Building scheme for PAU

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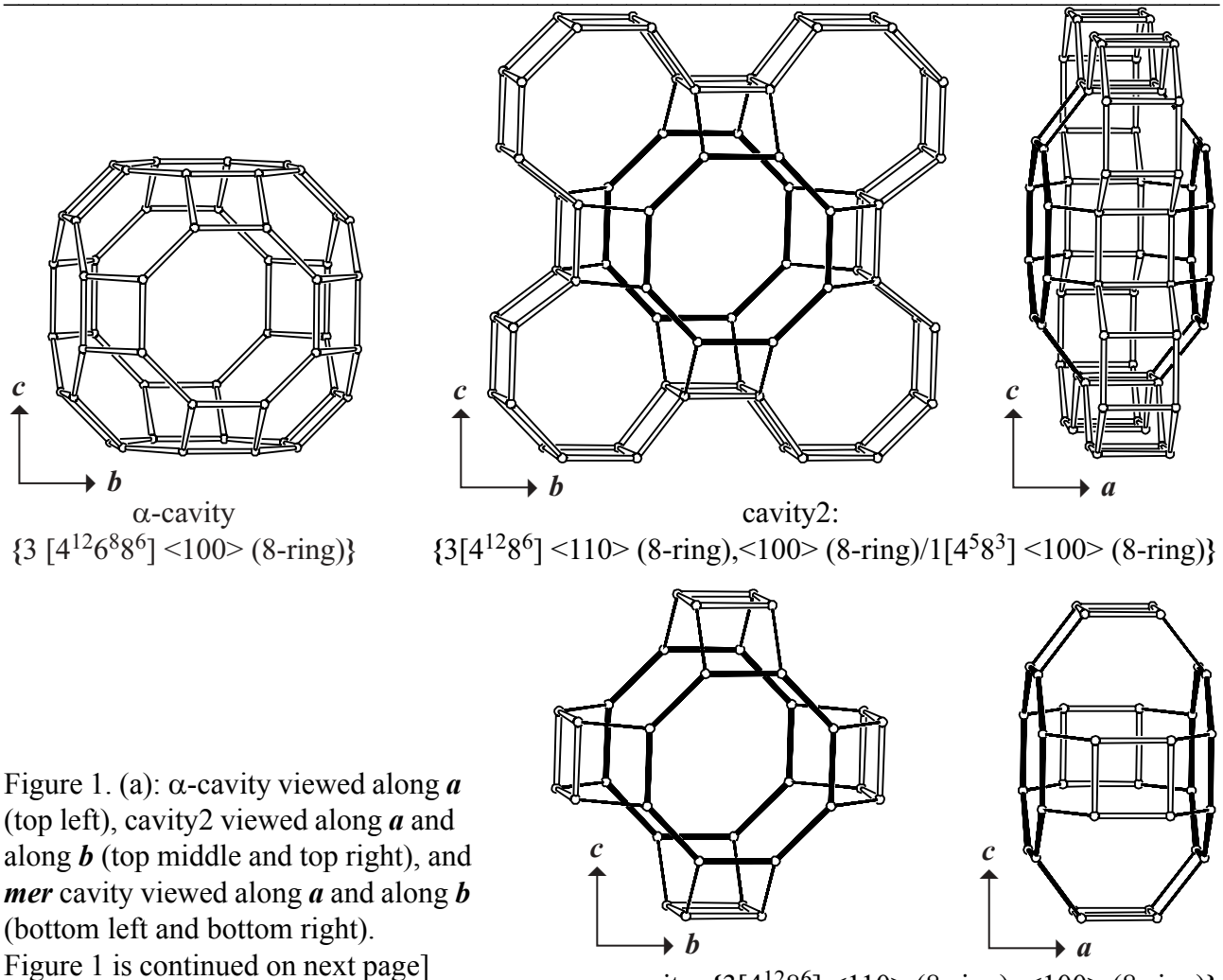
1. Periodic Building Unit:

