

Building scheme for ATS



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

ATS can be built using the zigzag chain (bold in Fig.1 (left)) running parallel to c . The repeat distance along the zigzag chain is about 5.2 Å. The repeat unit consists of 2 T atoms. The one-dimensional Periodic Building Unit (PerBU) is obtained when six zigzag chains are connected into two bands of fused 6-ring boats that are connected through a double zigzag chain. The repeat unit of the PerBU contains 12T atoms and is composed of two doubly connected 6-ring boats (bold in Fig.1 (right)).

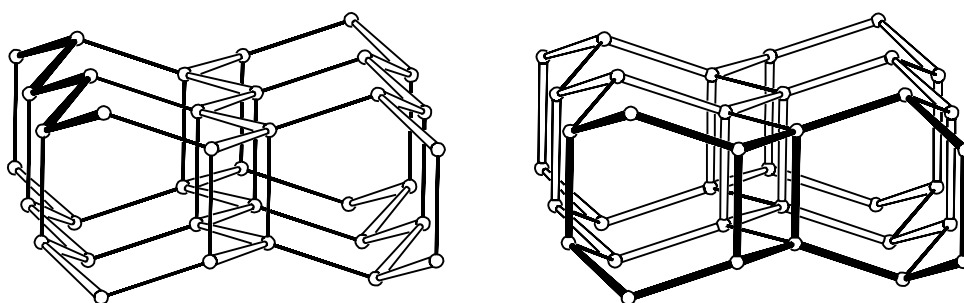


Figure 1. PerBU constructed from six zigzag chains (left) and PerBU constructed from doubly connected 6-ring boats.



2. Connection mode:

Neighboring PerBUs, related by a shift of $\frac{1}{2}(a + b)$, are connected through T4-rings. Double zigzag chains are formed.

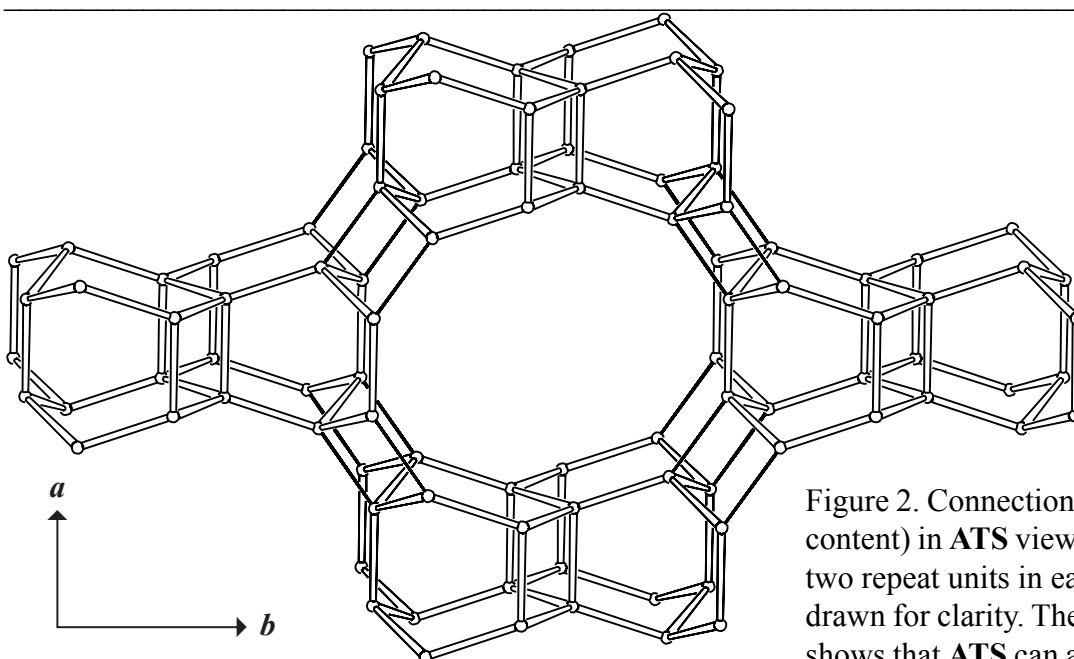


Figure 2. Connection mode (and cell content) in ATS viewed along c . Only two repeat units in each PerBU are drawn for clarity. The Figure also shows that ATS can as well be built using 4-rings or 12-rings.



