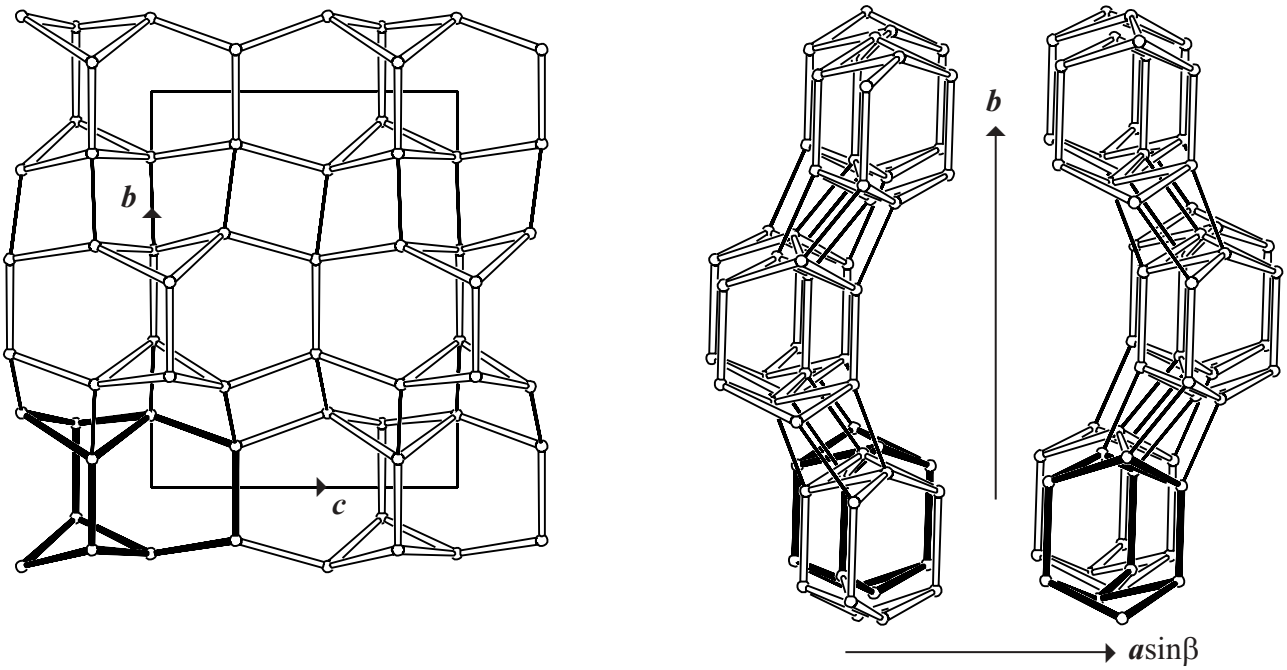
Building scheme for USI

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

1. Periodic Building Unit:

USI can be built using units of 10 T atoms. The T10-unit consists of doubly (1,3)-connected double 4-rings decorated with T2-dimers (or two 4-1 units; bold in Figure 1). T10-units, related by pure translations along ***c***, are connected along ***c*** into a chain of (fused) 6-rings with T2-dimer "handles". Neighboring chains, related by a rotation of 180º about ***b*** and a shift of ½***b***, are linked into the undulating ***bc*** layer. This two-dimensional Periodic Building Unit (PerBU) is depicted in Figure 1.



(a) **(b)**

Figure 1. (a): PerBU in **USI** viewed along ***a***; (b): PerBU viewed along ***c***. The PerBUs in (b) differ by a rotation of 180º about ***b***.

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2. Connection mode:

Neighboring PerBUs, related by a rotation of 180º about ***b***, are connected along ***a*** through 4-rings as shown in Figure 2 on next page. 12-Ring channels parallel to ***c*** and 10-ring channels parallel to ***b*** are formed.

