Building scheme for CGS and ETR

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:

CGS and **ETR** can be built using as one-dimensional Periodic Building Unit (PerBU) the chain depicted in Figure 1. The chain is composed of units of 16 T atoms (in bold) related by pure translations along **z**. The T16-unit consists of two two-fold (1,2)-connected double 4-rings or, alternatively, of a double 6-ring and a double 4-ring (sharing a face) with two "open" T-T bonds (see **Alternative description**)

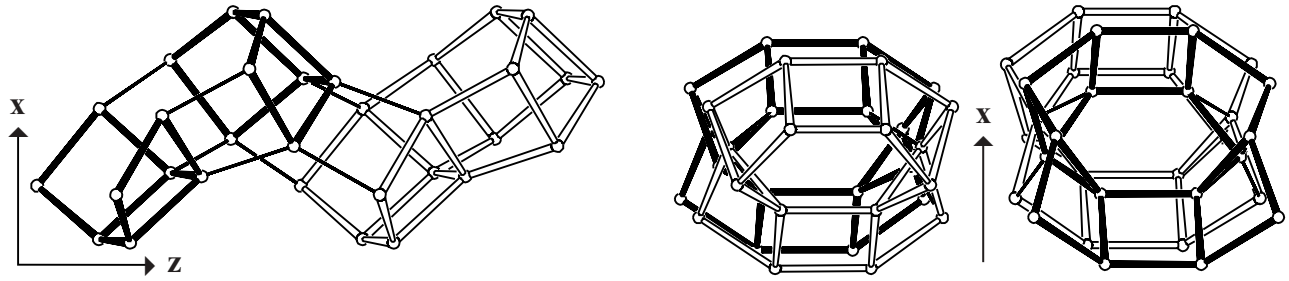
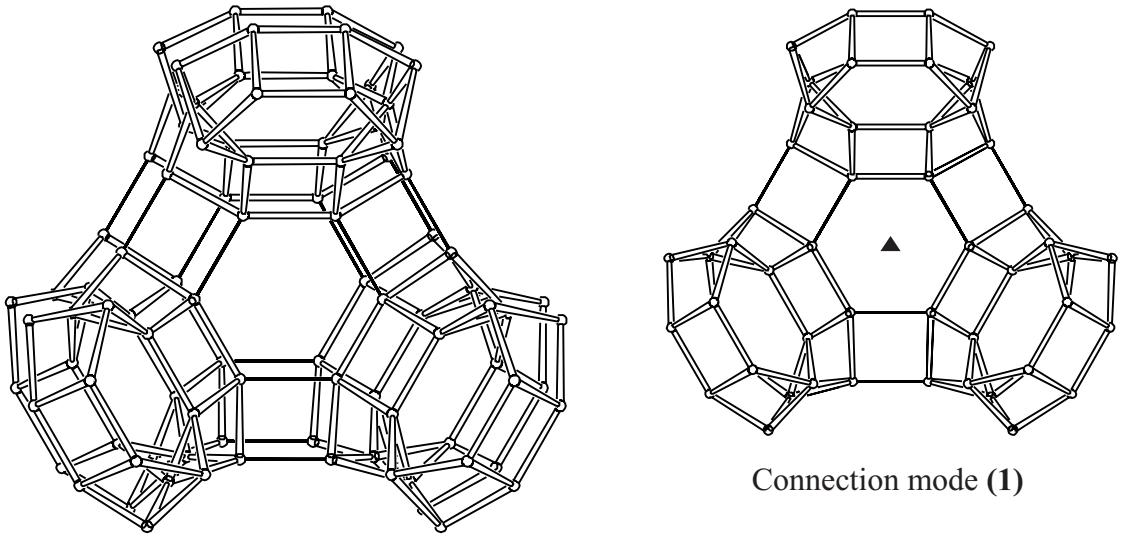


Figure 1. PerBU composed of T16-units (left) and perspective views of the PerBU along the chain axis **z** (right). The two PerBUs at the right are equal and are related by a rotation of 180º about **x**.

2. Connection mode:

Neighboring PerBUs can be connected in two different ways through 4-rings:
(1): neighboring PerBUs are related by a 3-fold rotation axis parallel to the chain axis **z**;
(2): neighboring PerBUs are related by a rotation of 180° about **x** and a shift of ½**y**.



