)\ldots</td>
<td>Pma2</td>
<td>8.4</td>
<td>28.78</td>
<td>24.70</td>
<td>-</td>
</tr>
</tbody>
</table>

\(^1\) \(a = 24.70\) Å (See Fig.1 and Section 4); the pore axis \(b = 8.4\) Å; \(n\) is parallel to \(a \times b\).

\(^2\) 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].

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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].

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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