

Building scheme for SOF



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1. Periodic Building Unit

Orthorhombic SOF can be built using units of 10 T atoms: a double 4-ring with two “dangling” T atoms (or two 4-1 units; bold in Figure 1). The D4Rs of the T10-units, related along $(a + b)$ by translations of $1/2(a + b)$, are connected through the “dangling” T atoms into a chain along $(a + b)$. Non-connected chains, related along b by pure translations along b , form the two-dimensional PerBU shown in Figure 1. [Compare this PerBU with the one in STW]

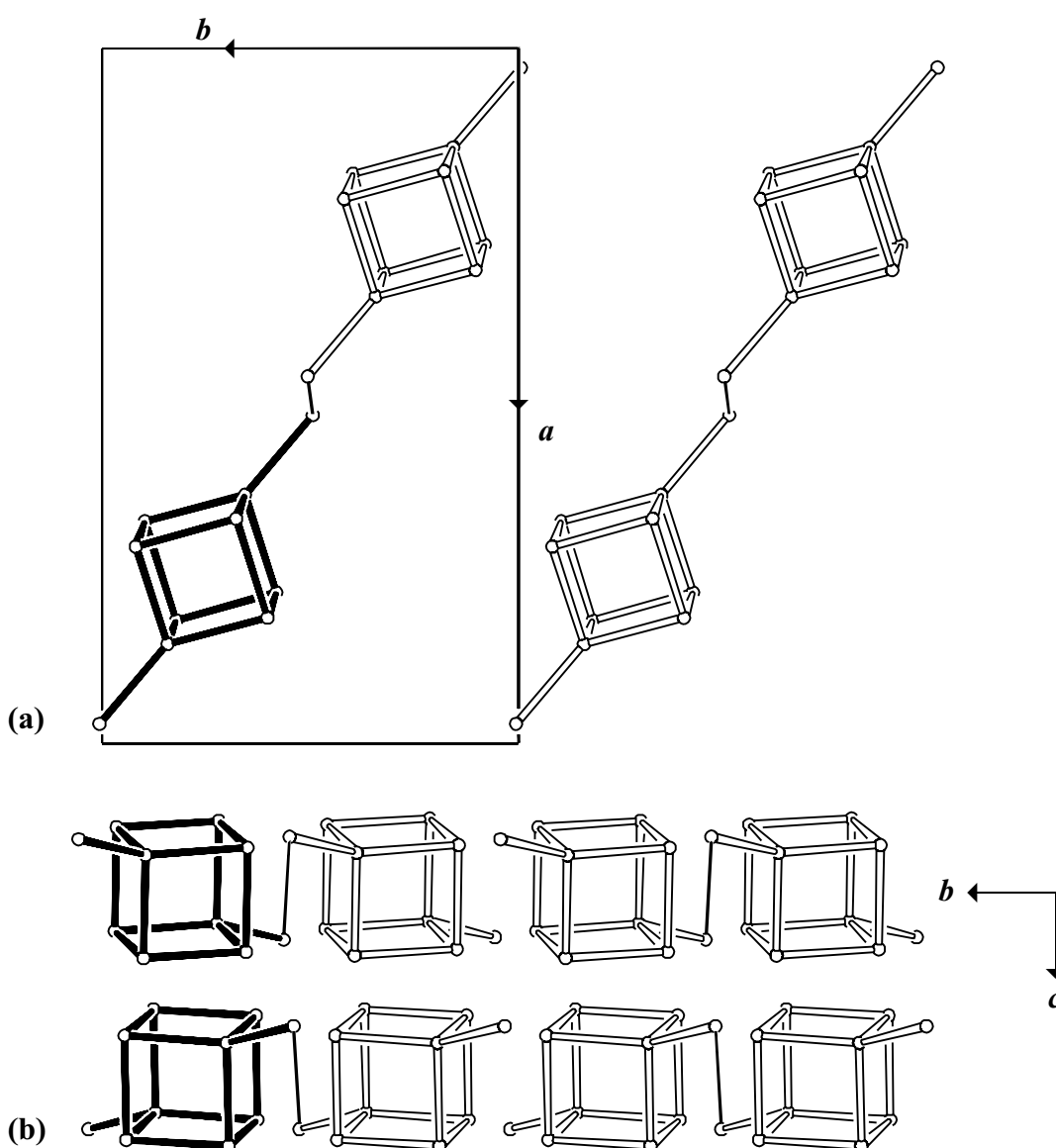


Figure 1. PerBU constructed from T10-units viewed along c (a) and along a (b). The PerBUs shown at the bottom are related by a rotation of 180° about b . For clarity, only two T10-units along $(a + b)$ are drawn.



