Building scheme for YUG

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:

The Periodic Building Unit (PerBU) equals the layer of units of 8 T atoms depicted in Figure 1. These T8-units (one in bold), consisting of two singly connected 4-rings and related by pure translations along ***a***, and ***c***, are connected through 5-rings that have a (deformed) zigzag chain in common.

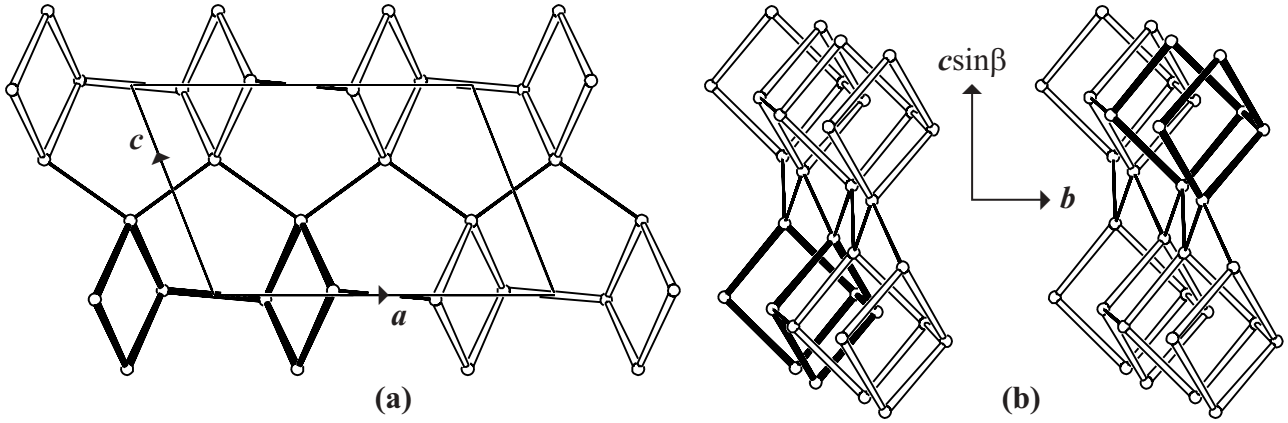


Figure 1. (a): PerBU in **YUG** viewed along ***b***; (b): PerBU viewed along ***a***. The two PerBUs shown in (b) differ by a rotation of 180º about ***b***.

2. Connection mode:

Neighboring PerBUs, related by a rotation of 180º about ***b*** (or by a mirror plane perpendicular to ***b***), are connected along ***b*** through 4-rings as shown in Figure 2. Intersecting 8-ring channels along ***a*** and ***c*** are formed.

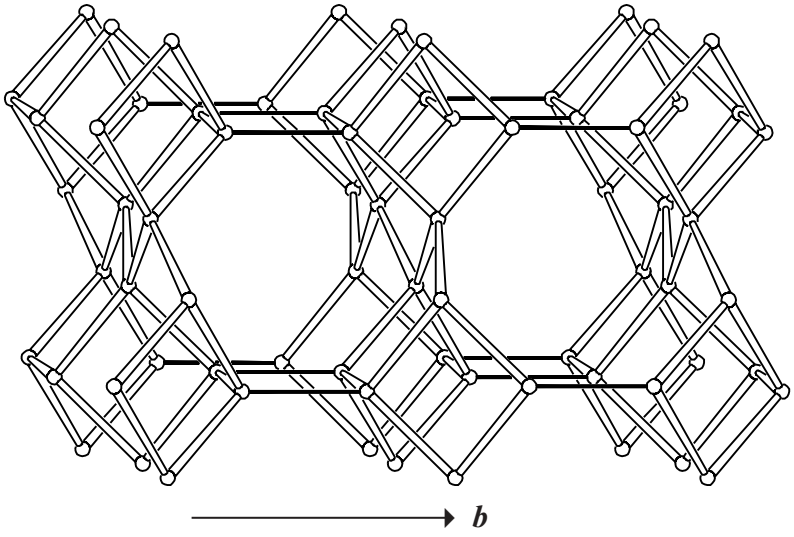


Figure 2. Connection mode viewed along ***a***. Only 1½ of the repeat distance along ***a*** is drawn for clarity.

