

# Building scheme for MEL and MFI



- 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:

**MEL** and **MFI** can be built using units of 12 T atoms (one in bold in Figure 1). T12-units consist of two 5-1 units (bold Figure 1(left)). T12-units, related by a rotation of  $180^\circ$  about  $c$ , form left- and right-handed chains along  $c$ . Chains, related by a mirror plane perpendicular to  $b$ , are connected into the Periodic Building Unit (PerBU). The PerBU equals the  $bc$  pentasil layer shown in Figure 1.

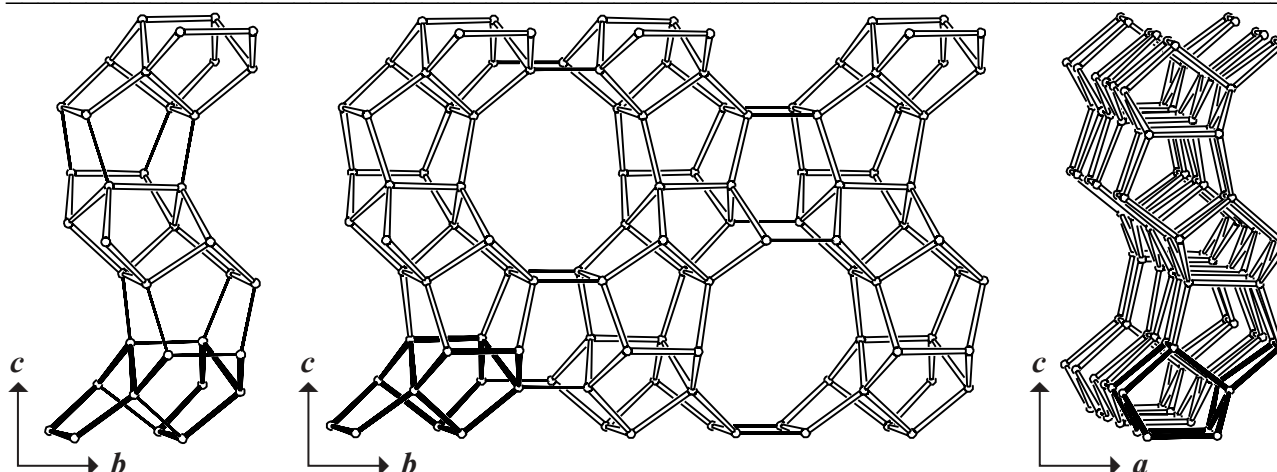


Figure 1. Polar chain (left) viewed along  $a$ , and PerBU viewed along  $a$  (middle) and along  $b$  (right). 

## 2. Connection mode:

Neighboring PerBUs are connected along  $a$  in two different ways as depicted in Figure 2:

- (1): neighboring layers are related by a rotation of  $180^\circ$  about  $a$  and a shift of  $1/2b$ .
- (2): neighboring layers are related by a rotation of  $180^\circ$  about  $c$  and a shift of  $1/2b$ .

