Building scheme for CGF

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) in **CGF** equals the layer shown in Figure 1. The PerBU is composed of T9-units (in bold): a double 4-ring (D4R) and a single T atom (a 4-4-1 unit). The T9-units are related along ***c*** by pure translations, and along ***a*** by a rotation of 180º about ***b***.

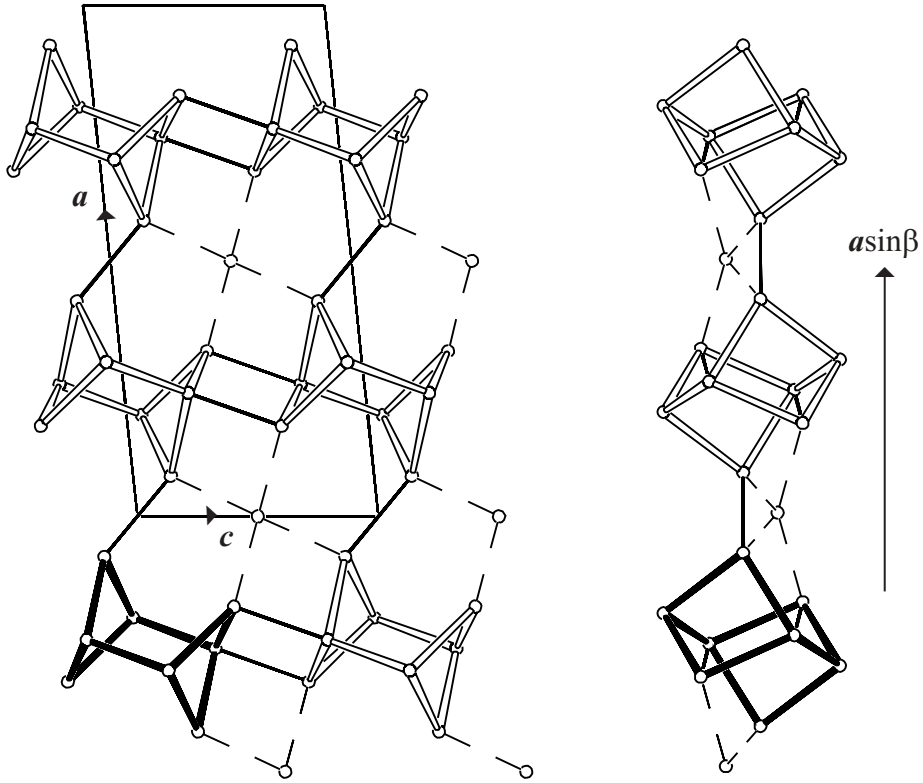

Figure 1. PerBU constructed from D4Rs and single T atoms (left), and parallel projection of the PerBU along ***c*** (right). T-T connections to single T atoms are striped.

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2. Connection mode:

Neighboring PerBUs, related by a shift of ½***a*** (or by a mirror plane perpendicular to ***b***), are connected along ***b*** through single T-T connections as shown in Figure 2 on next page. 8- and 10-Ring channels parallel to ***c*** and 8-ring channels parallel to ***a*** are formed.

