Building scheme for CAS

1. Periodic Building Unit – 2. Connection mode – 3. Projections of the unit cell content
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1. Periodic Building Unit:

CAS can be built using the zigzag (zz) chain (bold in Fig.1) running parallel to ***a***. The repeat distance along the zigzag chain is about 5.2 Å. The repeat unit consists of 2 T atoms. Three zz chains are connected to an infinite building unit. A two-dimensional Periodic Building Unit (PerBU) is obtained when infinite building units, related by a 2-fold axis parallel to the plane of the paper (pointing from top to bottom) are connected along ***c*** into a layer of (fused) 6-ring chairs and 6-ring boats decorated with additional zz chains as shown in Figure 1. [Compare this PerBU with those in **BIK** and **NSI**]

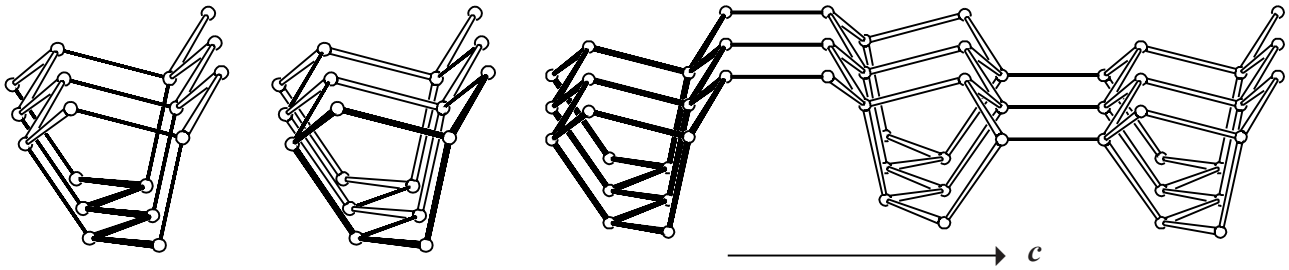

Figure 1. Infinite building unit constructed from three zz chains (left) and from 5-1-units (middle; see also: **Alternative description**) seen along the chain axis ***a***. Right: PerBU in **CAS**.

2. Connection mode:

Neighboring PerBUs, related by a shift of ½***a***, are connected along ***b*** through 5-rings. Two zz chains of the infinite building unit are involved in the (fused) 6-ring layer and the third zz chain (in bold) connects the 6-ring layers. [Compare this connection mode with those in **BIK** and **JBW**]

