Building scheme for ITE and RTH

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:

ITE and **RTH** can be built using units of 16 T atoms consisting of two sets of three (fused) 4-rings that are related by a rotation of 90º about **y**. T16-units (one in bold in Figure 1), related by pure translations along **y**, are connected into a chain along **y** through 5-rings. A chain of (fused) $[4^45^4]$-cages is formed. Chains, related by a shift of ½**y** (or by a mirror plane perpendicular to **x**) are linked along **x** through 4-rings. The Periodic Building Unit (PerBU) equals the **xy** layer shown in Figure 1.

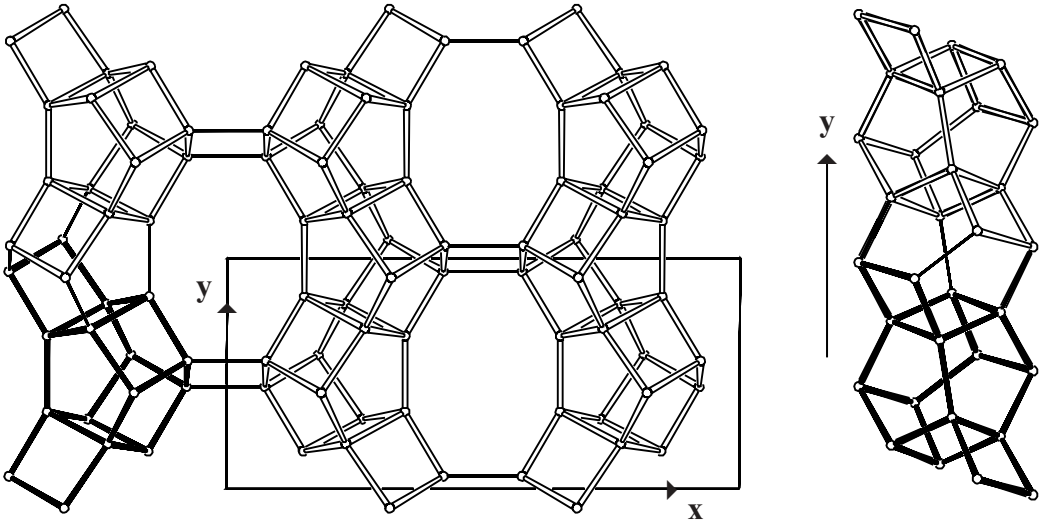

Figure 1. PerBU viewed along **z** (left) and projected along **x** (right).

2. Connection mode:

Neighboring PerBUs are related in two different ways as depicted in Figure 2:
(1): neighboring layers are related by a pure translation along **z** or,
(2): neighboring layers are related by a rotation of 180º about **z** and a shift of 1/2**x**.

