Building scheme for HEU and RRO

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:

HEU and **RRO** can be built using T9-units: a double 4-ring (D4R) with an additional bridging T atom (the 4-4=1 unit; bold in Figure 1). D4Rs, related by a rotation of 180º about an axis parallel to **y** and passing through the bridging T atom (or by mirroring the D4R in the plane of the paper), are connected into chains parallel to **z**. Neighboring chains, related by pure translations along **x** are connected through (fused) 4- and 5-rings into the Periodic Building Unit (PerBU; the **xz** layer).

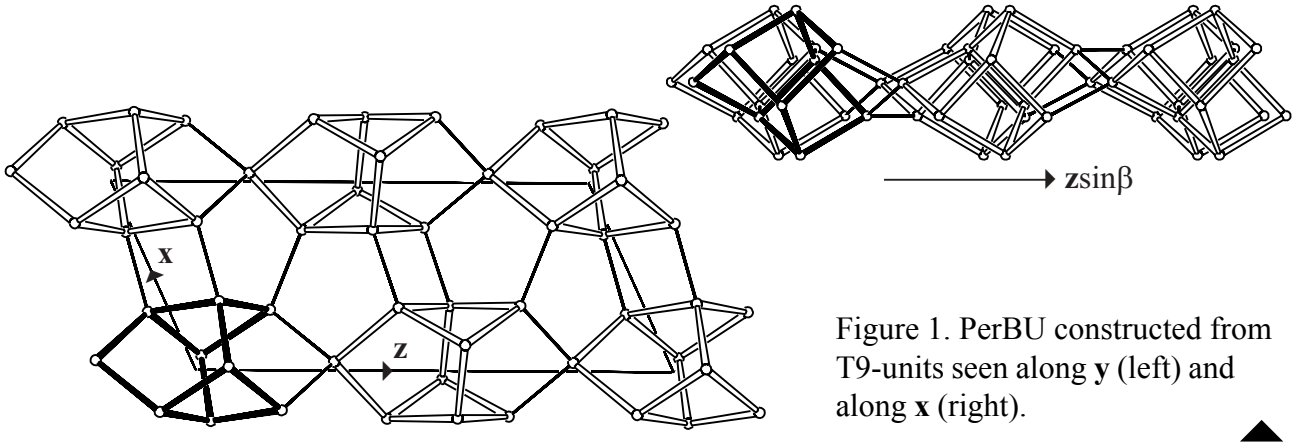


Figure 1. PerBU constructed from T9-units seen along **y** (left) and along **x** (right).

2. Connection mode:

Neighboring PerBUs can be connected along the PerBU plane normal **y** in two different ways:
(1): PerBUs, related by a pure translation along **y**, are connected through single T-T bonds;
(2): PerBUs, related by a rotation of 180º about **y**, are connected through single T-T bonds.
In both connection modes 8- and 10-rings are formed (see Figure 2).

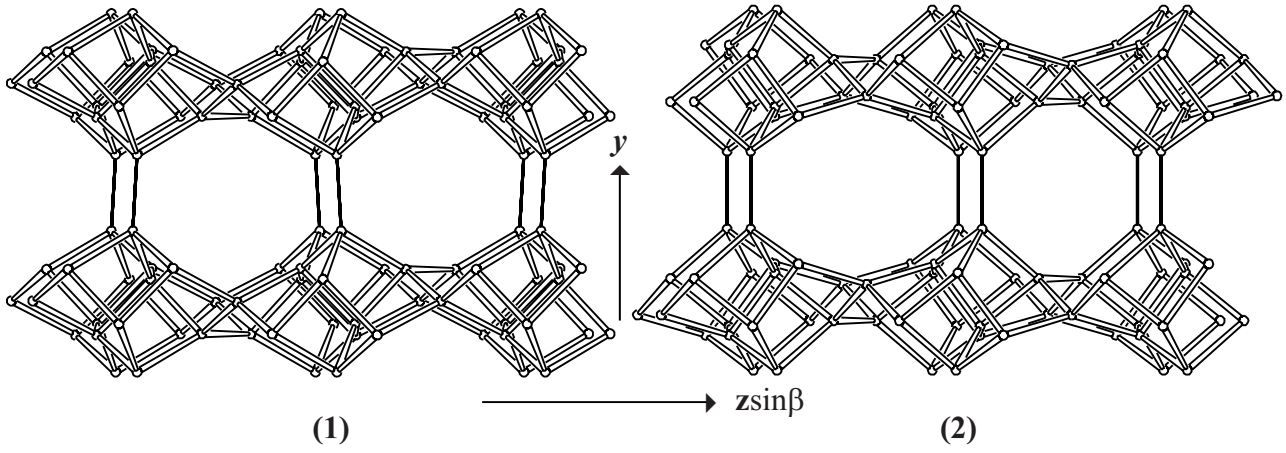


Figure 2. Connection mode **(1)** in **RRO** and connection mode **(2)** in **HEU** viewed along **x**.

