

Building scheme for SBE



1. Periodic Building Unit – 2. Connection mode – 3. Projections of the unit cell content
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1. Periodic Building Unit:

Tetragonal **SBE** can be built using the *sbe* cavity, composed of 64 T atoms, as zero-dimensional Periodic Building Unit (PerBU). The cavity consists of eight 8-rings (one in bold) connected around the 4-fold *c* axis. 4- and 12-Rings are formed as shown in Figure 1.

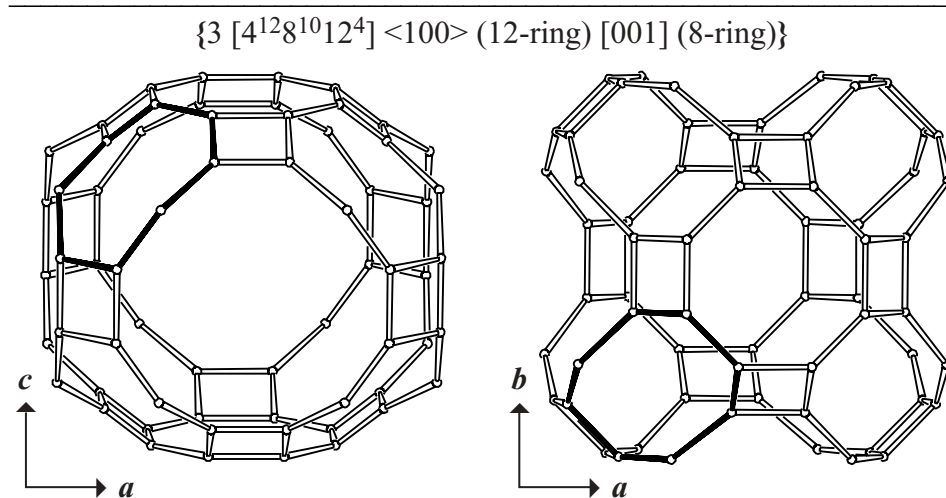


Figure 1. PerBU in **SBE** viewed perpendicular to the 4-fold axis (left) and along the 4-fold axis (right).



2. Connection mode:

The three-dimensional **SBE** framework is obtained when PerBUs, related by pure translations along *a* and *b* and by a translation of $\frac{1}{2}(a + b + c)$, are connected through 4-rings as shown in Figure 2.

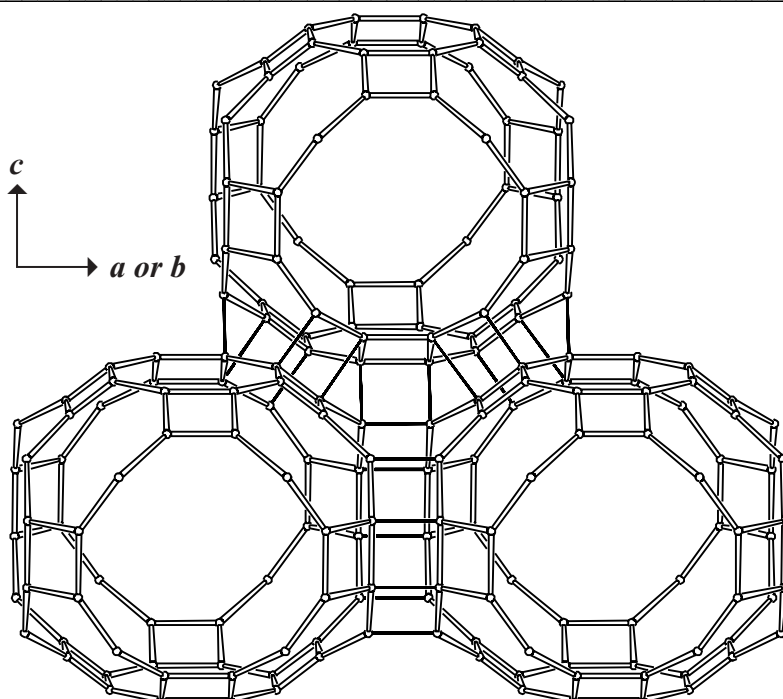


Figure 2. Connection mode viewed along *b* (or *a*). Only three PerBus are drawn for clarity.