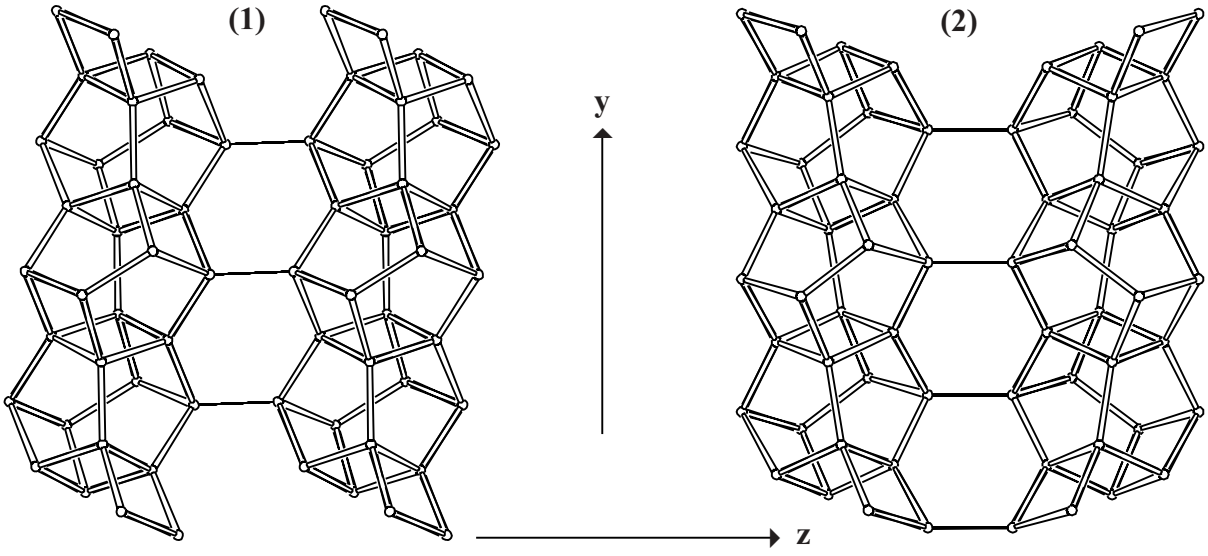

Figure 2. Connection mode **(1)** of the PerBUs observed in **RTH** and connection mode **(2)** observed in **ITE** viewed along **x**.

