Building scheme for -CLO

1. Periodic Building Unit:

The cubic interrupted framework of **-CLO** can be built using two types of Building Units: BU1 and BU2. BU1 equals an α-cavity that has all twelve 4-rings replaced by double 4-rings (D4Rs; Figure 1(a)). BU2 equals a slice of BU1 and consists of four D4Rs (Figure 1(b)). Each D4R is singly connected to two neighboring D4Rs. In each D4R two oxygen atoms are terminal oxygen atoms where the framework is not fully connected. A zero-dimensional Periodic Building Unit (PerBU) is obtained when one BU1 and three BU2s are connected through 6-rings as shown in Figure 1(c).
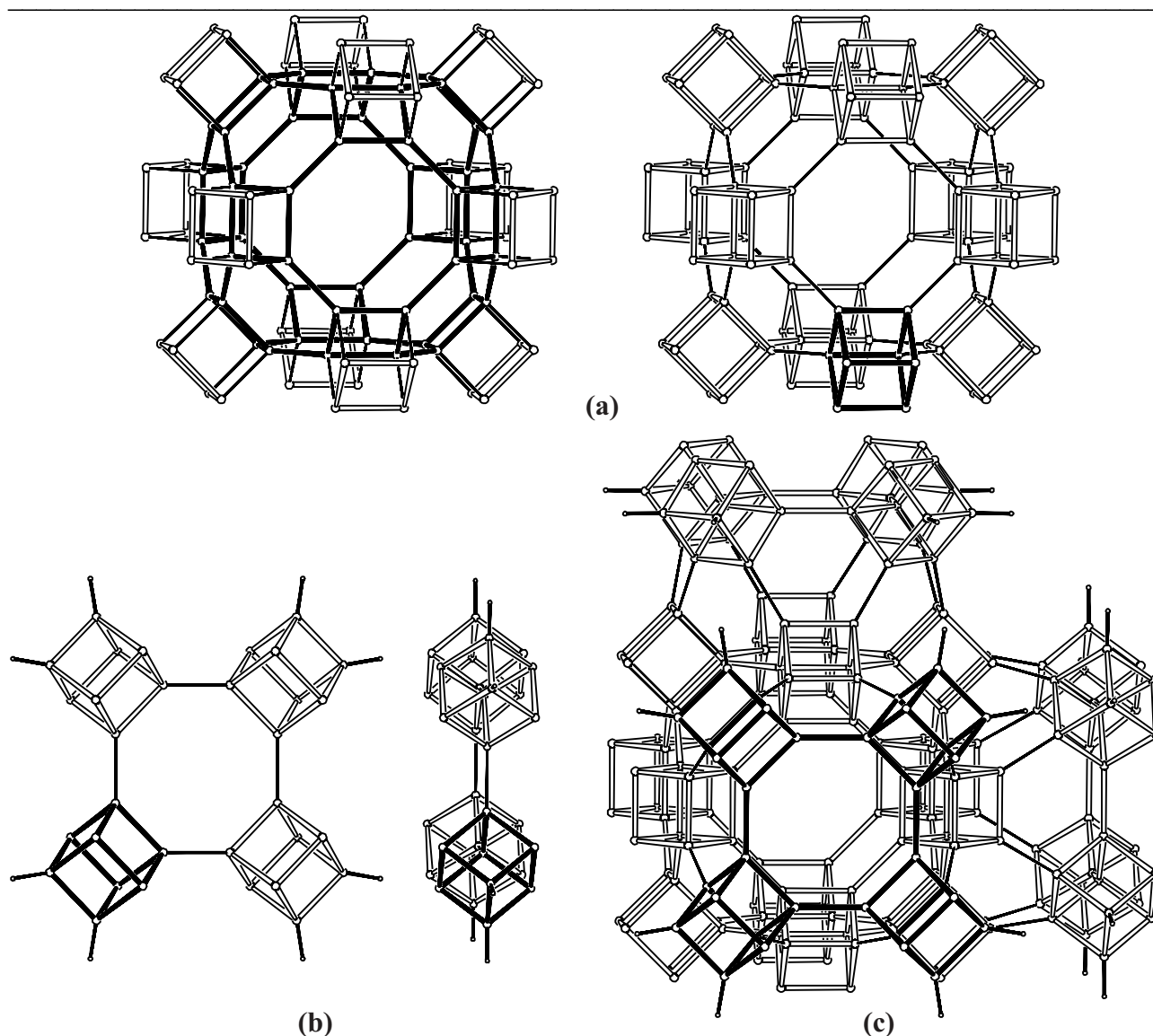

(a)

(b)

(c)

Figure 1. (a): BU1 constructed from the α-cavity with additional T4-rings (left) and BU1 constructed from D4Rs (right); (b): BU2 constructed from four D4Rs seen in top- (left), and side-view (right). Terminal O atoms are (bold bonded) small circles; (c): PerBU constructed from BU1 and three BU2s. For clarity, the BU2 towards the viewer is heavy bold.