2. Connection mode

Neighboring PerBUs, related by a screw rotation of 180° about b , are connected along c through 5-rings as shown in Figure 2.

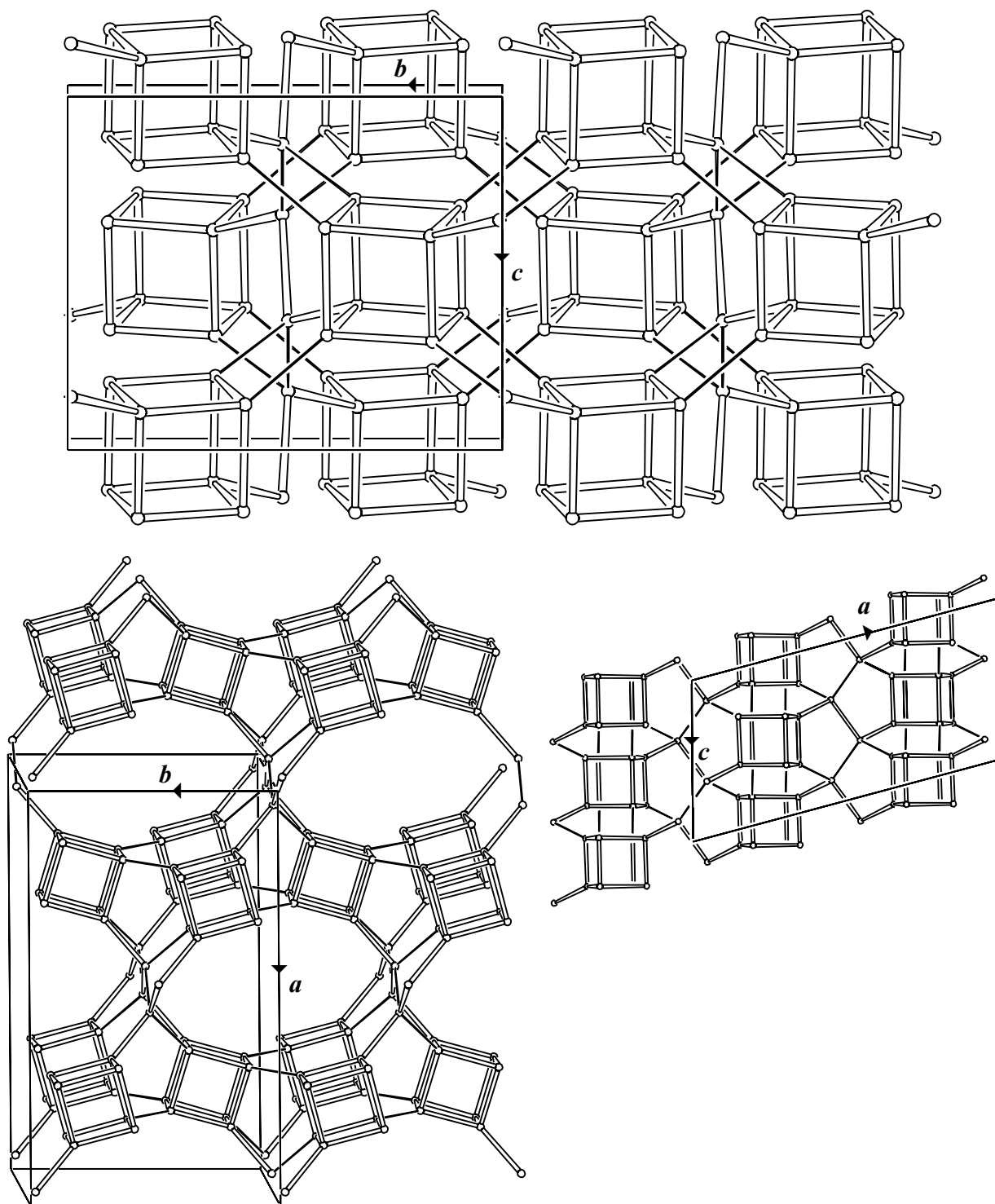


Figure 2. Connection mode and unit cell content viewed along a (top) and along c (bottom left). Bottom right: Unit cell content projected along b . For clarity, only two T10-units along $(a + b)$ are shown in the drawing at the top.



3. Channels and/or cages

12-Ring channels are parallel to c . The 12-ring channels are interconnecting through 9-rings. The interconnecting cavity and the 12-ring channel are illustrated in Figure 3. The **pore descriptors** are added.

