Building scheme for *STO

1. Periodic Building Unit – 2. Connection mode – 3. Parallel projections of the unit cell
4. Channels and/or cages – 5. Supplementary information

1. Periodic Building Unit:

The two-dimensional PerBUs in ***STO** are equal to the layers (PerBU1 and PerBU2) shown in Figure 1. The layers are built from tubular pores of fused 6-rings. The tubular pore is obtained when six crankshaft chains are linked into a channel with a 12-ring aperture (Figure 1(a)). Pores, related by pure translations along $\boldsymbol{a}_1$, are connected through crankshaft chains of the narsarsukite type into PerBU1. Pores, related by a translation along $\boldsymbol{a}_2$ and a shift along the pore axis of 1/2$\boldsymbol{b}$, are connected through double crankshaft chains of the feldspar type into PerBU2 (Figure 1(b and c)).

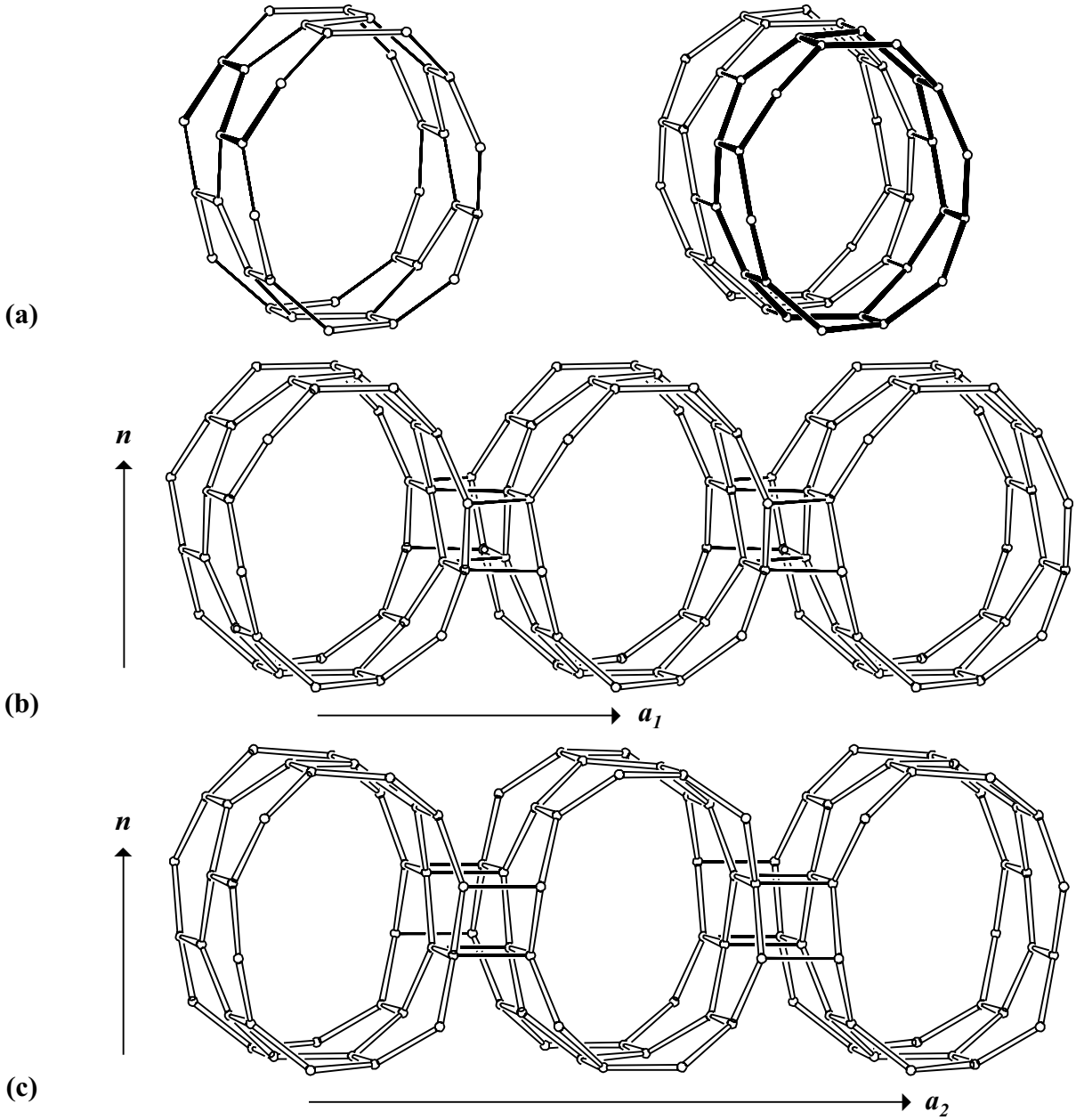


Fig. 1. (a) Tubular pore (top) constructed from crankshaft chains (left) and from 6-ring bands (right) viewed along the pore axis parallel to ***b***; (b) PerBU1 viewed perpendicular to the plane normal ***n*** and along the pore axis parallel to ***b***; (c) PerBU2 viewed as in (b).

2. Connection modes

