

# Building scheme for ATN and BCT



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:

ATN and BCT 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 four zigzag chains are connected into a cylindrical pore with an 8-ring window. The repeat unit of the PerBU is an 8-ring (bold in Fig.1(right)). The cylinder wall consists of fused 6-rings.

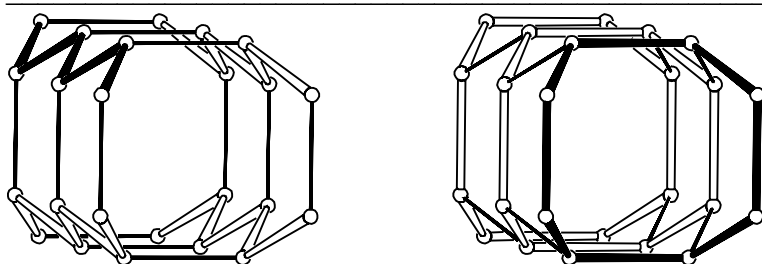


Figure 1. PerBU constructed from four zigzag chains (left) and PerBU constructed from 8-rings (right).



## 2. Connection mode:

Neighboring PerBUs can be connected along  $a$  and  $b$  in two different ways:

- (1): PerBUs, related by a shift of  $\frac{1}{2}(a + b + c)$ , are connected through double zigzag chains which form (fused) *atn* cavities.  
(2): PerBUs, related by pure translations along  $a$  and  $b$ , are connected through 4-rings.  
[Compare these connection modes with the connection modes in **ATO** and **CAN**]

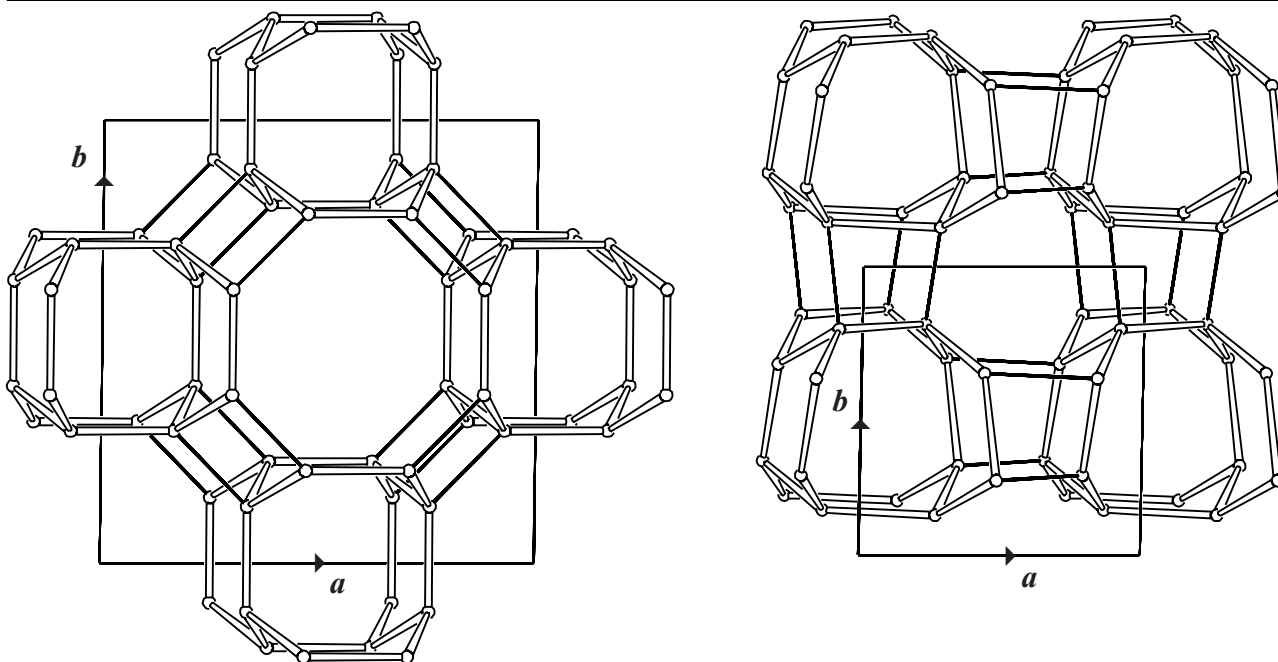


Figure 2. Connection mode (1) in ATN (left), and mode (2) in BCT (right) viewed along  $c$ .  
[Both structure types can as well be built using 4-rings as can be seen from the Figure]



