Building scheme for SFF and STF

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

The Periodic Building Unit (PerBU) in triclinic **SFF** and monoclinic **STF** is composed of units of 16 T atoms and equals the **xz** layer shown in Figure 1. The T16-unit consists of two 5-3 units (bold in Figure 1). T16-units, related by translations along **x** and **z** and are linked through 4-rings and zigzag chains, respectively.

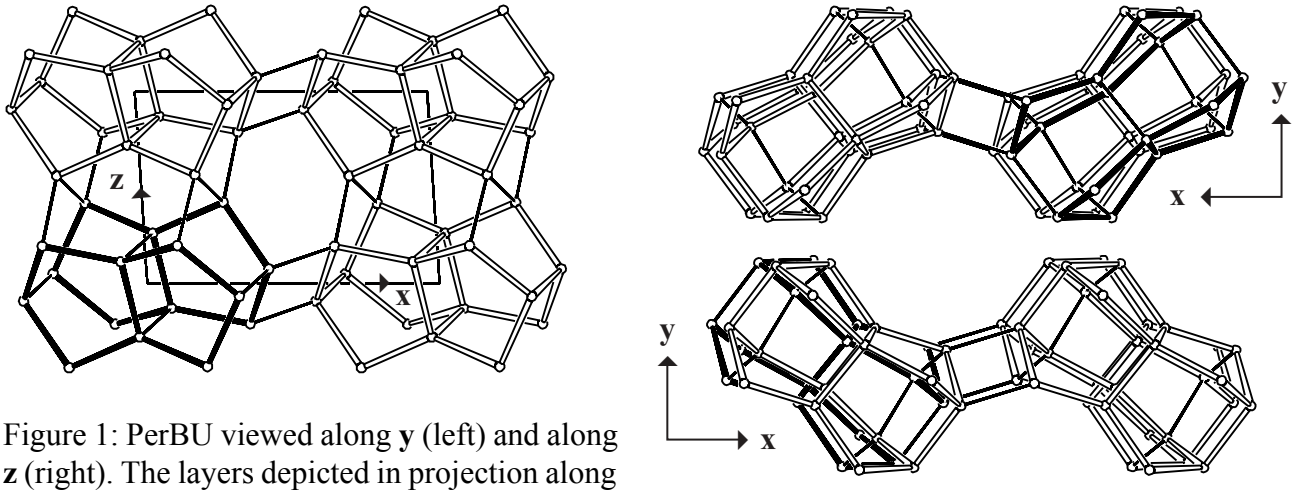
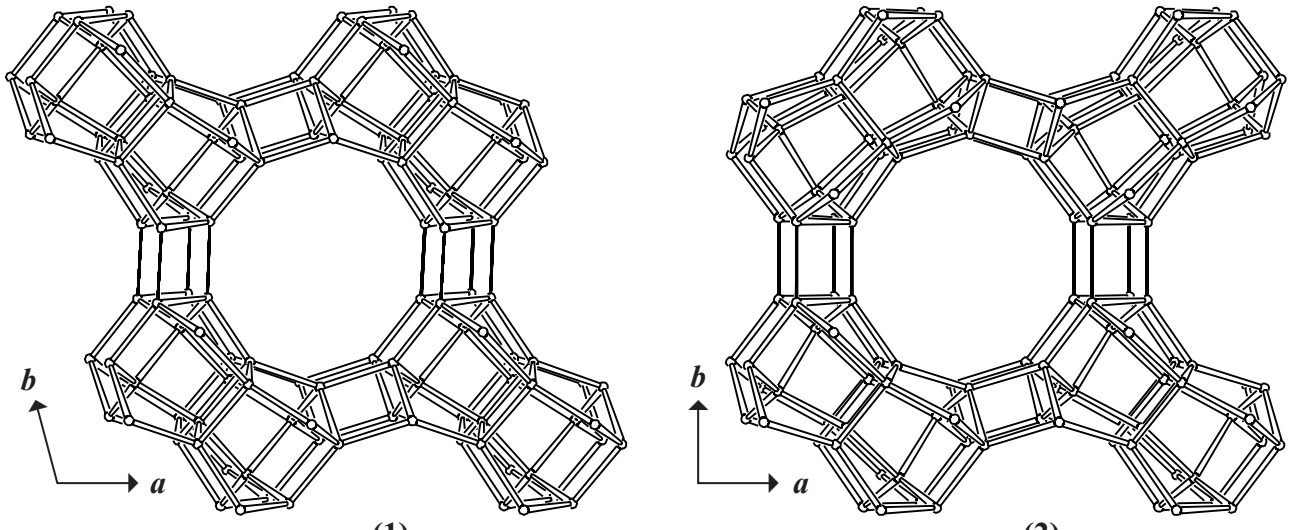


