Building scheme for LTL, MOZ and OFF

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:

LTL, **MOZ** and **OFF** can be built using the saw chain (bold in Fig.1) running parallel to ***c***. The repeat distance along the saw chain is about 7.5 Å. The repeat unit in the chain consists of 3 T atoms. Six saw chains are connected into an one-dimensional Periodic Building Unit (PerBU) consisting of a column of cancrinite (***can***) cages that are connected through double 6-rings.

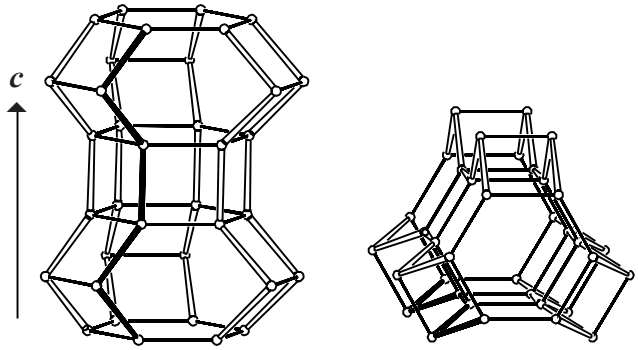
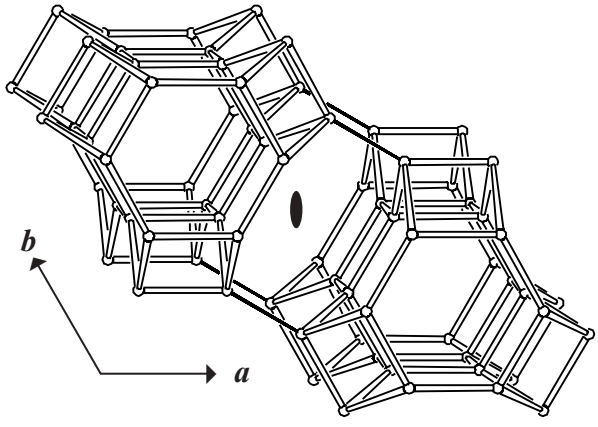


Figure 1. PerBU, composed of six saw chains that form a column of ***can*** cages, viewed perpendicular to ***c*** (left) and along ***c*** (right). Each ***can*** cage consists of three 6-rings or three 4-2 units.

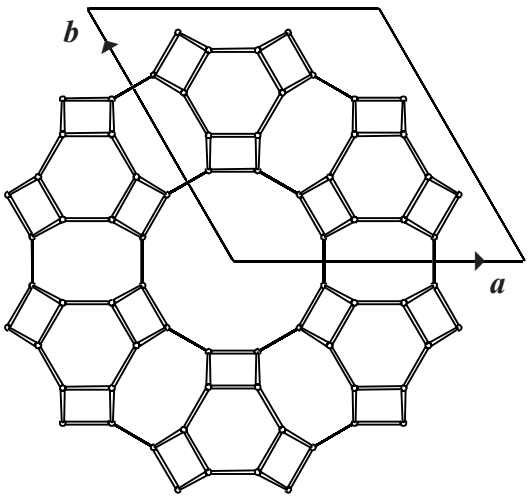
2. Connection mode:

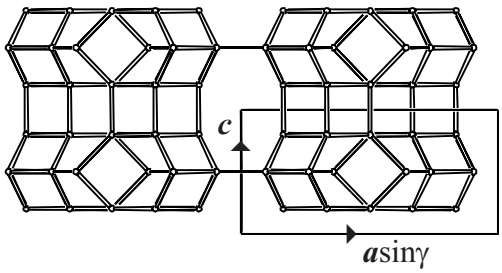
Neighboring PerBUs can be connected into the ***ab*** plane in three different ways:
(1): The PerBUs are related by a 2-fold axis parallel to ***c***. 8-Rings are formed.
(2): The PerBUs are related by a 3-fold axis parallel to ***c***. 8-Rings and 12-rings are formed.
(3): The PerBUs are related by a combination of modes **(1)** and **(2)**.



