

Building scheme for PHI



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1. Periodic Building Unit:

PHI can be built using the 4-ring and the crankshaft chain (bold in Fig.1 (left)) running parallel to a . The repeat distance along a crankshaft chain varies between 8.4-9.9 Å. The repeat unit consists of 4 T atoms. A one-dimensional Periodic Building Unit (PerBU) is obtained when two crankshaft chains and two 4-rings are connected in such a way that a channel with an 8-ring aperture is formed. The channel wall consists of 4-, 8- and 16-rings. The repeat unit of the PerBU consists of a 6-fold (1,2,3,4,5,6)-connected double 8-ring (D8R) (bold in Fig.1 (right)). [The 6-fold connection in the D8R in **PHI** is quite different from the 4-fold connection in the D8R in **APC**, **APD**, **GIS** and **MER**]

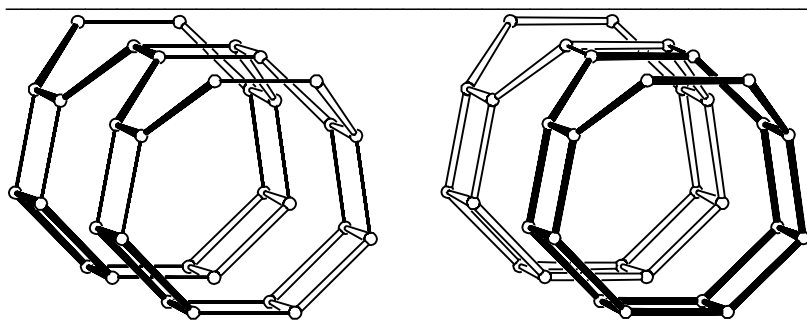


Figure 1. PerBU, viewed along a , constructed from crankshaft chains and 4-rings (or from 4-rings; left), and from 6-fold connected D8Rs (right).



2. Connection mode:

Neighboring PerBUs, related by a rotation of 180° about a accompanied by a shift of $\frac{1}{2}a$, are connected through 4-rings which form double-crankshaft chains as shown in Figure 2.

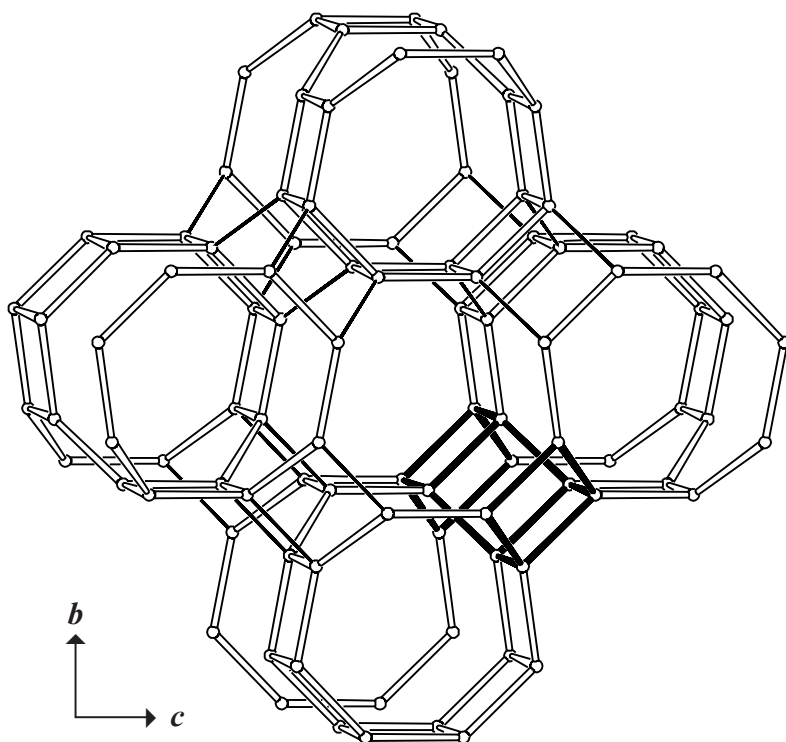
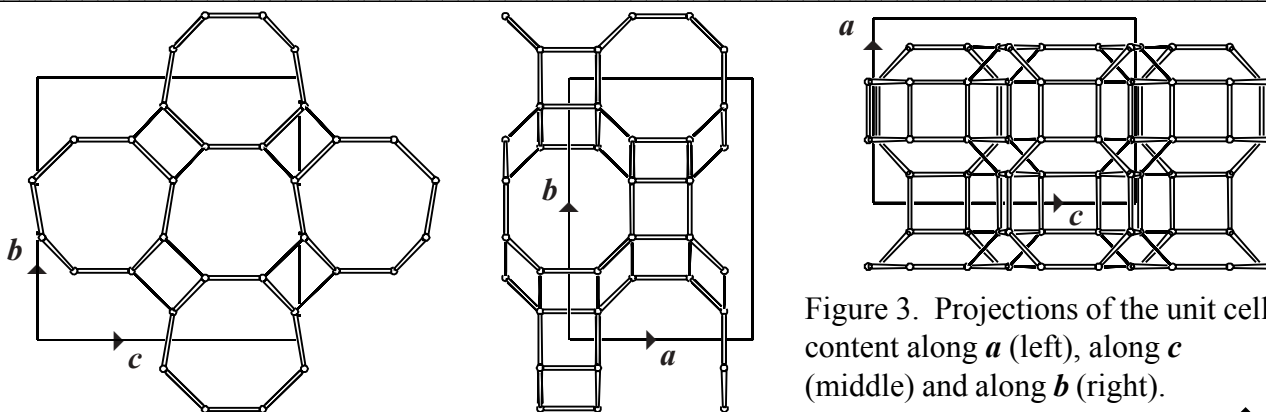


Figure 2. Connection mode in **PHI** viewed along a . For clarity, only $1\frac{1}{2}$ repeat units of the PerBUs along a are drawn. One double crankshaft chain, consisting of 2-fold (1,2)-connected double 4-rings, is indicated in bold (see **Supplementary information**).



