Building scheme for CHA

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1. Periodic Building Unit:

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

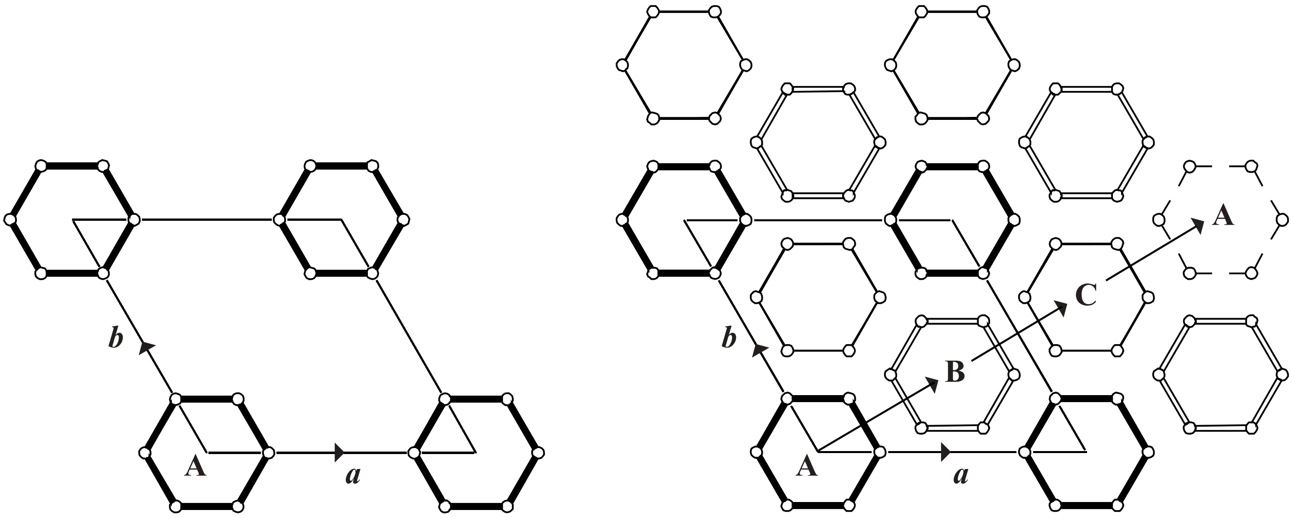


Figure 1: PerBU in **CHA** (left) and definition of 6-ring positions with respect to each other (right).

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 +(2/3***a*** + 1/3***b***) 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) +(2/3***a*** + 1/3***b***). 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 (2***a*** + ***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 -(2/3***a*** + 1/3***b***) 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).