The stacking of PerBUs along ***n*** requires a lateral shift of the PerBUs along ***a*** (and ***b***). It is convenient to describe the stacking sequence of the PerBUs along ***n*** using the same coordinate system in both PerBUs. Therefore the unit cell length along ***a*** is equal to $2|\boldsymbol{a}_1|$ in PerBU1 and equal to $|\boldsymbol{a}_2|$ in PerBU2. For both PerBUs the lateral shifts along ***a*** are then given as ± 1/6***a***.
Neighboring PerBUs can be stacked along ***n*** through 4-rings or crankshaft chains in several ways:
(1): the lateral shift of the top layer along ***a*** and ***b*** is -1/6***a*** and zero; denoted as (-1/6, 0);
(2): the lateral shift of the top layer along ***a*** and ***b*** is +1/6***a*** and zero; denoted as (1/6, 0);
(3): the lateral shift of the top layer along ***a*** and ***b*** is -1/6***a*** and 1/2***b***; denoted as (-1/6, 1/2);
(4): the lateral shift of the top layer along ***a*** and ***b*** is +1/6***a*** and 1/2***b***; denoted as (1/6, 1/2).

One example of the connection modes is depicted in Figure 2. The PerBUs are connected along ***n*** through 4-rings or crankshaft chains depending on whether the shift along ***b*** between neighboring pores is zero or 1/2***b***, respectively. The gaps between the pores are filled with T-T dimers. Once the distribution of the lateral shifts between the PerBUs stacked along ***n*** is known, the three-dimensional framework is defined. For a description of other connection modes see: **Disordered Structures**