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

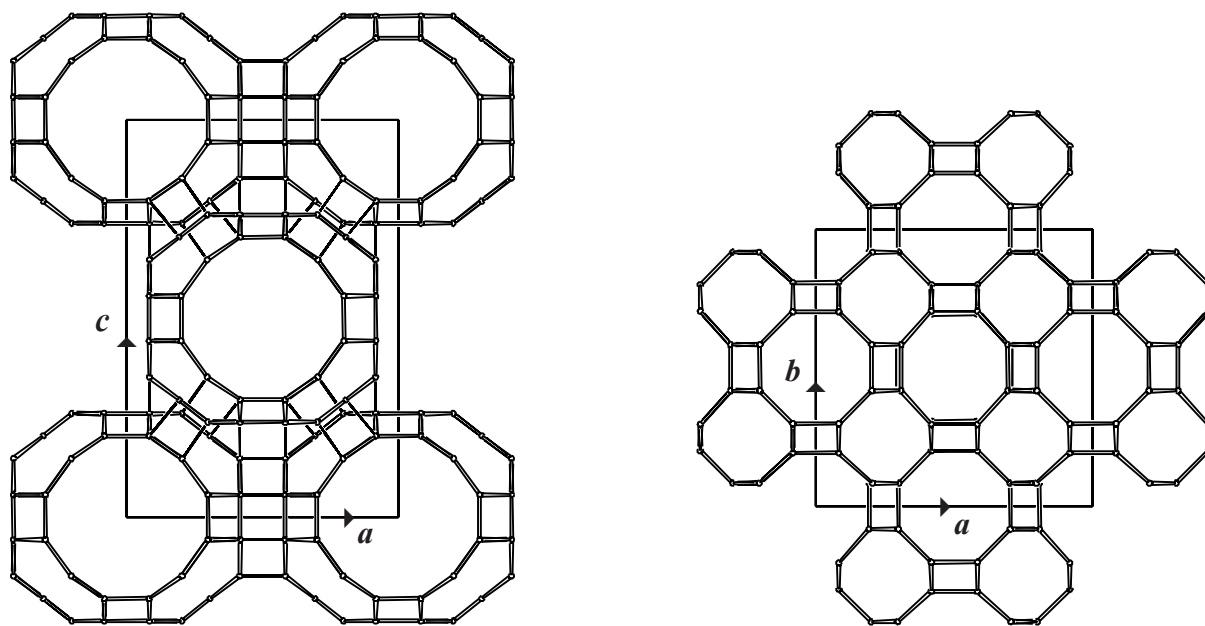


Figure 3. Unit cell content projected along $\langle 010 \rangle$ (left), and along c (right). ▲

4. Channels and/or cages:

In tetragonal **SBE** 12-ring channels are parallel to $\langle 100 \rangle$ and 8-ring channels are parallel to $[001]$. The channel intersections are equal to PerBU depicted in Figure 1. The linkage of complete PerBUs generate "double" *atn* cavities shown in Figure 4. The **pore descriptor** is added in Figures 1 and 4. The location of the "double" *atn* cavities within the framework is illustrated in Figure 5.

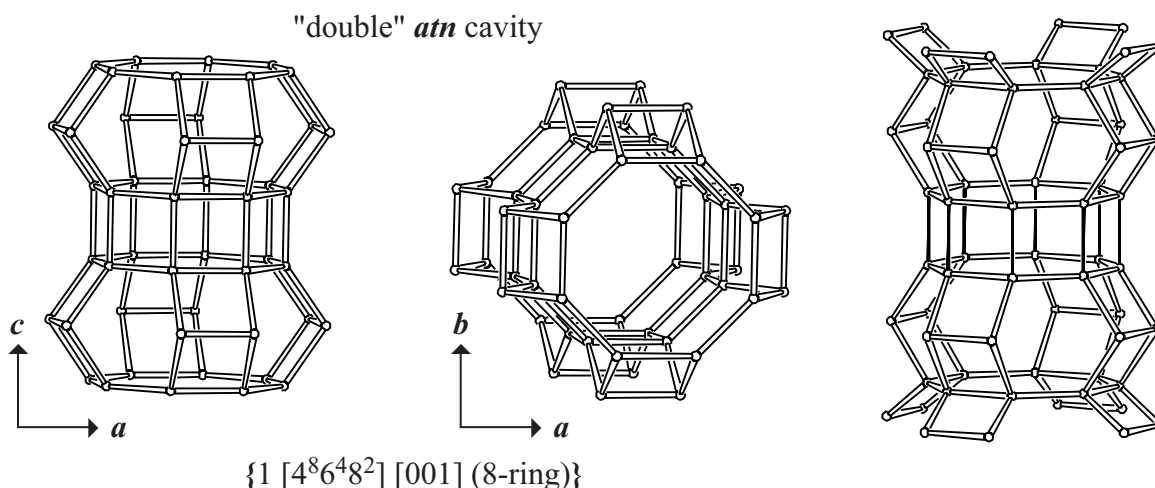


Figure 4. "Double" *atn* cavity viewed along $\langle 010 \rangle$ (left) and along c (middle). **SBE** can as well be built using the "double" *atn* cavities with "handles" shown at the right viewed along $[110]$. This alternative PerBU can be built using 4-rings.