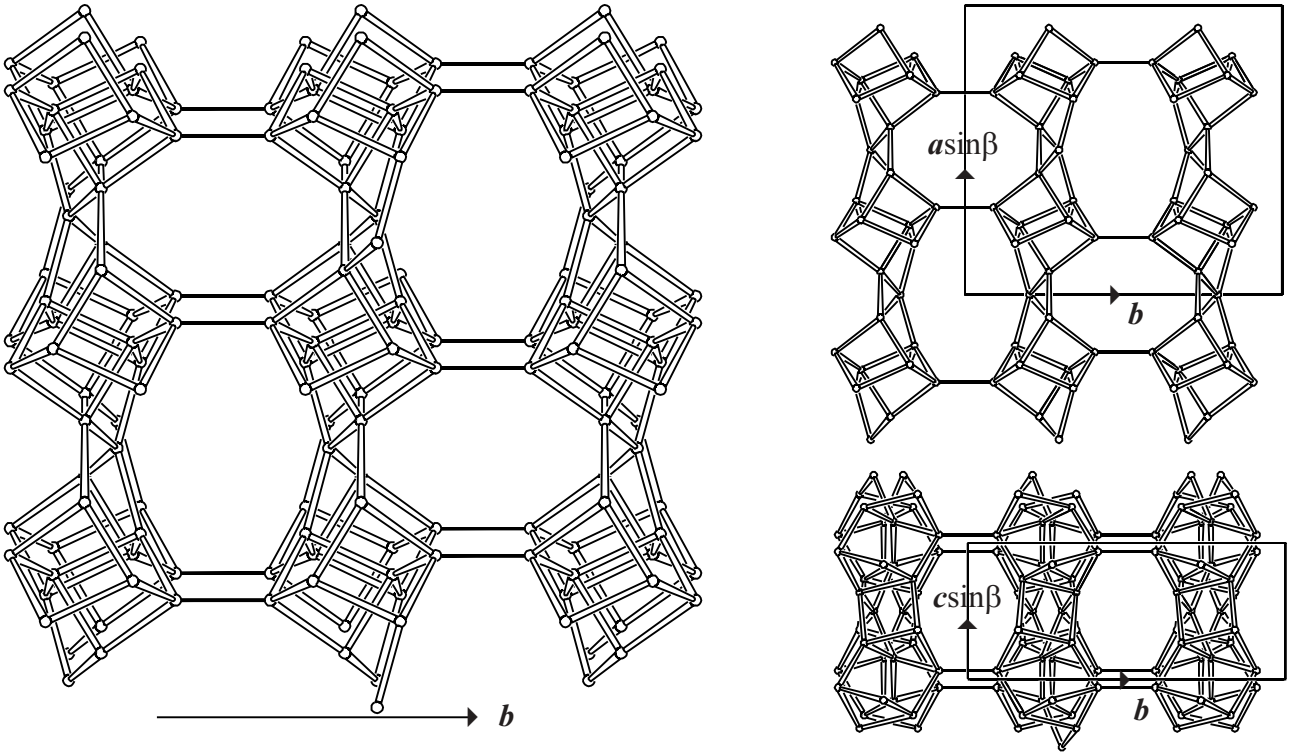

Figure 2. Connection mode in **CGF** viewed along ***c*** (left), and parallel projection of the unit cell content along ***c*** (top right), and along ***a*** (bottom right).

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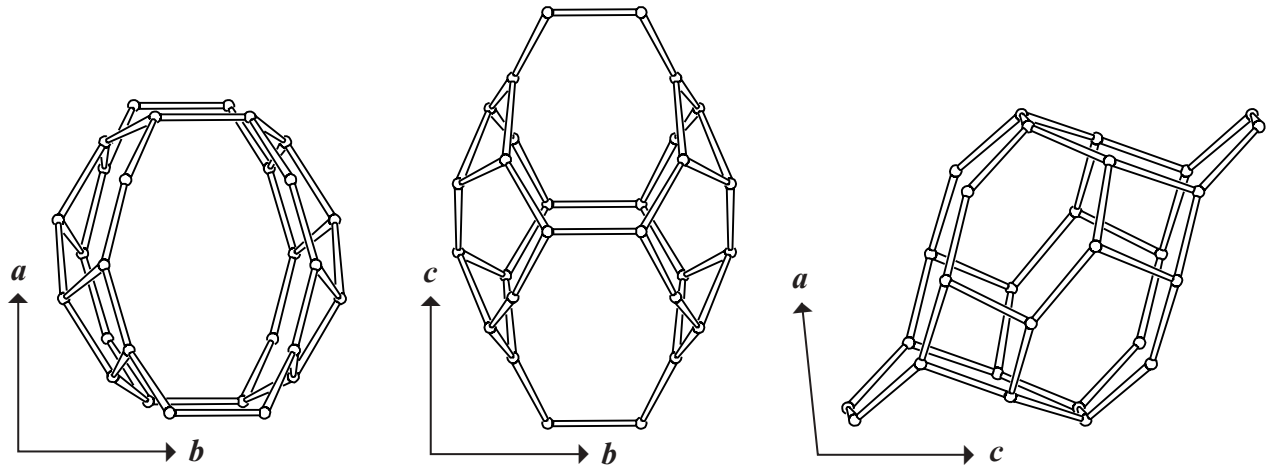
3. Projections of the unit cell content: See Figure 2.

