

Building scheme for SAO



1. Periodic Building Unit – 2. Connection mode – 3. Parallel projections of the unit cell
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1. Periodic Building Unit:

Tetragonal SAO can be built using units of 28 T atoms. The unit consists of two 4-fold (1,2,4,5)-connected 6-ring ‘boats’ (Figure 1(a); in bold) which are tetrahedral connected to four 4-rings. Alternatively, the T28-unit can be built using two 4-4- and two 4-2 units or using seven 4-rings. The two-dimensional Periodic Building Unit (PerBU) is obtained when T28-units, related by pure translations along a , and b are connected into the ab layer shown in Figure 1(b).

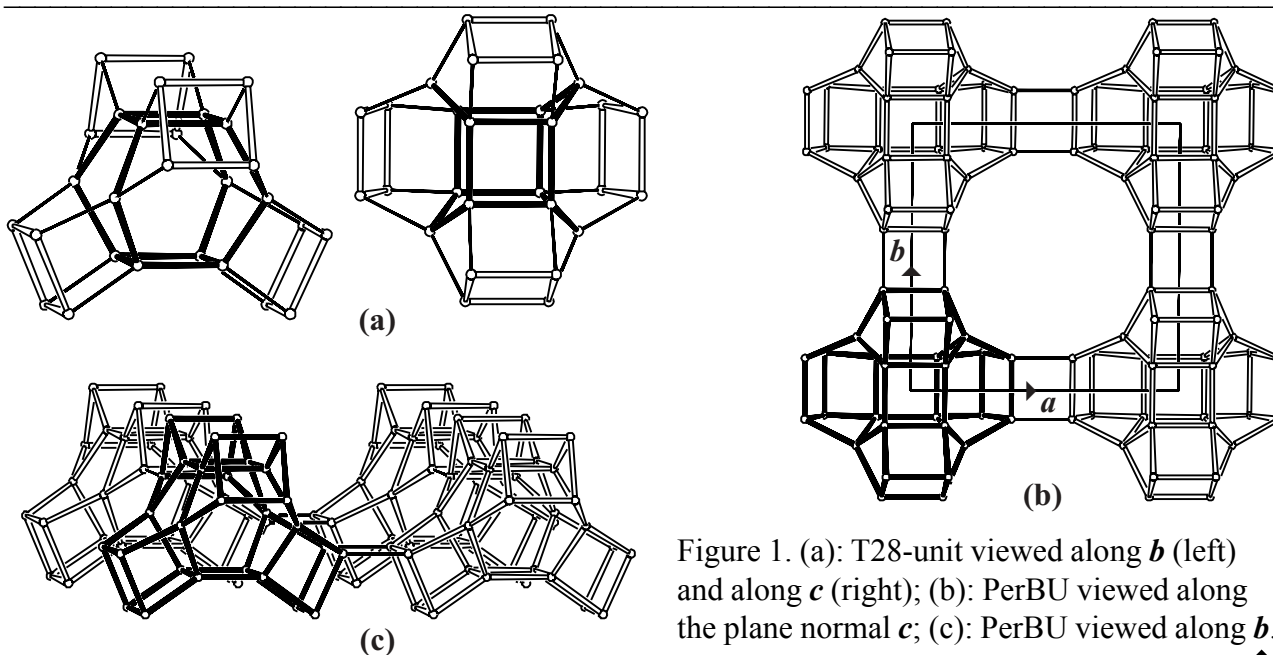


Figure 1. (a): T28-unit viewed along b (left) and along c (right); (b): PerBU viewed along the plane normal c ; (c): PerBU viewed along b .



2. Connection mode:

Neighboring PerBUs, related by a shift of $\frac{1}{2}(a + b + c)$, are connected along c as shown in Figure 2.

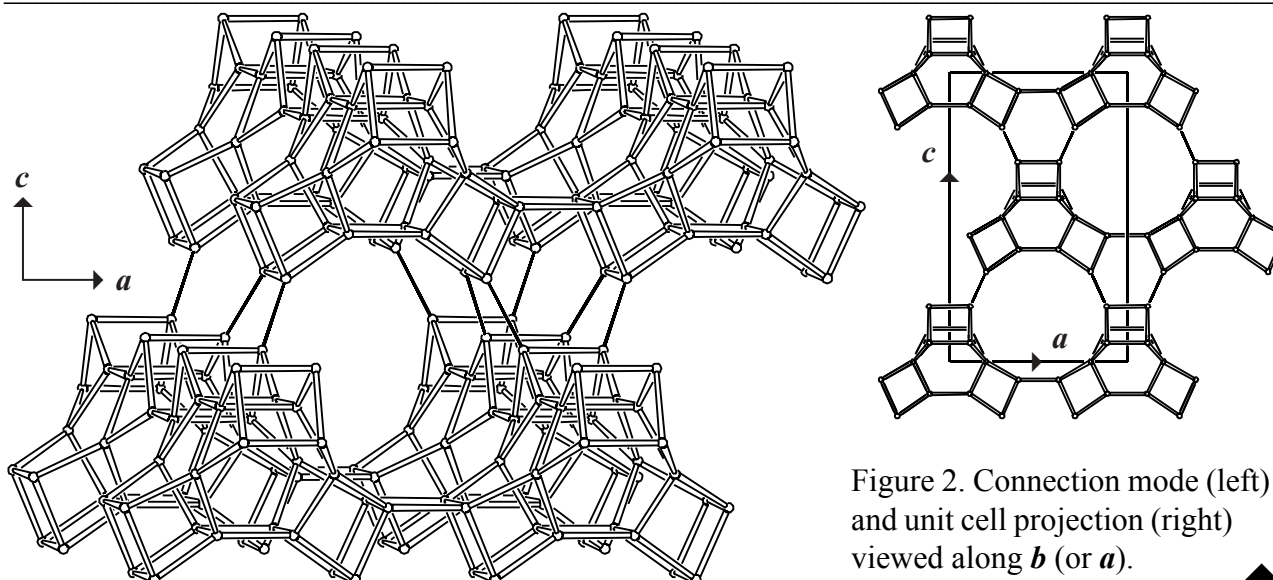


Figure 2. Connection mode (left) and unit cell projection (right) viewed along b (or a).



