Building scheme for OFF

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 **OFF** consists of an 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.

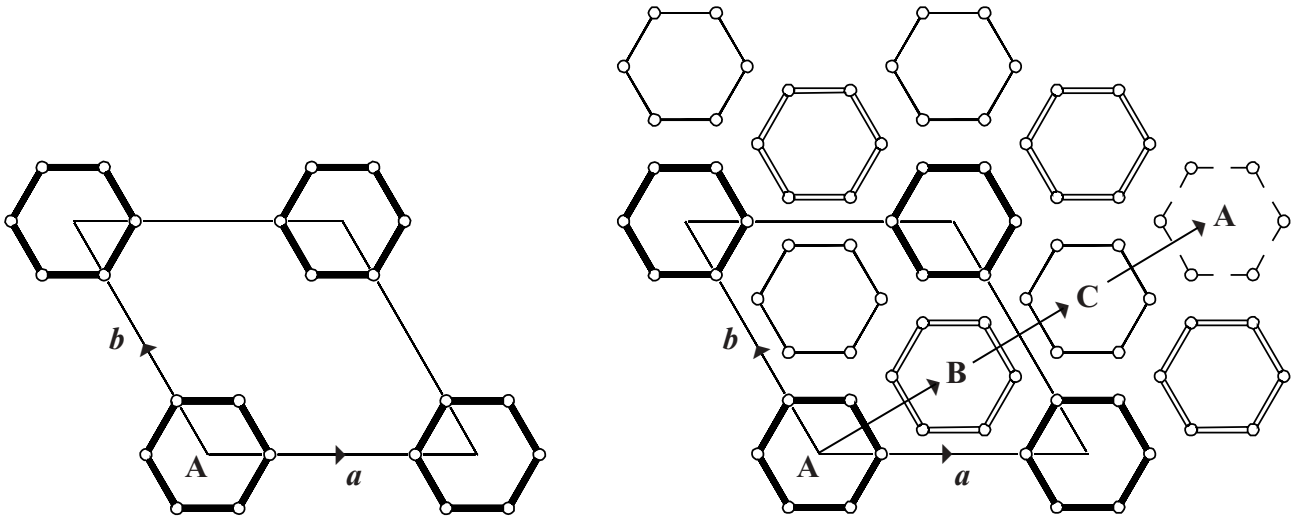


Figure 1: PerBU in **OFF** (left) and definition of 6-ring positions with respect to each other (right).

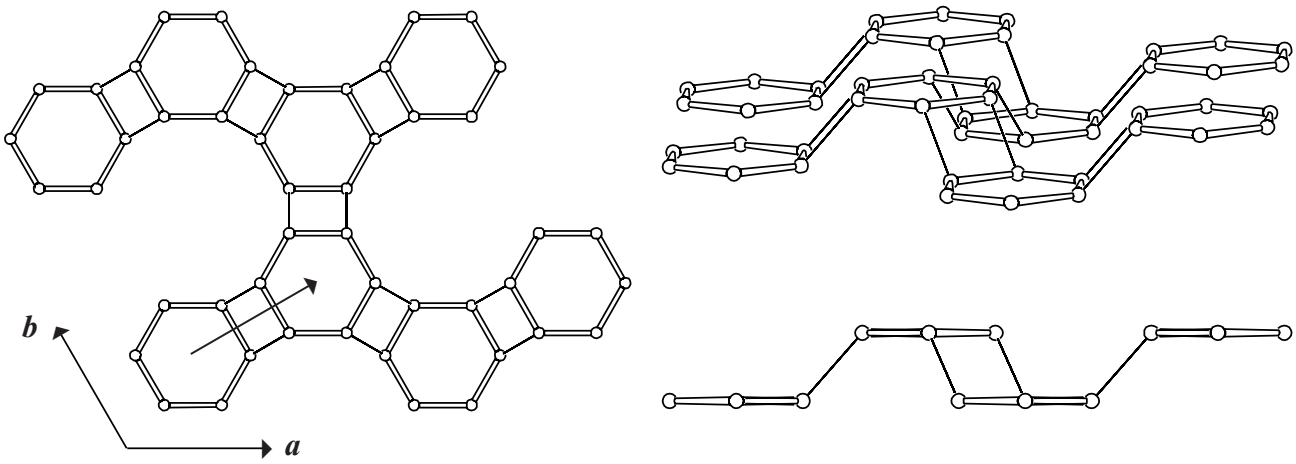
2. Connection mode:

