

# Building scheme for MER



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 **MER** 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. A one-dimensional Periodic Building Unit (PerBU) is obtained when four crankshaft chains are connected in such a way that a channel with an 8-ring aperture is formed. The channel wall consists of 4- and 8-rings. The repeat unit of the PerBU consists of a 4-fold (1,2,5,6)-connected double 8-ring (D8R) (bold in Fig.1 (right)). The PerBU is topologically equivalent to the channel in **ACO**. [The 4-fold connection in the D8R in **APC**, **APD** and **GIS** is different]

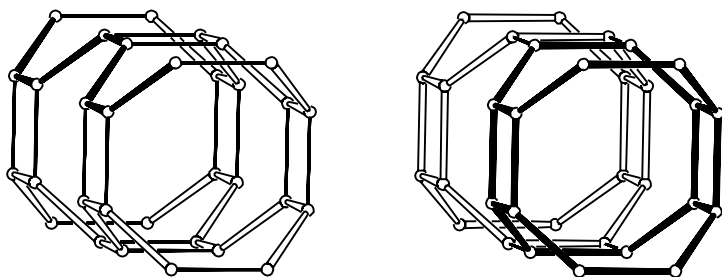


Figure 1. PerBU constructed from four crankshaft chains (left) and PerBU constructed from 4-fold connected D8Rs (right).



## 2. Connection mode:

Neighboring PerBUs, related by a shift of  $\frac{1}{2}(\pm a \pm b \pm c)$ , are connected through double crankshaft chains that form *mer* cavities [see **Alternative description**].

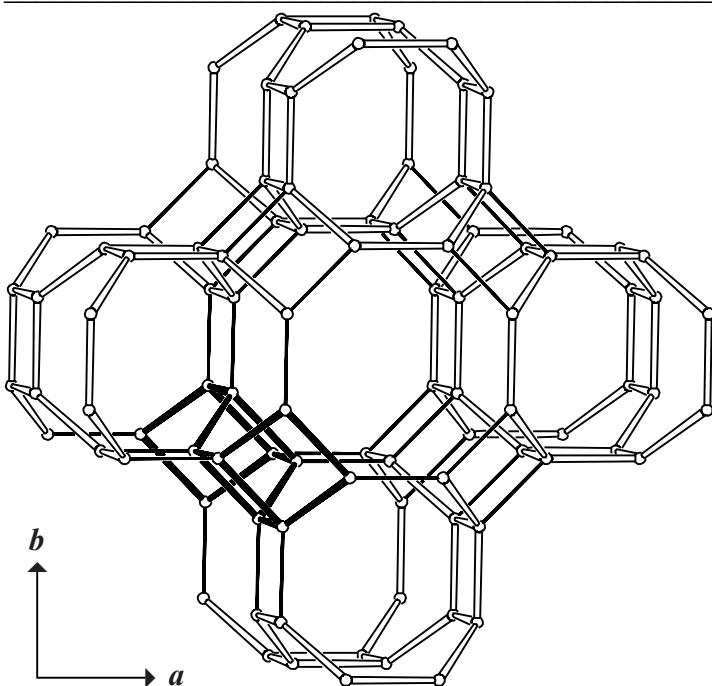


Figure 2. Connection mode viewed along  $c$ . For clarity, only  $1\frac{1}{2}$  repeat units of the PerBUs along  $c$  are drawn. One double crankshaft chain, consisting of 2-fold (1,2)-connected D4Rs, is indicated in bold (see **Alternative description**).