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

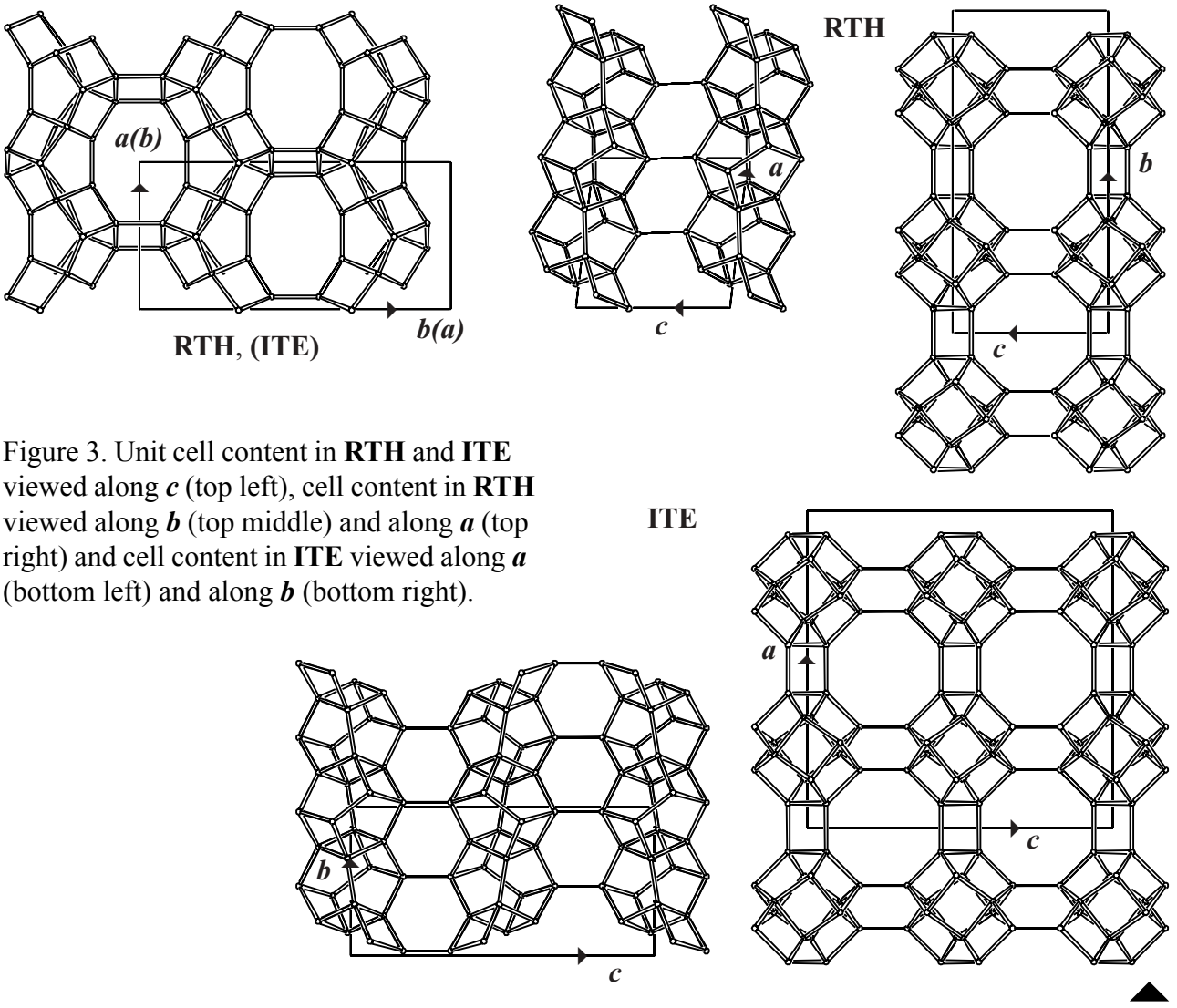

Figure 3. Unit cell content in **RTH** and **ITE** viewed along ***c*** (top left), cell content in **RTH** viewed along ***b*** (top middle) and along ***a*** (top right) and cell content in **ITE** viewed along ***a*** (bottom left) and along ***b*** (bottom right).

4. Channels and/or cages:

The intersections of 8-ring channels (or cavities) in both framework types are depicted in Figure 4. The **pore descriptors** are added. The fusion of cavities is illustrated in Figure 5.

Pore descriptor in **RTH**: {2 [$4^6 5^8 6^4 8^4$] [100] (8-ring), [001] (8-ring)}

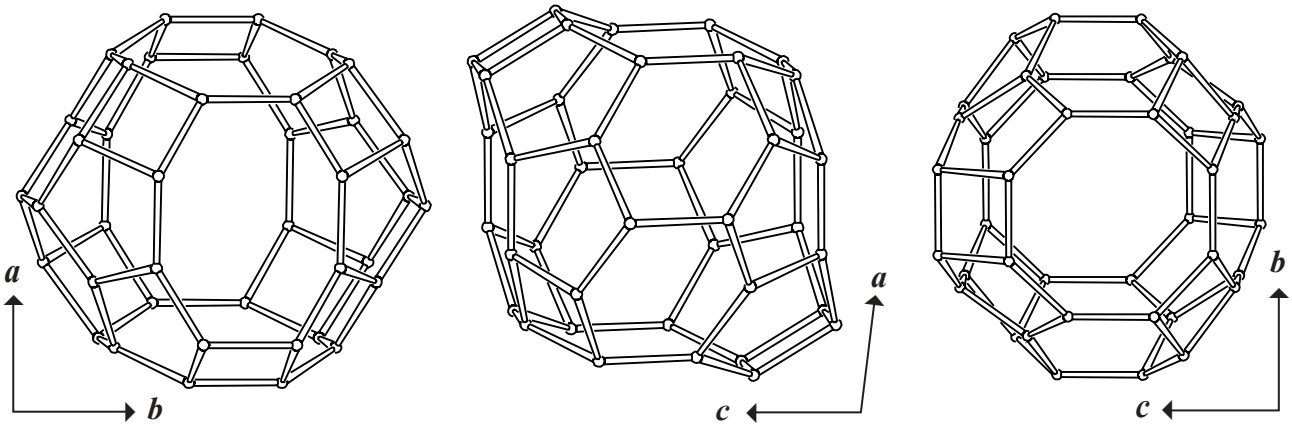

Figure 4. Cavity in **RTH** viewed (from left to right) along ***c***, ***b***, and ***a***.[Figure 4 is continued on next page]

Pore descriptor in **ITE**: {2 [$4^6 5^8 6^4 8^4$] [010] (8-ring), [001] (8-ring)}