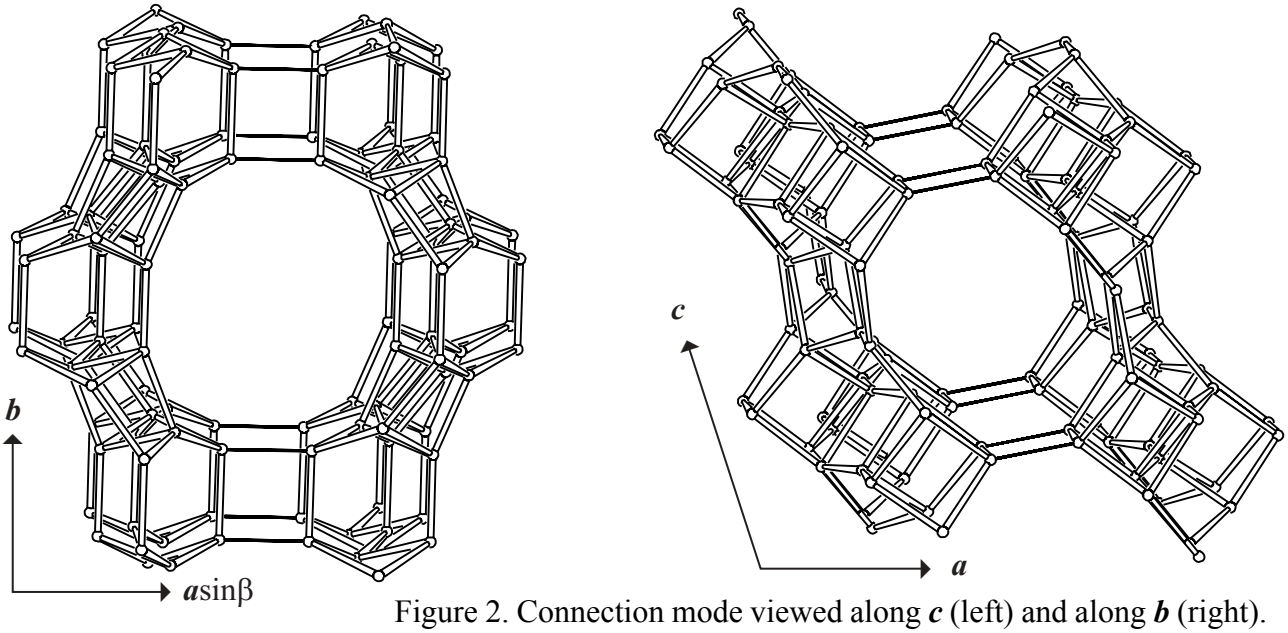

Figure 2. Connection mode viewed along ***c*** (left) and along ***b*** (right).

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

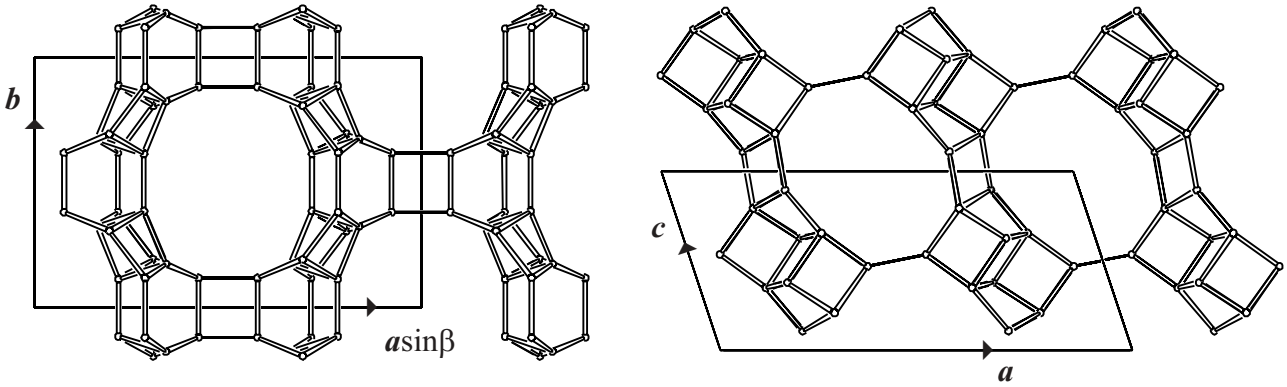

Figure 3. Parallel projections of the unit cell content seen along ***c*** (left) and along ***b*** (right).

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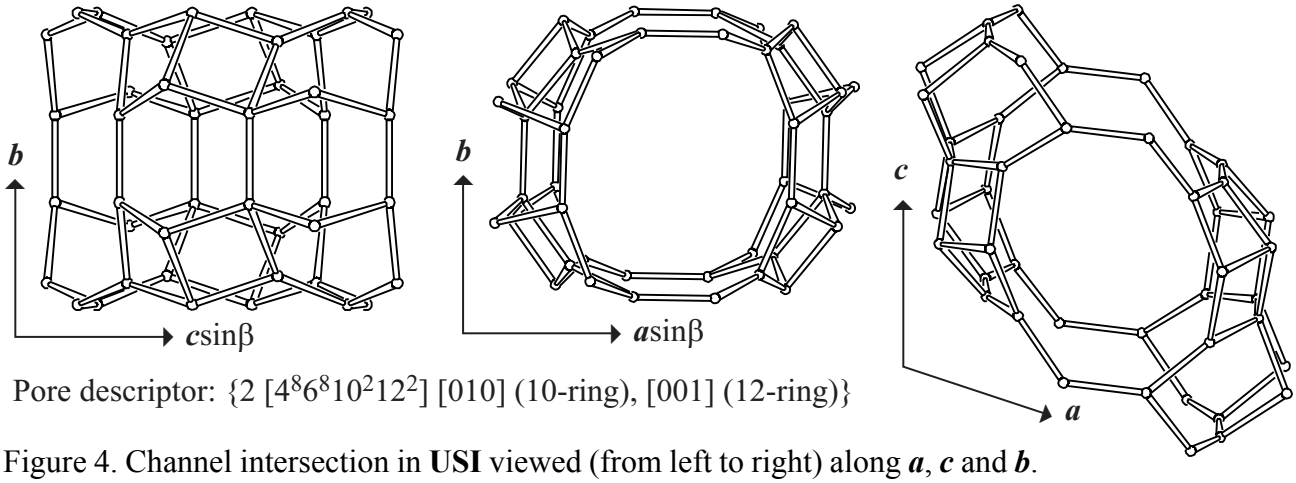
4. Channels and/or cages:

Channel intersection, **pore descriptor** and fusion of intersections into channels are shown in Fig. 4.