3. Projections of the unit cell content:

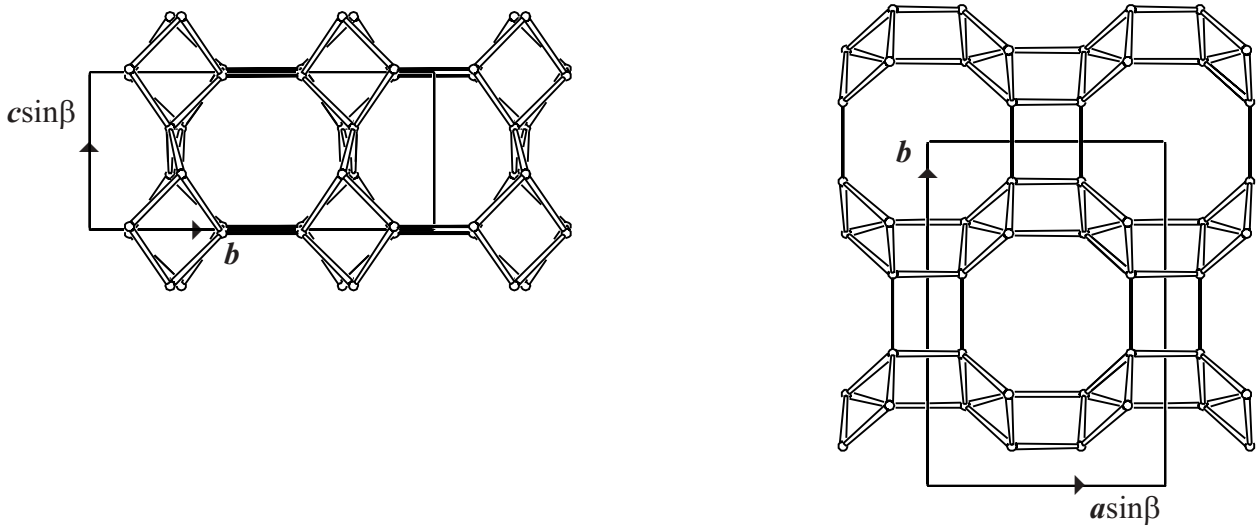
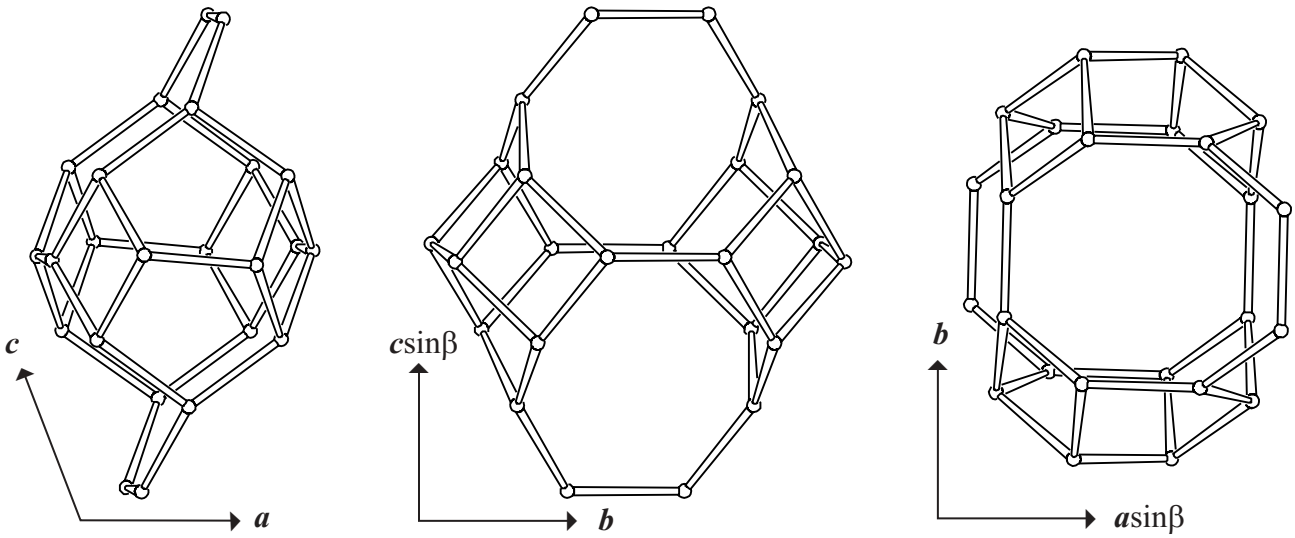


Figure 3. Unit cell content projected along ***a*** (left), and along ***c*** (right). **YUG** can also be built using 8-rings, as can be seen from the cell projection along ***c*** (right)

4. Channels and/or cages:

8-Ring channels along ***a***, and 8-ring channels along ***c*** intersect. The channel intersection and **pore descriptor** of the cavity is depicted in Figure 4.