Connection mode **(1)**

Figure 2. Connection mode **(1)** in **ETR** viewed along the 3-fold axis (left), and projected along the 3-fold axis (right). [Figure 2 is continued on next page]

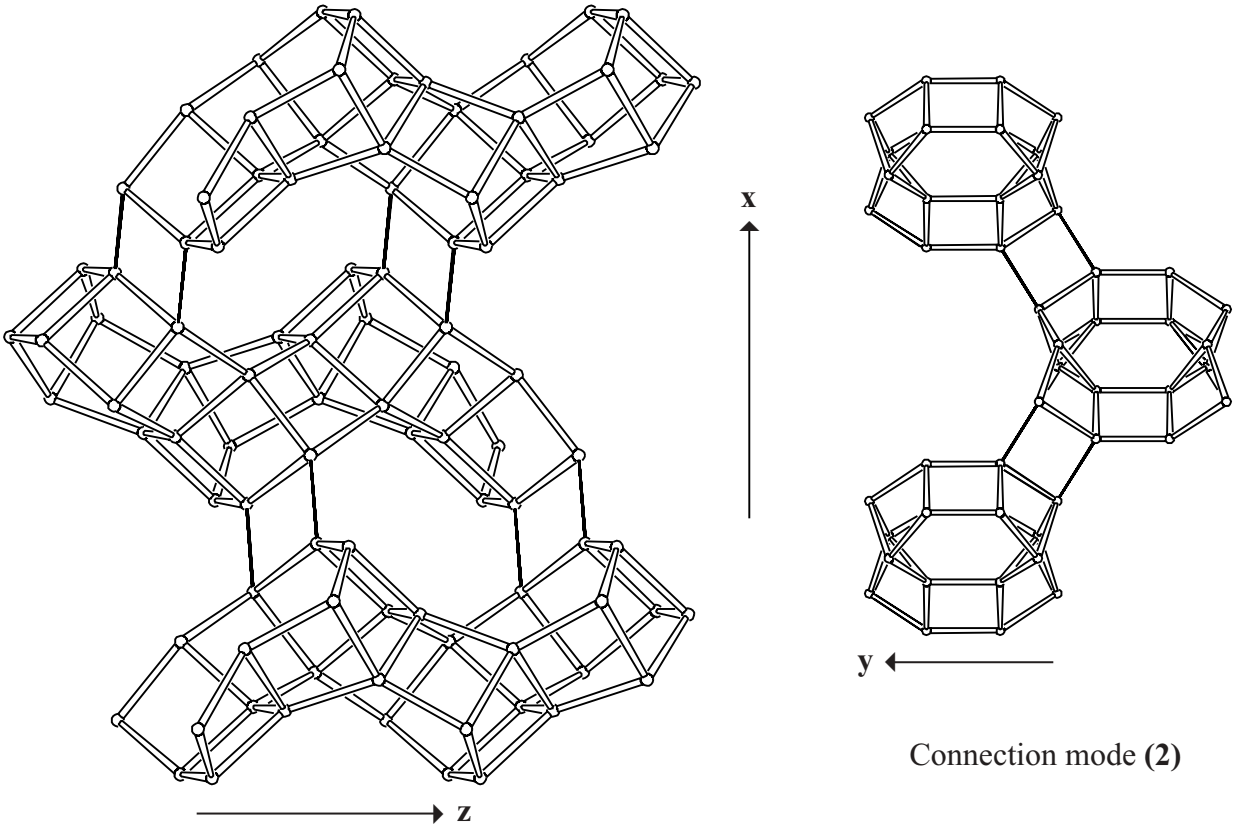


Figure 2 [Cont'd]. Connection mode **(2)** in **CGS** viewed along **y** (left), and projected along **z** (right).

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3. Projections of the unit cell content:

Pure **CGS** and **ETR** are obtained when neighboring PerBUs are exclusively related by 2-fold screw axes parallel to **x** and by 3-fold rotation axes parallel to **z**, respectively.