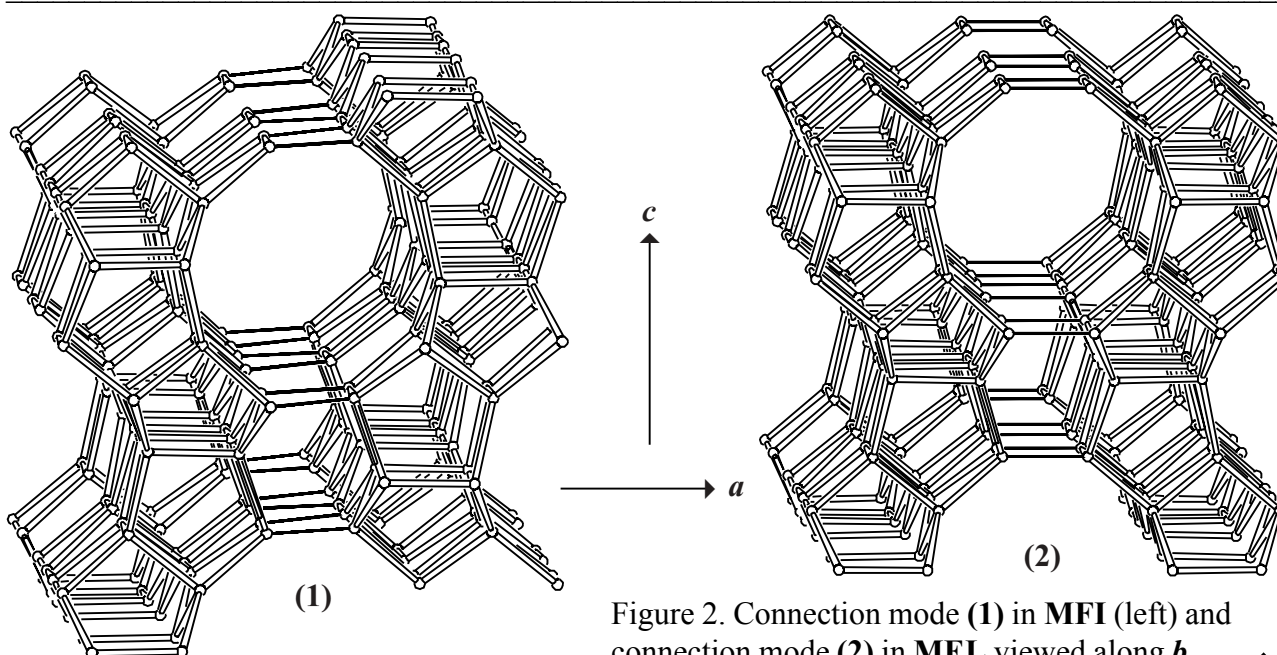



Figure 2. Connection mode (1) in **MFI** (left) and connection mode (2) in **MEL** viewed along  $b$ . 