Pore descriptor: {2 [$4^8 6^8 10^2 12^2$] [010] (10-ring), [001] (12-ring)}

Figure 4. Channel intersection in **USI** viewed (from left to right) along ***a***, ***c*** and ***b***.
[Figure 4 is continued on next page]

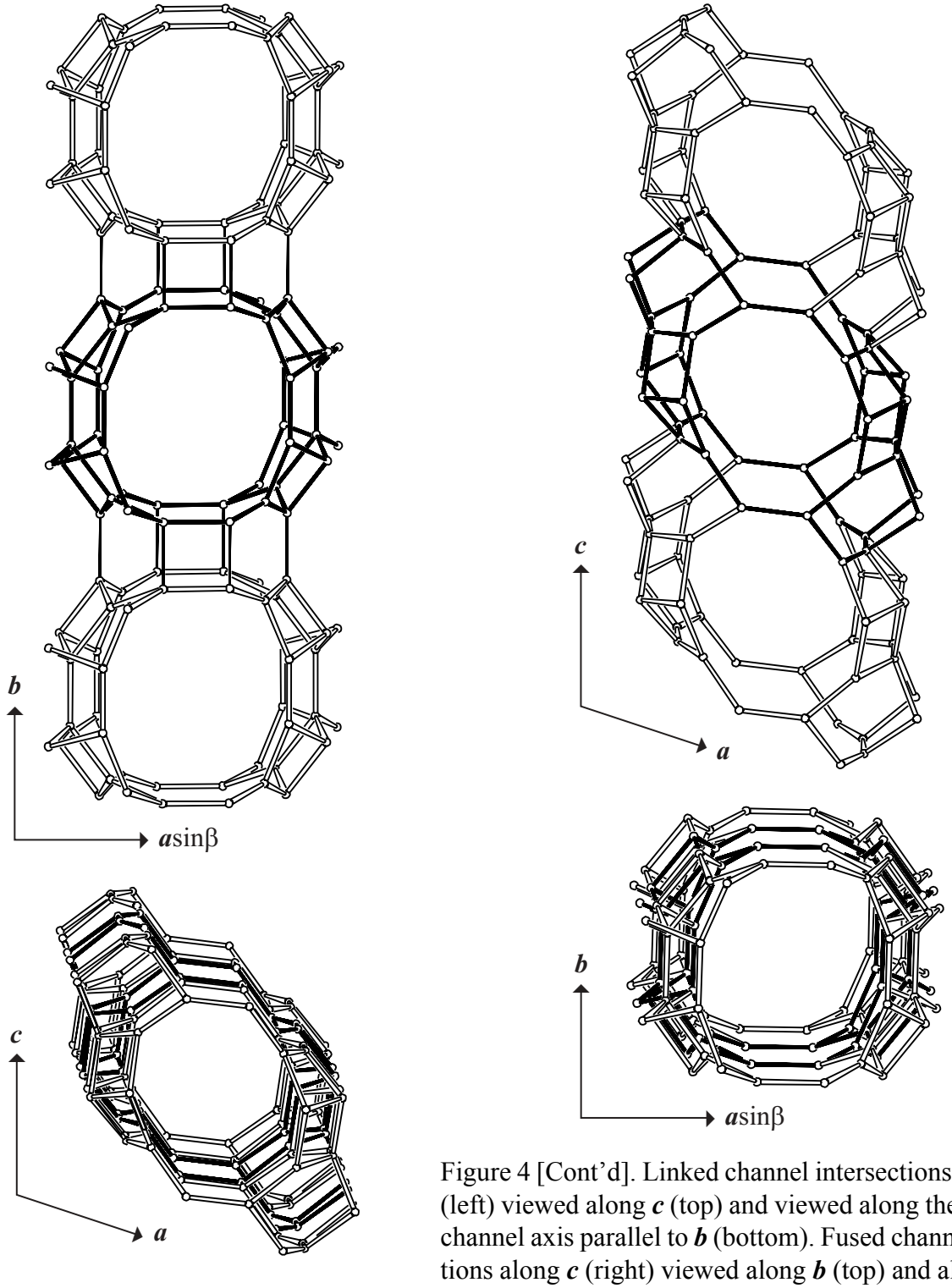


Figure 4 [Cont'd]. Linked channel intersections along ***b*** (left) viewed along ***c*** (top) and viewed along the 10-ring channel axis parallel to ***b*** (bottom). Fused channel intersections along ***c*** (right) viewed along ***b*** (top) and along the 12-ring channel axis parallel to ***c*** (bottom).

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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**).