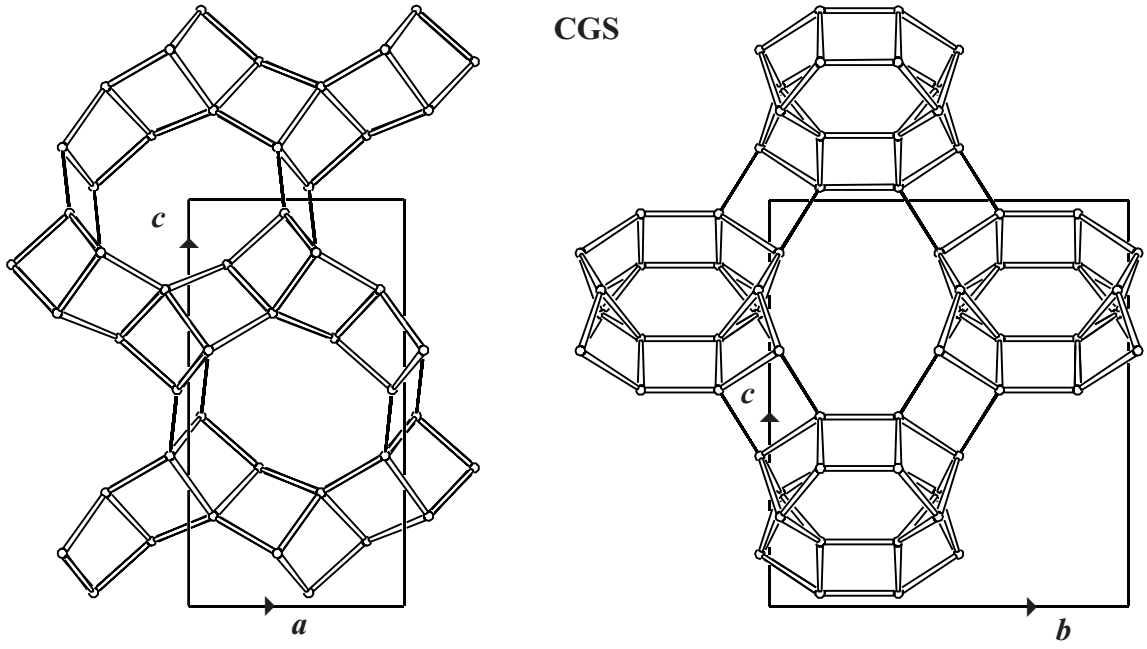


Figure 3. Cell content in **CGS** projected along ***b*** (left), and along ***a*** (right).
[Figure 3 is continued on next page]