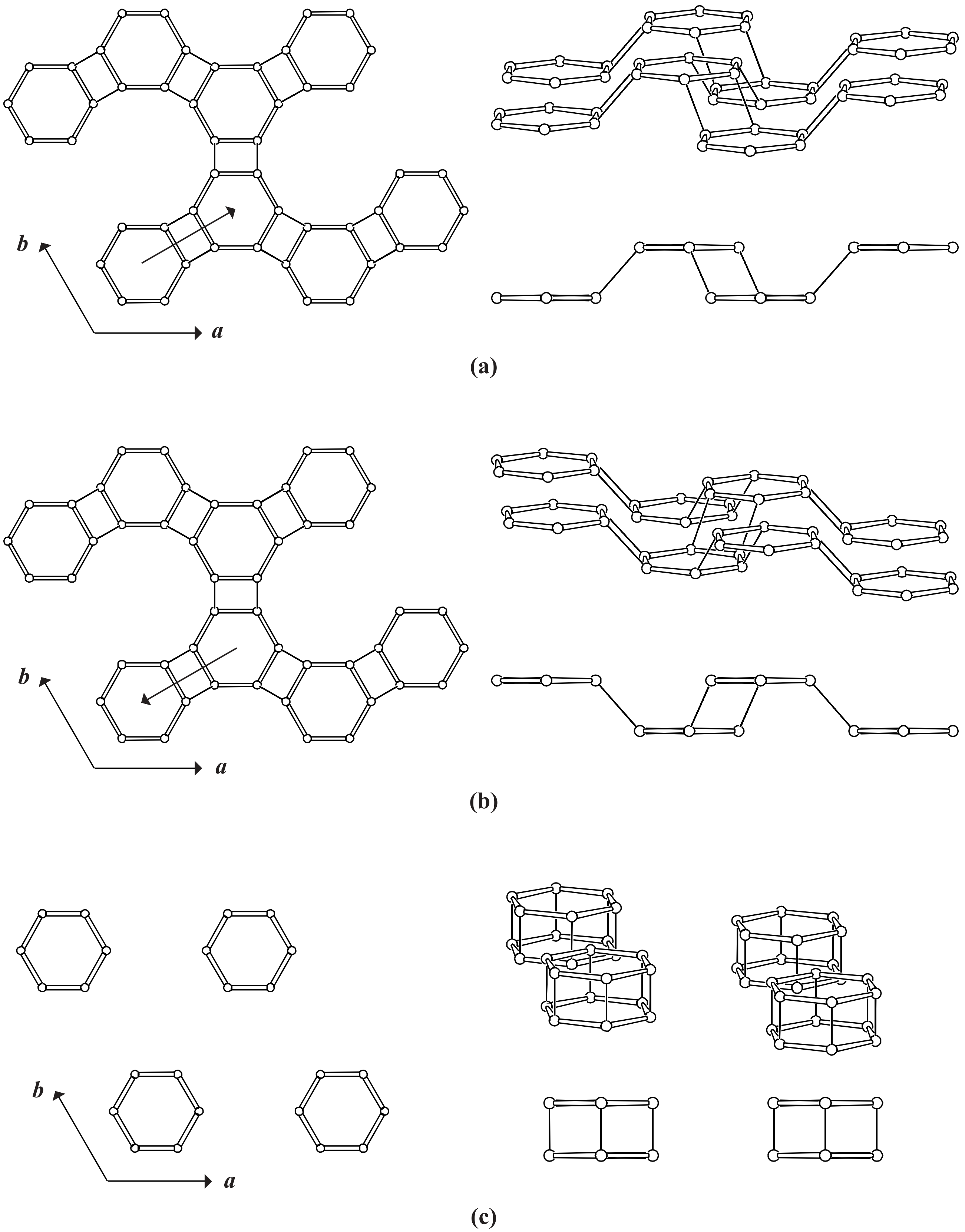


Figure 2. (a): Connection mode **(1)** viewed down [001] (left), nearly along [010] (top right), and along [010] (right bottom); (b): Connection mode **(2)** viewed as in (a); (c): Idem for connection mode **(3)**. In **CHA** all three connection modes between the PerBUs are observed.

3. Projections of the unit cell content:

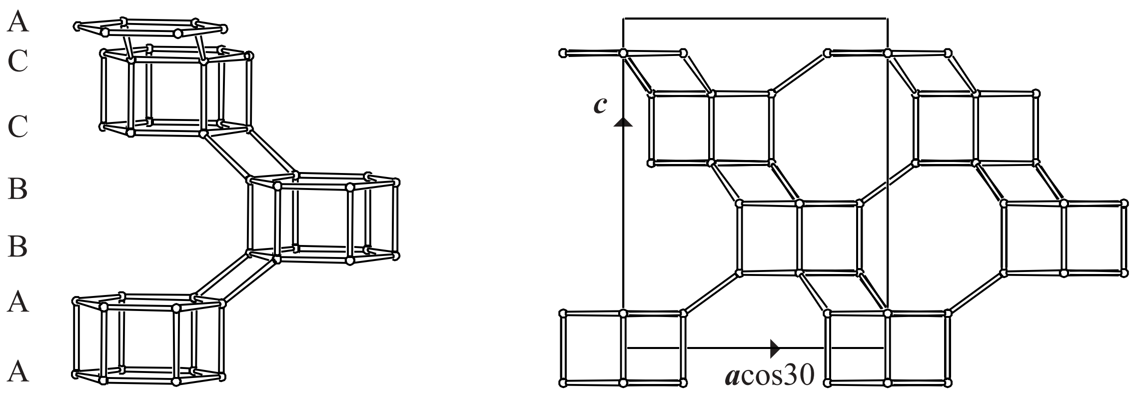
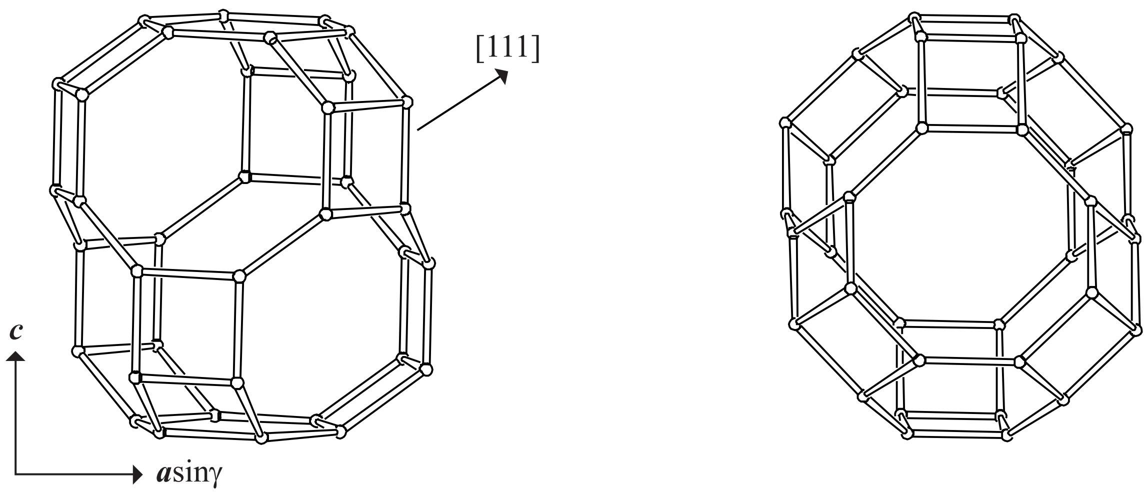