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

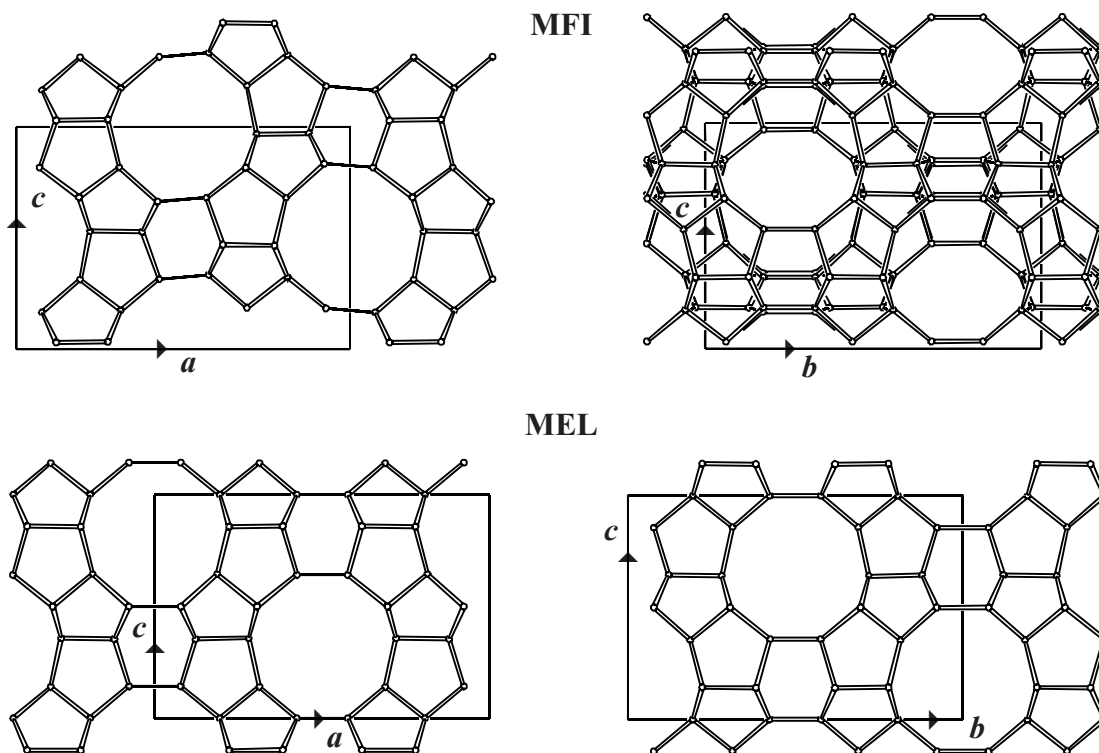


Figure 3. Unit cell content in **MFI** (top) and in **MEL** (bottom) projected along **b** (left) and along **a** (right). [Both projections in **MEL** are equal] ▲

4. Channels and/or cages:

The cavities that describe the intersections of 10-ring channels in both framework types are depicted in Figure 4. The **pore descriptors** are added. The connection of the cavities is illustrated in Figure 5.

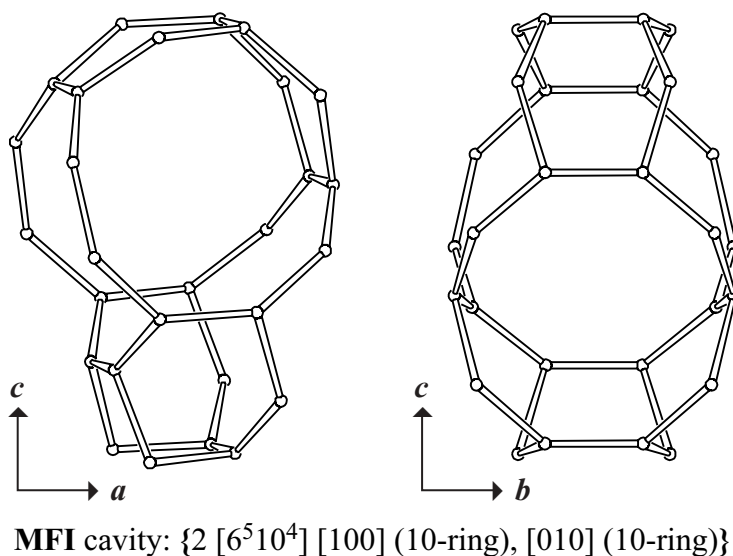
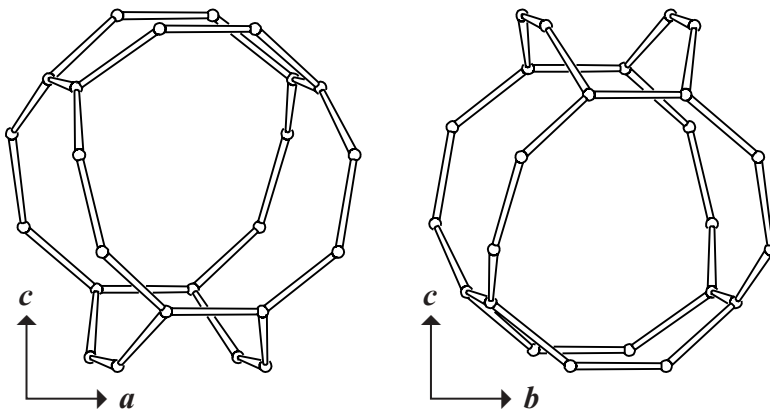
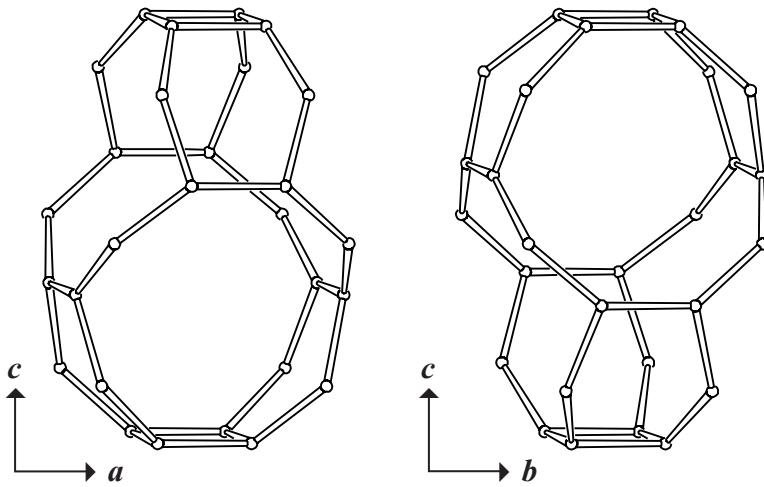