2. Connection mode:

Neighboring PerBUs, related by pure translations along the three cube axes, are connected into the three-dimensional framework. The connection mode within one cube face of the framework is illustrated in Figure 2.
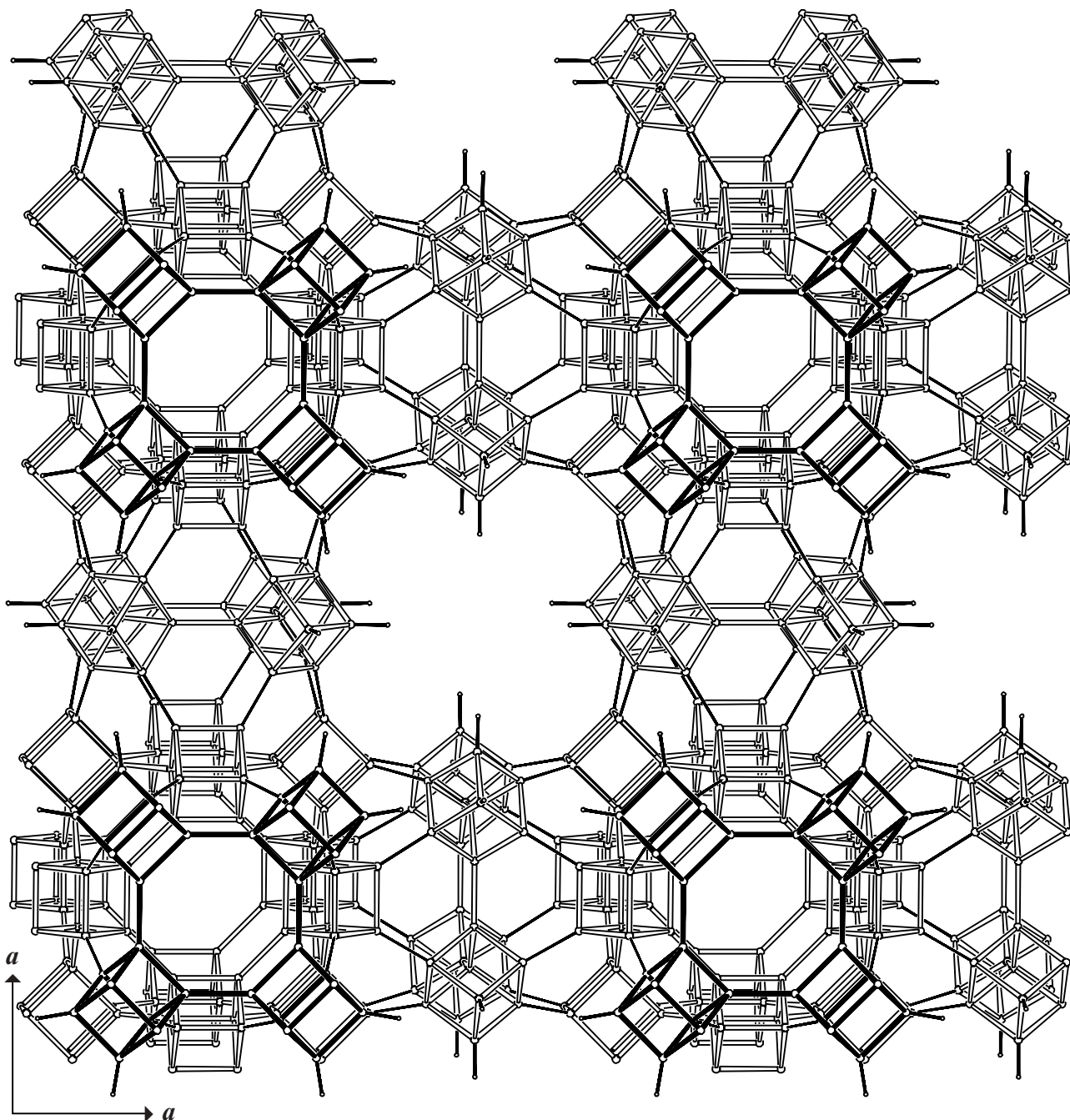

