

Building scheme for GIS



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

GIS can be built using the crankshaft chain (bold in Fig.1 (left)) running parallel to a . The repeat distance along a crankshaft chain varies between 8.4-9.9 Å. The repeat unit consists of 4 T atoms. A one-dimensional Periodic Building Unit (PerBU) is obtained when two crankshaft chains and two 4-rings are connected in such a way that a channel with an 8-ring aperture is formed. The channel wall consists of 4- and 12-rings. The repeat unit of the PerBU consists of a 4-fold (1,2,3,4)-connected double 8-ring (D8R) (bold in Fig.1 (right)). [The 4-fold connection in the D8R in **GIS** is different from the connection in the D8R in **APC**, **APD** and **MER**]

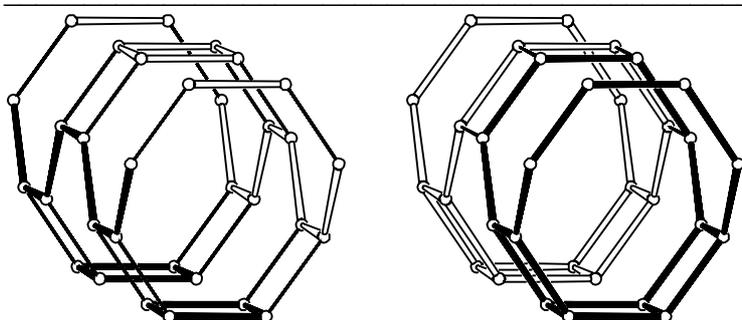


Figure 1. PerBU constructed from crankshaft chains and 4-rings (left) and PerBU constructed from 4-fold connected D8Rs (right).



2. Connection mode:

Neighboring PerBUs, related along b and c by pure translations, are connected through 4-rings that form double-crankshaft chains.

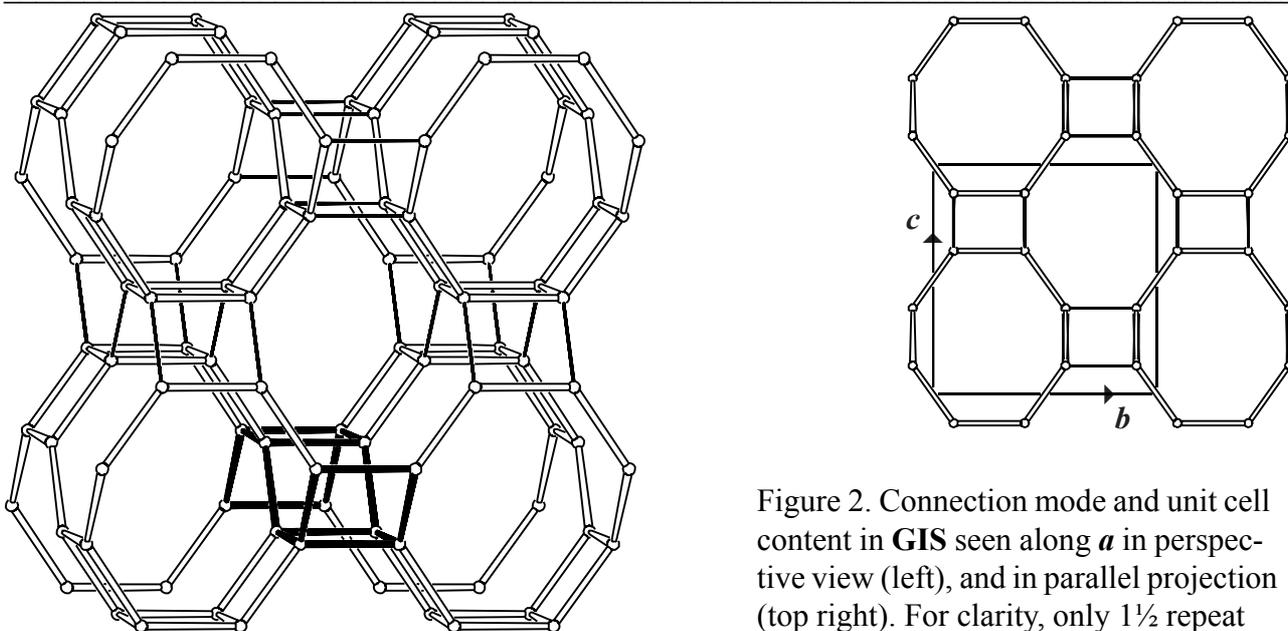


Figure 2. Connection mode and unit cell content in **GIS** seen along a in perspective view (left), and in parallel projection (top right). For clarity, only $1\frac{1}{2}$ repeat units of the PerBUs along a are drawn.

