

Building scheme for IFR



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1. Periodic Building Unit:

IFR can be built using units composed of 16 T atoms: a 4-fold (1,2,4,5)-connected double 6-ring with "handles" (or two 6-2 units; bold in Figure 1 (left)). The one-dimensional Periodic Building Unit (PerBU) is obtained when T16-units, related along c by pure translations, are connected through 4-rings into a chain along c as shown in Figure 1 (left). Alternatively, the PerBU can be obtained by connecting T16-units consisting of five (fused) 4-rings with four additional bridging T atoms (one unit in bold in Figure 1 (right)). The first type of T16-units is used in the present description.

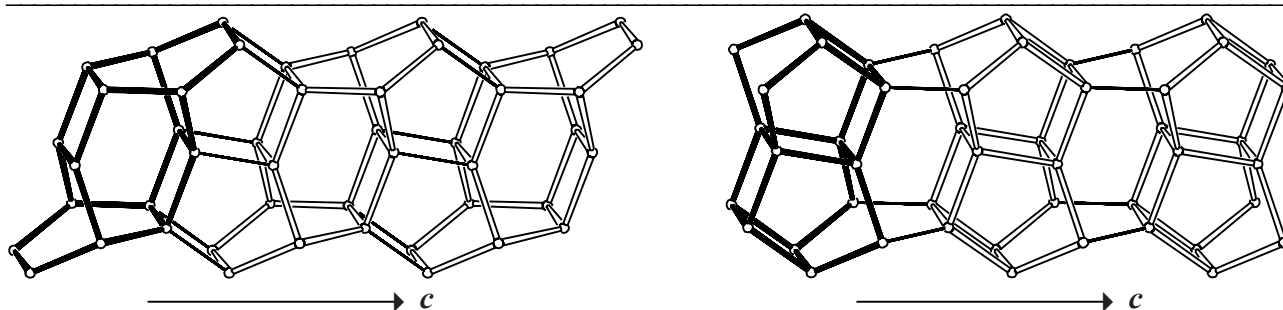


Figure 1. PerBU in **IFR** constructed from D6Rs with "handles" (left) and from (fused) 4-rings and four additional T atoms (right). View normal to the chain axis c .



2. Connection mode:

Neighboring PerBUs, related by a translation of $\frac{1}{2}(a \pm b)$, are connected along $\{110\}$ by 4-rings.

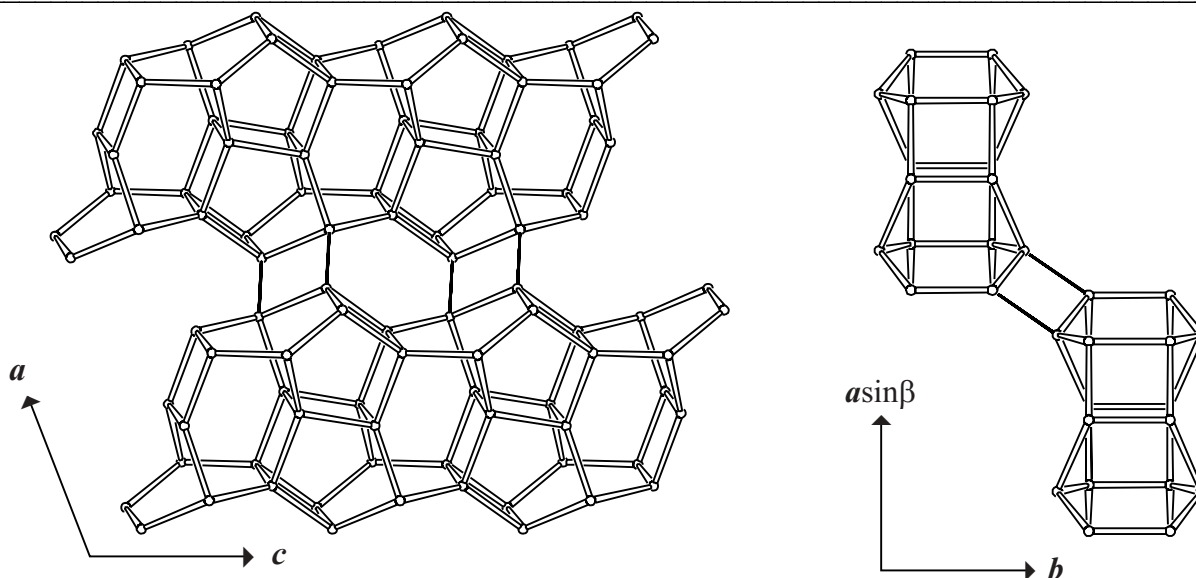


Figure 2. Connection mode viewed along b (left) and along c (right)