Figure 2. Connection mode within a cube face. [The connection mode in the other cube faces is the same]
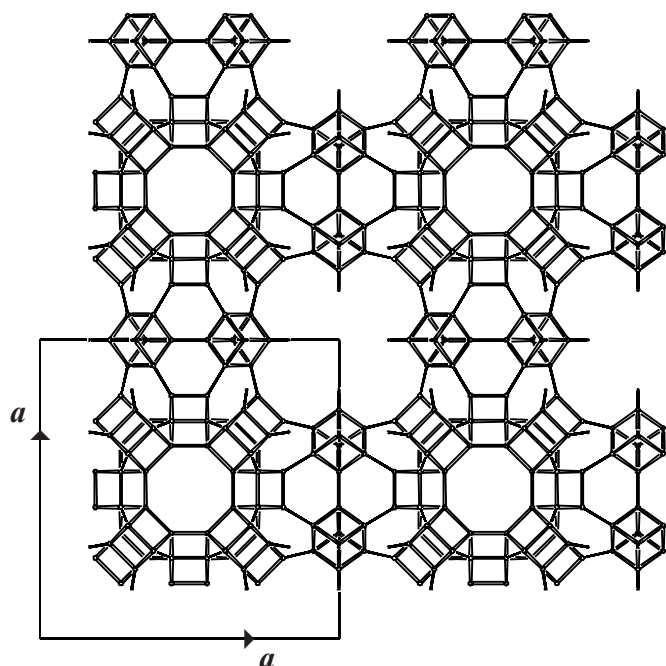
3. Projections of the unit cell content:

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a ↑

a →

Figure 3. Parallel projection of the unit cell content along a cube axis. ▲

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4. Channels and/or cages:

Intersecting 8-ring channels and intersecting 20-ring channels are parallel to the cube axes. There is no direct access from the 8-ring channels to the 20-ring channels. The **pore descriptor** for each of the two channel intersections is added in Figure 4.
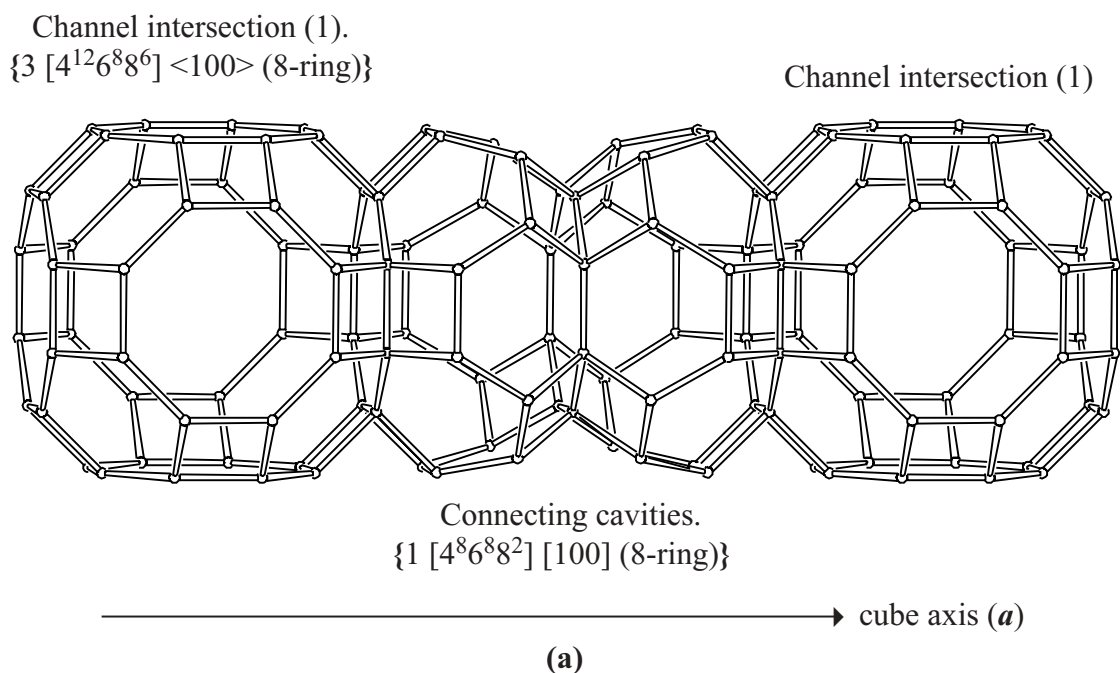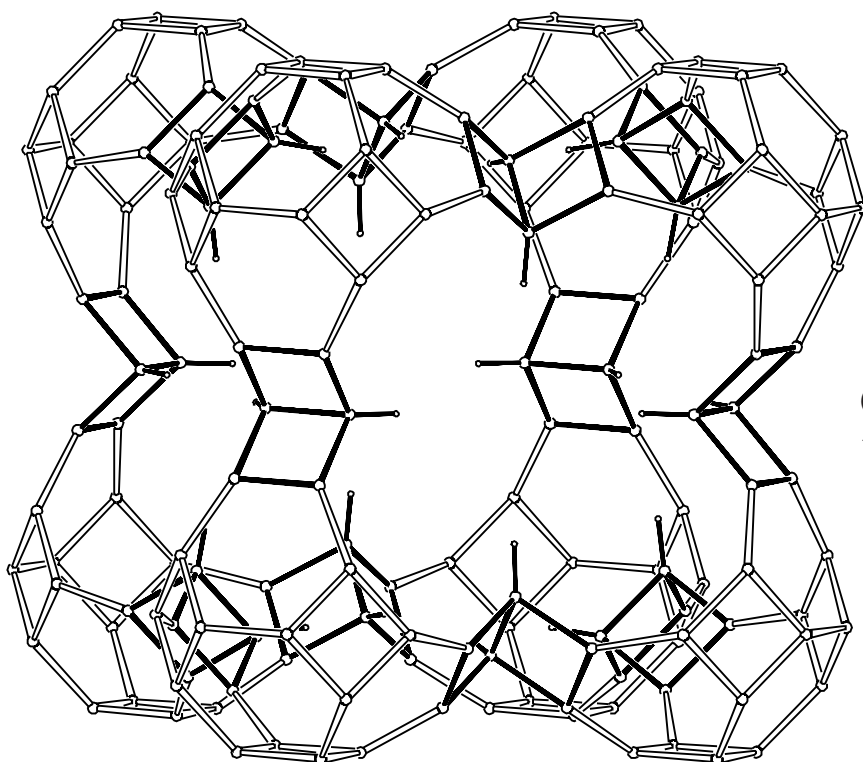
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Channel intersection (1).
$\{3\ [4^{12}6^{8}8^{6}]\ <100>\ (8\text{-ring})\}$