One double crankshaft chain, consisting of 2-fold (1,2)-connected double 4-rings, is indicated in bold (see **Alternative description**).



3. Projections of the unit cell content: See Figure 2. [Projections along *a* and *b* are equivalent]

4. Channels and/or cages:

The channel intersection is shown in Figure 3(a). The **pore descriptor** is added. Fused intersections form interconnecting channels parallel to [100] and [010] as depicted in Figure 3(b).

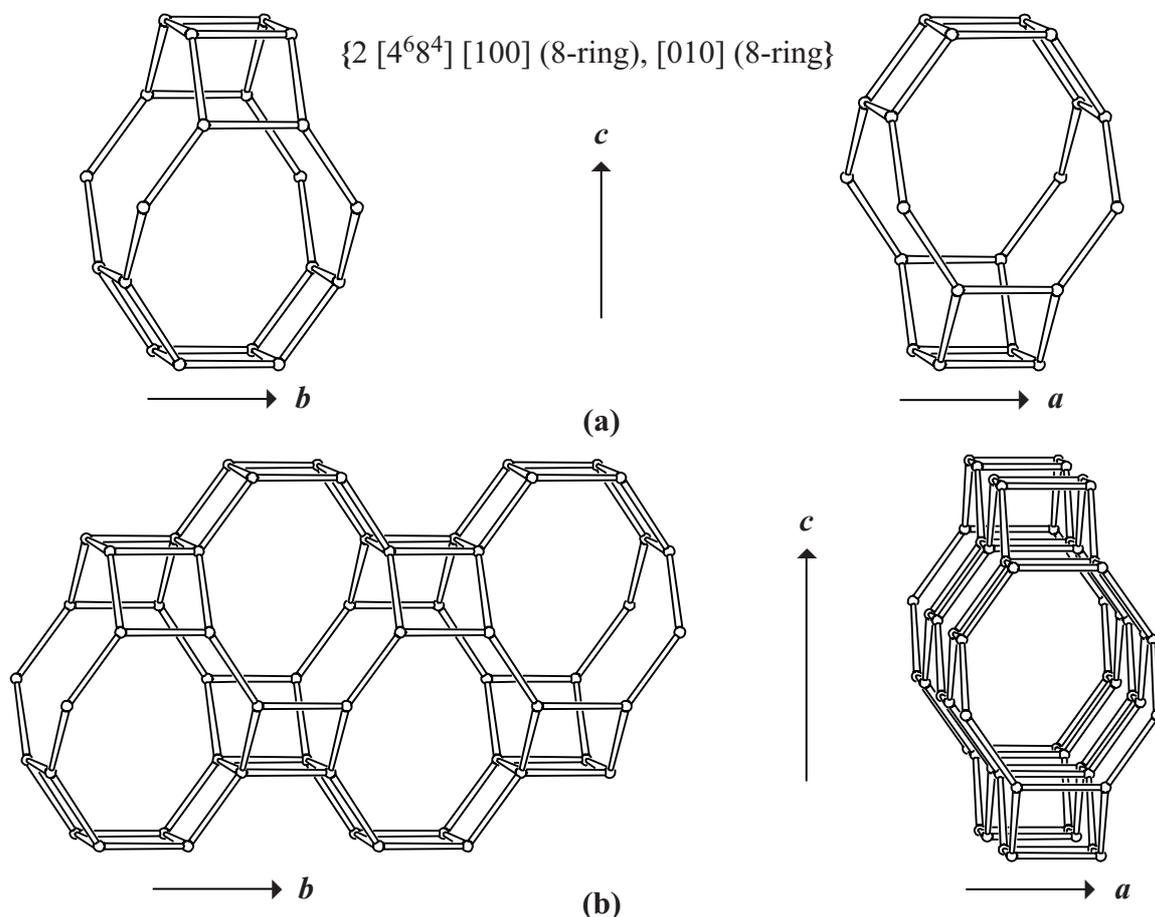


Figure 3. (a): Channel intersection viewed along *a* (left), and along *b* (right); (b): Fused cavities, (connected along *b* (or *a*)), viewed along *a* (or *b*) (left), and along *b* (or *a*) (right).

5. Supplementary information:

Other framework types containing crankshaft chains

In several framework types at least one of the unit cell dimensions is between 8.4 and 9.9 Å. In many cases this indicates the presence of crankshaft chains.

In the **INTRO** pages links are given to detailed descriptions of these framework types (choose: **Crankshaft chains**). 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 3**).

Alternative description of GIS using (modified) double 4-rings (D4Rs)

Several framework types, like GIS, can be built using double crankshaft chains of the feldspar type consisting of 2-fold (1,2)-connected D4Rs (see Figure 2).

In the **INTRO** pages links are given to descriptions of other framework types containing (modified) D4Rs (choose: **Double 4-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 5**).