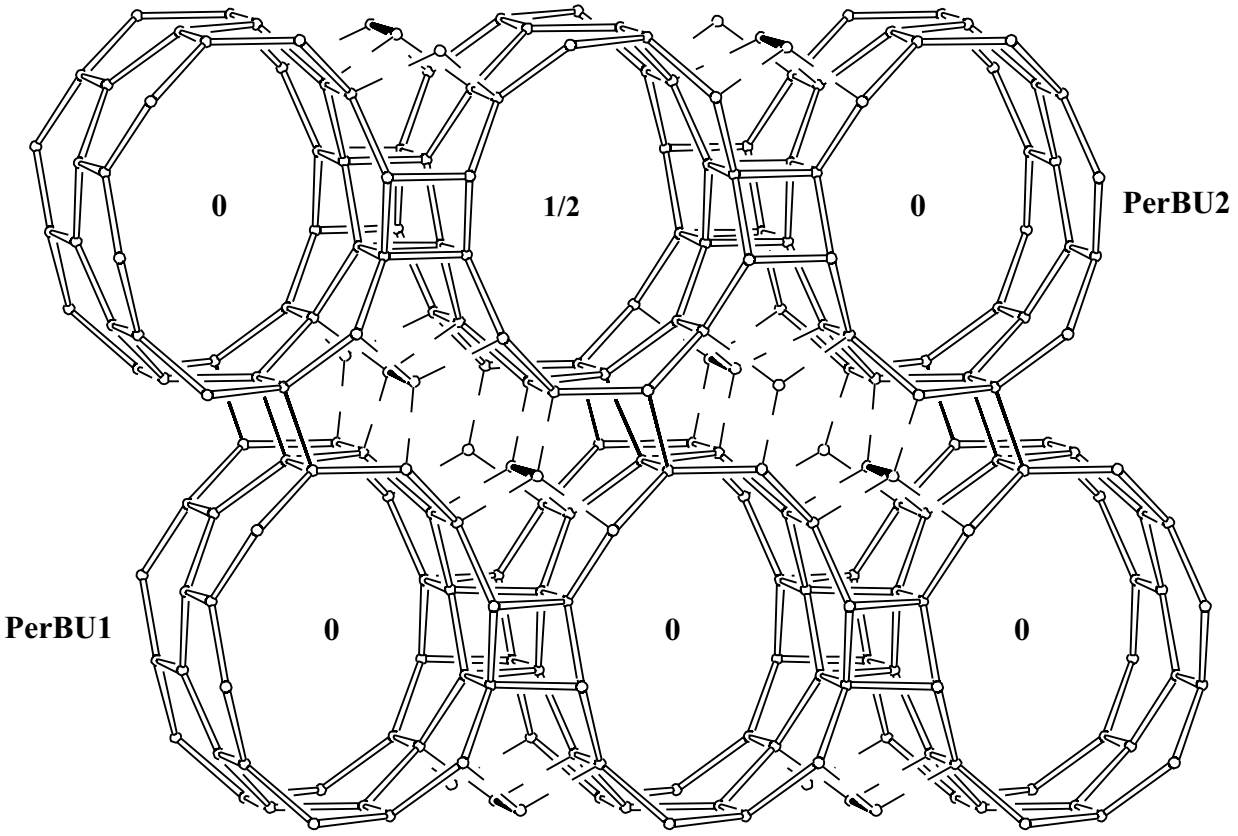


Fig. 2. Connection mode **(1)** in ***STO** between PerBU1 and PerBU2, viewed along the pore axis ***b***. Connecting T-T modes between PerBUs are drawn as single lines. The connections to the T-T dimers (heavy bold), which fill the space between the tubular pores, are striped. The number in the pore gives the fractional shift of the pore along ***b***.

3. Projections of the unit cell content:

In ***STO** the strictly alternating PerBU1 and PerBU2 are connected along ***n*** through 4-rings and crankshaft chains. The unit cell content is shown in Figure 3 on next page.