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

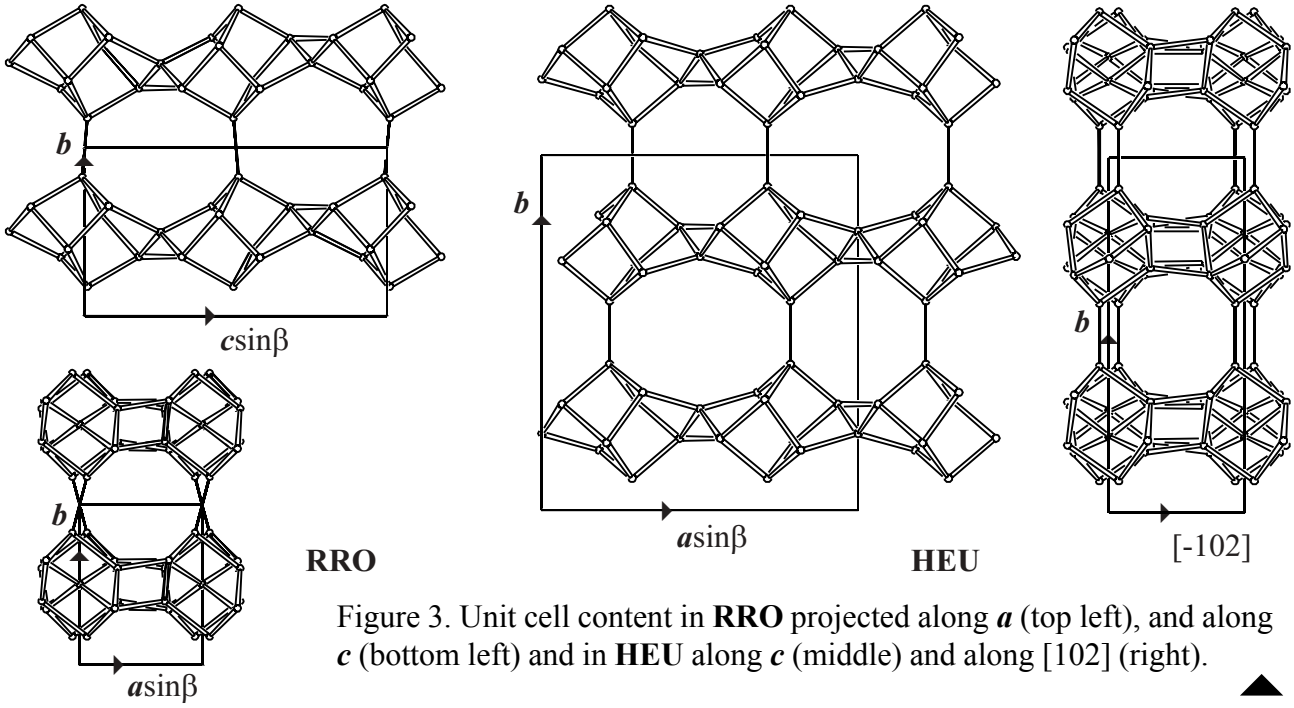
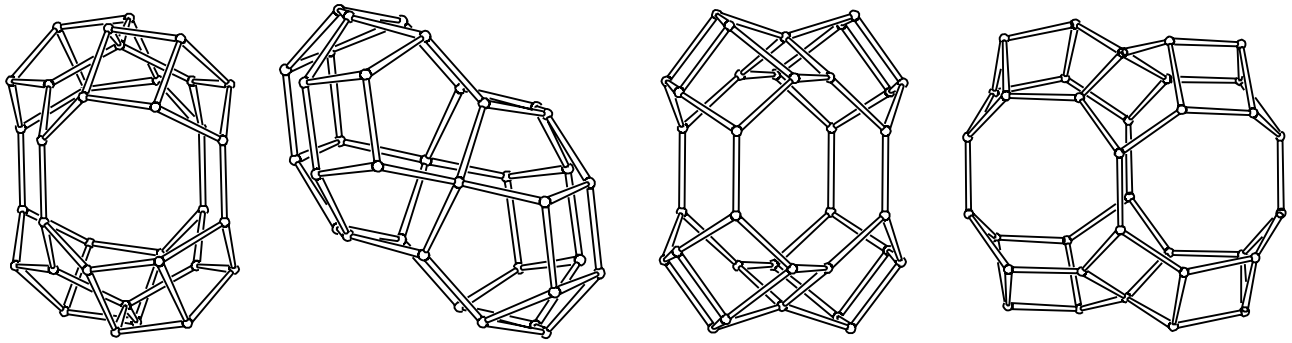