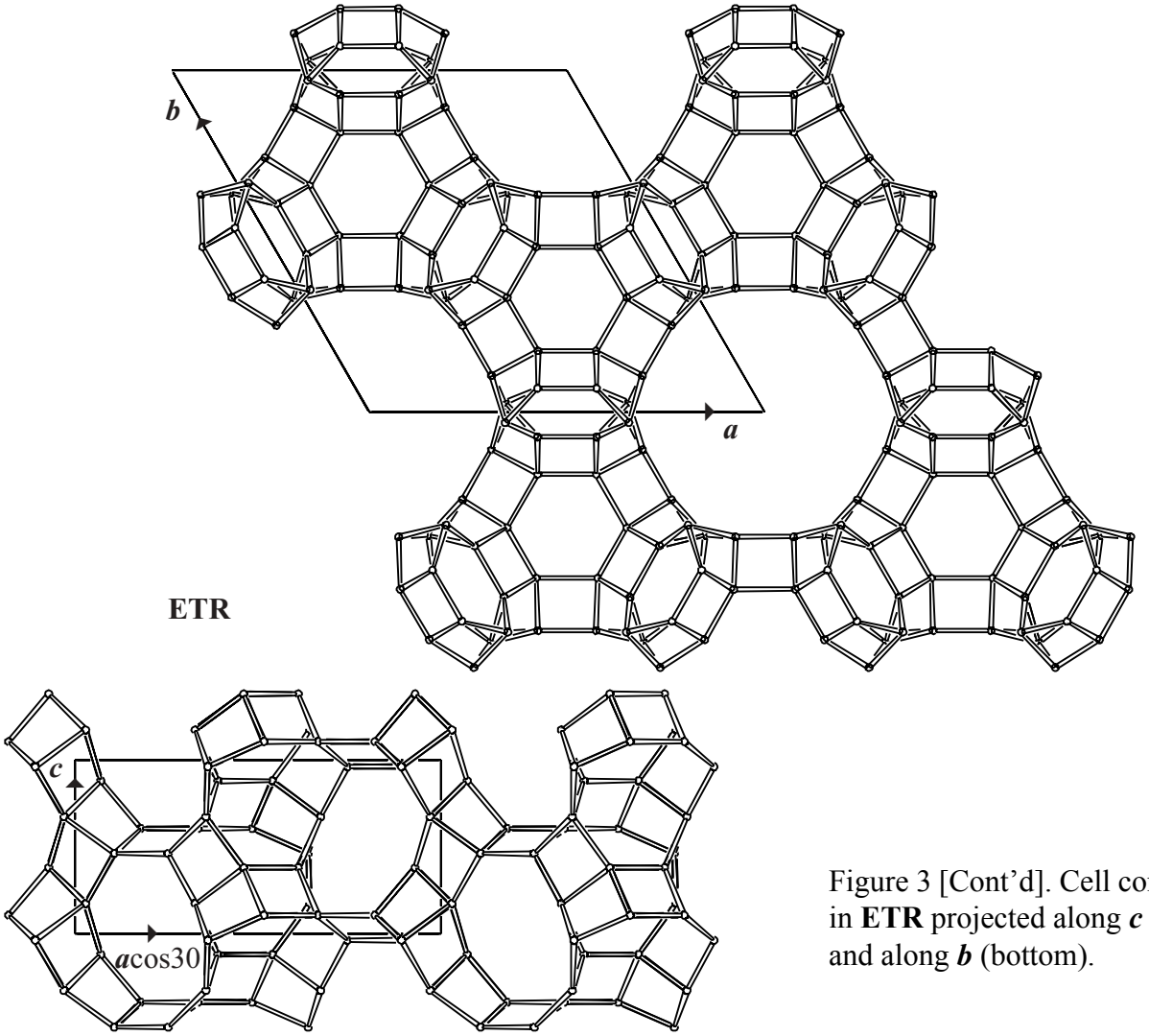
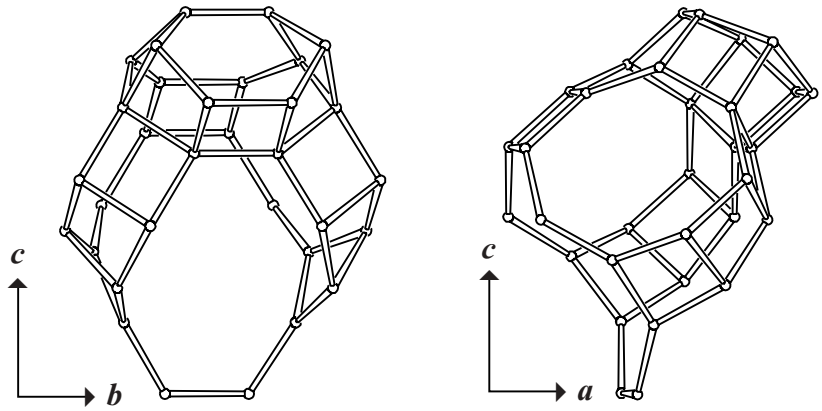


Figure 3 [Cont'd]. Cell content in **ETR** projected along ***c*** (top), and along ***b*** (bottom).