Connection mode **(1)**

LTL





(a)

Figure 2. (a): Connection mode **(1)** in **LTL** viewed along ***c*** (left) and parallel projection of the unit cell content along ***c*** (top right) and along ***b*** (or along three (symmetry) equivalent other directions; bottom right). [Figure 2 is continued on next page]

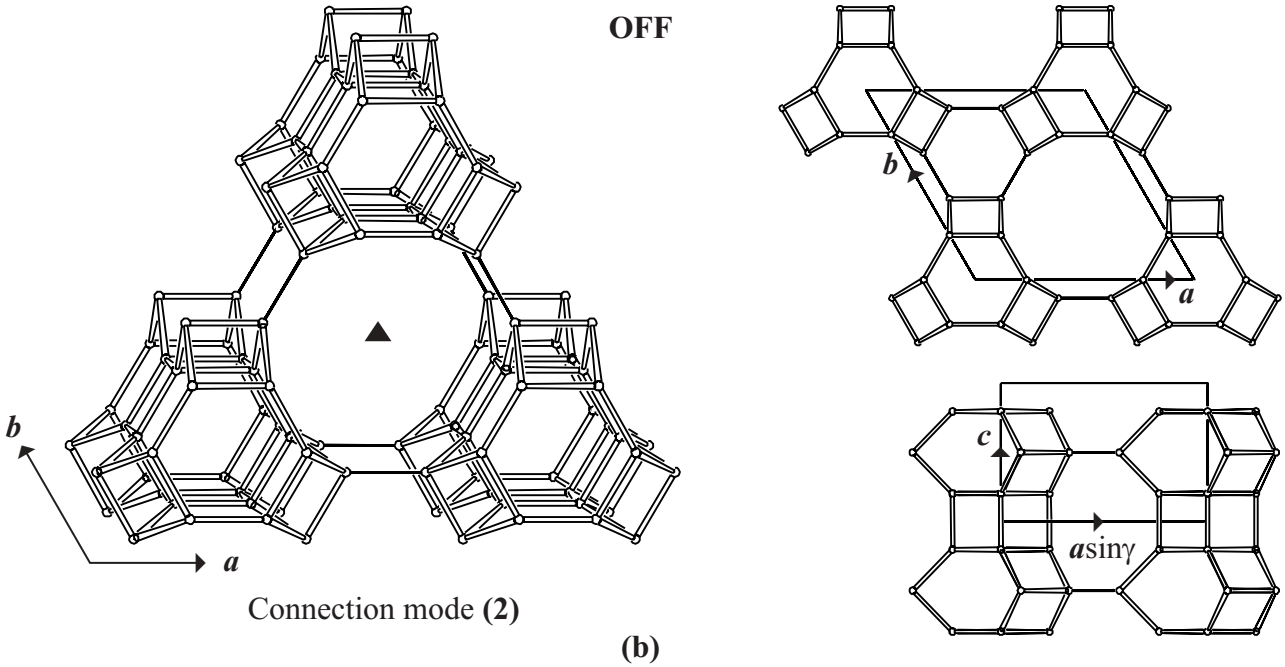


Figure 2 [Cont'd]. (b): Connection mode **(2)** in **OFF** viewed along ***c*** (left) and parallel projection of the unit cell content along ***c*** (top right) and along ***b*** (bottom right).