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:

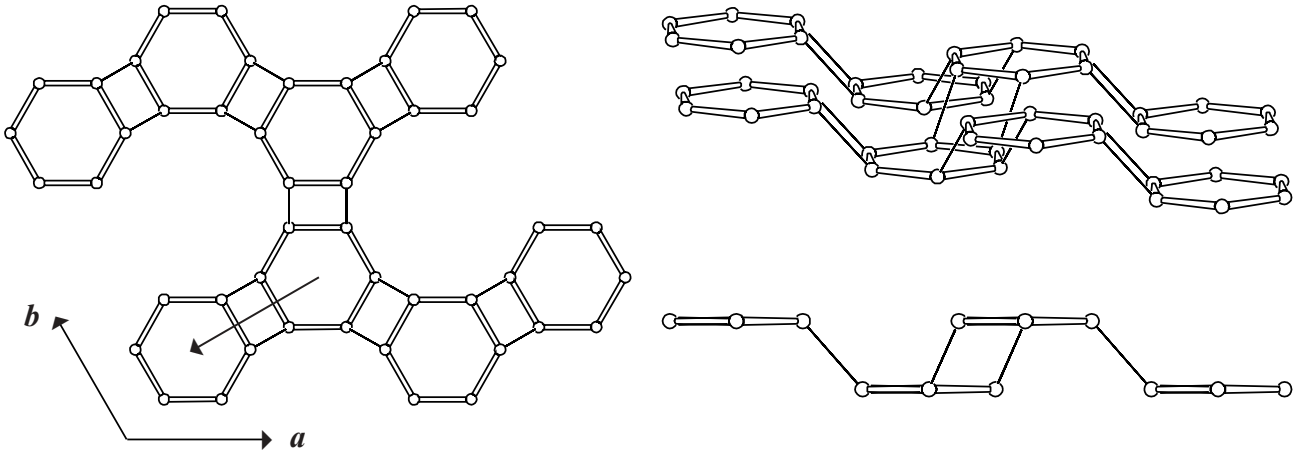
(1) the next layer (second layer) is shifted by +(2/3***a*** + 1/3***b***) before connecting it to the first layer. The 6-rings in the second layer are centered at (2/3, 1/3). This position is usually denoted as the B position as illustrated in Figure 1. The same connection mode can be repeated: a third 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).

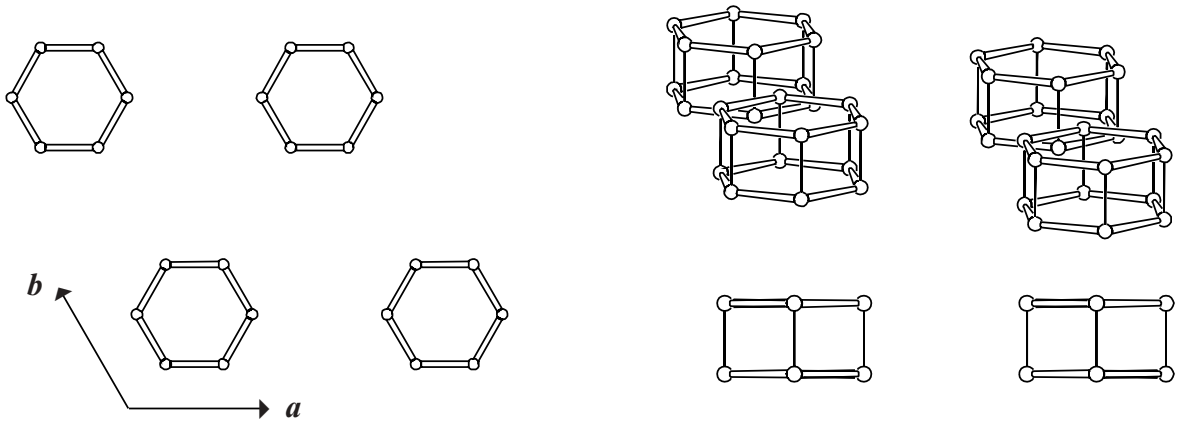
(3) the added layer has a zero lateral shift along ***a*** and ***b***. This connection mode leads to an AA, BB or CC stacking sequence depending on whether the added layer is connected to a layer with 6-rings in the A, B or C position, respectively (see Fig. 2(c) on next page).