### 3. Projections of the unit cell content:

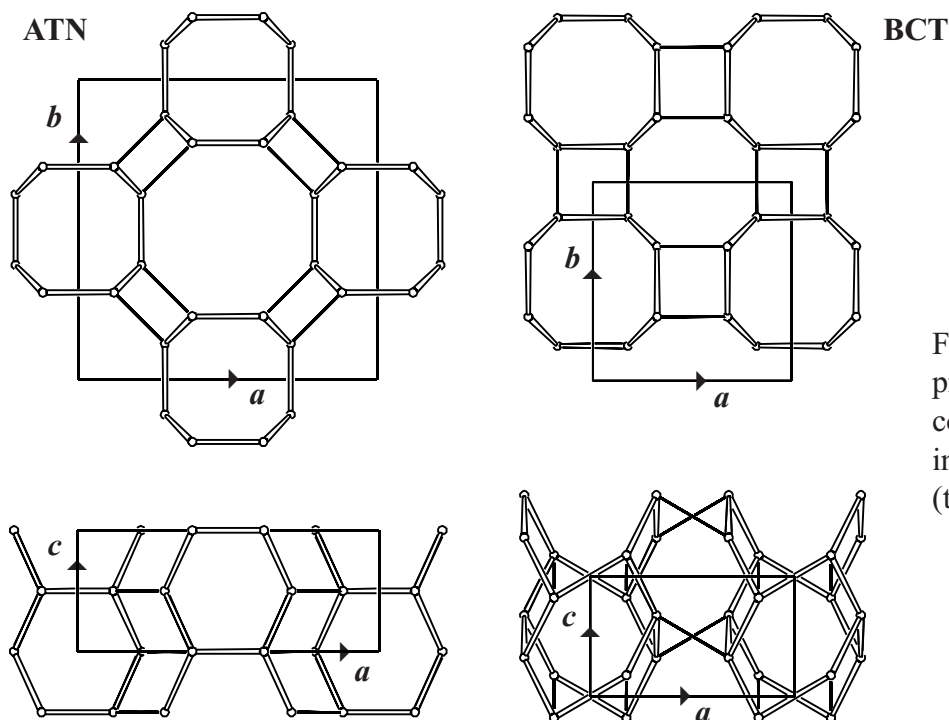


Figure 3. Parallel projections of the unit cell content in **ATN** (left), and in **BCT** (right), along  $c$  (top), and along  $b$  (bottom).

### 4. Channels and/or cages:

There are two types of channels parallel to  $c$ . The first type equals the PerBU and is present in **ATN** as well as in **BCT**. The channel wall consists of fused 6-rings. The second type, only present in **ATN**, is obtained when *atn* cavities are connected through common 8-rings as depicted in Figures 4 and 5.