Channel intersection (1)

Connecting cavities.
$\{1\ [4^{8}6^{8}8^{2}]\ [100]\ (8\text{-ring})\}$

→ cube axis (**a**)

(a)

Figure 4. (a): The intersection of 8-ring channels (intersection (1)) equals the α-cavity (left). α-Cavities are connected along the cube axes by sharing 8-rings with smaller cavities.
[Figure 4 is continued on next page]

(b): Channel intersection (2).
{3 [$4^{40}6^{32}20^6$] <100> (20-ring)}
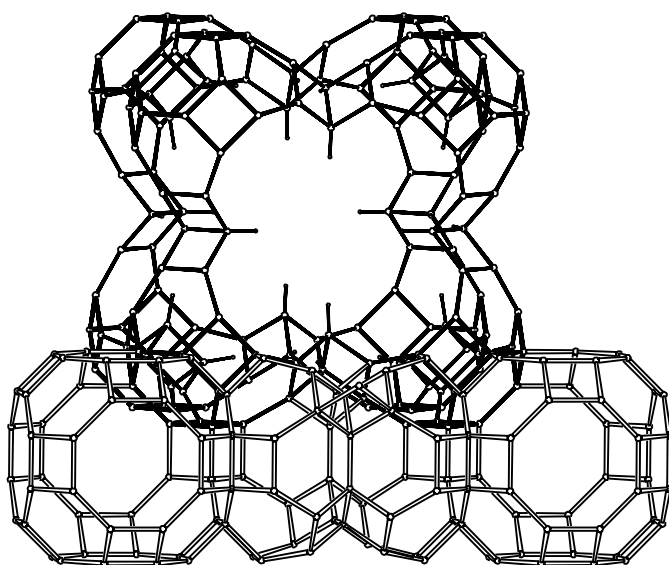
(c): Fused cavities.

Figure 4 [Cont'd]. (b): Channel intersection (2) with 20-ring windows viewed along a cube axis; (c): Fused channel intersections viewed along a cube axis. ▲

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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**).

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