Figure 4. Cavity in **MFI** viewed along **b** (left) and along **a** (right). [Fig. 4 is continued on next page]



MEL cavity 1:  $\{2 [8^2 10^4] \langle 100 \rangle (10\text{-ring})\}$



MEL cavity 2:  $\{2 [4^2 6^4 10^4] \langle 100 \rangle (10\text{-ring})\}$

Figure 4 [Cont'd]. The two different channel intersections in MEL viewed along *b* (left) and along *a* (right).

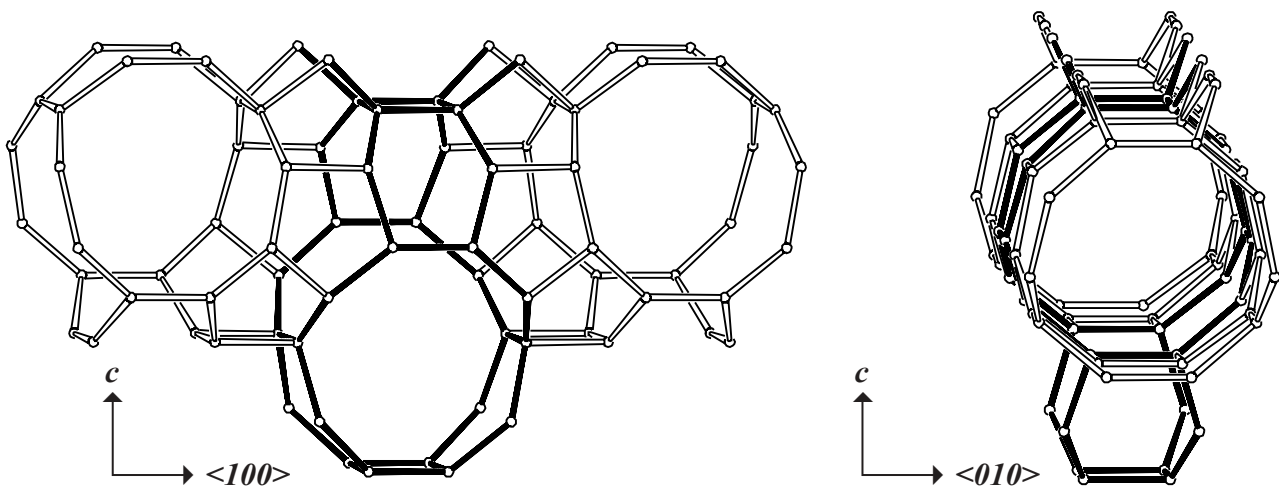


Figure 5. Linkage of the two types of cavities in tetragonal MEL into straight 10-ring channels parallel to *a* (or *b*) viewed along *b* (or *a*; left) and along the straight 10-ring channel axis parallel to *a* (or *b*; right). [Figure 5 is continued on next page]