3. Projections of the unit cell content: See Figure 2. ▲

4. Channels and/or cages:

Interconnecting 12-Ring channels are parallel to $\langle 100 \rangle$. The channel is depicted in Figure 3 together with the **pore descriptor**. The fusion of channels is illustrated in Figure 4. Diffusion along the 16-ring channels parallel to $[001]$ is obstructed as can be seen from the drawings of the (fused) channels at the bottom of Figure 3.

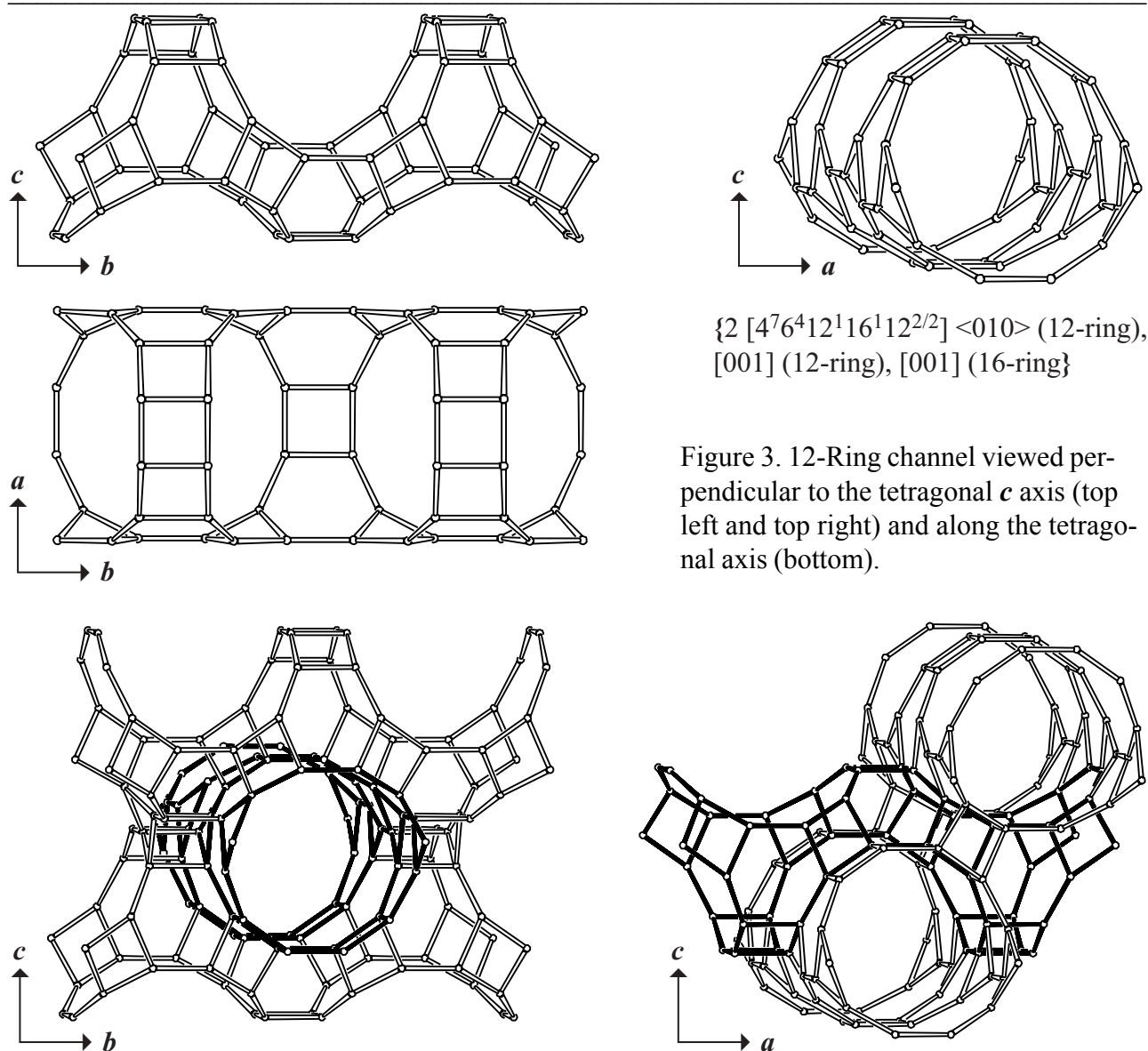


Figure 3. 12-Ring channel viewed perpendicular to the tetragonal c axis (top left and top right) and along the tetragonal axis (bottom).

Figure 4. Fusion of channels viewed along a (left), and along b (right). ▲

5. Supplementary information:

Other framework types containing (modified) double 6-rings (D6Rs)

Several other framework types can be built using (modified) D6Rs.

In the **INTRO** pages links are given to descriptions of other framework types containing (modified) D6Rs (choose: **Double 6-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 7**). ▲