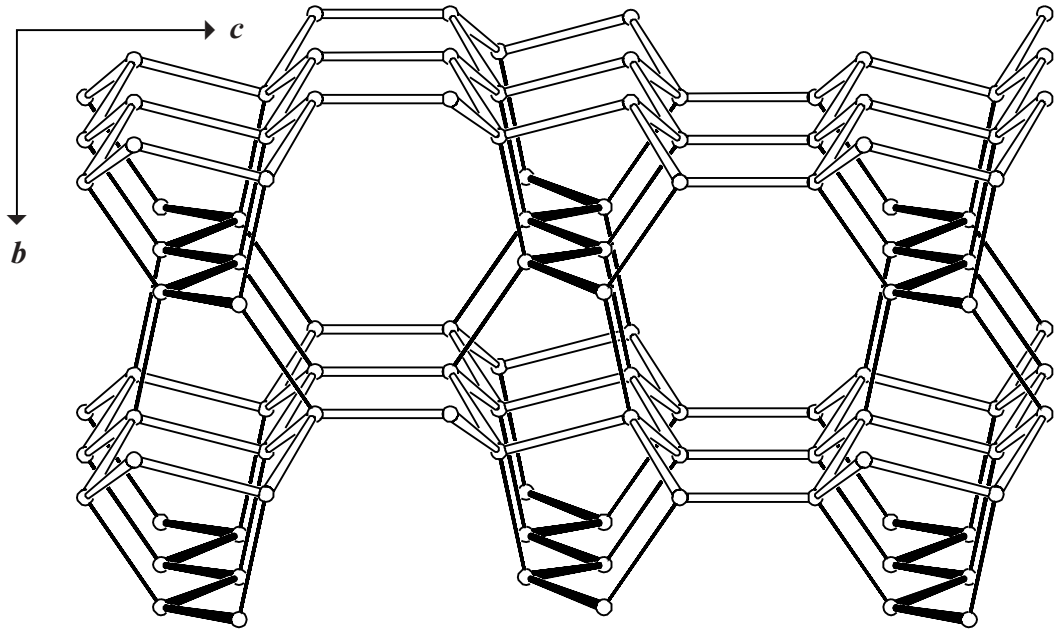

Figure 2. Connection mode in **CAS** viewed along ***a***.