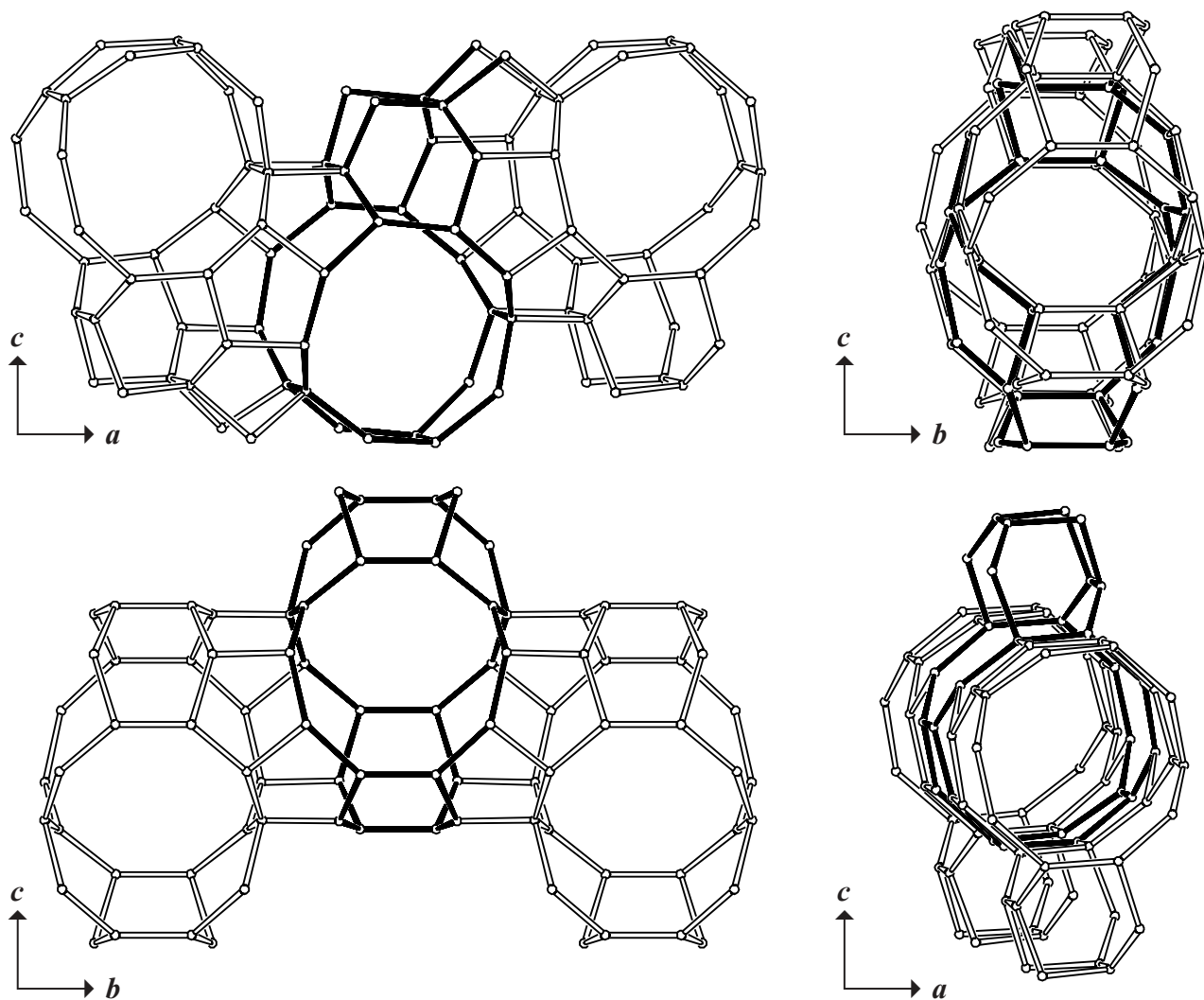


Figure 5 [Cont'd]. Linkage of one type of cavities in orthorhombic **MFI** into sinusoidal 10-ring channels parallel to **a** (top) viewed along **b** (left) and along the sinusoidal channel axis parallel to **a** (right); linkage of the cavities into straight channels parallel to **b** (bottom) viewed along **a** (left) and along the straight 10-ring channel axis parallel to **b** (right). ▲

## 5. Supplementary information:

### *Other framework types containing (modified) 5-rings*

5-Rings can be connected in several other ways. In all cases 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) 5-rings (choose: **5-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 6**). ▲