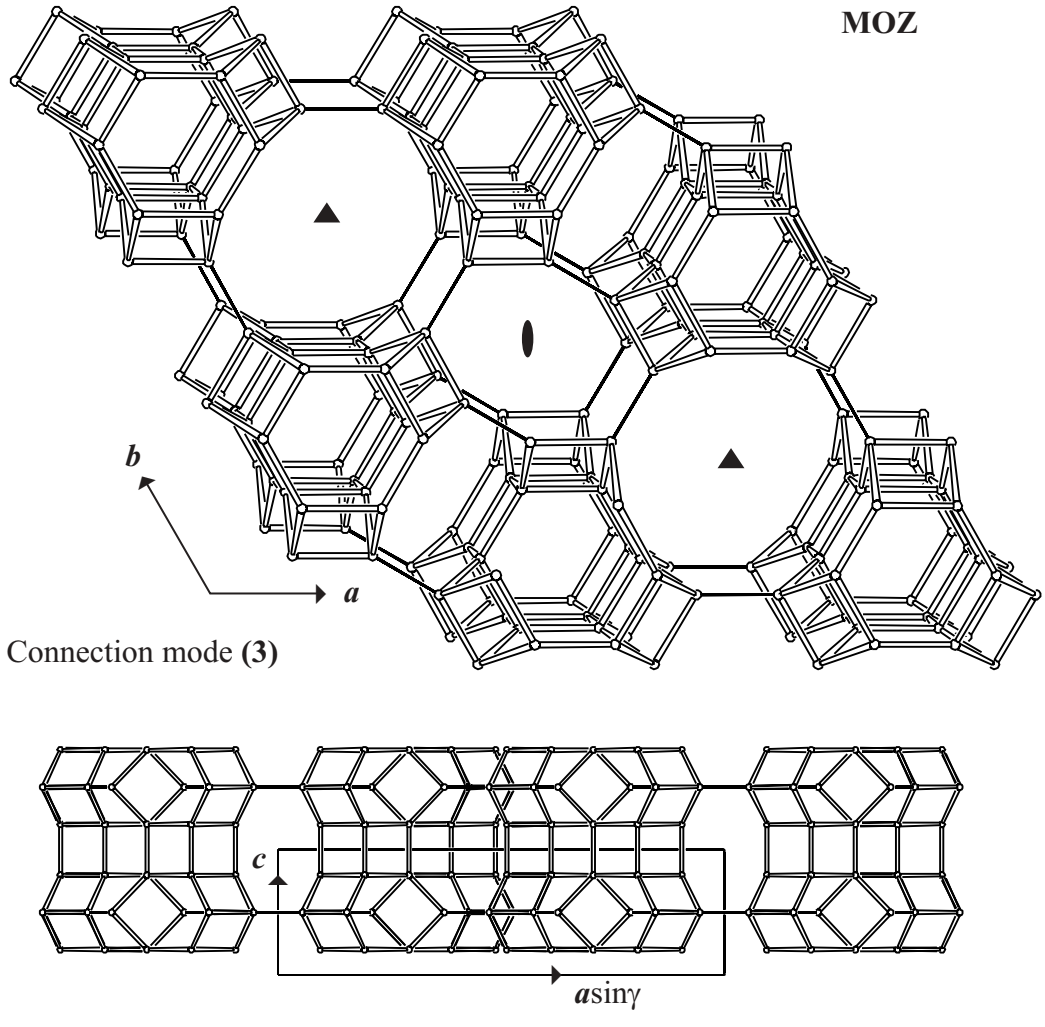
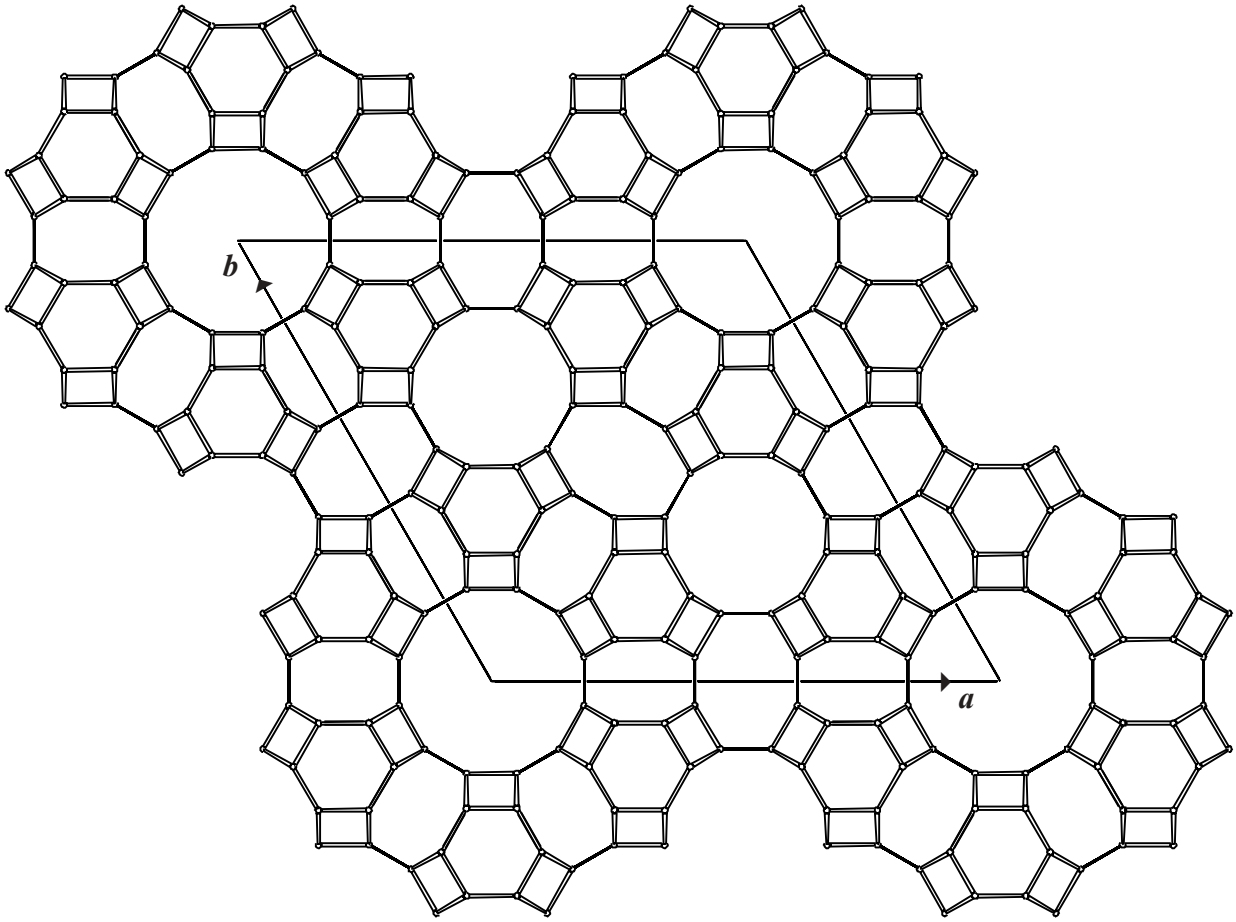