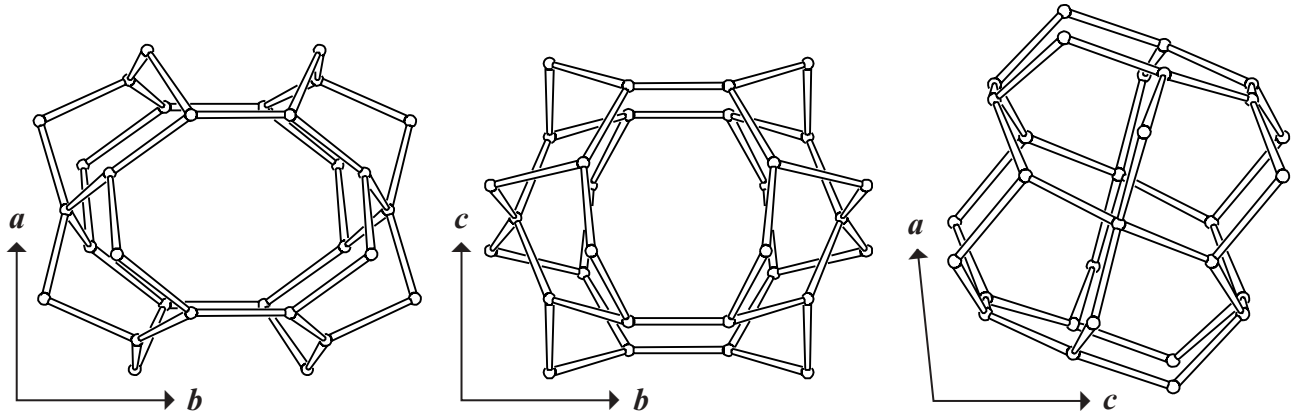
4. Channels and/or cages:

8-Ring channels parallel to ***a*** do intersect with (interconnected) 10- and 8-ring channels parallel to ***c***. The intersections are shown in Figure 3. For each intersection the **pore descriptor** is added in Figure 3. Fusion of intersections in the ***ac*** plane is illustrated in Figure 4.



Cavity 1: {2 [$4^4 6^4 8^2 10^2$] [100] (8-ring), [001] (10-ring)}

Figure 3. First channel intersection, with pore descriptor, viewed along (from left to right) ***c***, ***a*** and ***b***.
[Figure 3 is continued on next page]



Cavity 2: {2 [$6^8 8^4$] [100] (8-ring), [001] (8-ring)}

Figure 3 [Cont'd]. Second channel intersection, with pore descriptor, viewed along (from left to right) ***c***, ***a*** and ***b***.

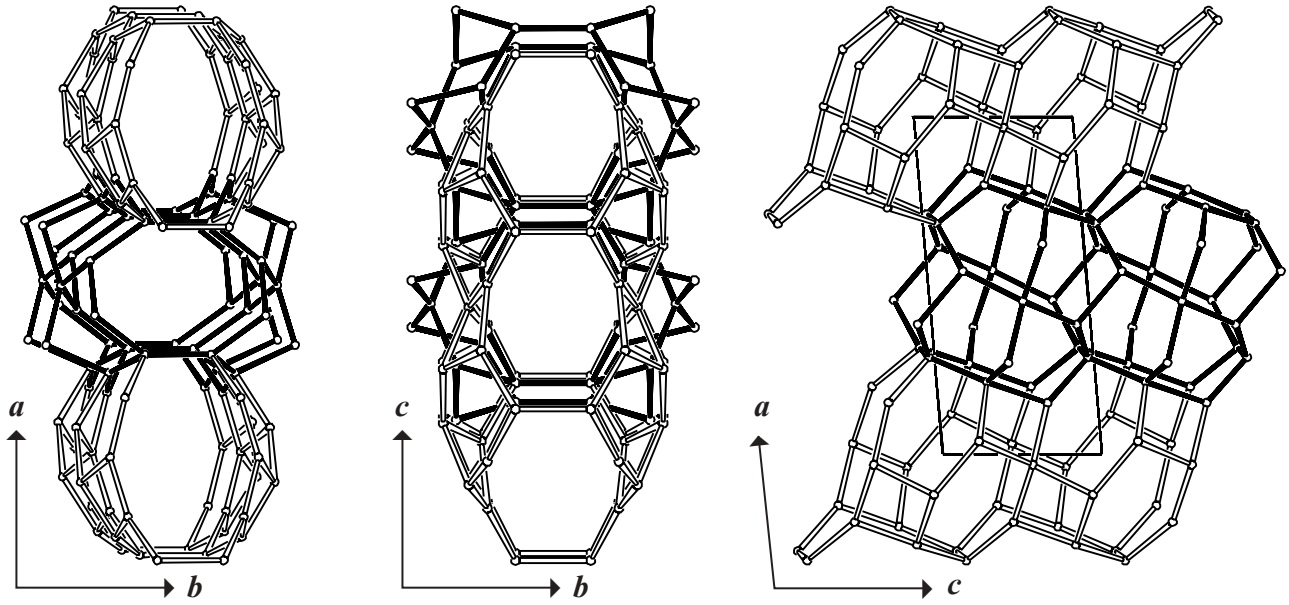


Figure 4. Fused channel intersections viewed along (from left to right) ***c***, ***a*** and ***b*** illustrating the 8- and 10-ring channels formed.

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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**).