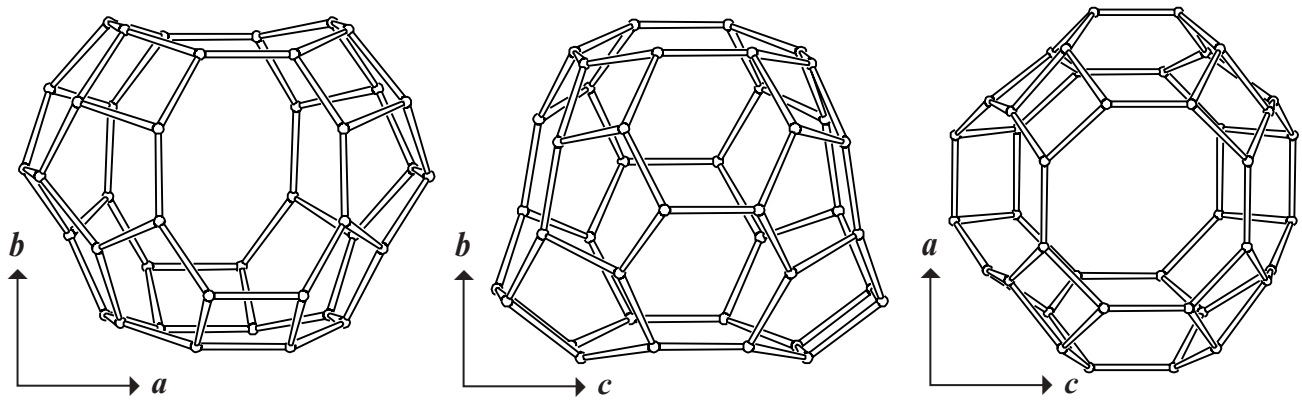

Figure 4 [Cont'd]. Cavity in **ITE** viewed (from left to right) along ***c***, ***a***, and ***b***.

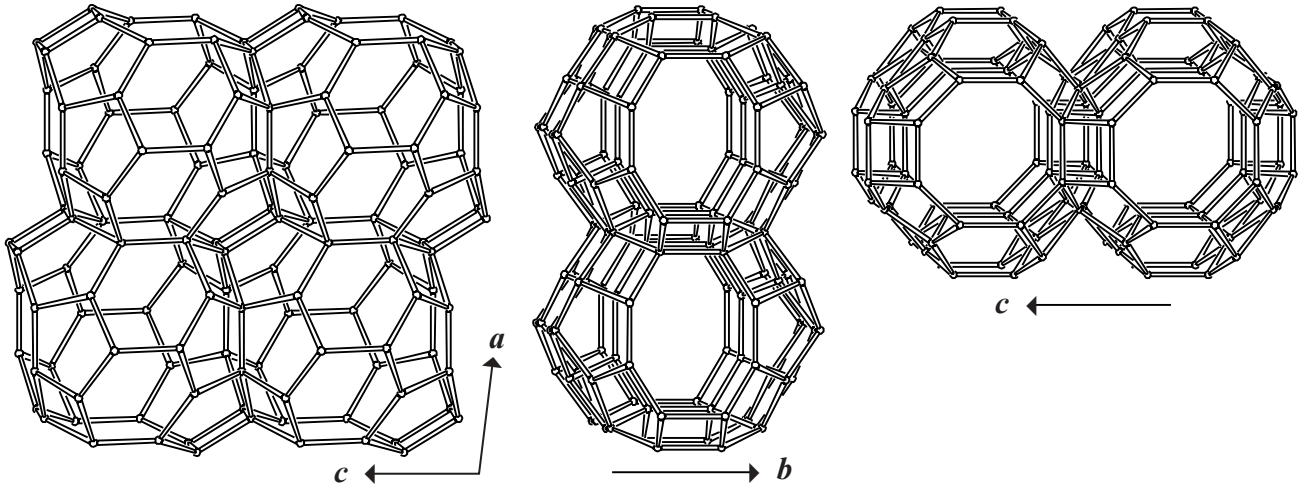

Figure 5. (a): Fusion of cavities in **RTH** into 8-ring channels parallel to ***a*** and ***c*** viewed along ***b*** (left), along the 8-ring channel axis parallel to ***c*** (middle) and along the 8-ring channel axis parallel to ***a***.

