



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:

DFO can be built using a building unit of 22T atoms (bold in Figure 1(a)) that consists of two sets of 2-fold (1,3)-connected double 4-rings with “handles” (or of two 4-1 and two 1-4-1 units). The T22-unit very much resembles the building unit in **LAU**. T22-units, related by pure translations along c , are connected through 4-rings into chains along c . Chains are connected along a 6-fold axis parallel to c into the tubular Periodic Building Unit (PerBU) shown in Figure 1(b and c).

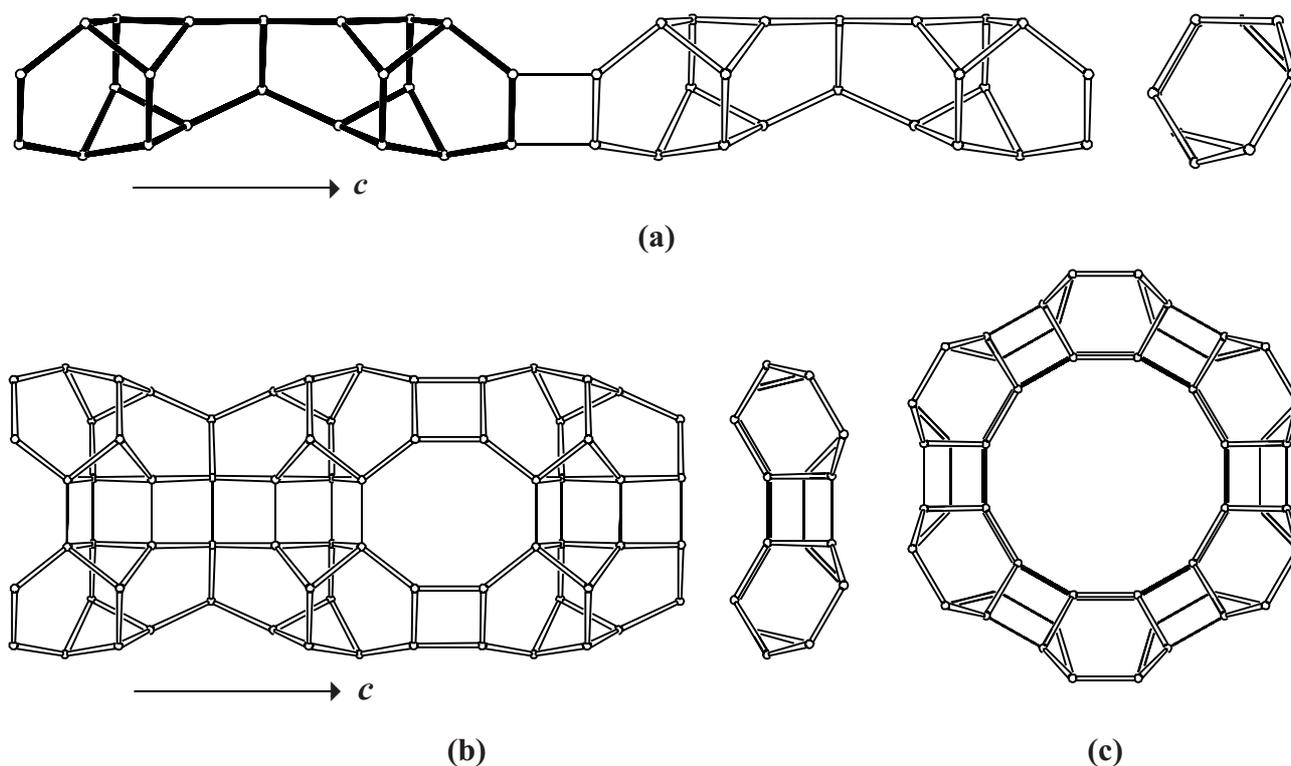


Figure 1.

- (a): Chain, constructed from T22-units, viewed perpendicular to c (left) and along c (right);
 (b): Connection mode of two chains in the PerBU viewed perpendicular to the 6-fold axis. 8-Rings are formed. The chain length along c has been limited to $1\frac{1}{2}$ of the repeat unit for clarity reasons;
 (c): Parallel projection of the PerBU along the 6-fold axis.



2. Connection mode:

Neighboring PerBUs, related by pure translations along a and b , are connected along a and b (and $(a + b)$) through single- and double 4-rings (and 6-rings) as shown in Figure 2. In the perspective drawing only one chain of each PerBU is shown for clarity reasons. 10-Rings are formed.

