

# Building scheme for APD



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## 1. Periodic Building Unit:

**APD** can be built using the crankshaft chain (bold in Figure 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 [or 6-2 units] are connected in such a way that an 8-ring channel is formed. The channel wall consists of 4-, 6- and 8-rings. The repeat unit of the PerBU consists of a 4-fold (1,2,4,6)-connected double 8-ring (D8R) (bold in Fig.1(right)) [or two 6-2 units]. [The 4-fold connection in the D8R is different from the connection in the D8R in **ACO**, **APC**, **GIS** and **MER**]

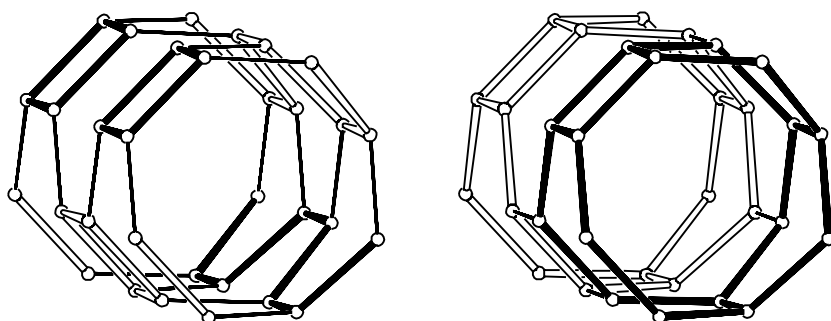


Figure 1. PerBU constructed from crankshaft chains and 4-rings (left) and PerBU constructed from 4-fold connected D8Rs (right). ▲

## 2. Connection mode:

Neighboring PerBUs, related along  $c$  by a pure translation and along  $b$  by a shift of  $\frac{1}{2}(a + b)$ , are connected through 4-rings which form double-crankshaft chains.

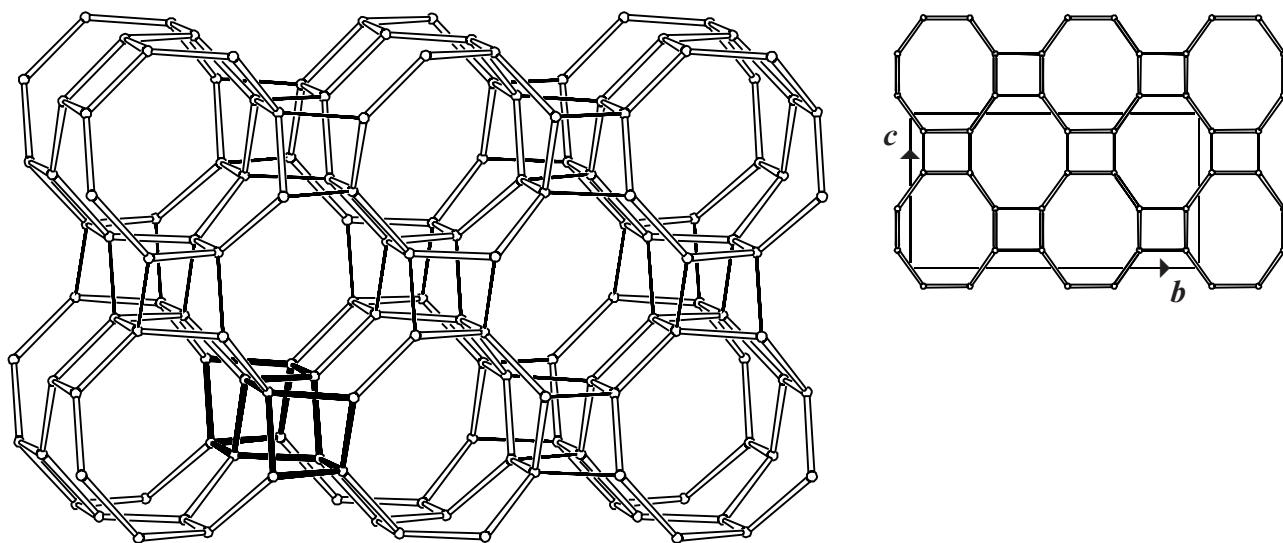


Figure 2. Connection mode and unit cell content in **APD** seen along  $a$  in perspective view (left) and in parallel projection (top right). For clarity, only  $1\frac{1}{2}$  repeat units of the PerBUs along  $a$  are drawn. One double crankshaft chain, consisting of 2-fold (1,3)-connected double 4-rings, is indicated in bold (see **Alternative description**). ▲

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



#### 4. Channels and/or cages:

The channel intersection (or cavity) is depicted in Figure 3 together with the **pore descriptor**. Fused cavities form pairs of interconnecting channels parallel to **a** as depicted in Figure 4.

