

# Building scheme for DFT



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:

Tetragonal **DFT** can be built using the crankshaft chain (bold in Fig.1 (left)) running parallel to  $c$ . The repeat distance along a crankshaft chain varies between 8.4-9.9 Å. The repeat unit consists of 4 T atoms. Two of these chains are connected into a one-dimensional Periodic Building Unit (PerBU) with a 4-ring pore. The pore wall consists of fused 6-rings. The repeat unit of the PerBU is a 2-fold (1,3)-connected double 4-ring (bold in Fig.1 (right)).

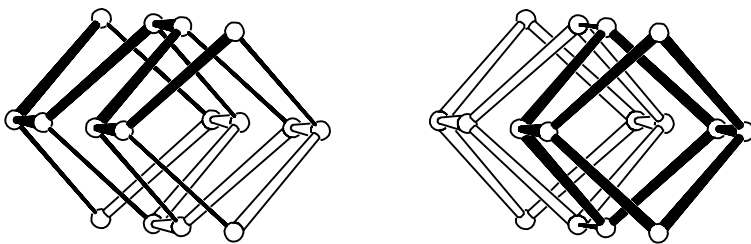


Figure 1. PerBU (seen along  $c$ ) constructed from two crankshaft chains (left) and PerBU constructed from 2-fold (1,3)-connected double 4-rings (right; see [Alternative description](#))

## 2. Connection mode:

Neighboring PerBUs, related by a pure translation along  $a$  and  $b$ , are connected through 4-rings. 8-Rings perpendicular to  $[100]$ ,  $[010]$  and  $[001]$  are formed.