3. Projections of the unit cell content:

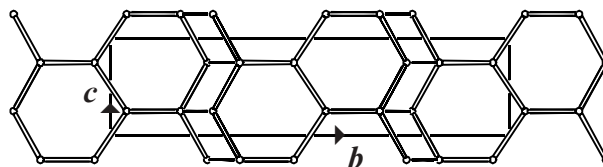
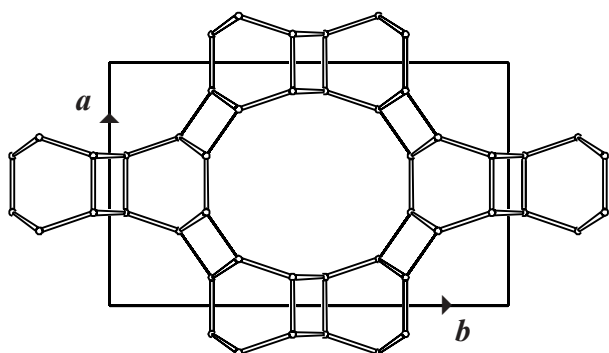
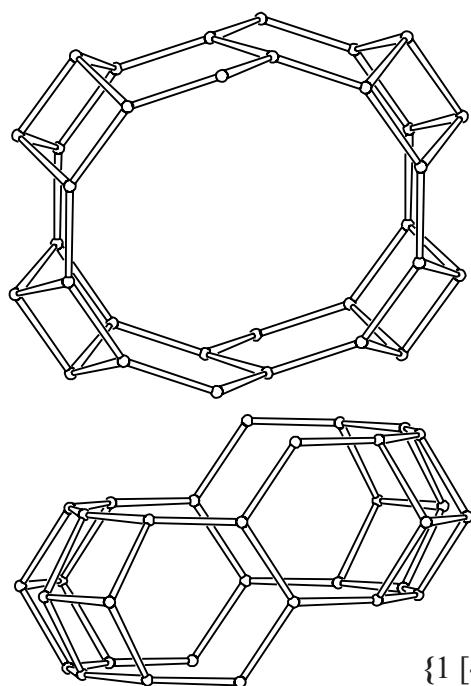


Figure 3. Parallel projection of the unit cell content in ATS along c (left), and along a (right).

4. Channels and/or cages:

Cavities with side-pockets, consisting of 6- and 4-rings, are connected through common 12-rings to channels running parallel to c as depicted in Figure 4. The **pore descriptor** is added.



{1 [4⁸6⁶12^{2/2}] [001] (12-ring)}

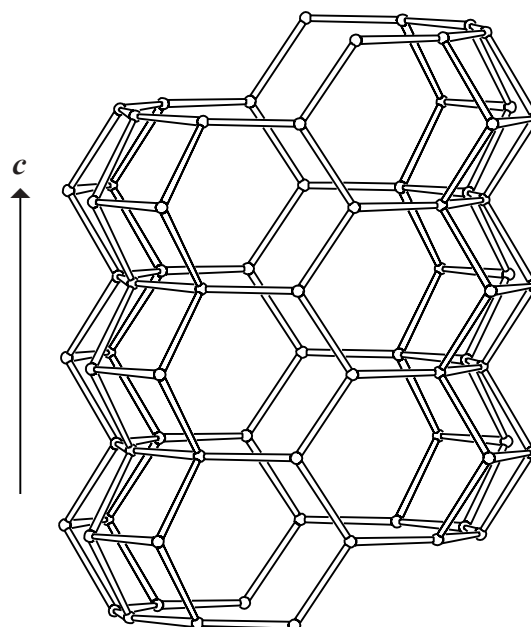


Figure 4. Cavity in ATS in viewed along c (top left) and normal to c (bottom left). Fused cavities form non-interconnecting 12-ring channels parallel to c (right).

5. Supplementary information:

Other framework types containing zigzag chains

In several framework types at least one of the unit cell dimensions is about $n \cdot 5.2 \text{ \AA}$ (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**).