Figure 1: PerBU viewed along **y** (left) and along **z** (right). The layers depicted in projection along **z** are identical and related by a rotation of 180º about **y** or by a mirror plane perpendicular to **y**.

2. Connection mode:

Neighboring PerBUs are connected along ***b*** through 4-rings in two different ways shown in Figure 2.
(1): neighboring PerBUs are related by a pure translation along ***b***.
(2): neighboring PerBUs are related by a rotation of 180º about ***b***.



(1) **(2)**

Figure 2. Connection mode **(1)** in **STF** (left) and connection mode **(2)** in **SFF** viewed along ***c***.

3. Projections of the unit cell content:

Pure **SFF** and **STF** are obtained when neighboring PerBUs along ***b*** are exclusively related by reflection or inversion, respectively (Figure 3).

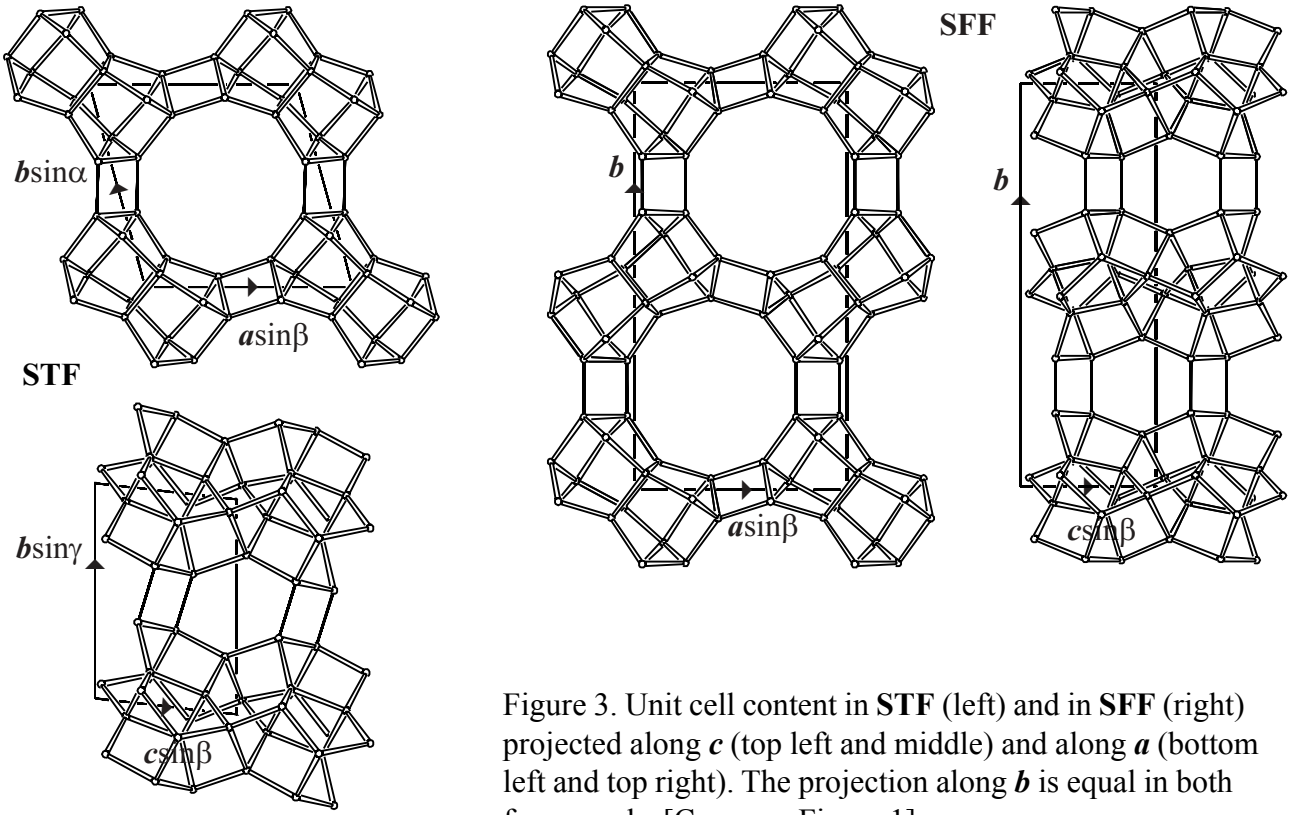