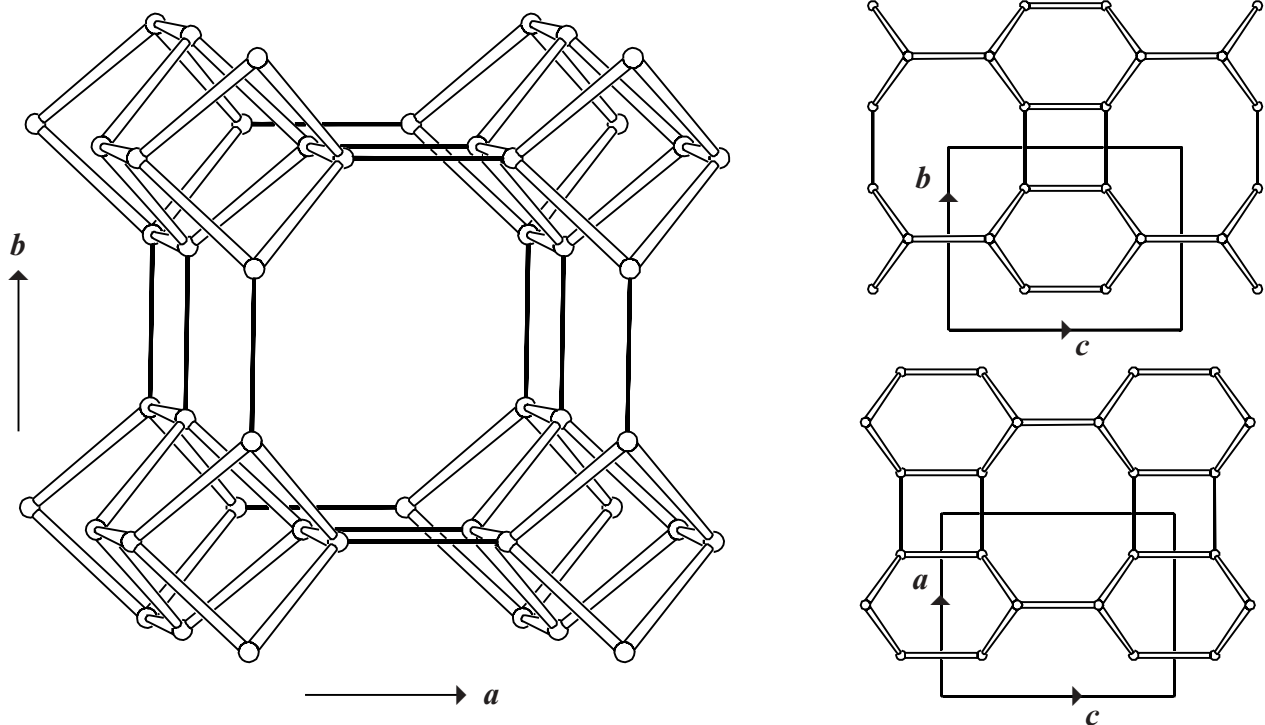


Figure 2. Connection mode viewed along  $c$  (left) and parallel projection of the unit cell content along  $a$  (top right), and along  $b$  (bottom right). In the perspective drawing, only  $1\frac{1}{2}$  repeat units of the PerBUs along  $c$  are shown for clarity.

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

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

One-dimensional, interconnecting 8-ring channels are parallel to  $c$  and  $a$  (and  $b$ ). The channel intersection is depicted in Figure 3. The **pore descriptor** is added. The connection of channel intersections is illustrated in Figure 4.

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$\{2 [4^28^4] \langle 100 \rangle (8\text{-ring}), [001] (8\text{-ring})\}$

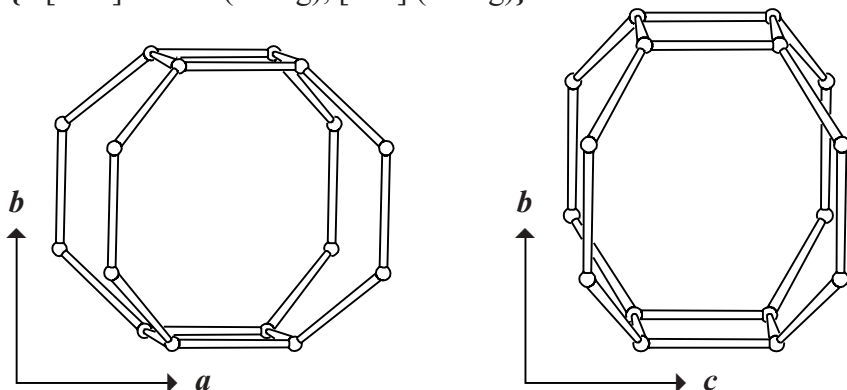


Figure 3. Intersection of channels viewed along  $c$  (left), and along  $a$  (or  $b$ ) (right).

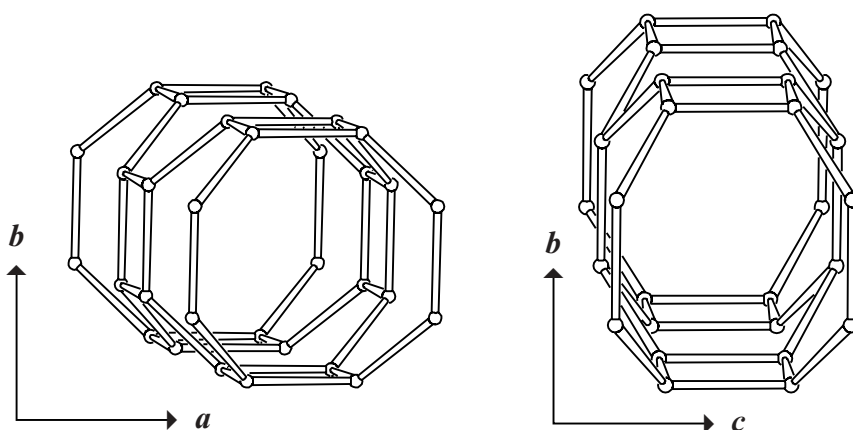


Figure 4. Connection of intersections viewed along  $c$  (left), and along  $a$  (or  $b$ ) (right). ▲

#### 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 DFT using (modified) double 4-rings (D4Rs)***

Several framework types, like **DFT**, can be built using double crankshaft chains of the narsarsukite type consisting of 2-fold (1,3)-connected D4Rs (see Figure 1).

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**). ▲