Compare Figure 5 on next page.

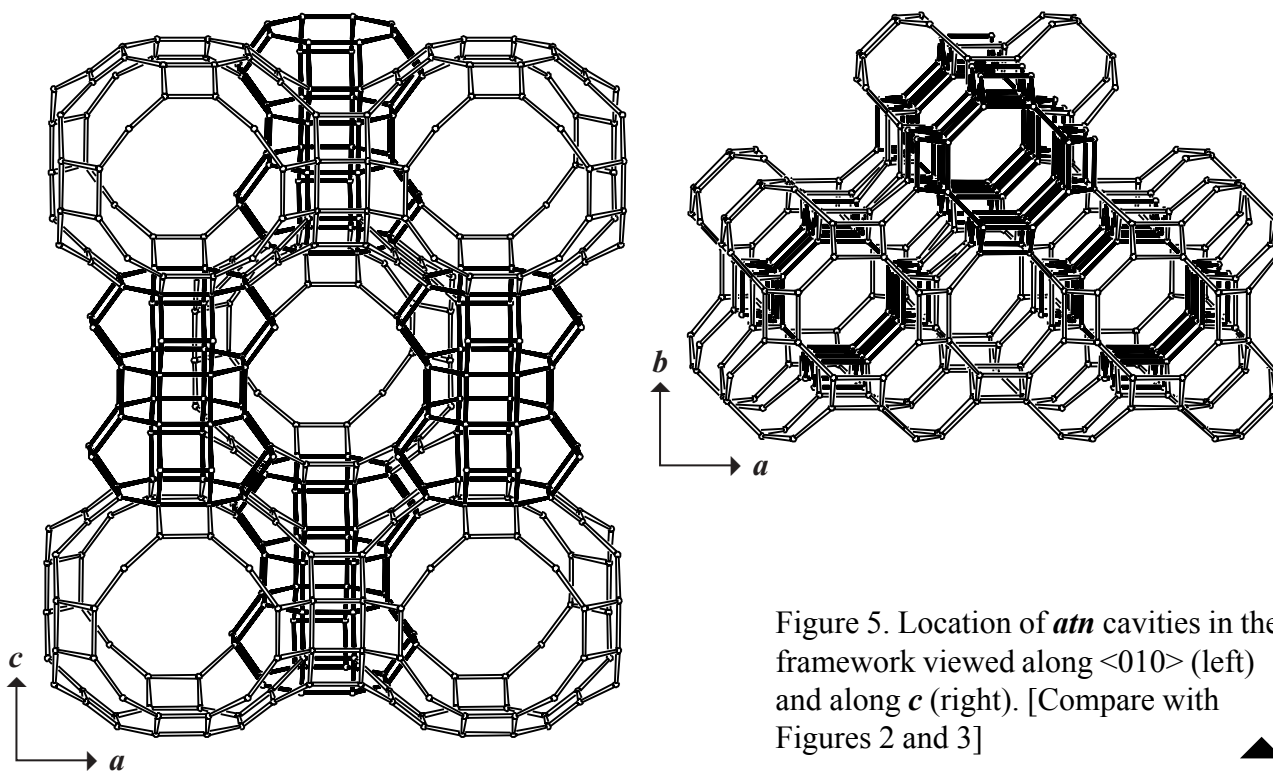


Figure 5. Location of *atn* cavities in the framework viewed along $\langle 010 \rangle$ (left) and along *c* (right). [Compare with Figures 2 and 3] ▲

5. Supplementary information:

Other framework types containing (modified) cavities

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

In the [INTRO](#)-pages links are given to a detailed description of a sub-set of framework types that contain (modified) cavities (choose: **Cages**). There is also a link provided to a summary of the PerBUs used in the building schemes of these framework types (choose: **Appendix; Figure 11**). ▲