(a)



(b)



(c)

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 **OFF** all three connection modes between the PerBUs are observed.

3. Projections of the unit cell content:

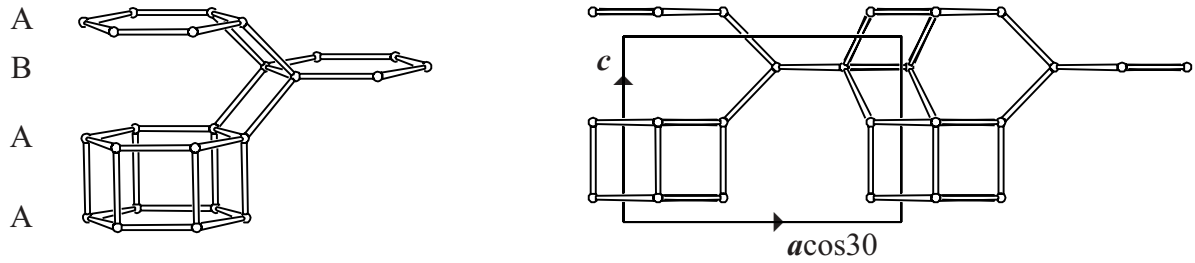


Figure 3. Perspective drawing (left) and projection of the unit cell content (right) along ***b***. The stacking sequence is given. In the perspective drawing each PerBU is represented by one 6-ring. [**OFF** can also be built using 4-2 units; see **LTL** building scheme]

▲

4. Channels and/or cages:

Cage, cavity and channel are depicted in Figure 4. The **pore descriptors** are added. ***can*** Cages and ***gme*** cavities are connected along ***c*** through double 6-rings and common 6-rings, respectively. A fused system of cages and channel is shown in Figure 5. A one-dimensional channel with a 12-ring window is obtained when (fused) ***gme*** cavities or ***can*** cages are connected around a 3-fold axis.

can cage	***gmel* cavity**	***12-ring channel***
{0 [$4^6 6^5$]}	{2 [$4^9 6^2 8^3$] <100> (8-ring)}	{3 [$4^3 6^3 8^3 12^{2/2}$] [001] (12-ring), <100>, (8-ring)}