In cubic **PAU** three types of cavities can be distinguished. The α-cavity (Figure 1(a)) consists of 48 T atoms: six 8-rings, eight 6-rings or twelve 4-rings. The second cavity (cavity2) contains 64 T atoms: eight 8-rings or sixteen 4-rings connected into a double 24-ring 'capped' on both sides with an 8-ring (Figure 1(a); 8-rings in bold). The ***mer*** cavity is equal to cavity2 without the 'side-pockets' and contains 32 T atoms: four 8-rings or eight 4-rings as shown in Figure 1(a). The cavities are connected into two different building units. The first building unit (BU1; Figure 1(b)) consists of six cavities2 which are connected to an α-cavity through double 8-rings (and contains 48 + 6*64 = 432T atoms). The second building unit (BU2; Figure 1(b)) consists of six ***mer*** cavities which are connected to an α-cavity through double 8-rings (and contains 48 + 6*32 = 240T atoms). Neighboring BU1s, related by pure translations along the cube axes, are connected into cubic faces through double 8-rings as shown in Figure 1(c). The Periodic Building Unit (PerBU) is obtained when the "empty spaces" in the BU1-cubic faces are filled with BU2 units. The BU1 and BU2 units, shifted with respect to each other over ½(***a*** + ***b*** + ***c***), are connected through 4-rings as shown in Fig.1(c,d).

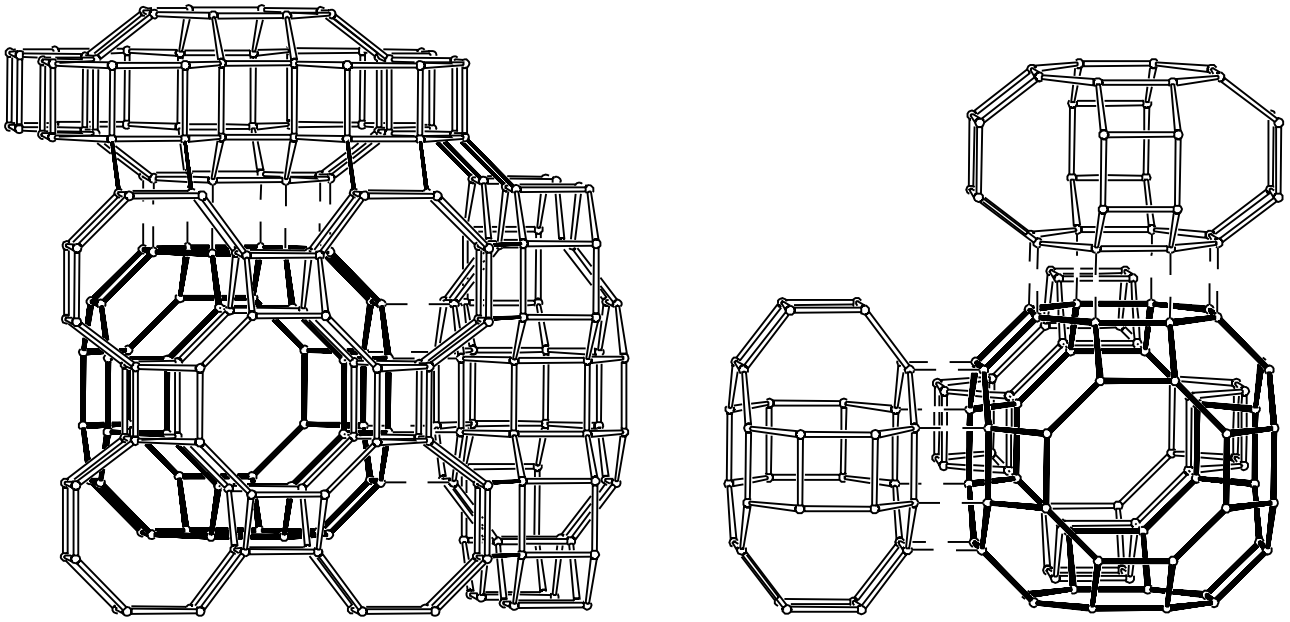


α-cavity
{3 [$4^{12}6^8 8^6$] <100> (8-ring)}

cavity2:
{3[$4^{12}8^6$] <110> (8-ring),<100> (8-ring)/1[$4^5 8^3$] <100> (8-ring)}