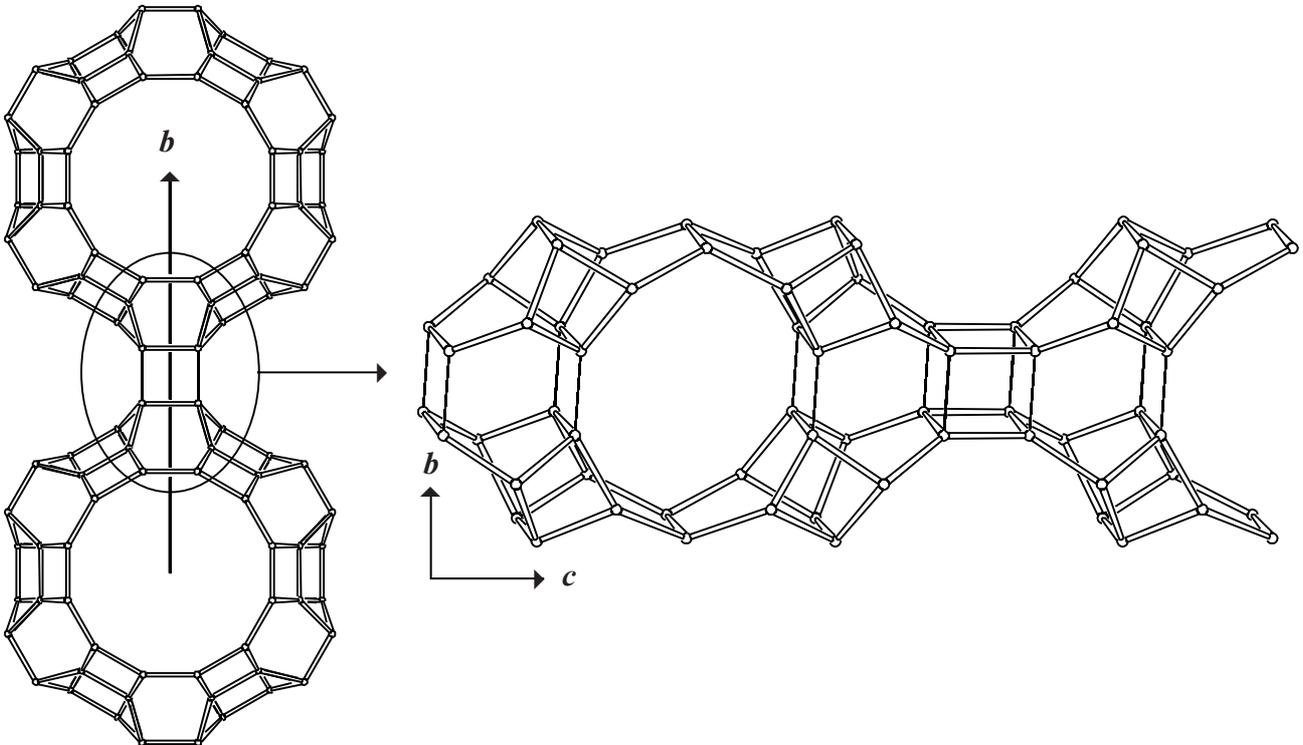


Figure 2. Connection mode between PerBUs in **DFO** viewed along c (left) and perspective view of the connection mode nearly along $[210]$ (right) (or, equivalently, along $[120]$ or $[-110]$). ▲