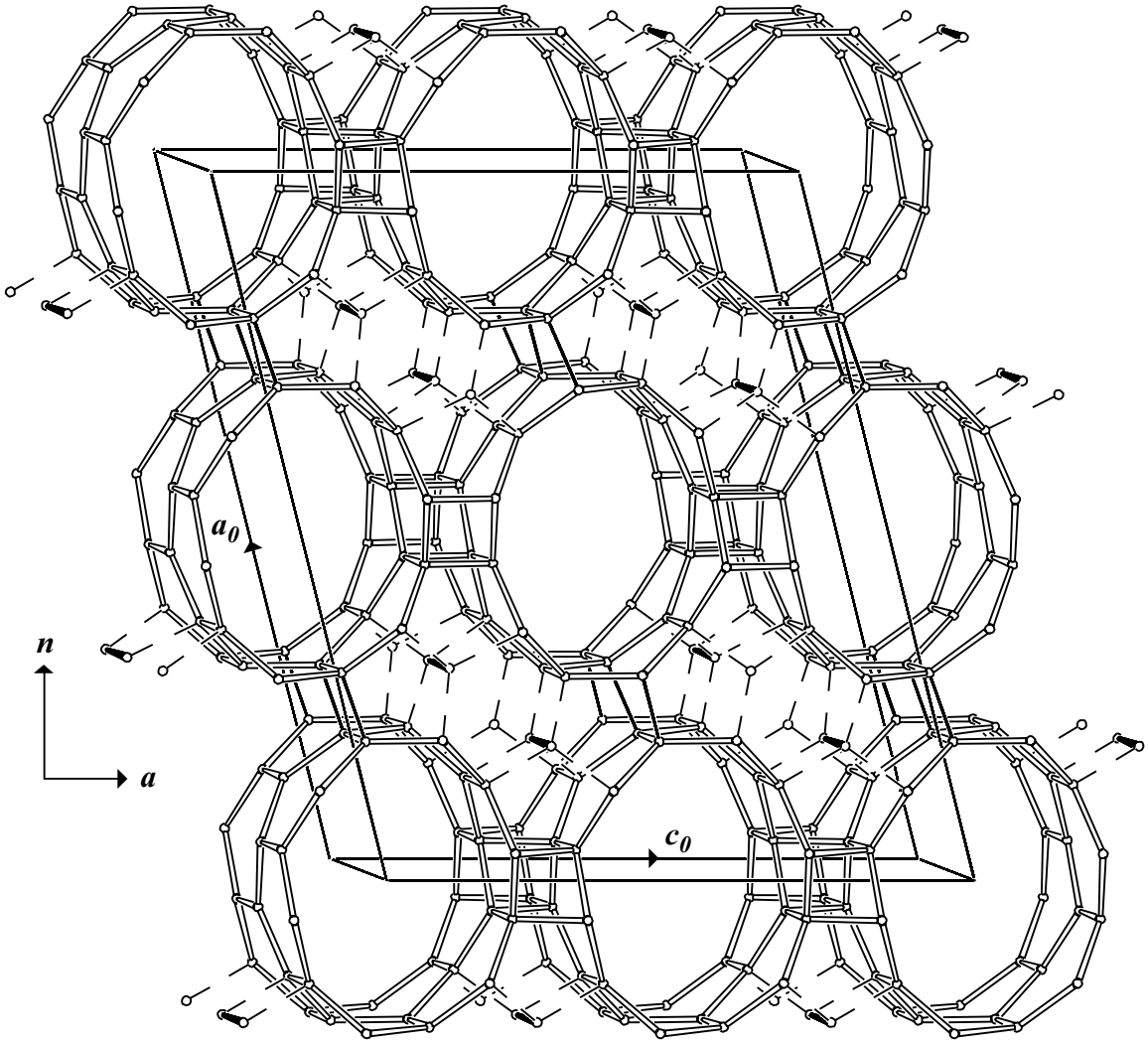


Fig. 3. The ordered end-member ***STO** viewed along the pore axis. The unit cell is given in standard setting. T-T connections to dimer units are striped.

4. Channels and/or cages:

Non-interconnecting one-dimensional 12- ring channels are parallel to ***b***. The channel, topologically equivalent to the channel in **AFI**, is depicted in Figure 4 together with the **pore descriptor**.

{1 [$6^{12}12^{2/2}$] [001] (12-ring)}

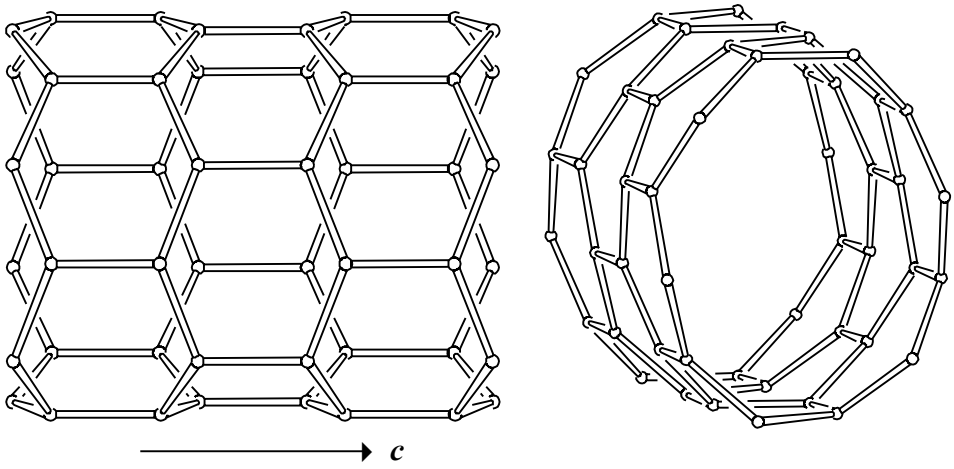
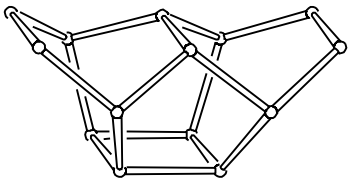