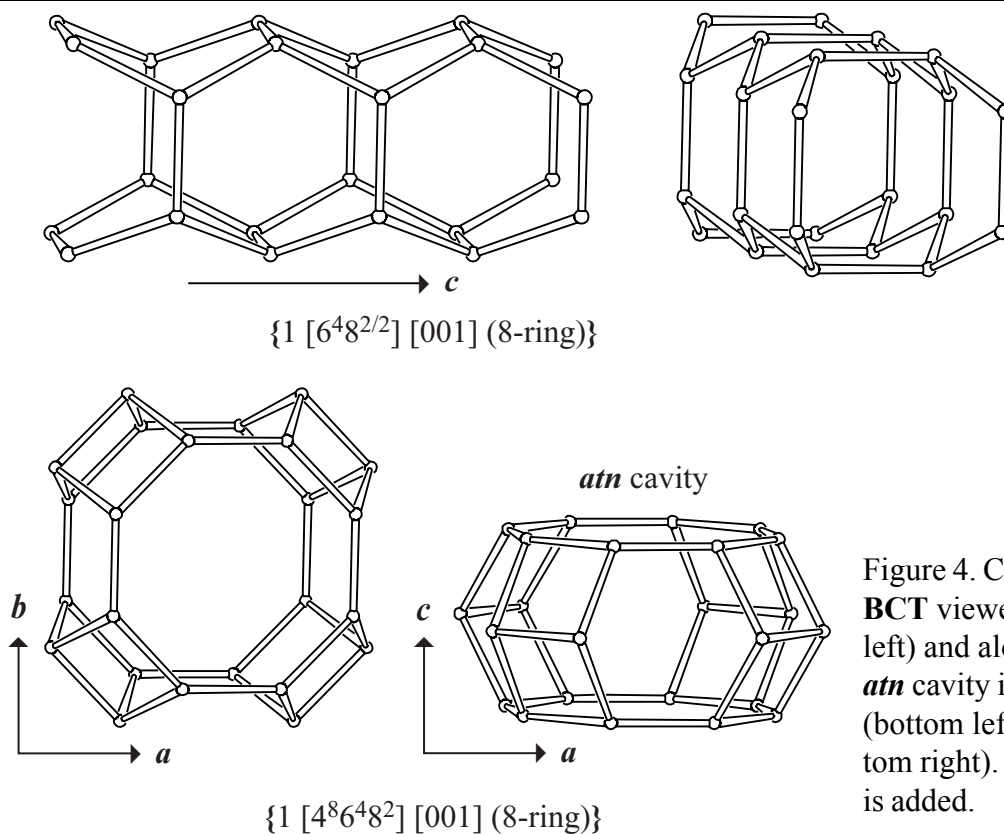


Figure 4. Channel in **ATN** and **BCT** viewed normal to  $c$  (top left) and along  $c$  (top right) and *atn* cavity in **ATN** seen along  $c$  (bottom left) and along  $b$  (bottom right). The **pore descriptor** is added.

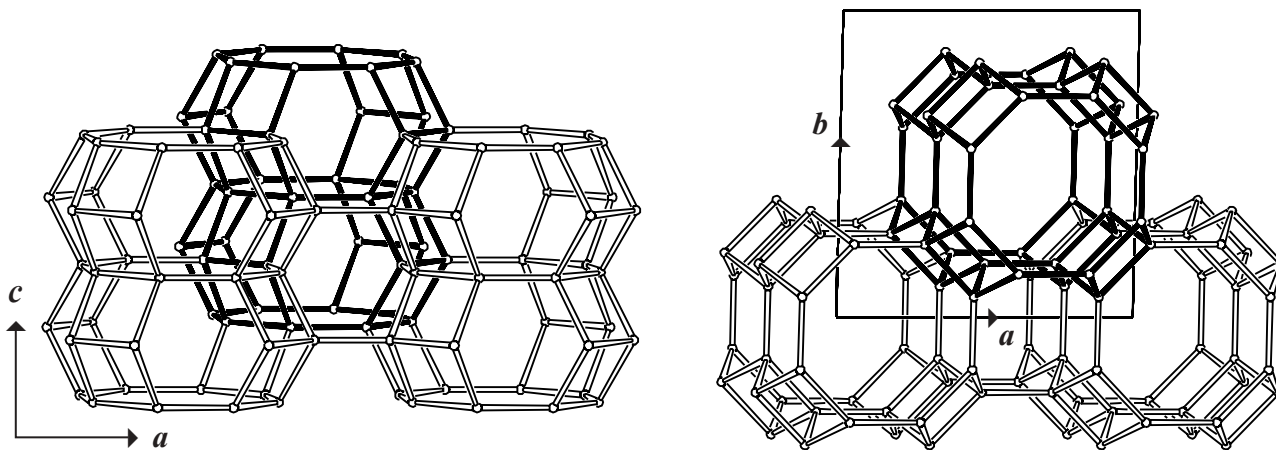


Figure 5. Fused *atn* cavities seen along *b* (left) forming the second type of 8-ring channels along *c* in ATN (right). ▲

## 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  $n = 1, 2, 3, \text{ etc.}$ ). 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**). ▲