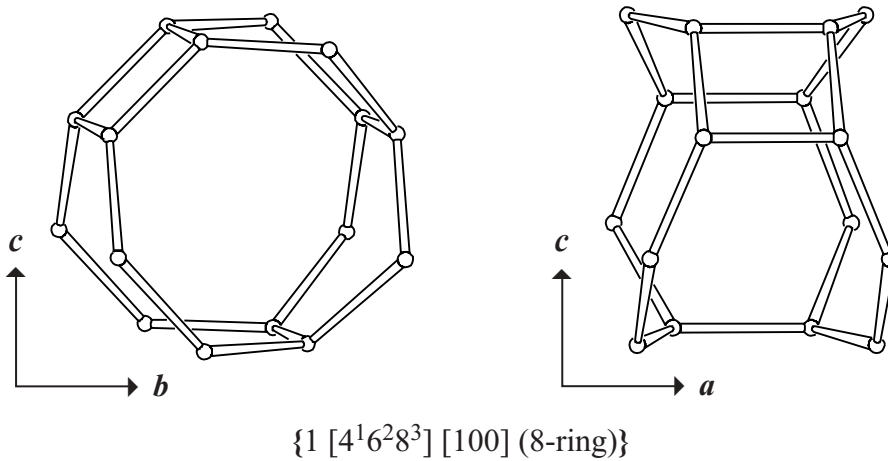
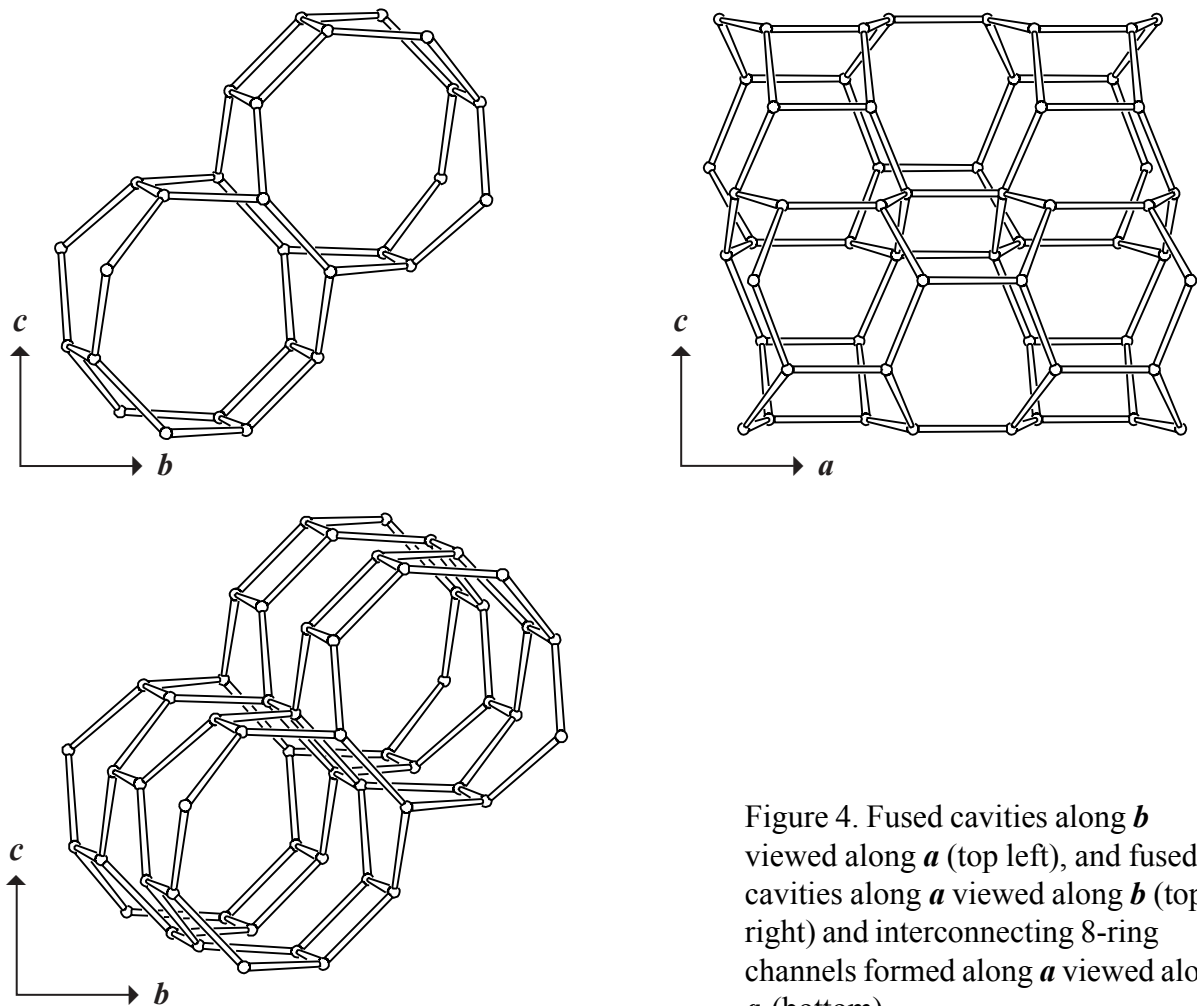


Figure 3. Intersection of channels viewed along **a** (left), and along **b** (right).



## 5. Supplementary information:

### *Other framework types containing crankshaft chains*

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 APD using (modified) double 4-rings (D4Rs)*

Several framework types, like **APD**, can be built using double crankshaft chains of the narsarsukite type consisting of 2-fold (1,3)-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**). ▲