Fig. 4. Channel in ***STO** viewed perpendicular to ***b***(left) and along ***b*** (right).

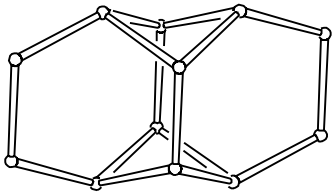
5. Composite Building Unit:

$[4^1 5^2 6^4]$ **10**



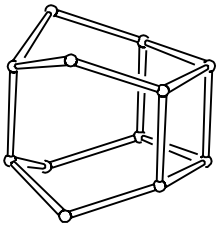
CON, DON, ITH, IWR, IWW, MEL, MFI, MWW, SFG, SSF, *STO

$[4^2 6^4]$-b **18**



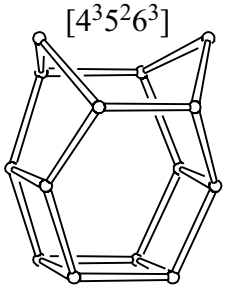
AEL, AET, AFI, AFO, AHT, ATV, BOG, CGF, DFO, LAU, *STO, TER, USI, VFI

$[4^2 6^4]$-c **19**



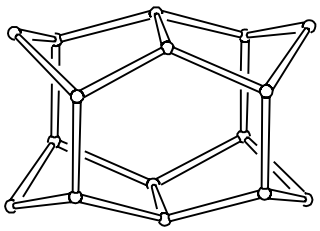
ATS, IMF, OSI, *STO

$[4^3 5^2 6^3]$ **24**



DON, *STO

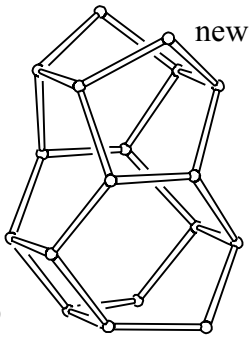
$[5^4 6^4]$-a **61**



***STO, TUN**

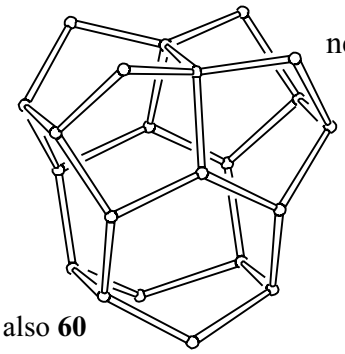
[The numbering is used in the Appendix to the "Building Schemes"-book]

$[4^1 5^2 6^6]$ new



***STO**

$[5^4 6^7]$ new



***STO;** see also **60**

5. Supplementary information:

Other framework types containing crankshaft chains

In several framework types at least one of the unit cell dimensions is between 8.4 and 9.9 Å. In many cases this indicates the presence of crankshaft chains.

In the **INTRO**-pages links are given to detailed descriptions of these framework types (choose: **Crankshaft chains**). There is also a link provided to a summary of the Periodic Building Units used in the building schemes of these framework types (choose: **Appendix**; **Figure 3**).

Alternative description of* AFI *using (modified) double 4-rings (D4Rs)

Several framework types, like **AFI**, can be built using double crankshaft chains of the narsarsukite type consisting of 2-fold (1,3)-connected D4Rs (see Figure 2).

In the **INTRO** pages links are given to descriptions of other framework types containing (modified) D4Rs (choose: **Double 4-rings**). There is also a link provided to a summary of the Periodic Building Units used in the building schemes of these framework types (choose: **Appendix**; **Figure 5**).