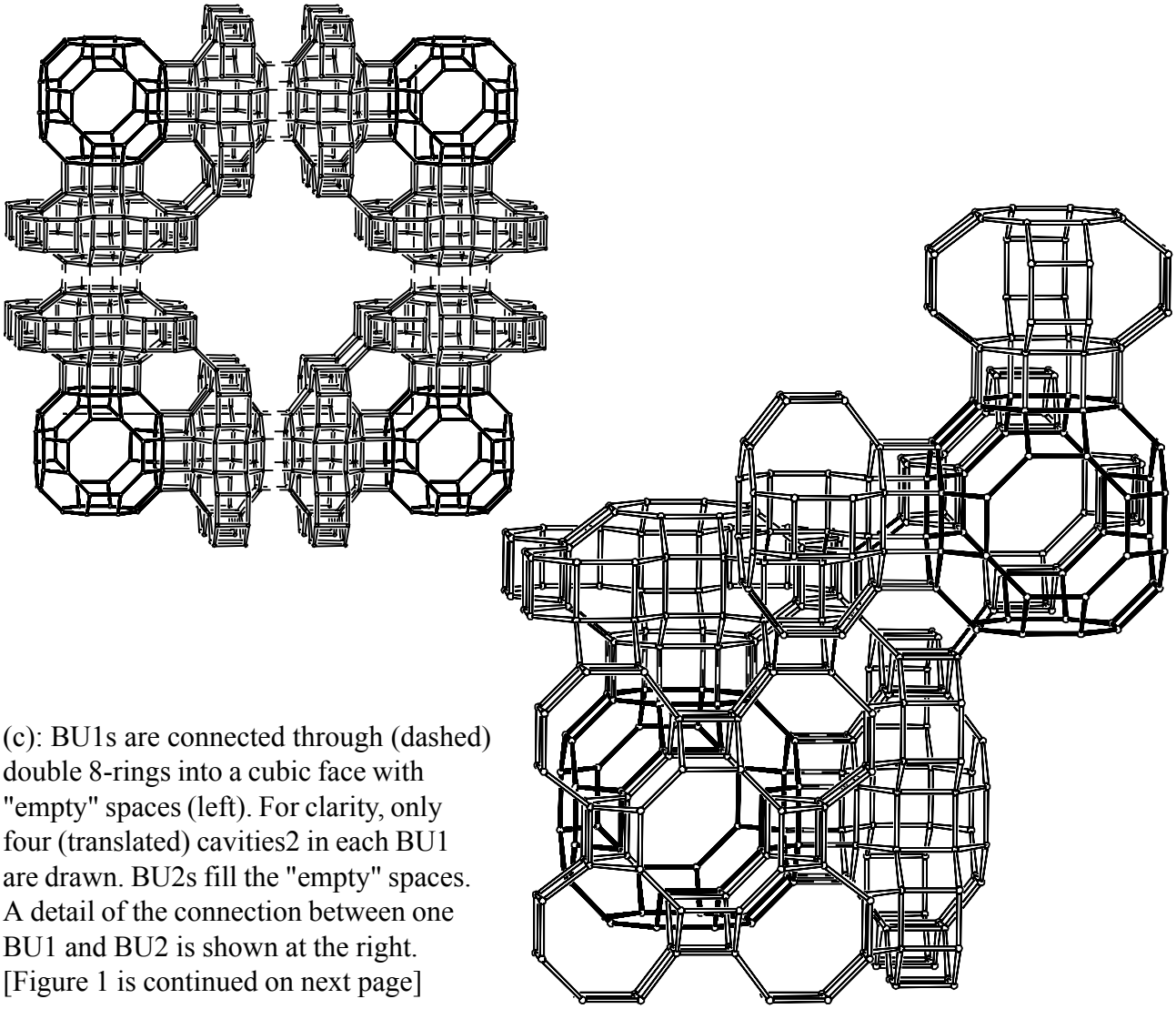
Figure 1. (a): α-cavity viewed along ***a*** (top left), cavity2 viewed along ***a*** and along ***b*** (top middle and top right), and ***mer*** cavity viewed along ***a*** and along ***b*** (bottom left and bottom right).
Figure 1 is continued on next page]

mer cavity: {3[$4^{12}8^6$] <110> (8-ring), <100> (8-ring)}



BU1 BU2

Figure 1[Cont'd].(b): BU1(left) and BU2 (right) viewed along a cubic axis. For clarity, only three of the six cavities2 (left) and three of the six ***mer*** cavities (right) are attached to a (bold) α-cavity; double 8-ring connections to the α-cavity are dashed and the additional connections (4-rings and a 6-ring) between cavities2 are in light bold.