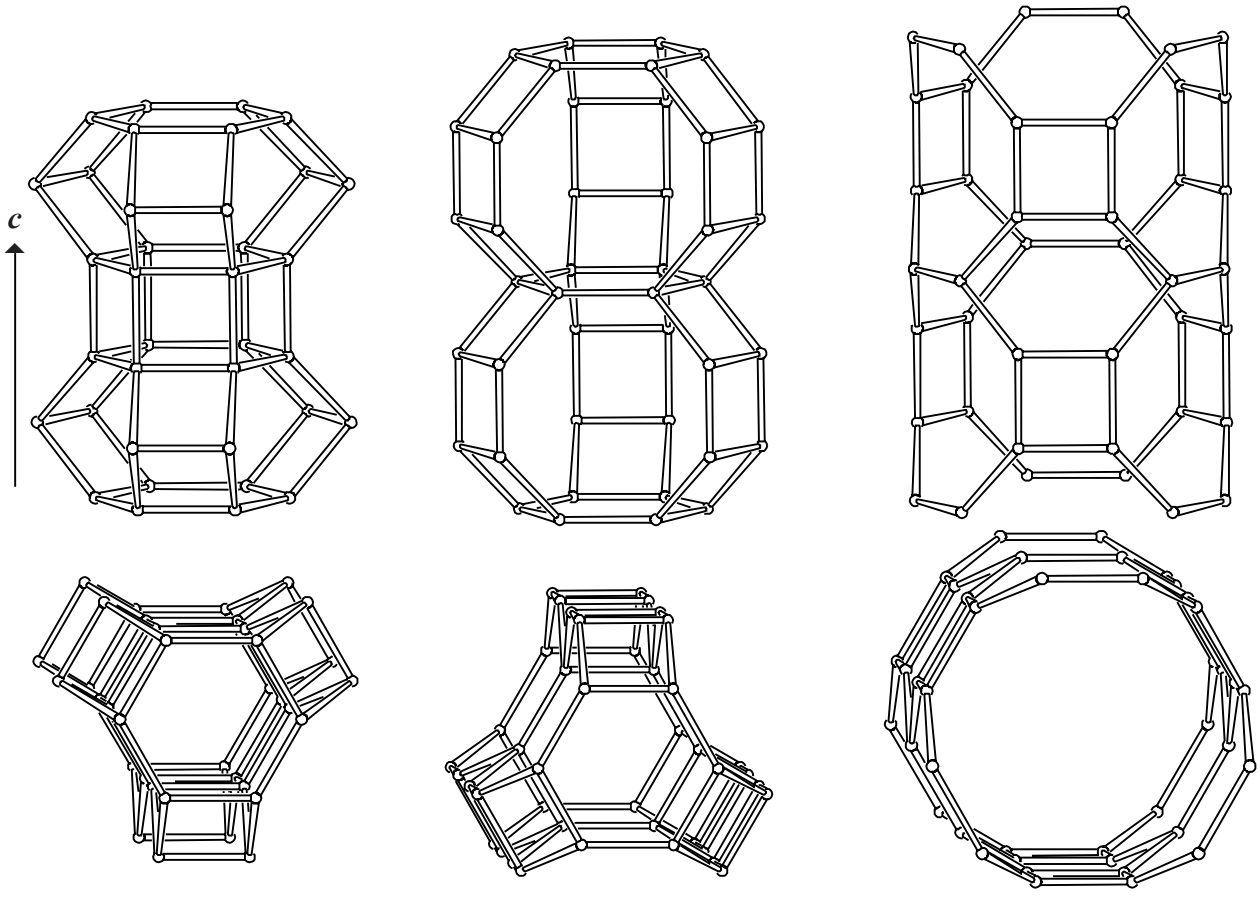


Figure 4. ***can*** Cages (left), ***gme*** cavities (middle) and 12-ring channel (right)) seen along <120> (top) and along ***c*** (bottom). [Figure 5 is on next page]