Figure 3. Unit cell content in **STF** (left) and in **SFF** (right) projected along ***c*** (top left and middle) and along ***a*** (bottom left and top right). The projection along ***b*** is equal in both frameworks [Compare Figure 1].

4. Channels and/or cages:

The cavities that describe the non-interconnecting 10-ring channels parallel to [001] in both framework types are depicted in Figure 4. The **pore descriptor**, the same for both channels, is added. The connection of the cavities is illustrated in Figure 5.

{1[$4^4 5^8 6^6 10^2$][001] (10-ring)}

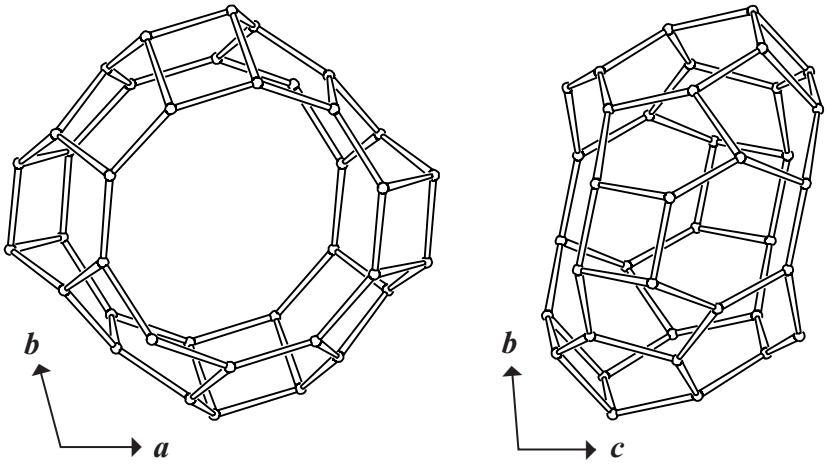


Figure 4. Cavity in **STF** viewed along ***c*** (left) and along ***a*** (right). [Fig. 4 is continued on next page]

{1[$4^4 5^8 6^6 10^2$][001] (10-ring)}

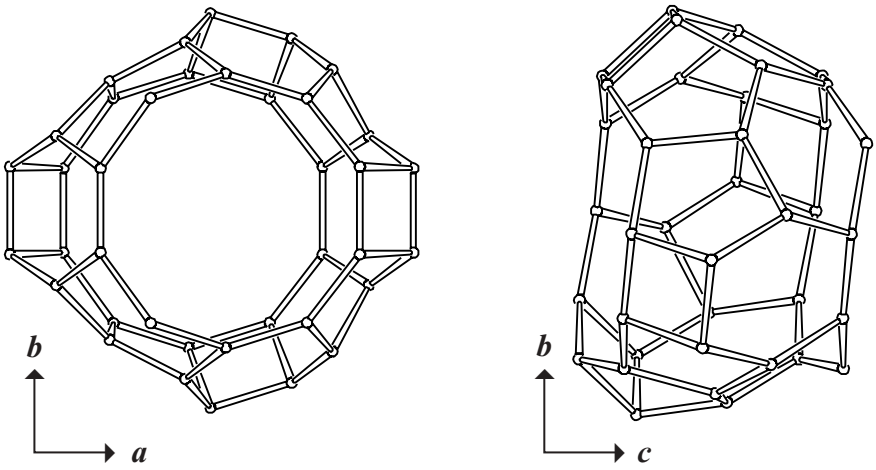


Figure 4. Cavity in **SFF** viewed along ***c*** (left) and along ***a*** (right).

