## **Building scheme for AFT**



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 two-dimensional Periodic Building Unit (PerBU) of **AFT** consists of a hexagonal array of non-connected planar 6-rings (bold in Figure 1), which are related by pure translations along  $\boldsymbol{a}$  and  $\boldsymbol{b}$ . The 6-rings are centered at (0,0) in the  $\boldsymbol{ab}$  layer. This position is usually called the A position.

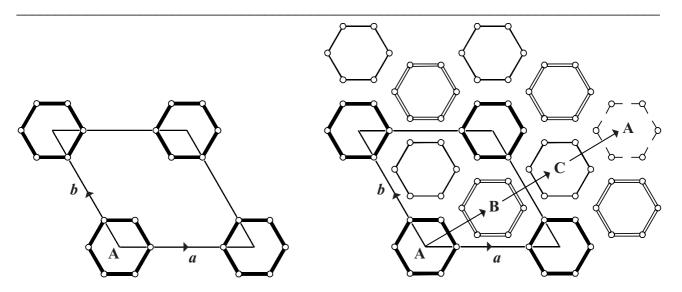


Figure 1: PerBU in AFT (left) and definition of 6-ring positions with respect to each other (right).

#### 2. Connection mode:

The distance between two neighboring PerBUs is about 2.55 Å. Neighboring PerBUs can be connected through tilted 4-rings along +[001] in three different ways:

- (1) the next layer (second layer) is shifted by +(2/3a + 1/3b) before connecting it to the first layer. The 6-rings in the second layer are centered at (2/3, 1/3). This position is usually denoted as the B position as illustrated in Figure 1. The same connection mode can be repeated: a third PerBU is shifted with respect to the second layer by (again) + (2/3a + 1/3b). The 6-rings are now centered at (4/3, 2/3) [or, equivalently, at (1/3, 2/3)]. This position is called the C position. Adding a fourth layer with the same connection mode gives a shift with respect to the first layer of (2a + b) [or zero] and an A position of the 6-rings is again obtained. The resulting stacking sequences, exhibiting the same connection mode, are denoted as AB, BC and CA, respectively (see Fig. 2(a) on next page).
- (2) the added layers are shifted by -(2/3a + 1/3b) before connecting them along +[001] to the previous layer. The resulting stacking sequences AC, CB and BA are obtained (see Fig. 2(b) on next page).
- (3) the added layer has a zero lateral shift along *a* and *b*. This connection mode leads to an AA, BB or CC stacking sequence depending on whether the added layer is connected to a layer with 6-rings in the A, B or C position, respectively (see Fig. 2(c) on next page).

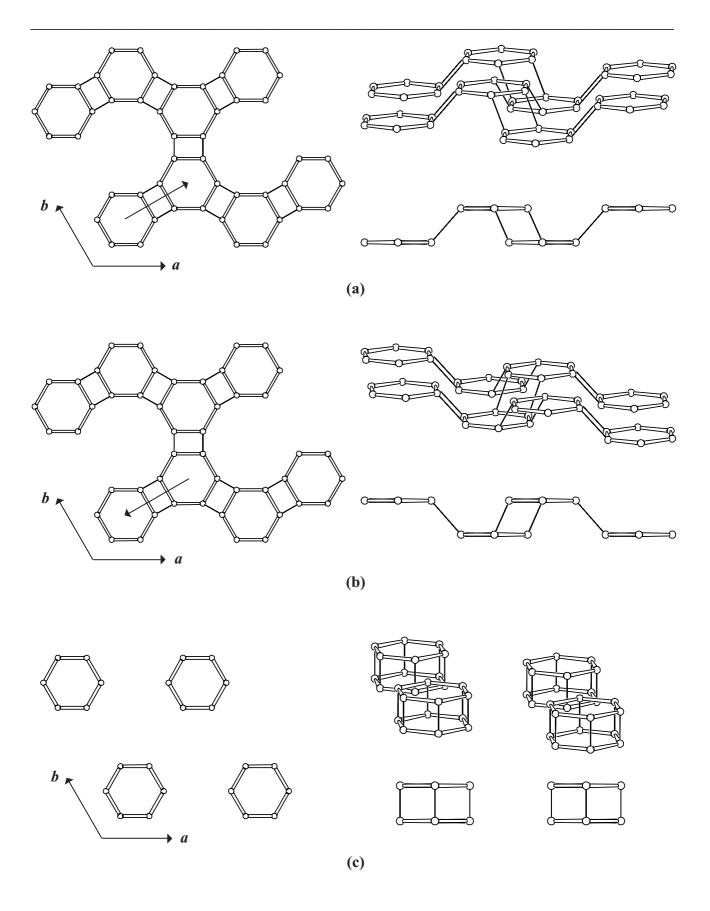


Figure 2. (a): Connection mode (1) viewed down [001] (left), nearly along [010] (top right), and along [010] (right bottom); (b): Connection mode (2) viewed as in (a); (c): Idem for connection mode (3). In **AFT** all three connection modes between the PerBUs are observed.