(c): BU1s are connected through (dashed) double 8-rings into a cubic face with "empty" spaces (left). For clarity, only four (translated) cavities2 in each BU1 are drawn. BU2s fill the "empty" spaces. A detail of the connection between one BU1 and BU2 is shown at the right.

[Figure 1 is continued on next page]

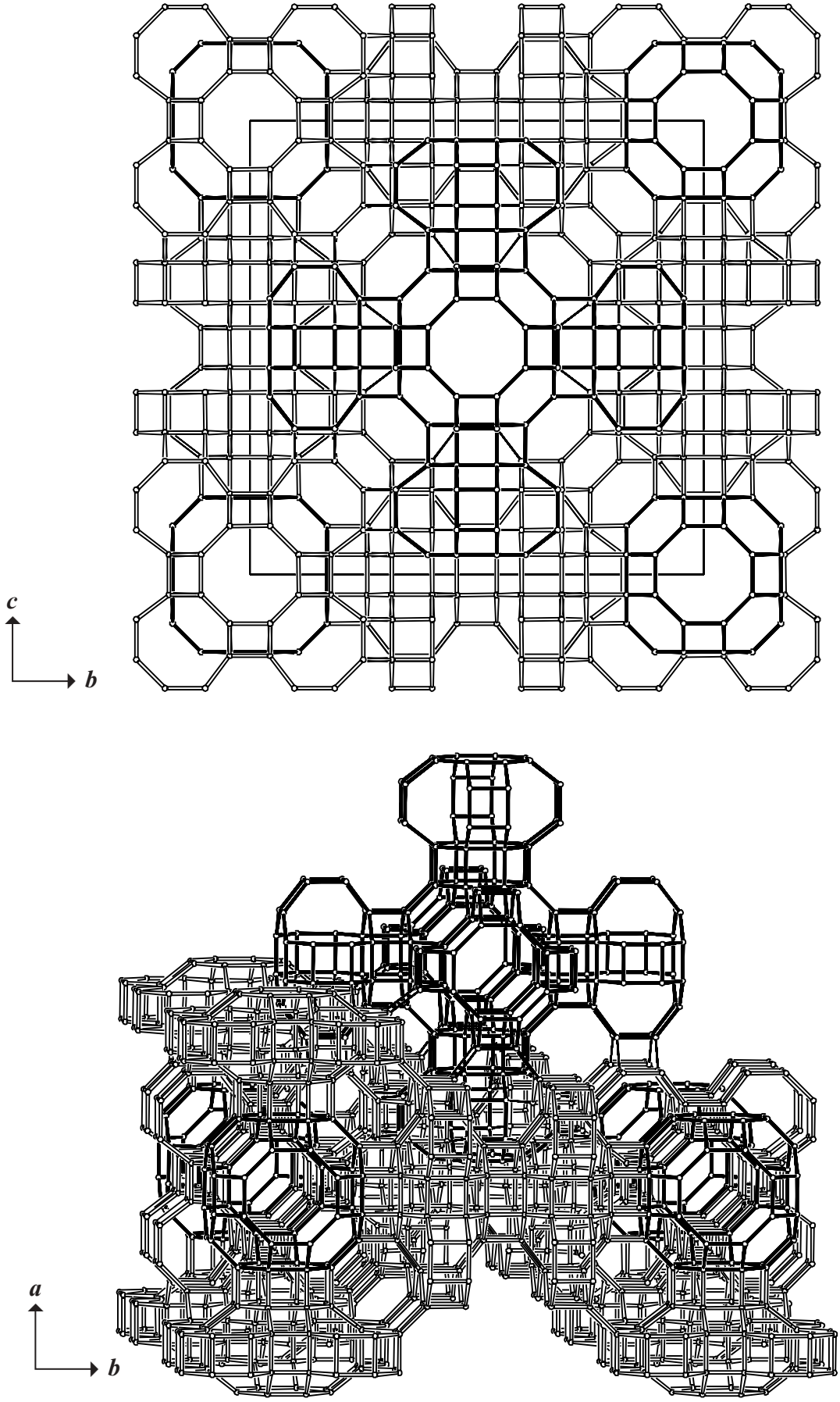


Figure 1 [Cont'd]. (d): PerBU in **PAU** viewed along ***a*** (top), and along ***c*** (bottom). For clarity, not all cavities2 are drawn. Bu2 and α-cavities are in bold.

