Building scheme for ATO and CAN

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:

The framework types **ATO** and **CAN** can be built using the zigzag chain (bold in Figure 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 a cylindrical pore with a 12-ring window. The repeat unit of the PerBU is a 12-ring (bold in Fig.1 (right)). The cylinder wall consists of fused 6-rings. [See also: **alternative description** of **CAN**]

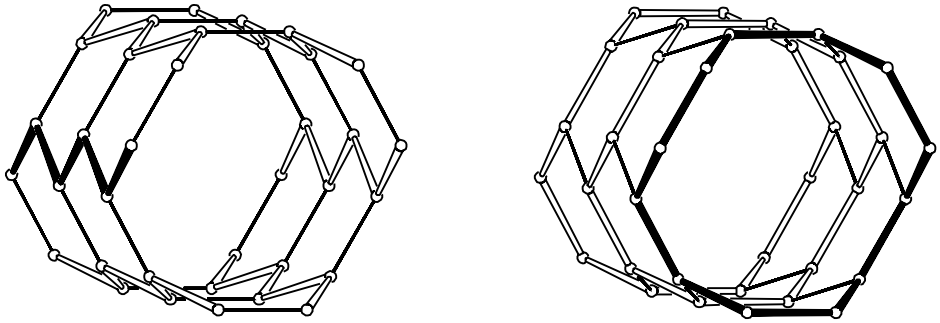

Figure 1. PerBU constructed from six zigzag chains (left) and PerBU constructed from 12-rings (right).

2. Connection mode:

Three neighboring PerBUs can be connected in two different ways:
(1): neighboring PerBUs are connected through 4-rings around a 3-fold screw axis parallel to ***c***;
(2): three neighboring PerBUs are connected through double zigzag chains around a 3-fold rotation axis parallel to ***c*** .[Compare the connection modes with those in **ATN** and **BCT**]

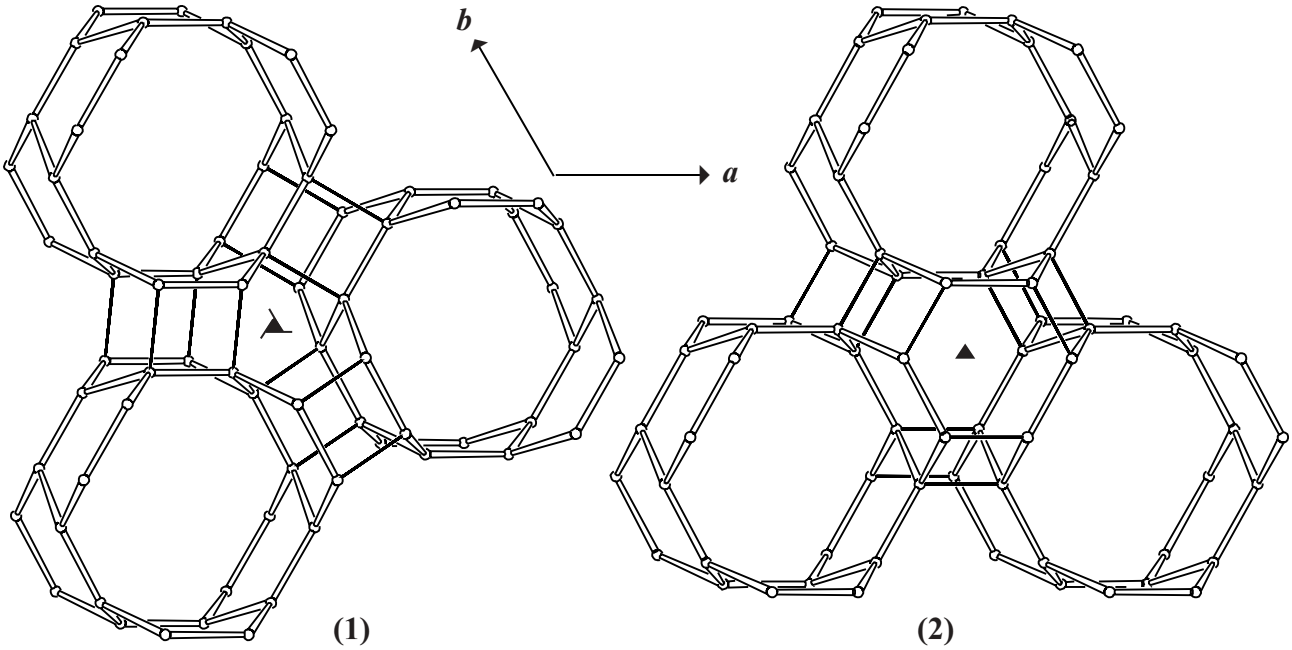

Figure 2. Connection mode **(1)** in **ATO** (left) and connection mode **(2)** in **CAN** (right) viewed along ***c***. Only two repeat units of the PerBUs are drawn for clarity.

3. Projections of the unit cell content:

Pure **ATO** and **CAN**, shown in Figure 3, are obtained when three neighboring PerBUs are exclusively related by 3-fold screw axes parallel to ***c*** and by 3-fold rotation axes parallel to ***c***, respectively.