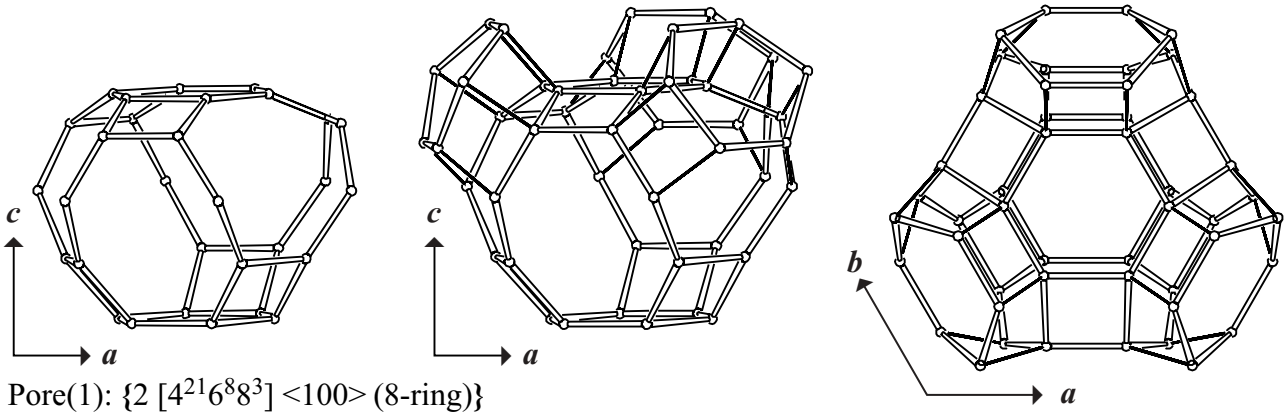
4. Channels and/or cages:

In **CGS**, 8-ring channels parallel to ***b*** and 10-ring channels parallel to ***a*** do intersect. In **ETR** two types of channel intersections (or cavities) are present. The first cavity is the intersection of 8-ring channels parallel to <100>; the second cavity is the intersection of the 18-ring channel parallel to ***c*** with the 8-ring channels. For each intersection the **pore descriptor** is added in Figure 4. The fusion of the cavities is illustrated in Figure 5.

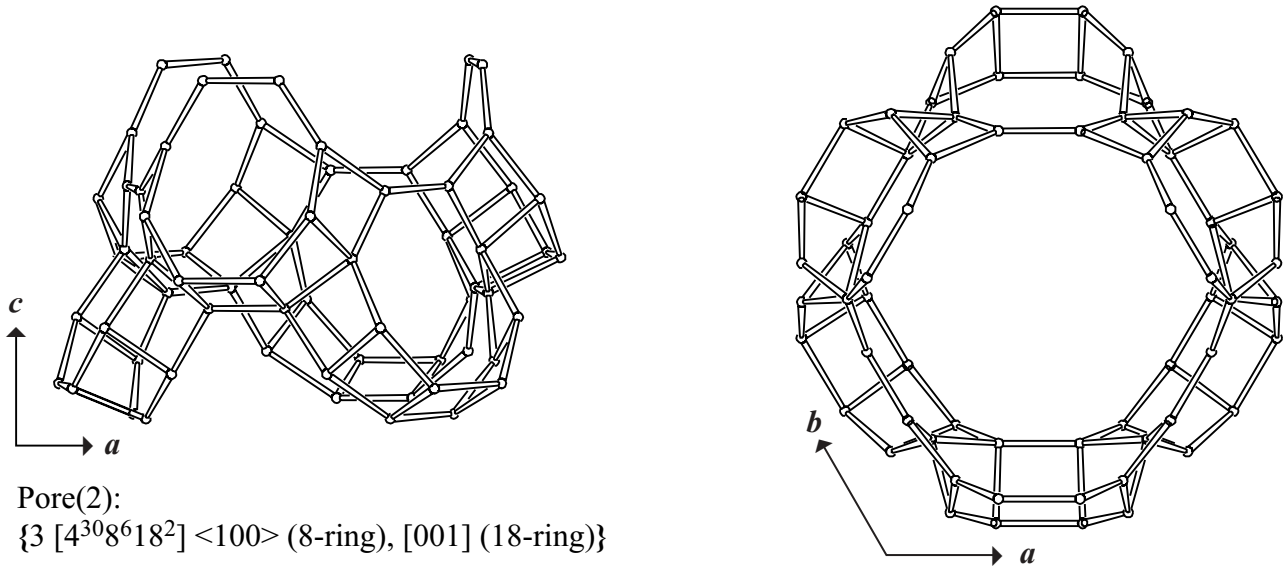


{2 [$4^{12}6^{2}8^{2}10^{2}$] [100] (10-ring), [010] (8-ring)}

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



Pore(1): {2 [$4^{21}6^{8}8^{3}$] <100> (8-ring)}



Pore(2):
{3 [$4^{30}8^{6}18^{2}$] <100> (8-ring), [001] (18-ring)}

Figure 4 [Cont'd]. The two channel intersections in **ETR**. Top: cavity(1) viewed along ***b*** (left and middle), and along ***c*** (right). The drawing at the left is added to illustrate that the free entrance to three of the six 8-rings of cavity(1) are "blocked" by additional 6-rings; Bottom: cavity(2) viewed along ***b*** (left), and along ***c*** (right).