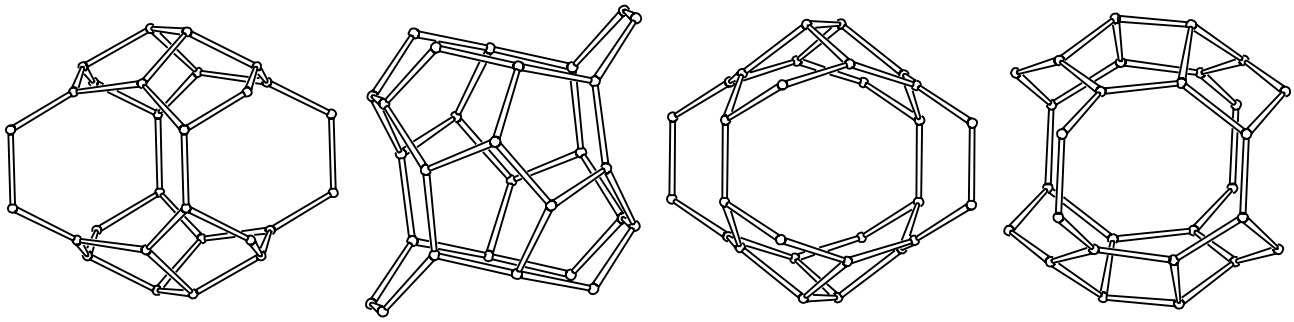
Figure 3. Unit cell content in **RRO** projected along ***a*** (top left), and along ***c*** (bottom left) and in **HEU** along ***c*** (middle) and along [102] (right).

4. Channels and/or cages:

In **HEU**, 8- and 10-ring channels parallel to ***a*** and 8-ring channels parallel to ***c*** form a two-dimensional channel system with two types of intersections that are interconnected through common 8-rings. The intersections are depicted in Figure 4. The fusion of intersections is shown in Fig. 5.



Intersection 1: {2 [$4^8 5^8 8^4$] [100] (8-ring), [001] (8-ring)}

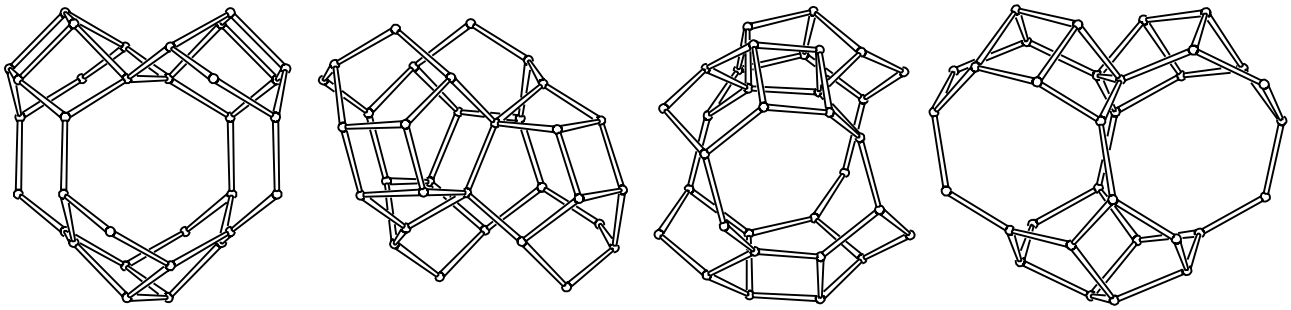


Intersection 2: {2 [$5^8 8^2 10^2$] [102] (8-ring), [100] (10-ring)}

(a)