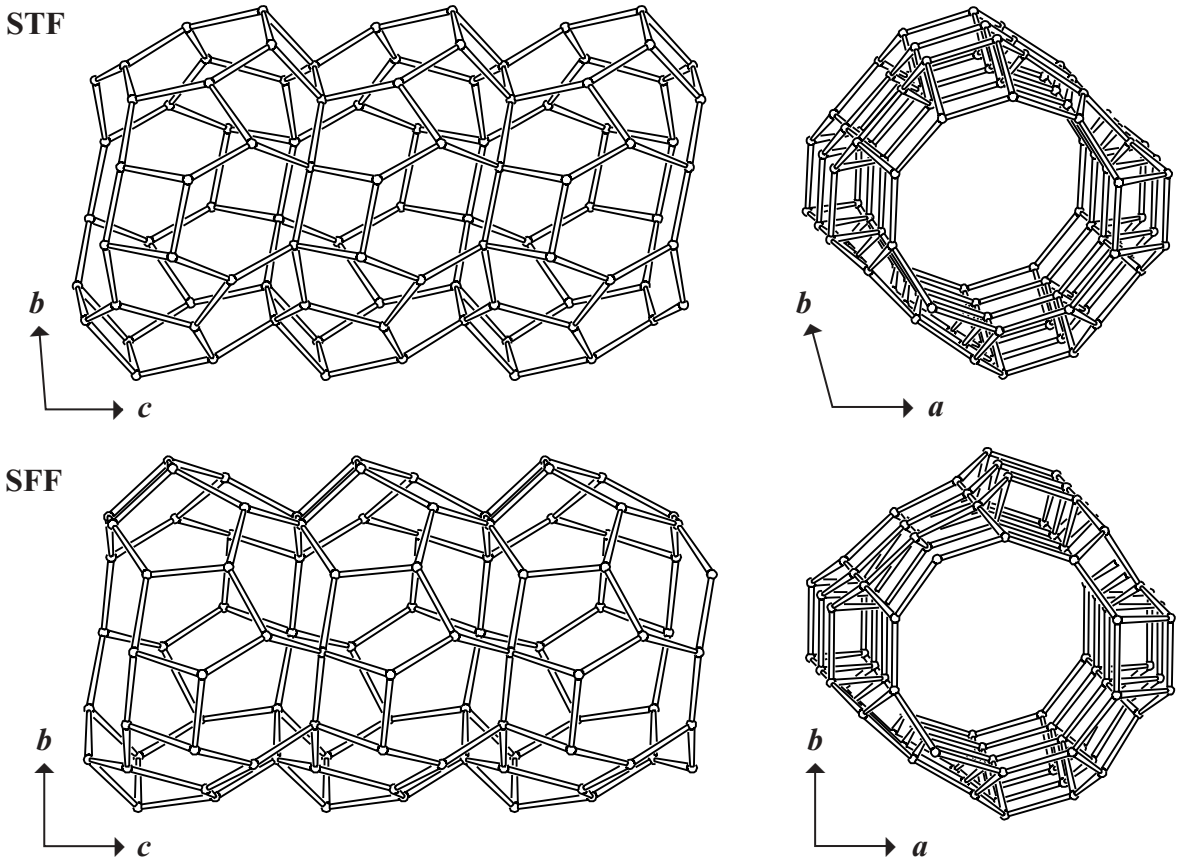


Figure 5. Linkage of the cavities in triclinic **STF** (top) and in monoclinic **SFF** (bottom) into 10-ring channels parallel to ***c*** viewed along ***a*** (left), and along the 10-ring channel axis parallel to ***c*** (right).

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5. Supplementary information:

Other framework types containing (modified) 5-rings

5-Rings can be connected in several other ways. In all cases additional T atoms are needed to build the framework.

In the **INTRO**-pages links are given to a detailed description of a sub-set of framework types that contain (modified) 5-rings (choose: **5-Rings**). There is also a link provided to a summary of the PerBUs used in the building schemes of these framework types (choose: **Appendix**; **Figure 6**).