# 3. Projections of the unit cell content:

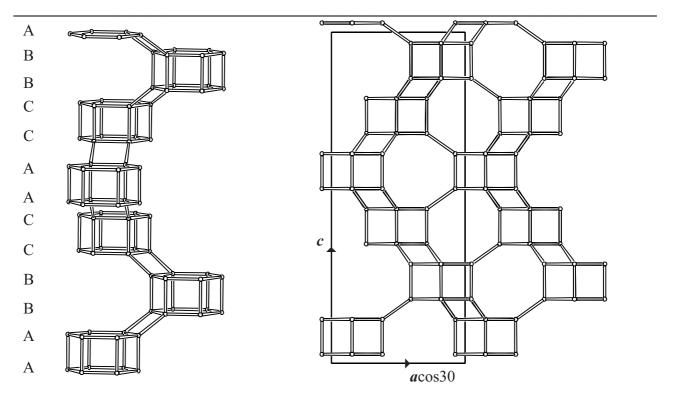


Figure 3. Perspective drawing (left) and projection of the unit cell content (right) along **b**. The stacking sequence is given. In the perspective drawing each PerBU is represented by one 6-ring. [AFT can as well be built using double 6-rings, 4-rings or 4-2 units; see Alternative description].

## 4. Channels and/or cages:

The three types of cavities in **AFT** (the *gmel*-, *chab*- and *aft*-cavities) are depicted in Figure 4. A three-dimensional channel system is obtained by connecting the cavities as illustrated in Figure 5.

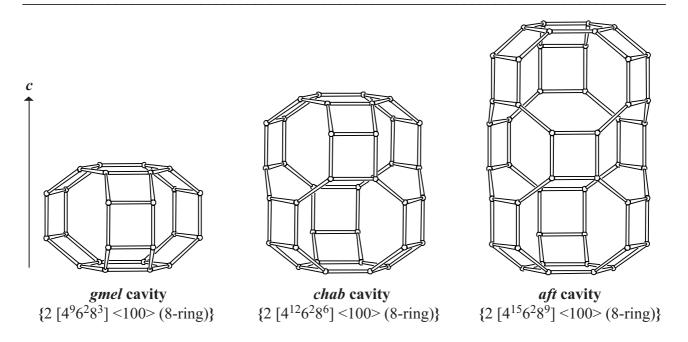


Figure 4. Cavities viewed along <120>. The **pore descriptors** are added.

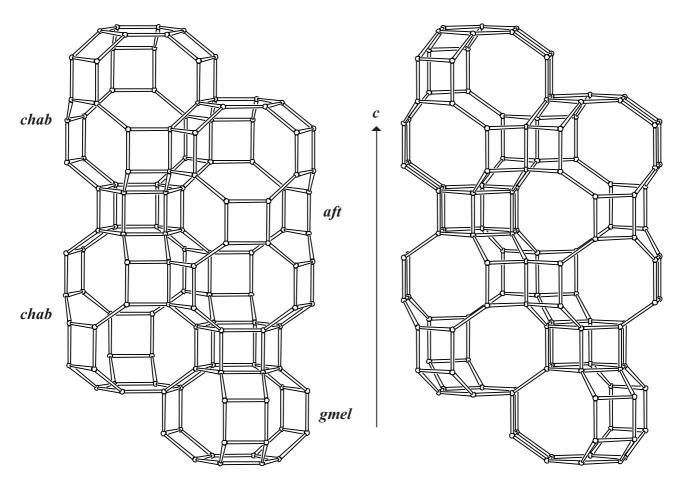


Figure 5 Connection of the cavities viewed along <120> (left) and along <010> (right). The twodimensional channels with 8-ring apertures are interconnected along *c* through 12-rings in the *chab*and *aft*-cavities leading to a three-dimensional channel system (See also Figure 4).

#### 5. Supplementary information:

# Other framework types containing a hexagonal array of non-connected 6-rings

A large number of framework types can be constructed using the hexagonal PerBU described in Section 1. They all belong to the ABC-6 family. In these framework types the unit cell dimension along the hexagonal axis is  $\approx (n^*)2.55$  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**).

### Alternative description of AFT using (modified) double 6-rings (D6Rs)

Several framework types, like AFT, can be built using (modified) D6Rs.

In the **INTRO** pages links are given to descriptions of other framework types containing (modified) D6Rs (choose: **Double 6-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 7**).