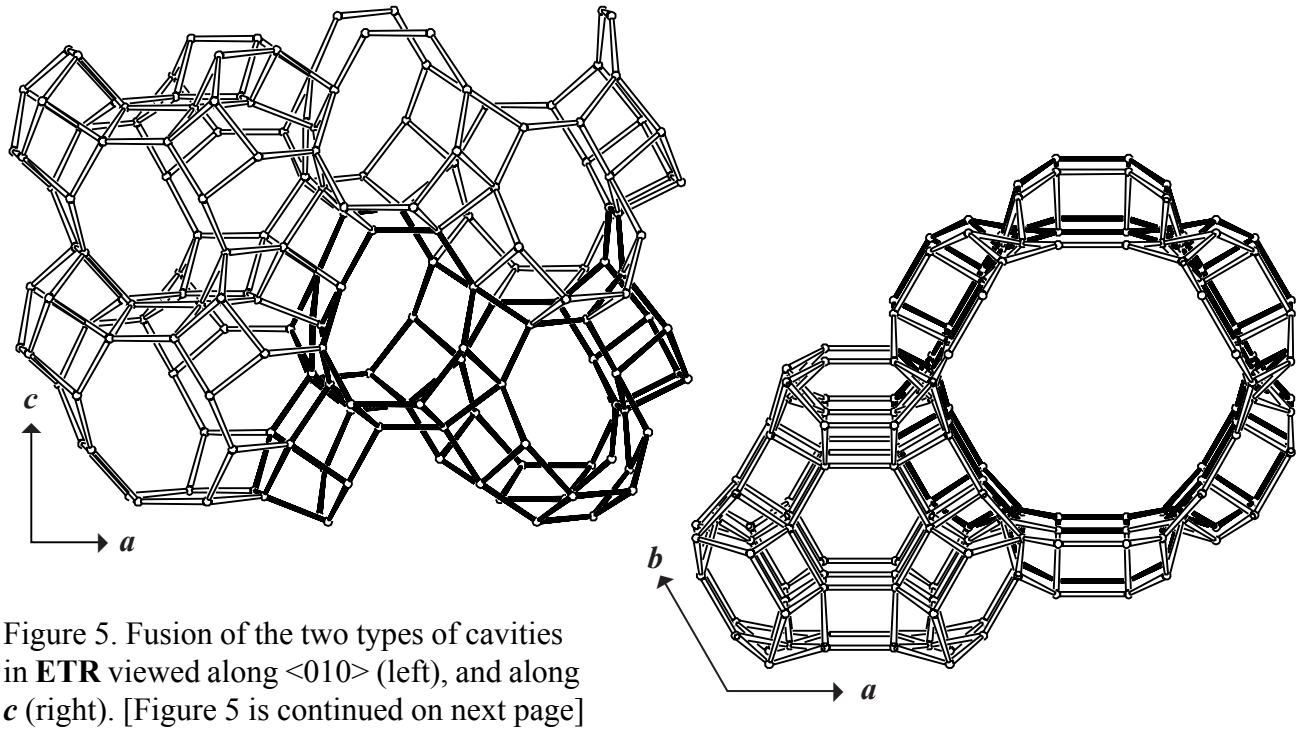


Figure 5. Fusion of the two types of cavities in **ETR** viewed along <010> (left), and along ***c*** (right). [Figure 5 is continued on next page]