Figure 2. (c1): Connection mode **(3)** in **MOZ** viewed along ***c*** (top) and parallel projection of the unit cell content along ***b*** (bottom). [Figure 2 is continued on next page]



(c2)

Figure 2 [Cont'd]. (c2): Parallel projection of the unit cell content in **MOZ** along ***c***.

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

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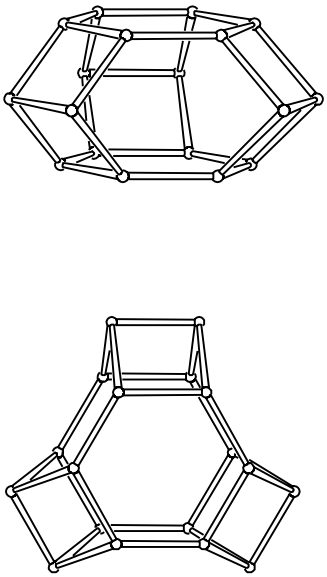
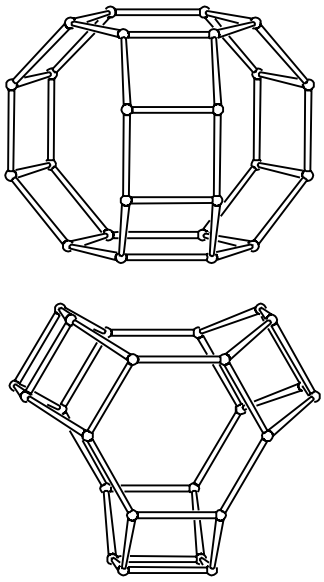
4. Channels and/or cages:

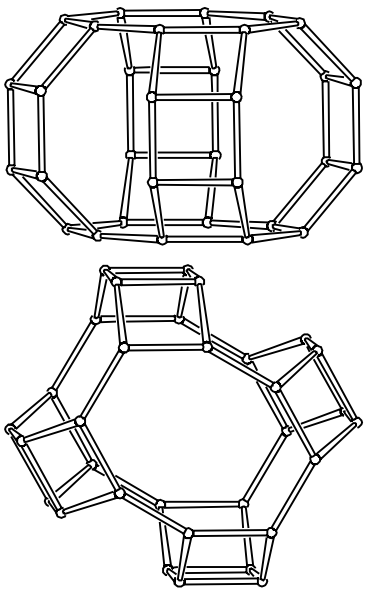
In **OFF** and **LTL** 12-ring channels, that are different in each framework type, are parallel to ***c***. In **MOZ** two different 12-ring channels are parallel to ***c***. They are topologically identical to the channels in **OFF** and in **LTL**. In **OFF**, ***can*** cages and ***gmel*** cavities interconnect the 12-ring channels. The 12-ring channels in **LTL** are interconnected through 8-ring channels parallel to ***c***. This 8-ring channel is topologically equivalent to the 8-ring channel in **DFT**, **LOV** and **RSN**. The two different 12-ring channels in **MOZ** are interconnected differently: the **OFF**-type 12-ring channels are interconnected through ***mer*** cavities and the **LTL**-type 12-ring channels are interconnected using both the ***mer*** cavity and (topologically) the same 8-ring channel that interconnects the 12-ring channels in **LTL**. Finally, in all three structure types two-dimensional 8-ring channels, intersecting the 12-ring channels, are perpendicular to ***c*** and run along three symmetrically equivalent directions: ***a***, ***b*** and [110], hereafter represented as along $<100>_{hex}$. Figure 3 on next page summarizes the channel intersections, the cavities and cages and lists the **pore descriptors**. Systems of fused channel intersections and cages are depicted in Figure 4 on next pages.



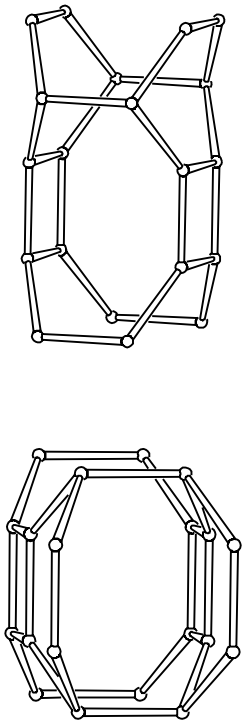
***can* cage in LTL, OFF and MOZ**
Pore descriptor:
{0 [$4^6 6^5$]}



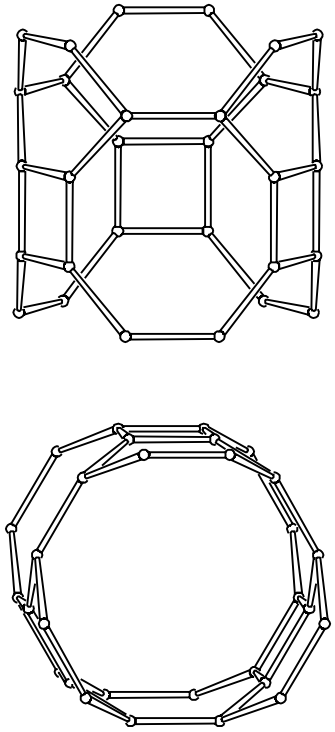
***gmel* cavity in OFF**;
8/8-ring intersection
Pore descriptor:
{2 [$4^9 6^2 8^3$] <100>$_{hex}$ (8-ring)}