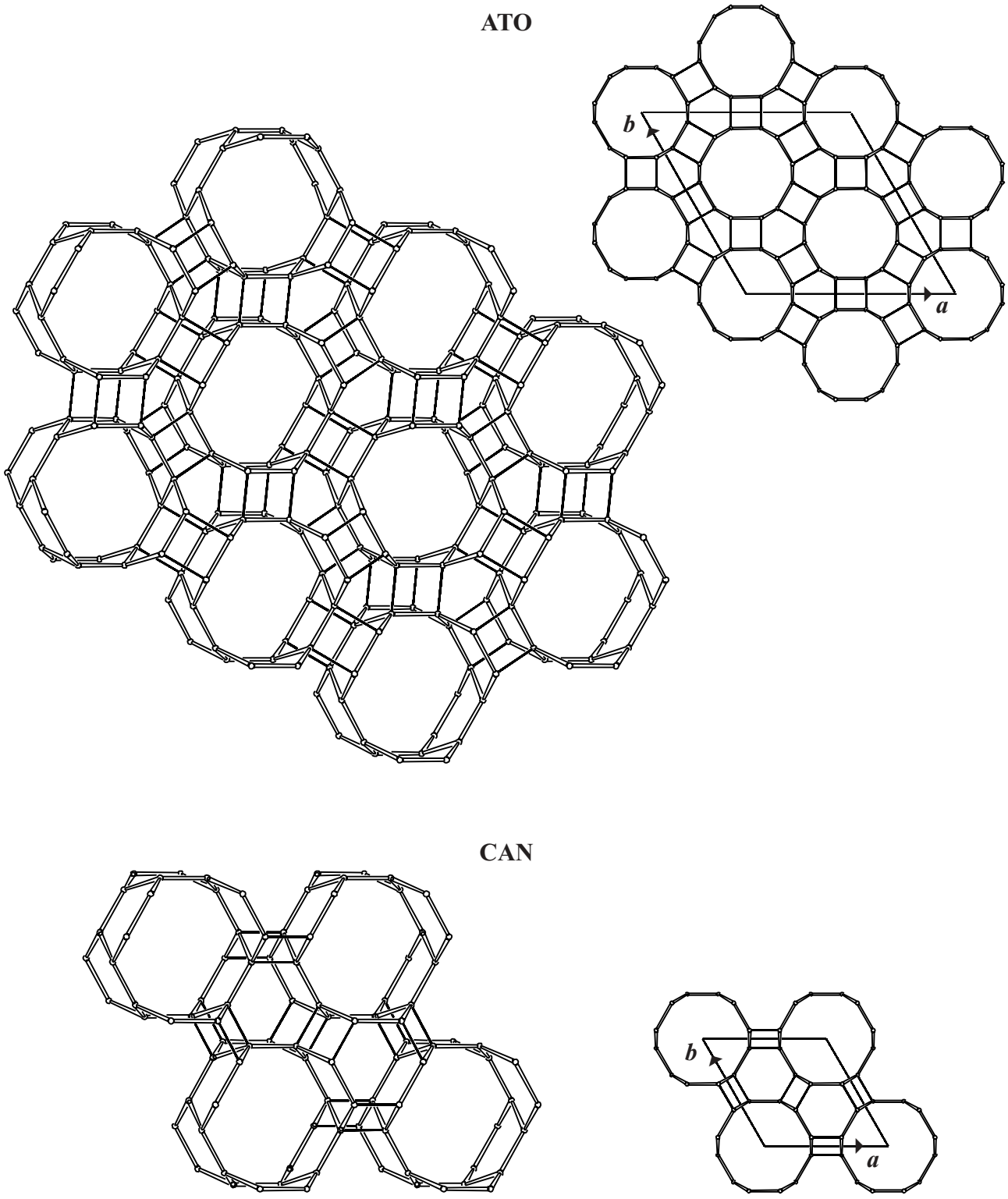

Figure 3. Cell content in **ATO** (top) and in **CAN** (bottom) viewed along ***c*** in perspective (left), and in projection (right). [Both structure types can as well be constructed using 4- or 6-rings as can be seen from the Figure]

4. Channels and/or cages:

Channels run parallel to ***c*** and are equal to the PerBU. The channel wall consists of fused 6-rings as depicted in Figure 4. The **pore descriptor** is added in Figure 4.

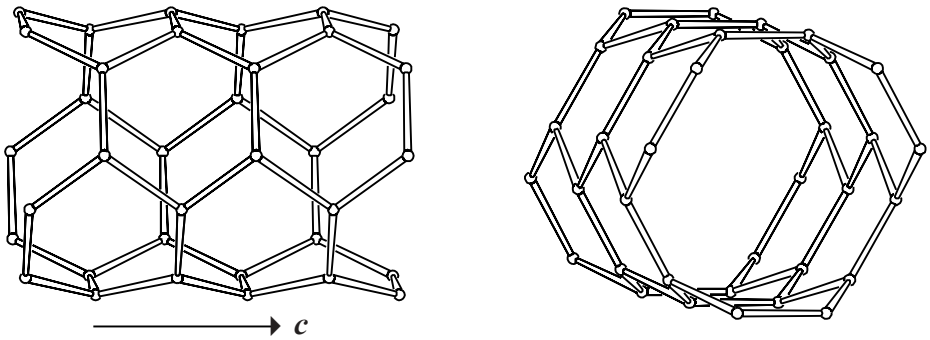

Figure 4. Channel in **ATO** and **CAN** viewed normal to the chain axis ***c*** (left), and along ***c*** (right).

{1 [$6^6 12^{2/2}$] [001] (12-ring)}

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 of* CAN *using a hexagonal array of non-connected 6-rings
A large number of framework types, like **CAN**, can be constructed using a hexagonal array of non-connected 6-rings as PerBU. They all belong to the ABC-6 family. In these framework types the unit cell dimension along the hexagonal axis is ≈(n*)2.55 Å where n is equal to the number of PerBUs that are connected along the hexagonal axis.
In the **INTRO** pages links are given to detailed descriptions of framework types belonging to the ABC-6 family (choose: **ABC-6 family**).