3. Projections of the unit cell content:

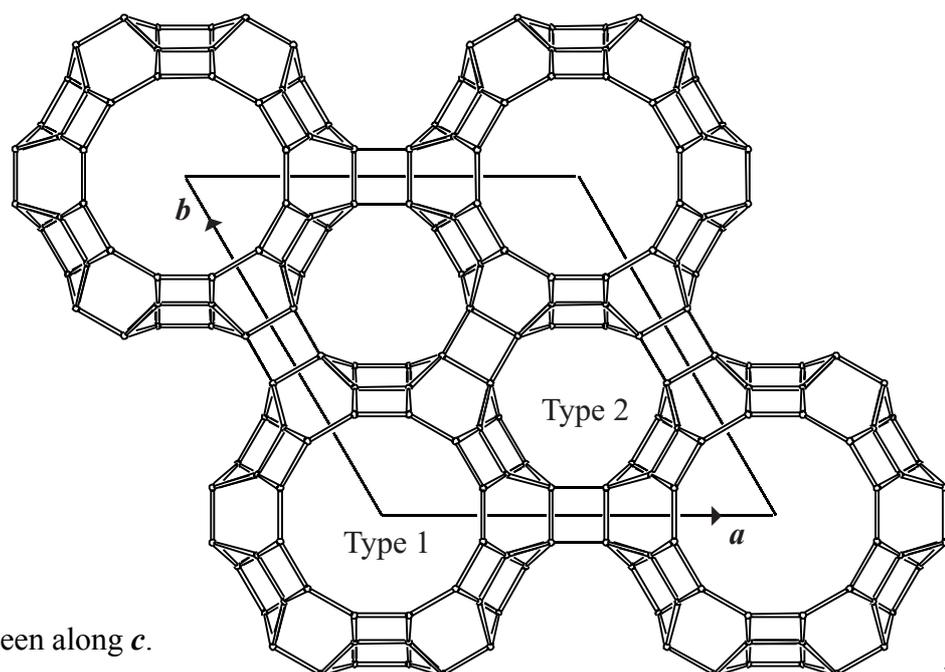
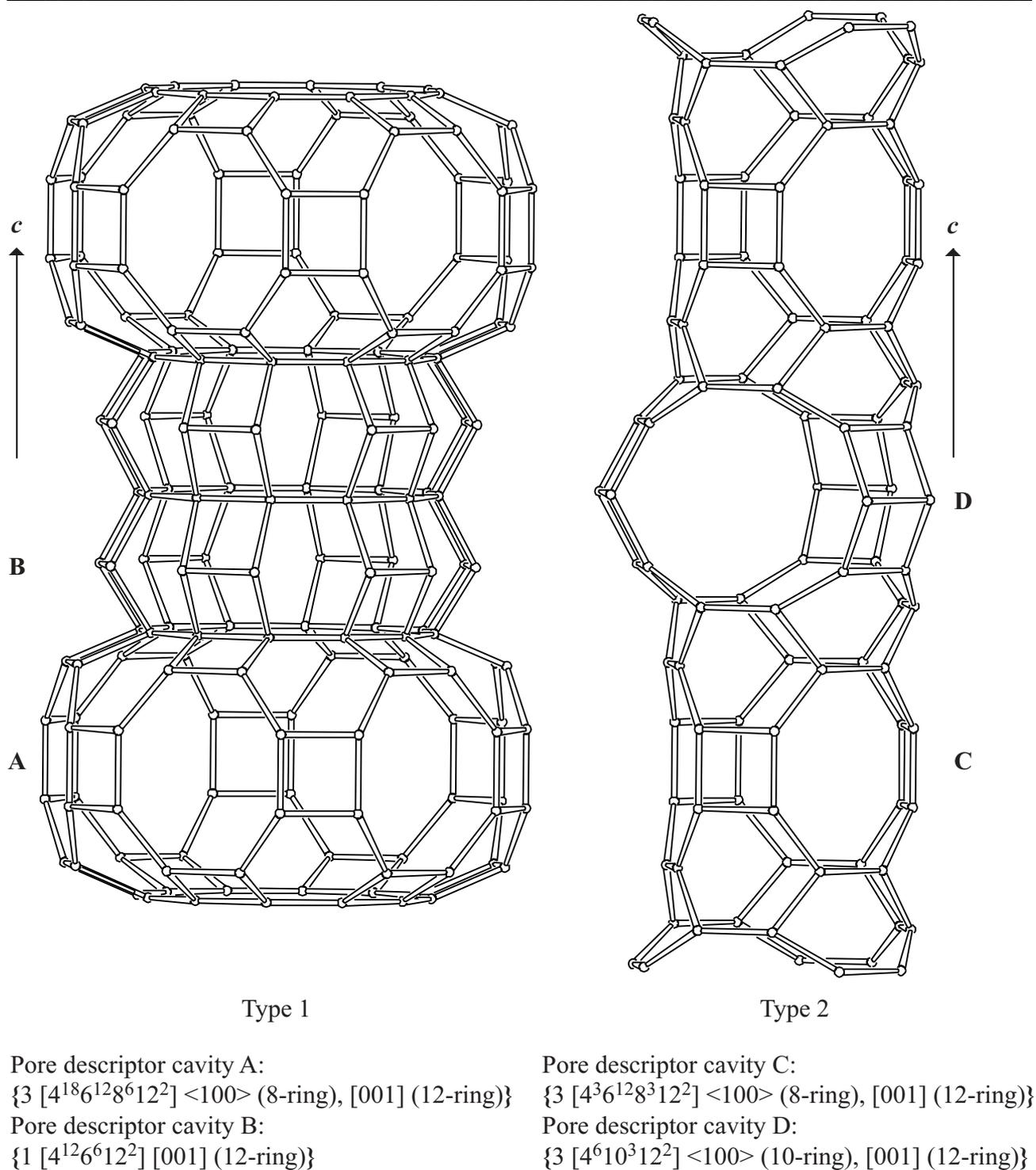