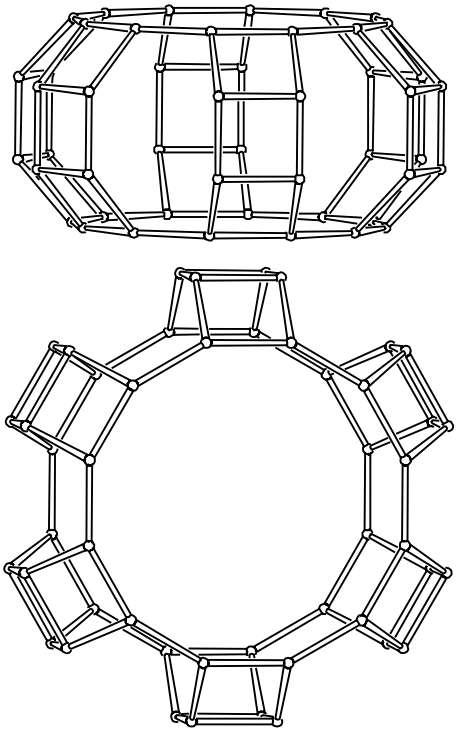
***mer* cavity in MOZ**;
8/8-ring intersection
Pore descriptor:
{3 [$4^{12} 8^6$] <100>$_{hex}$ (8-ring), [001] (8-ring)}



***8/8-ring intersection* in LTL and MOZ**
Pore descriptor:
{2 [$4^2 6^2 8^4$] [100] (8-ring)}



***8/12-ring intersection* in OFF and MOZ**
Pore descriptor:
{3 [$4^3 6^3 8^3 12^2$] <100>$_{hex}$ (8-ring), [001] (12-ring)}



***8/12-ring intersection* in LTL and MOZ**
Pore descriptor:
{3 [$4^{18} 8^6 12^2$] <100>$_{hex}$ (8-ring), [001] (12-ring)}

Figure 3. ***can*** Cage and channel intersections in **LTL**, **MOZ** and **OFF** viewed along <120>$_{hex}$ (top) and along ***c*** (bottom).

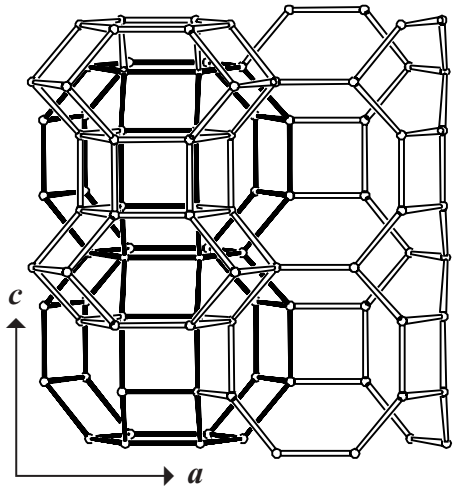
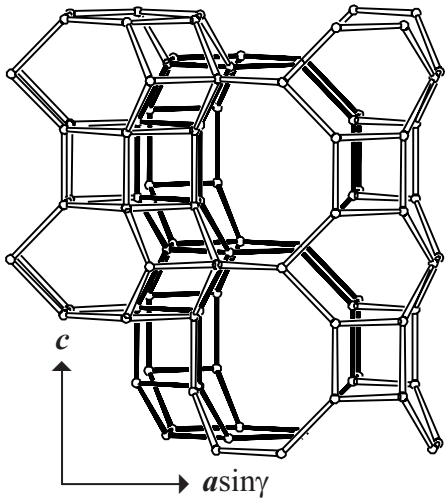
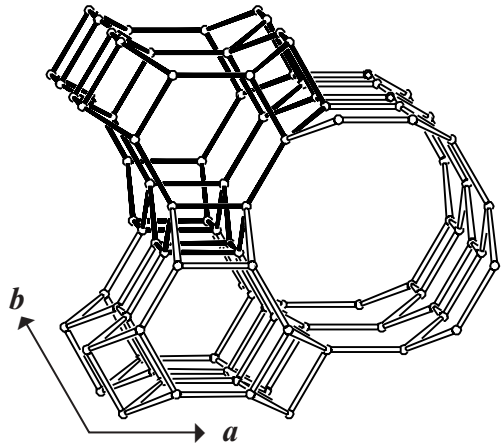
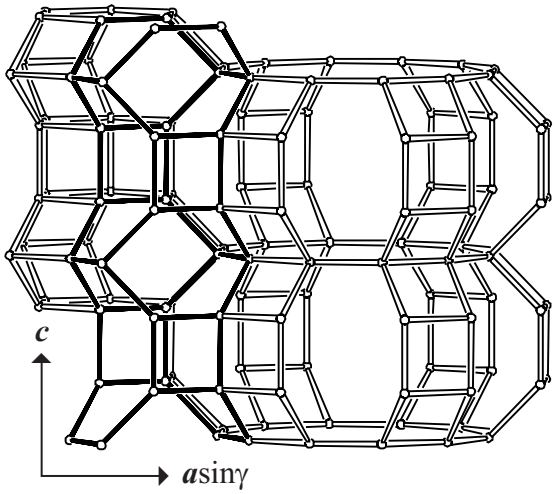
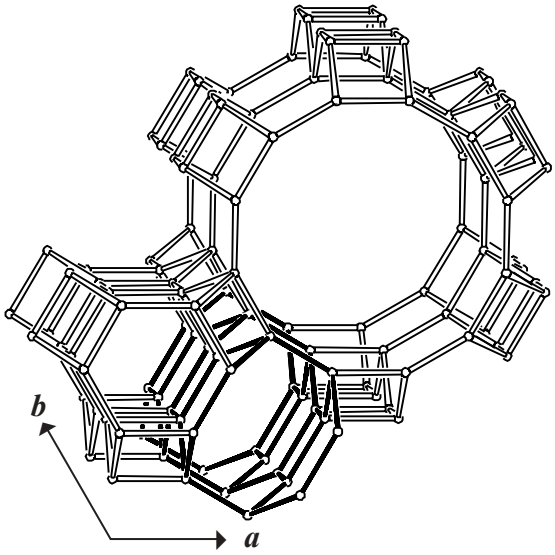