Pore descriptor: {2 [$4^4 5^4 8^4$] [100] (8-ring), [001] (8-ring)}



(a)

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

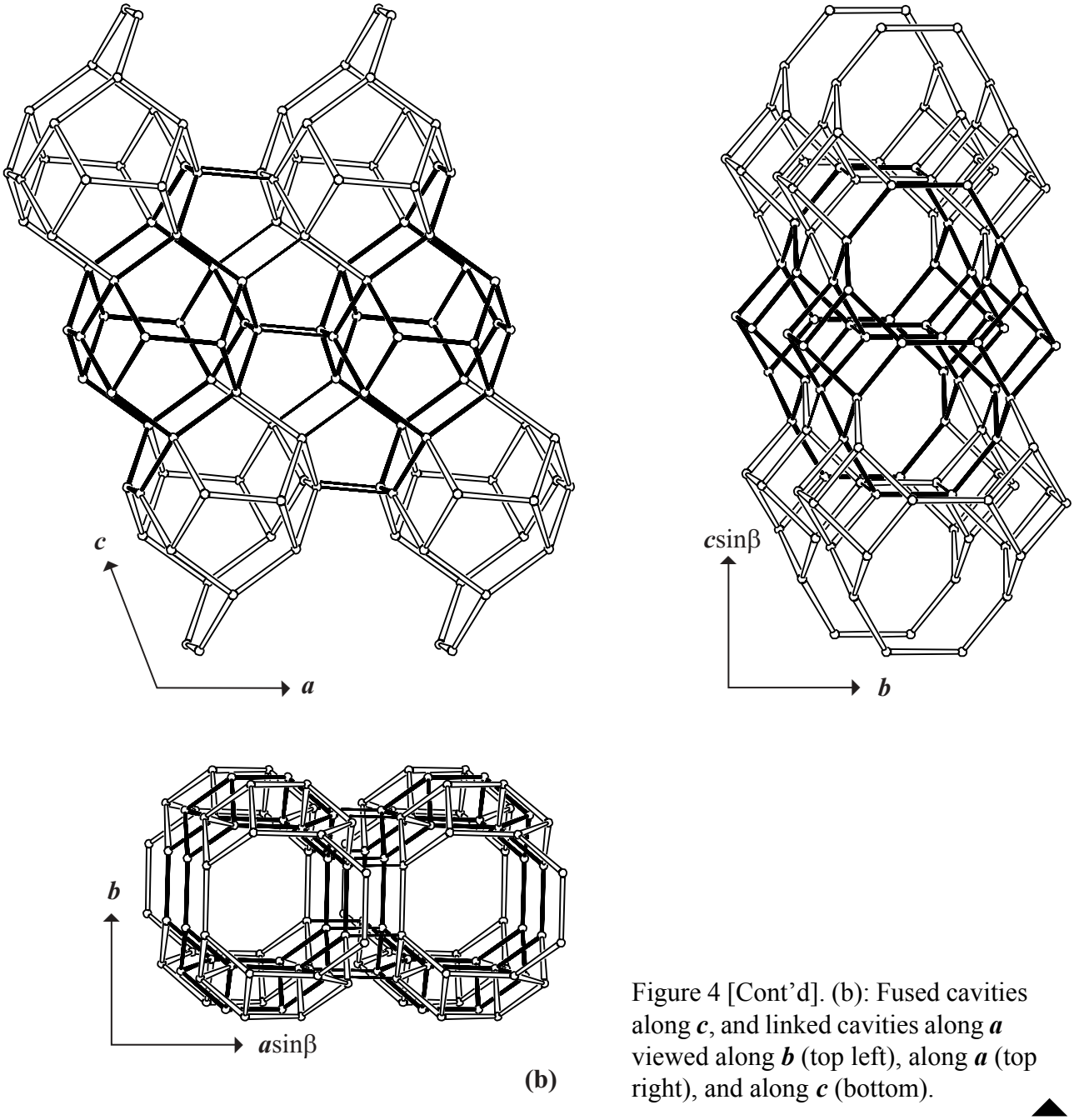


Figure 4 [Cont'd]. (b): Fused cavities along ***c***, and linked cavities along ***a*** viewed along ***b*** (top left), along ***a*** (top right), and along ***c*** (bottom).

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**).