Figure 3. Perspective drawing (left) and projection of the unit cell content (right) along ***b***. The stacking sequence is given. In the perspective drawing each PerBU is represented by one 6-ring. Figure 3 also illustrates that **CHA** can be built using double 6-rings (or two 4-2 units or three 4-rings).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

4. Channels and/or cages:

The ***chab*** cavity is depicted in Figure 4. A three-dimensional channel system is obtained by connecting the cavities through common 8-rings and double 6-rings (Figure 5).



chab **cavity**
{3 [$4^{12}6^{2}8^{6}$] <100> (8-ring), <111> (8-ring)}

Figure 4. Left: ***chab*** cavity viewed along <010>, and along <111> (right) . The **pore descriptor** is added.

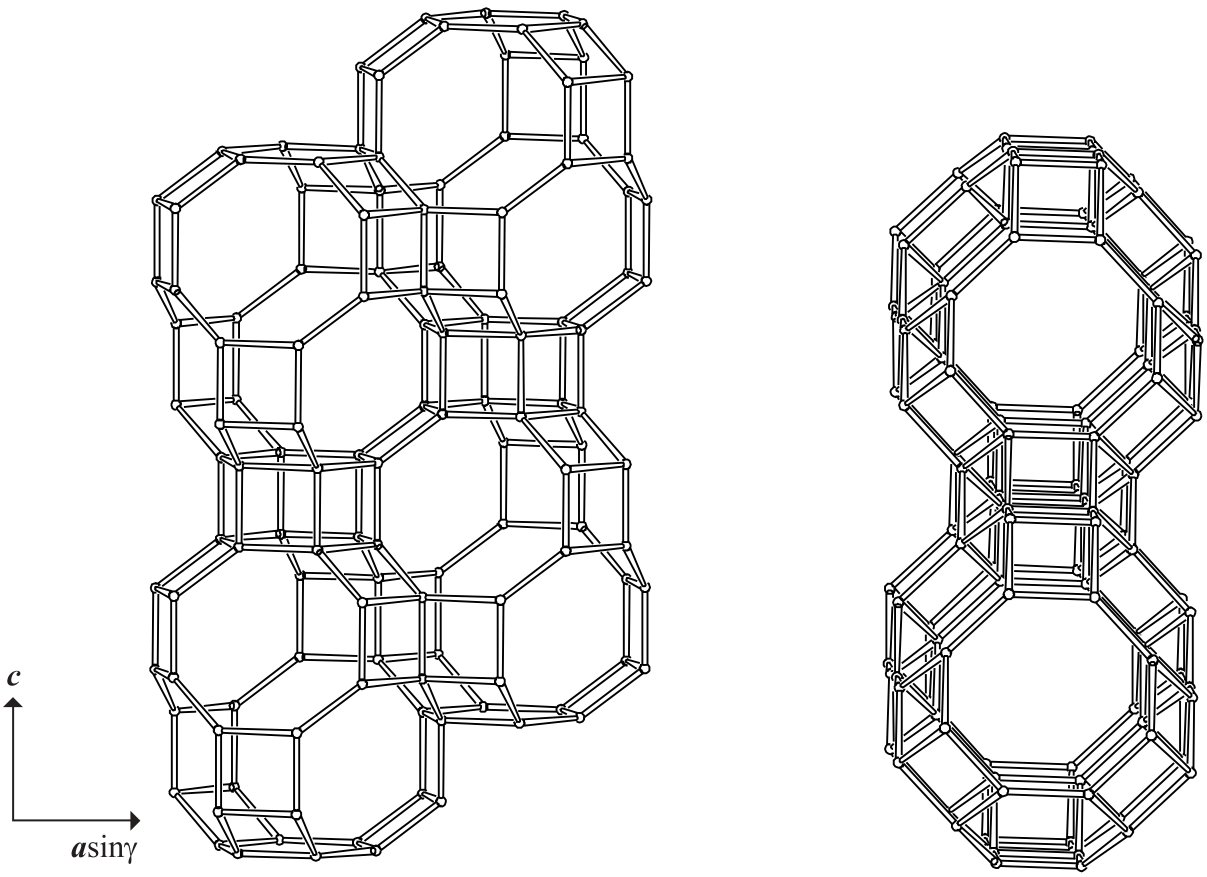


Figure 5. Channels in **CHA** viewed along <010> (left), and along <111> (right).

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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 ≈(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**).

Aternative description of* CHA *using (modified) double 6-rings (D6Rs)
Several framework types, like **CHA**, can be built using (modified) D6Rs. An alternative building scheme for **CHA** using D6Rs is given in the building scheme for **AEI**.
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).**