Figure 4(a). Fusion of channel intersections in **OFF** viewed along $<120>_{hex}$ (left), along $<010>_{hex}$ (top right) and along ***c*** (bottom right). The ***gmel*** cavities are in bold.









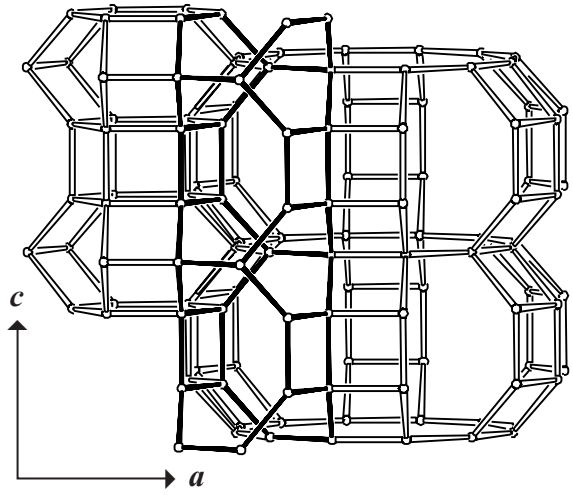


Figure 4(b). Fusion of channel intersections in **LTL** viewed along $<120>_{hex}$ (right), along $<010>_{hex}$ (top left) and along ***c*** (bottom left). The 8-ring channel parallel to ***c*** is in bold.

[Figure 4 is continued on next page]