### 3. Projections of the unit cell content:

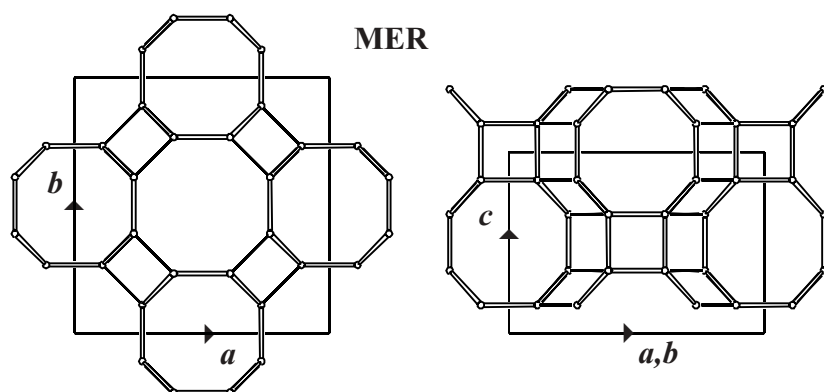


Figure 3. Projection of the unit cell content in **MER** viewed along *c* (left) and along *b* (or *a*; right). ▲

### 4. Channels and/or cages:

There are two types of channel intersections in tetragonal **MER**: the cavity equal to the repeat unit of the PerBU (see Fig.1 (right)) and the *mer* cavity. There are also two types of 8-ring channels parallel to *c*. The first type equals the PerBU and is topologically equivalent to the channel in **ACO**. The PerBU and the *mer* cavity are shown in Figure 4 together with their **pore descriptor**. The second type of 8-ring channels parallel to *c* is obtained when *mer* cavities are connected through double 8-rings. The linkage of channel and cavities is illustrated in Figure 5. Interconnecting 8-ring channels are parallel to [100], [010] and [001].