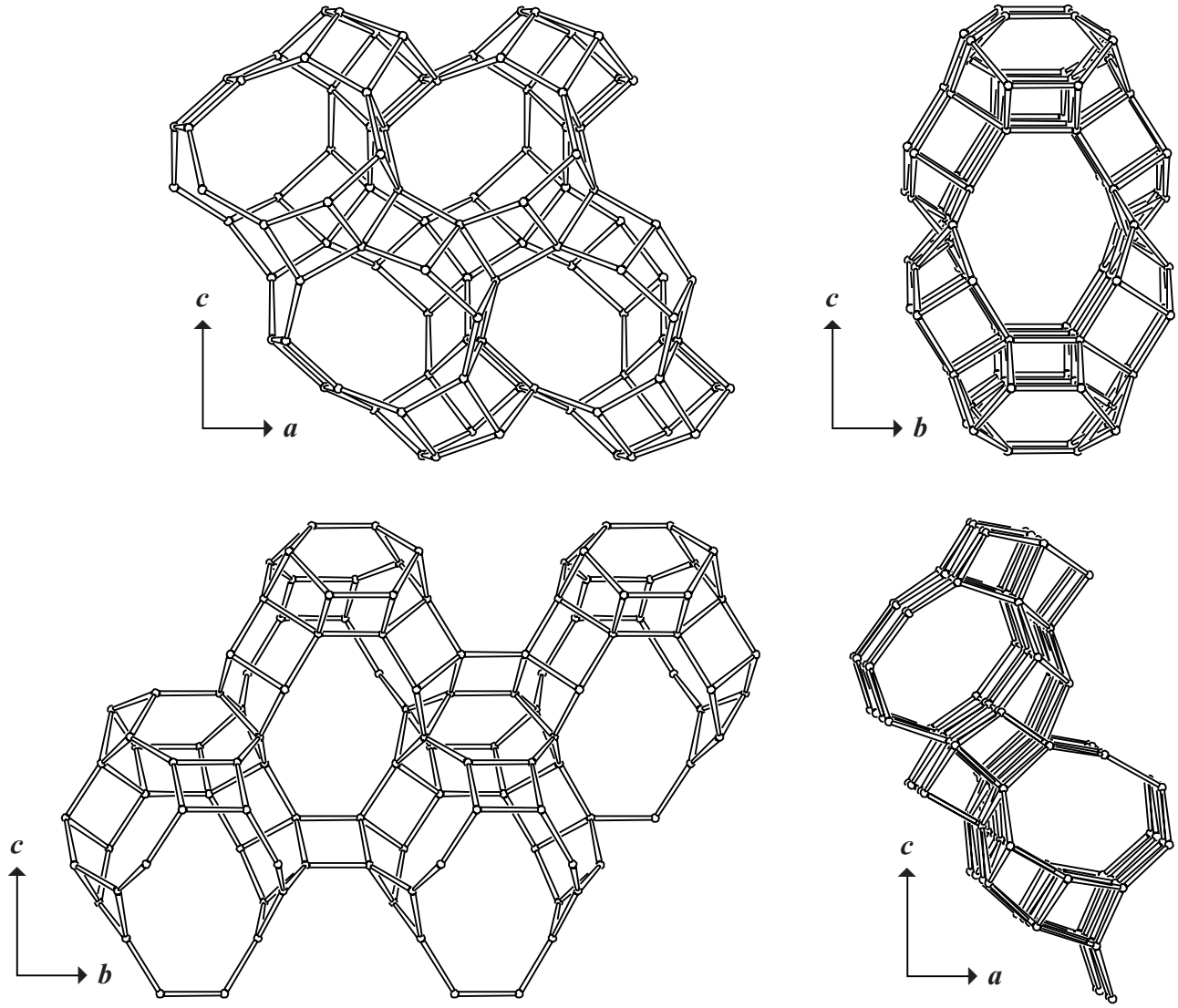


Figure 5 [Cont'd]. Fusion of cavities in **CGS**. Fusion in the ***ac*** layer (top) viewed along ***b*** (left) and along ***a*** (right), and fusion in the ***bc*** layer (bottom) viewed along ***a*** (left) and along ***b*** (right).

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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**).

Alternative description of* CGS *and* ETR *using (modified) double 6-rings (D6Rs)
Several framework types, like **CGS** and **ETR**, can be built using (modified) D6Rs (see Figure 1).
In the **INTRO** pages links are given to a detailed description of a sub-set of framework types that contain (modified) D6Rs (choose: **Double 6-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 7**).