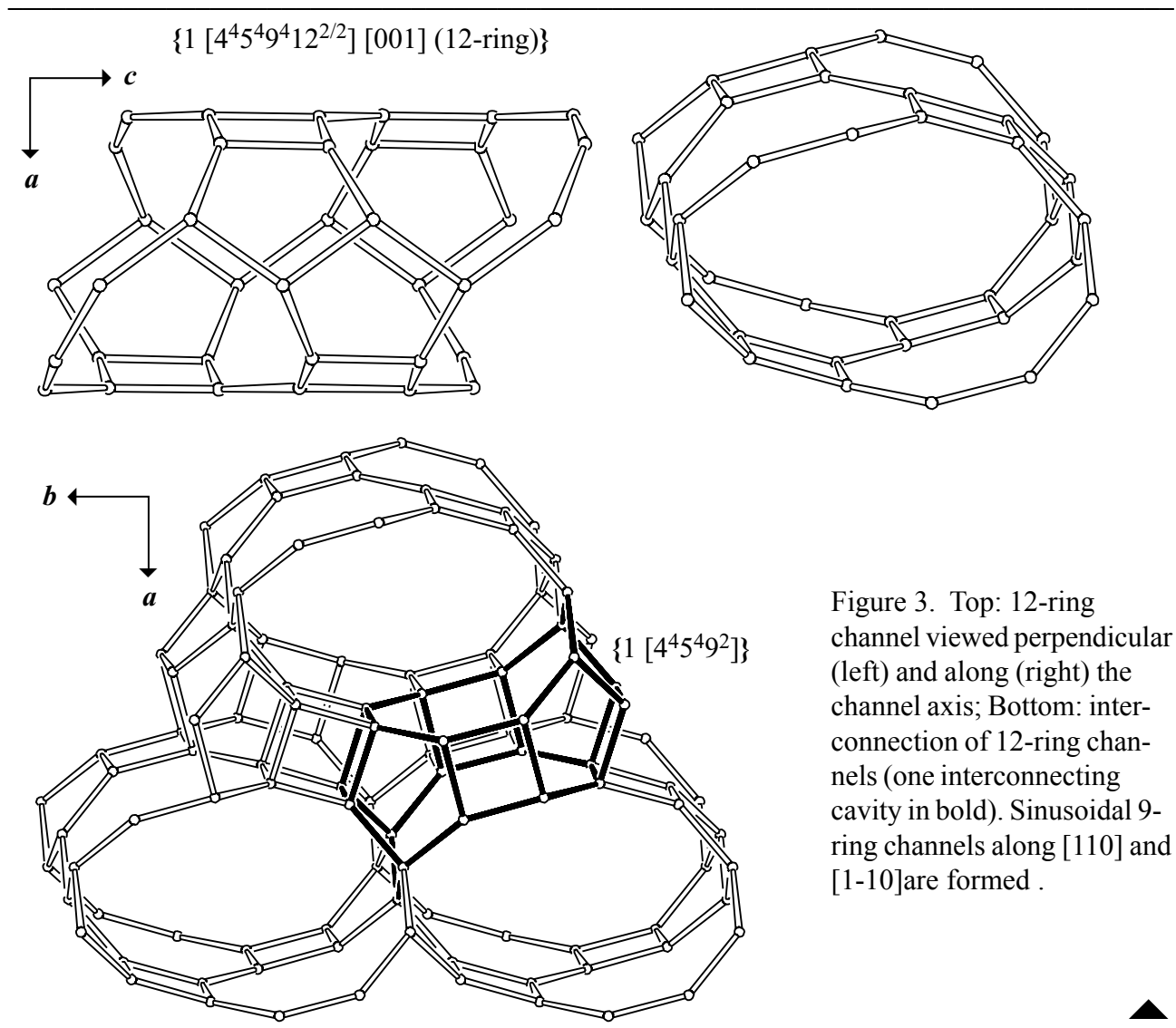
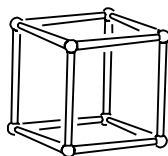


Figure 3. Top: 12-ring channel viewed perpendicular (left) and along (right) the channel axis; Bottom: interconnection of 12-ring channels (one interconnecting cavity in bold). Sinusoidal 9-ring channels along $[110]$ and $[1-10]$ are formed.

4. Composite Building Units

$d4r: [4^6]$



ACO, AFY, AST, ASV, BEC, -CLO, DFO, ISV, ITH, ITW, IWR, IWV, IWW, LTA, SOF, STW, UFI, UOZ, UTL

Figure 4. Composite Building Unit.

5. Supplementary information

Other framework types containing (modified) double 4-rings (D4Rs)

Double 4-rings (D4Rs) can be connected in several other ways. In some cases the 4-rings of the D4Rs are not 4-fold connected and/or 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) D4Rs (choose: **Double 4-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 5**).