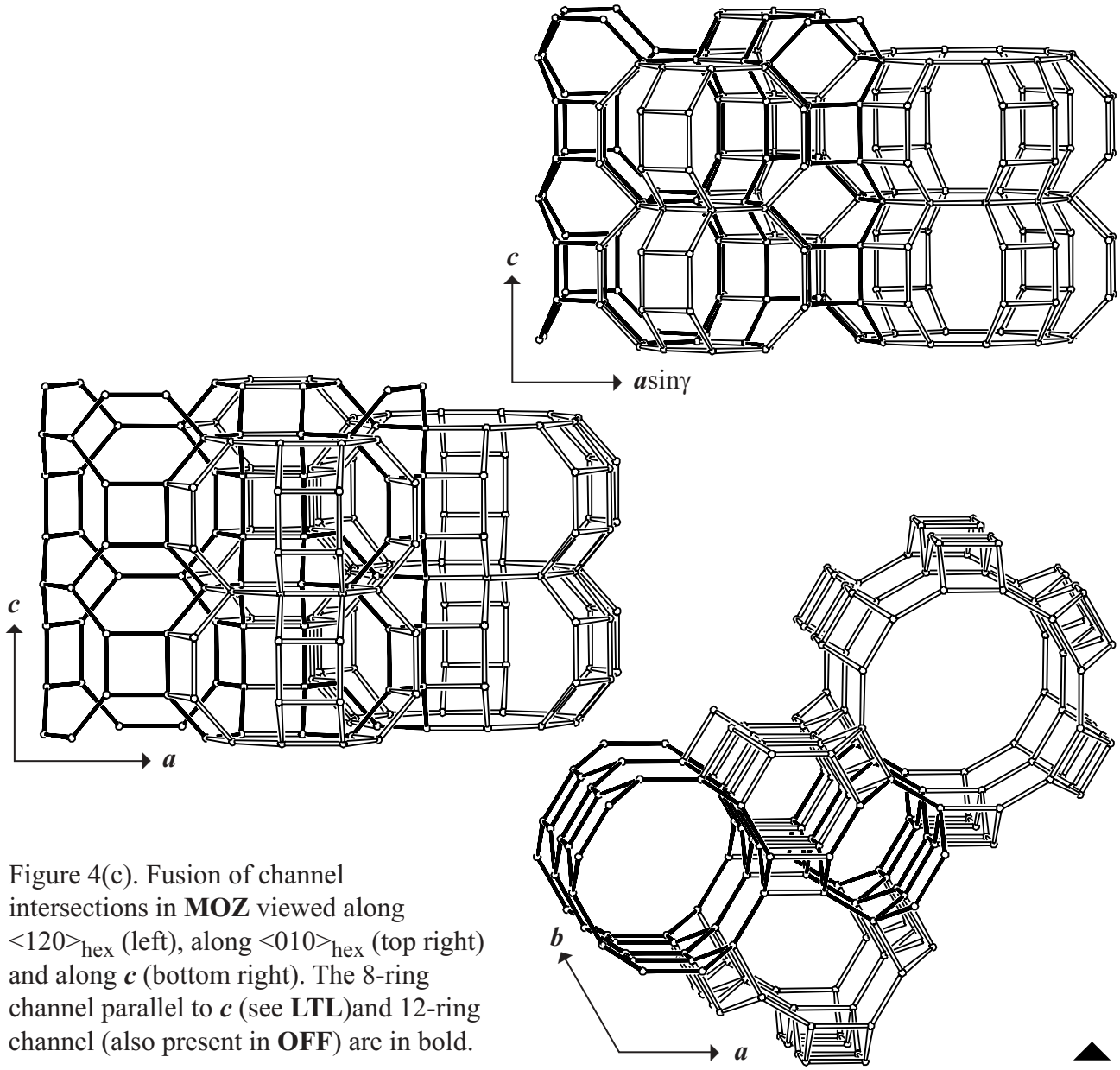


Figure 4(c). Fusion of channel intersections in **MOZ** viewed along $<120>_{hex}$ (left), along $<010>_{hex}$ (top right) and along ***c*** (bottom right). The 8-ring channel parallel to ***c*** (see **LTL**)and 12-ring channel (also present in **OFF**) are in bold.

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5. Supplementary information:

***Alternative description of* OFF**

A large number of framework types, like **OFF**, can be constructed using a hexagonal PerBU of non-connected 6-rings. They all belong to the ABC-6 family.

In the **INTRO** pages links are given to descriptions of framework types belonging to the ABC-6 family (choose: **ABC-6 family**).

Other framework types containing saw chains

In several framework types at least one of the unit cell dimensions is about n*7.5 Å (where n = 1, 2, 3... etc.). In many cases this indicates the presence of saw chains.

In the **INTRO** pages links are given to descriptions of other framework types containing (twisted) saw chains (choose: **Saw 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 2**).

Other framework types containing (modified) cavities

Several framework types can be built using (modified) cavities.

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**).