2. Connection mode:

Neighboring ***bc*** planes are related by pure translations along ***a***. The connection modes in the ***ab***- and ***ac***-planes are equivalent to those shown in Figure 1 for the ***bc*** plane.

3. Projections of the unit cell content: See Figure 1(d; top).

4. Channels and/or cages:

Cavities are shown in Figure 1(a). The **pore descriptors** are added in Figure 1(a). Two systems of equal, non-intersecting 8-ring channels are parallel to <100> (see Figure 2).

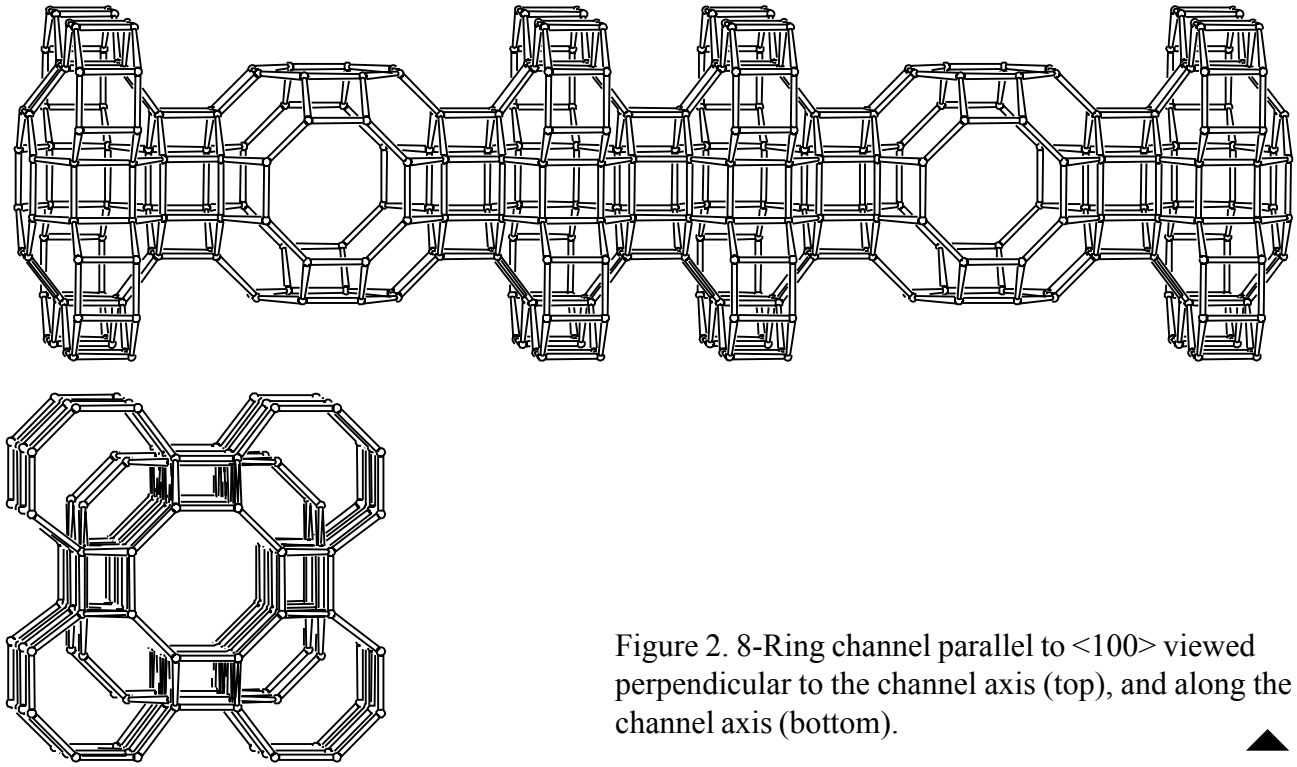


Figure 2. 8-Ring channel parallel to <100> viewed perpendicular to the channel axis (top), and along the channel axis (bottom).

5. Supplementary information:

Other framework types containing (modified) cavities
Several other 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**).