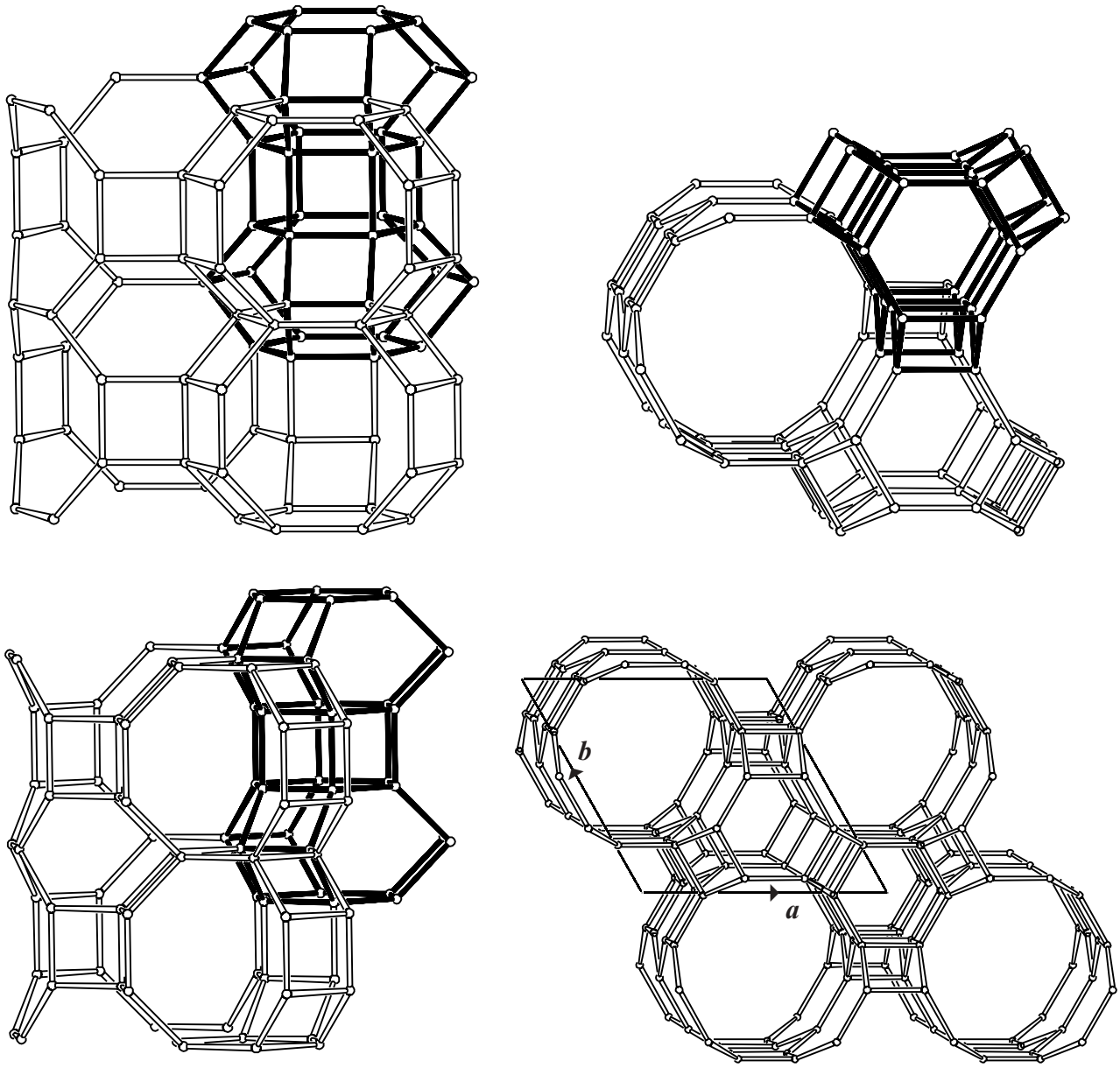


Figure 5. Fused cages and channel viewed along <120> (top left) and along ***c*** (top right). For clarity: ***can*** cages are drawn in bold lines and two-dimensional 8-ring channels viewed along <110> (bottom left) and one-dimensional 12-ring channels along ***c*** (bottom right). The two-dimensional channels intersect with the one-dimensional channels.

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5. Supplementary information:

***Alternative description of* OFF**

An alternative building scheme for **OFF**, using saw chains or ***can*** cages, is given in the building scheme of **LTL**.

Other framework types belonging to the* ABC-6 *family

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 the number of PerBUs along the hexagonal axis. In the **INTRO**-pages links are given to descriptions of other framework types belonging to the ABC0-6 family (choose: **ABC-6 family**).