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

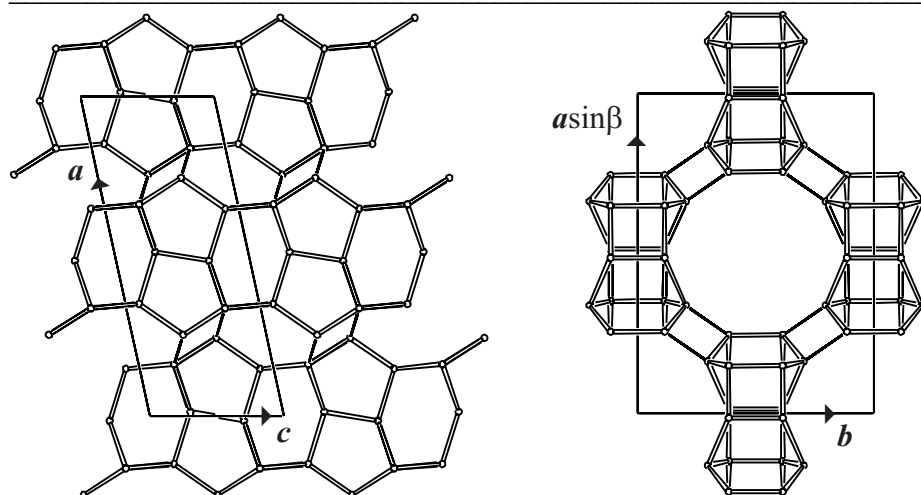


Figure 3. Unit cell content projected along *b* (middle) and along *c* (right).

4. Channels and/or cages:

12-Ring channels are parallel to *c*. The channels can be obtained by connecting cavities through common 12-rings. The cavity is depicted in Figure 4 together with its **pore descriptor**. The fusion of cavities is illustrated in Figure 5. [Compare with Figure 3 and Figure 4 in description of LAU]

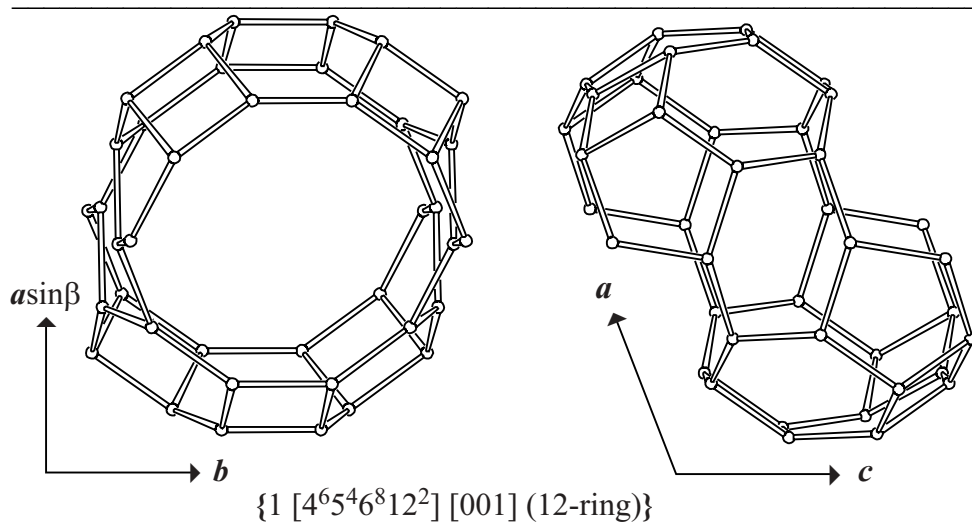


Figure 4. Cavity viewed along *c* (left) and along *b* (right).

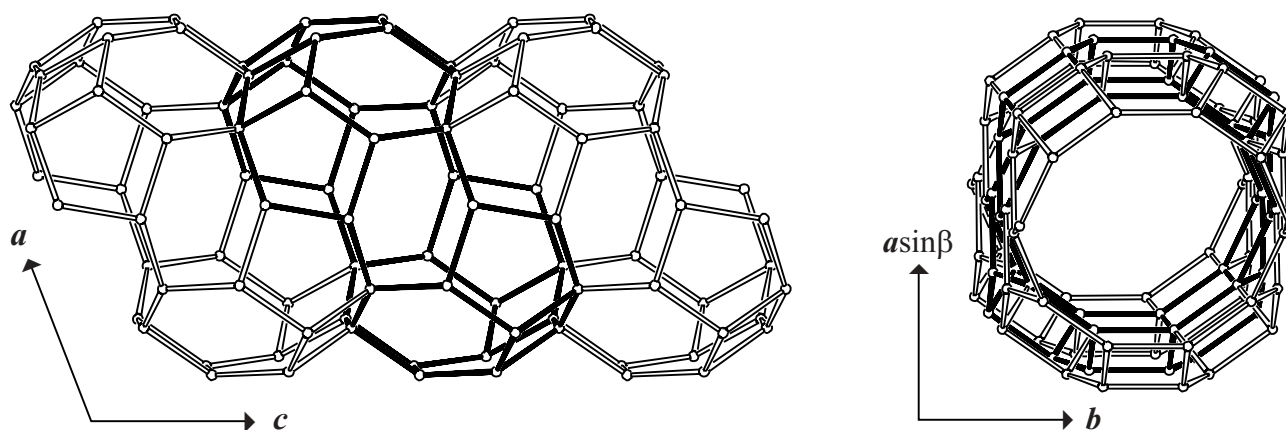


Figure 5. Fusion of cavities along *c* viewed along *b* (left) and along *c* (right). Non-interconnecting 12-Ring channels are parallel to *c*.

5. Supplementary information:

Other framework types containing (modified) double 6-rings (D6Rs)

Several other framework types can be built using (modified) D6Rs.

In the **INTRO** pages links are given to descriptions of other framework types containing (modified) D6Rs (choose: **Double 6-rings**). There is also a link provided to a summary of the Periodic Building Units used in the building schemes of these framework types (choose: **Appendix; Figure 7**).