Figure 3. Cell content seen along c . ▲

4. Channels and/or cages:

There are two types of 12-ring channels parallel to c (see Figure 3). They are interconnected through common 8-rings. The 12-ring channels of type 2 are interconnected through 10-rings. Cavities in both 12-ring channels are shown in Figure 4 together with the **pore descriptors**.



(a)

Figure 4. (a): Cavities, with their pore descriptors, in the 12-ring channels parallel to c of type 1 (left) and type 2 (right) viewed along $\langle 010 \rangle$ (i.e. along $[010]$ or $[100]$ or $[110]$). There are 8- and 10-ring channels parallel to $\langle 010 \rangle$. [Figure 4 is continued on next page]

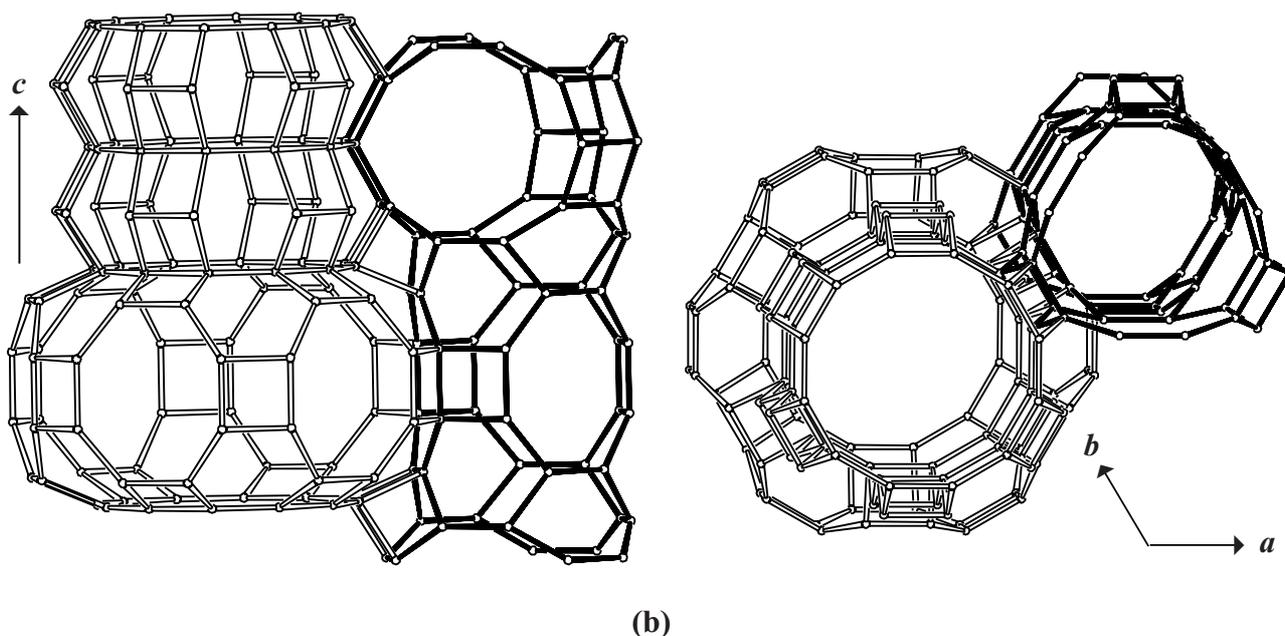


Figure 4 [Cont'd]. (b): Fused 12-ring channels viewed along $\langle 010 \rangle$ (left) and along c (right). 12-Ring channels of type 1 are interconnected to 12-ring channels of type 2 through common 8-rings (and 4-rings). The 12-ring channels of type 2 are interconnected through 10-rings.



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**).