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



4. Channels and/or cages:

Interconnecting channels are parallel to $[100]$ and $[001]$. The channel intersection is shown in Figure 4(a). The **pore descriptor** is added. Fusion of intersections is illustrated in Figure 4(b).

$\{2[4^{12}8^6] [100] (8\text{-ring}), [001] (8\text{-ring})\}$

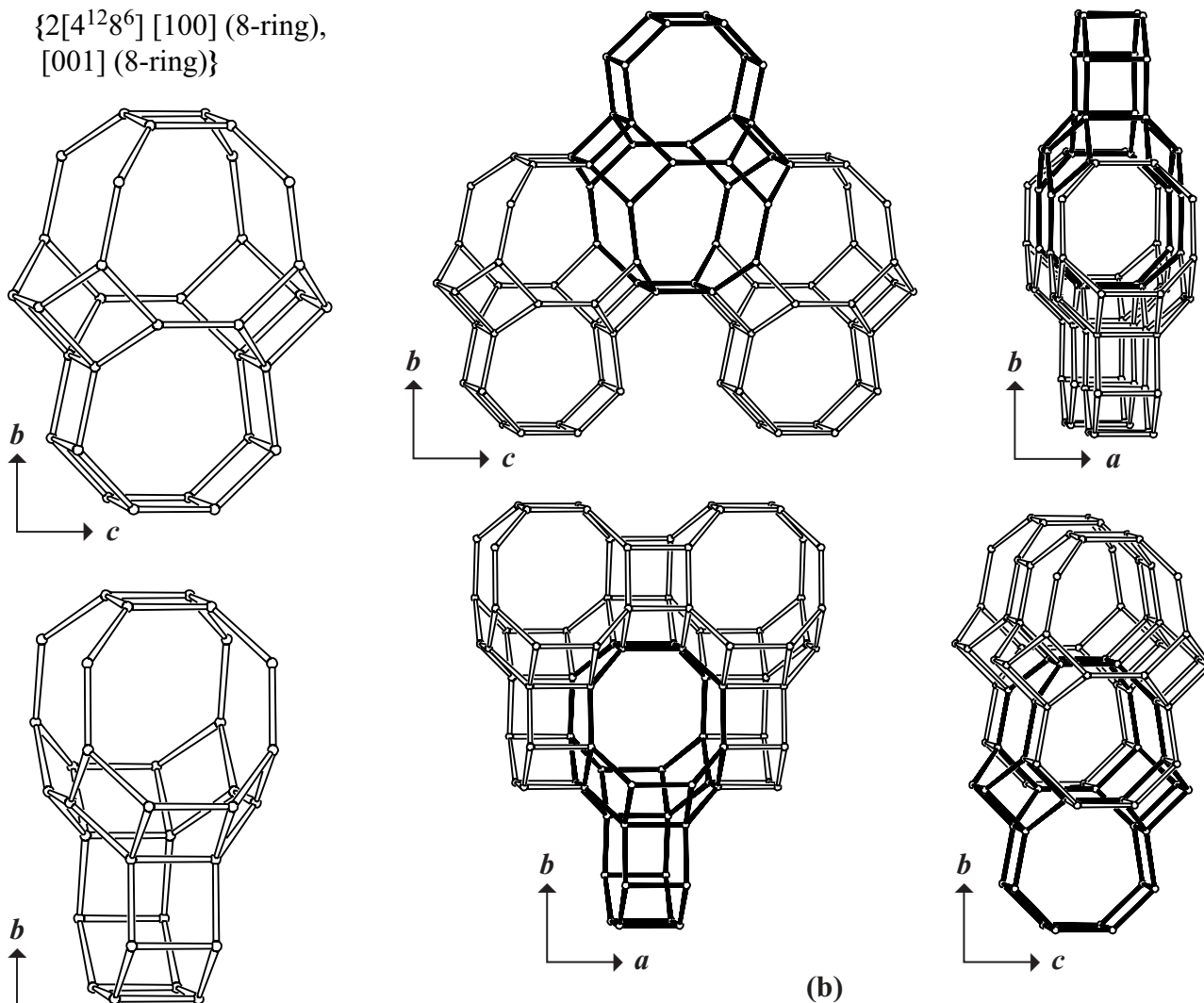


Figure 4. (a): Channel intersection viewed along a (top) and along c (bottom); (b): Fused cavities along c (top) viewed along a (left) and along c (right) and fused cavities along a (bottom) viewed along c (left) and along a (right).

5. Supplementary information:

In several framework types at least one of the unit cell dimensions is between 8.4 and 9.9 Å. In many cases this indicates the presence of crankshaft chains.

In the **INTRO** pages links are given to detailed descriptions of these framework types (choose: **Crankshaft chains**). 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 3**).

Alternative description of PHI using (modified) double 4-rings (D4Rs)

Several framework types, like **PHI**, can be built using double crankshaft chains of the feldspar type consisting of 2-fold (1,2)-connected D4Rs (see Figure 2).

In the **INTRO** pages links are given to descriptions of other framework types containing (modified) D4Rs (choose: **Double 4-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 5**). ▲