Figure 4. (a): Intersections of channels in **HEU**, with **pore descriptors**, viewed (from left to right) along ***a***, ***b***, ***c*** and [102]. [Figure 4 is continued on next page]

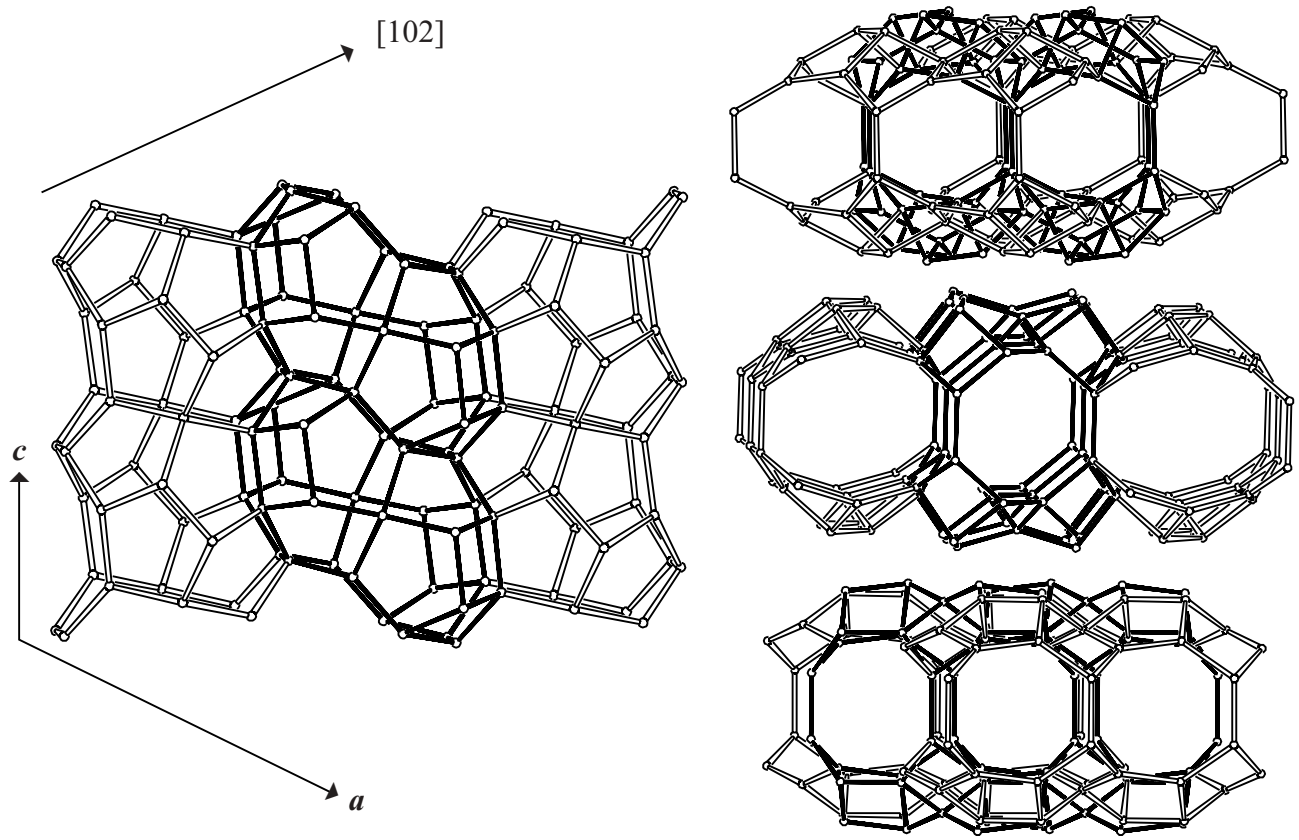
In **RRO**, 10-ring channels are parallel to ***a***, and 8-ring channels are parallel to ***c***. The intersecting two-dimensional channel system has one type of intersection shown in Figure 4(b). Figure 5 illustrates the fusion of intersections.