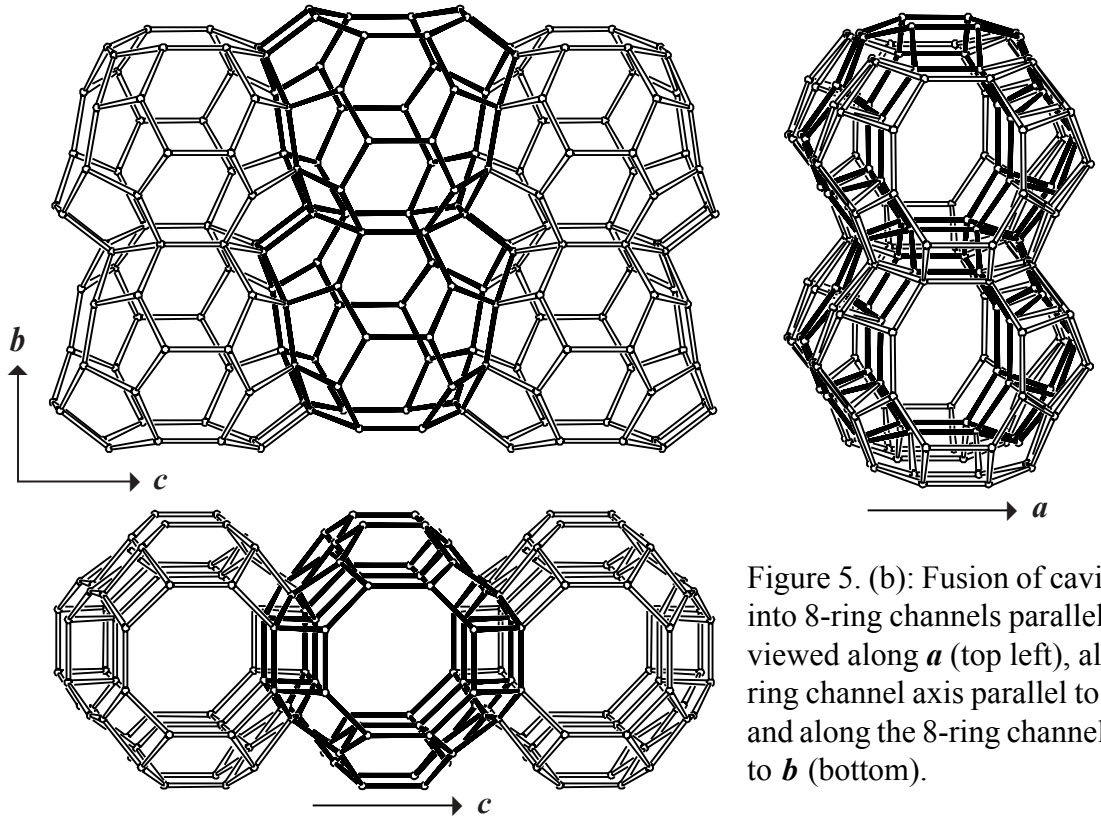

Figure 5. (b): Fusion of cavities in **ITE** into 8-ring channels parallel to ***b*** and ***c*** viewed along ***a*** (top left), along the 8-ring channel axis parallel to ***c*** (top right) and along the 8-ring channel axis parallel to ***b*** (bottom).

5. Supplementary information:

Other framework types containing (modified) single 3- and/or 4-rings

Single 3- and/or 4-rings can be connected in several other ways. In several 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) single 3- and/or 4-rings (choose: **Single 3- and/or 4-rings**). There is also a link to a summary of the Periodic Building Units used in the building schemes of these framework types (choose: **Appendix**; **Figure 4**).