3. Projections of the unit cell content:

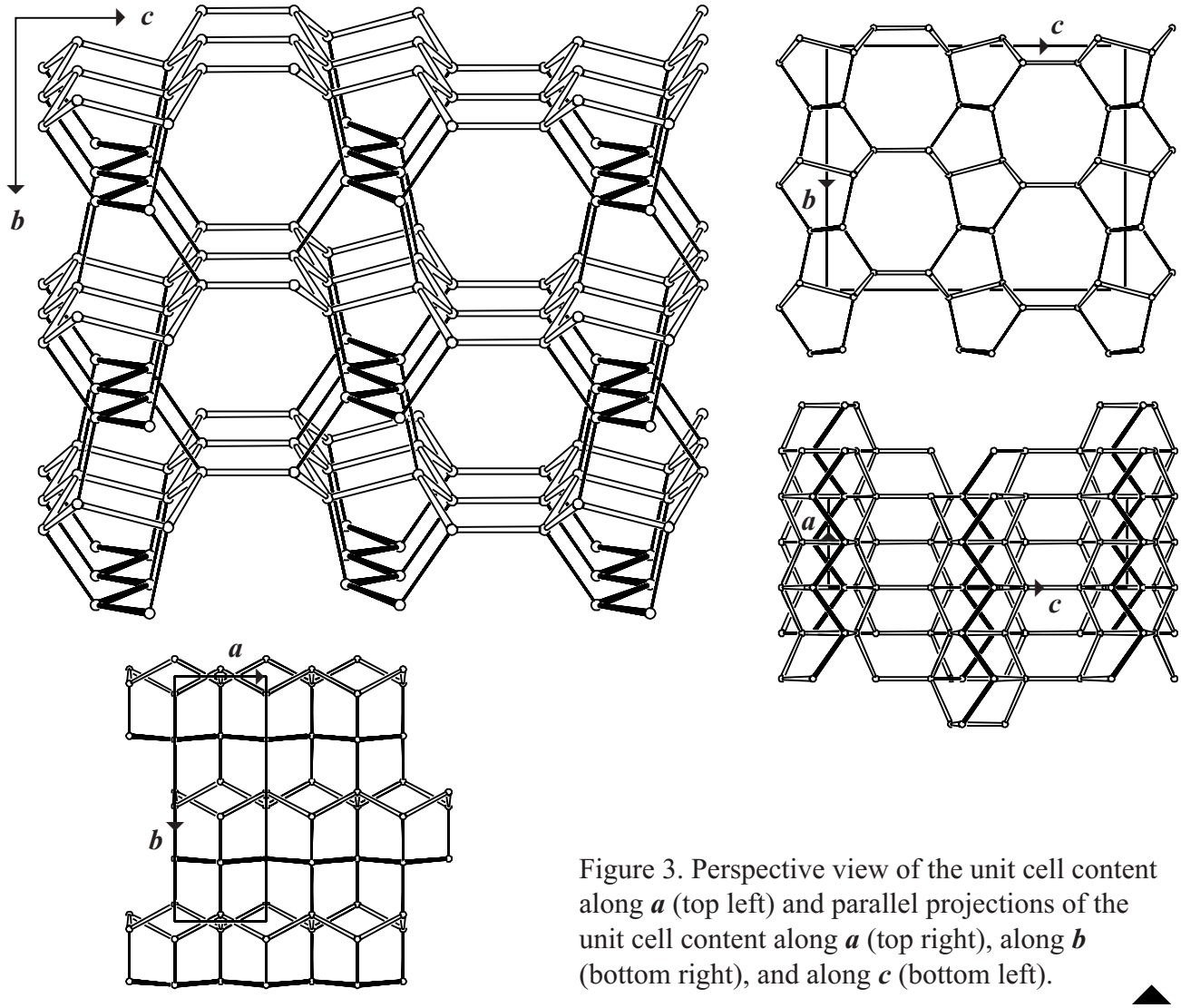

Figure 3. Perspective view of the unit cell content along ***a*** (top left) and parallel projections of the unit cell content along ***a*** (top right), along ***b*** (bottom right), and along ***c*** (bottom left).

4. Channels and/or cages:

The 8-ring channel in **CAS**, depicted in Figure 4, is parallel to ***a***.

{1 [$6^6 8^{2/2}$] [100] (8-ring)}

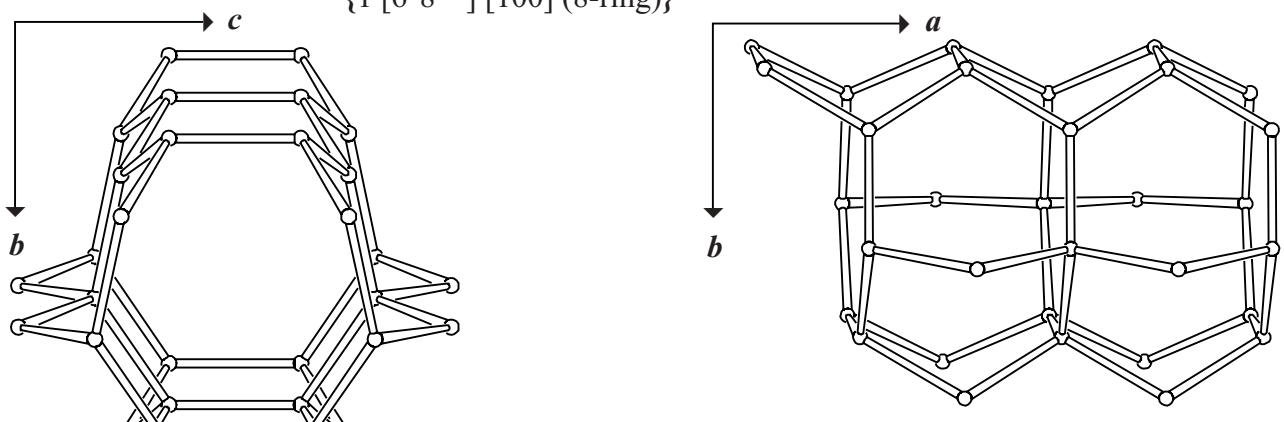

Figure 4. Channel in perspective view along ***a*** (left), and along ***c*** (right). The **pore descriptor** is added.

5. Supplementary information:

Other framework types containing zigzag chains
In several framework types at least one of the unit cell dimensions is about n*5.2 Å (where n = 1, 2, 3, etc.). In many cases this indicates the presence of zigzag chains.
In the **INTRO** pages links are given to detailed descriptions of these framework types (choose: **Zigzag chains**). 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 1**).

Alternative description using (modified) 5-rings
Several framework types, like **CAS**, can be constructed using (modified) 5-rings.
In the **INTRO** pages links are given to detailed descriptions of these framework types (choose: **5-Rings**). There is also a link provided to a summary of the Periodic Building Units used in the building schemes of these framework types (choose: **Appendix**; **Figure 6**).