{2 [$4^4 5^8 8^2 10^2$] [100] (10-ring), [001] (8-ring)}

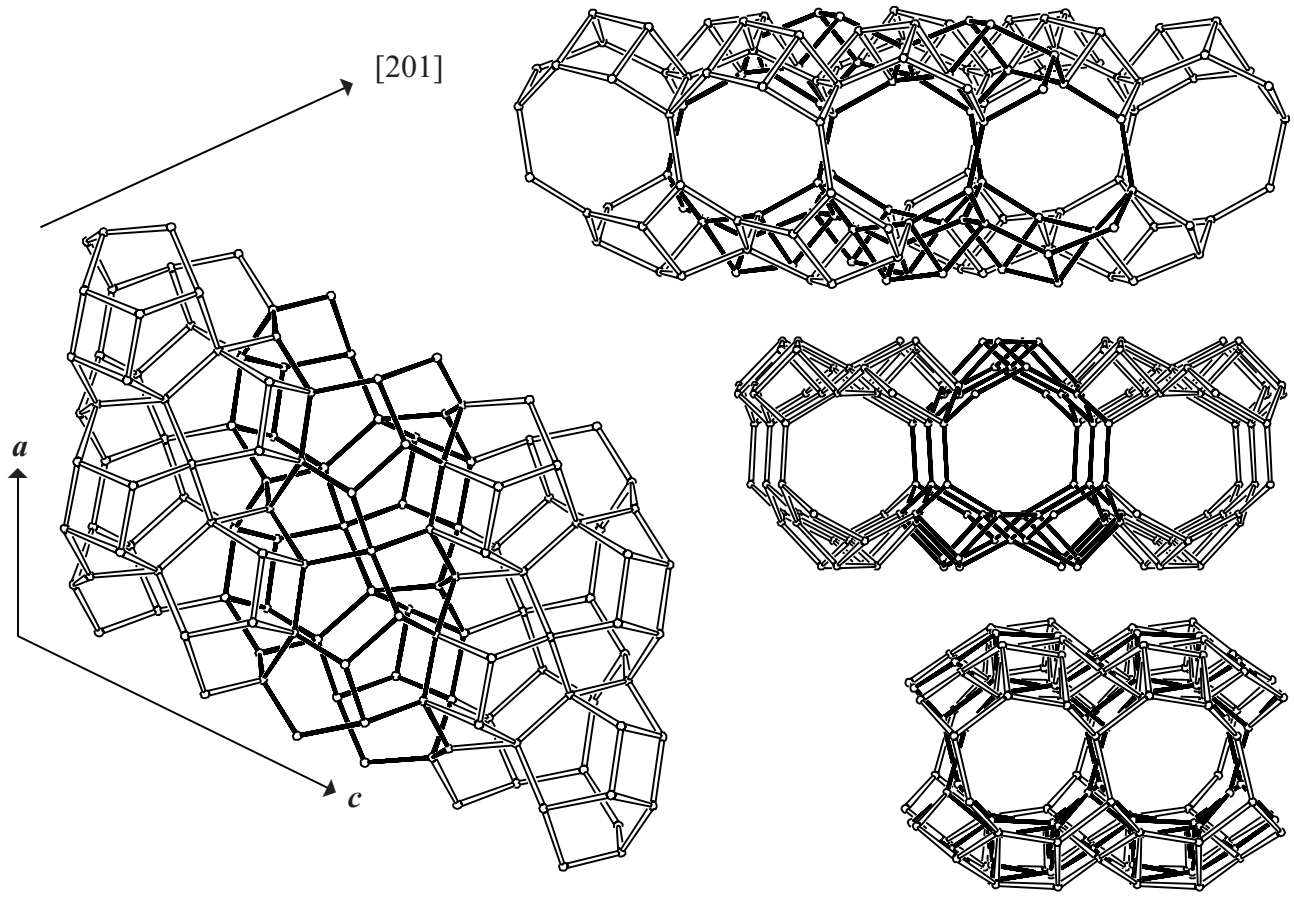
(b)

Figure 4 [Cont'd]. (b): Intersection of channels in **RRO**, viewed (from left to right) along ***a***, ***b***, ***c*** and [201].



(a)

Figure 5. (a): Fused channel intersections in **HEU** viewed along ***b*** (left), and (from top right to bottom right) along ***a***, ***c*** and [102]. [Figure 5 is continued on next page]



(b)

Figure 5 [Cont'd]. (b): Fused channel intersections in **RRO** viewed along ***b*** (left) and (from top right to bottom right) along [201], ***a*** and ***c***.

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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**).