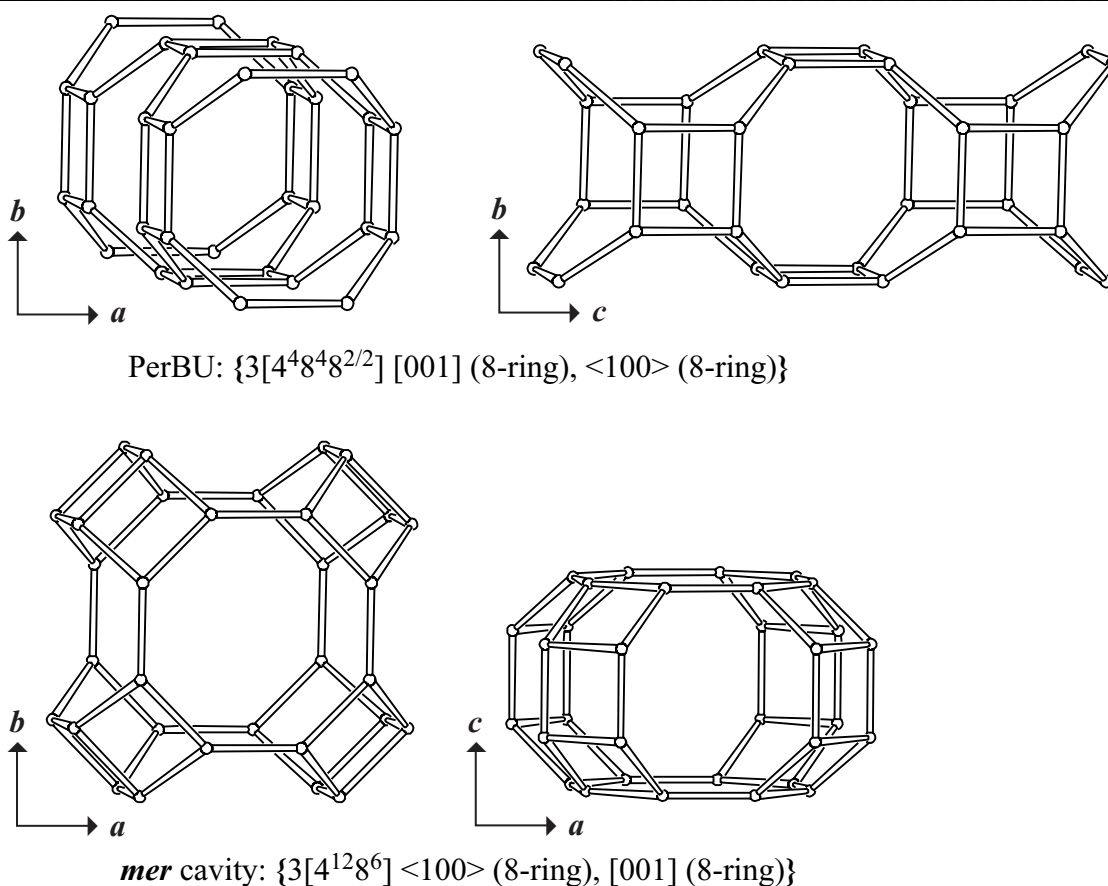


Figure 4. PerBU in **MER** (top) and *mer* cavity (bottom) viewed along *c* (left) and along *a* (or *b*) (right). [Figure 5 is on next page]

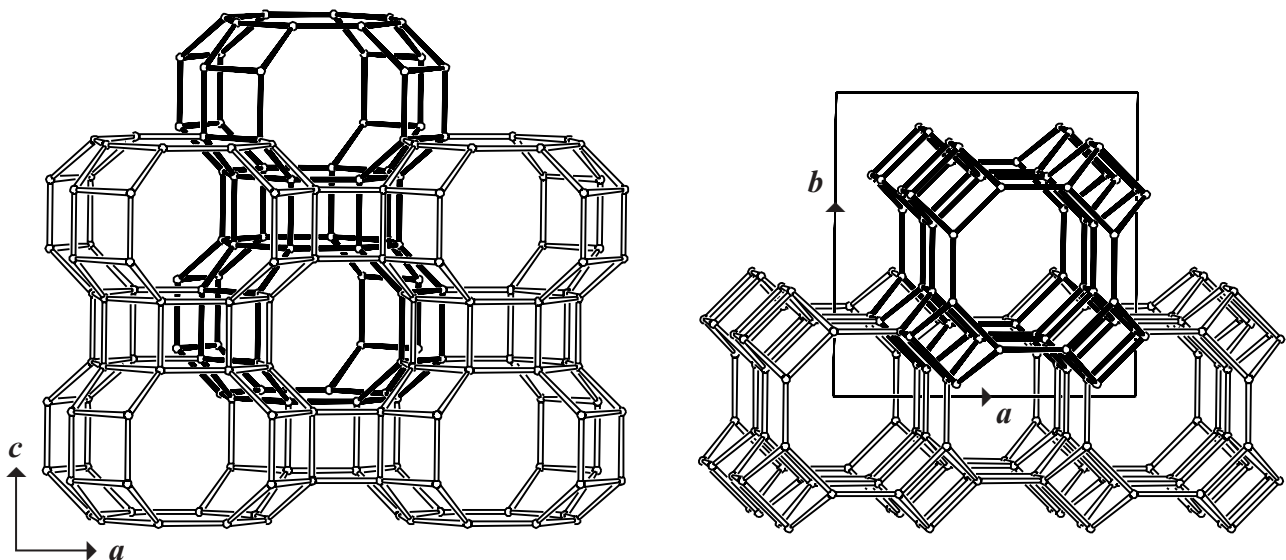


Figure 5. Linkage of channel and *mer* cavities (one in black for clarity) through (double) 8-rings viewed along *b* (or *a*) (left) and along *c* (right) illustrating the 8-ring channels along  $\langle 010 \rangle$  and the second type of 8-ring channels parallel to *c*. The Figure also illustrates that **MER** can as well be constructed using double 8-rings (See also Figure 2). ▲

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

Several framework types, like **MER**, 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**).

### *Alternative description of MER using (modified) cavities*

Several framework types, like **MER**, can be built using (modified) cavities (see Figure 5).

In the **INTRO**-pages links are given to a detailed description of a sub-set of framework types that contain (modified) cavities (choose: **Cages**). There is also a link provided to a summary of the PerBUs used in the building schemes of these framework types (choose: **Appendix; Figure 11**). ▲