Building scheme for LOS



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1. Periodic Building Unit:

The two-dimensional Periodic Building Unit (PerBU) of **LOS** consists of an 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.

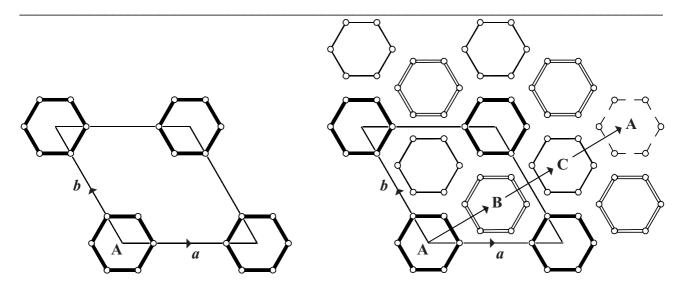


Figure 1: PerBU in LOS (left) and definition of 6-ring positions with respect to each other (right).

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).

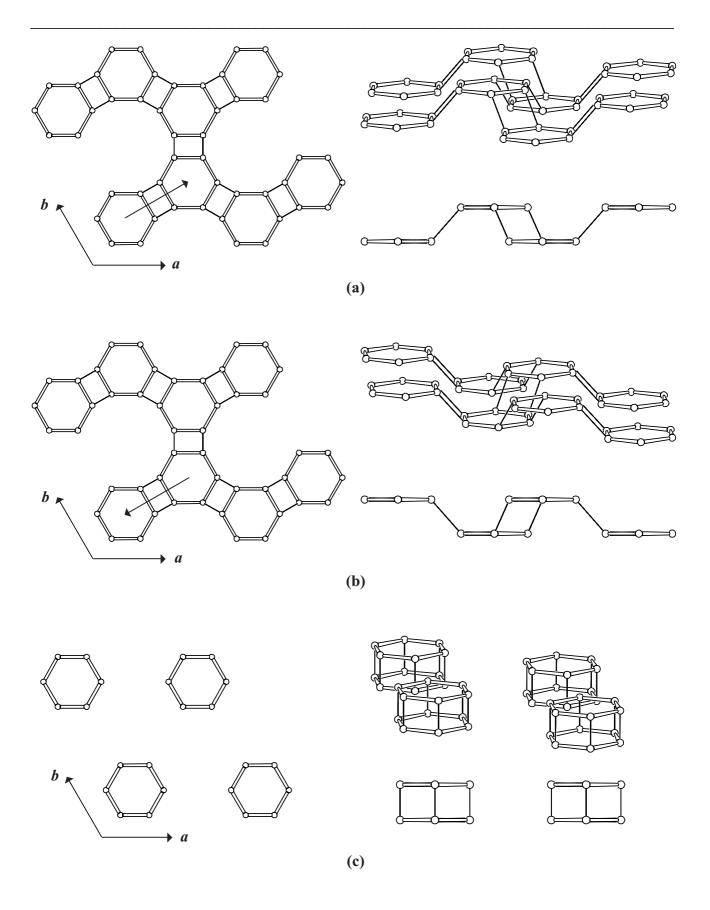


Figure 2. (a): Connection mode (1) viewed down [001] (left), nearly along [010] (top right), and along [010] (right bottom); (b): Connection mode (2) viewed as in (a); (c): Idem for connection mode (3). In LOS only connection modes (1) and (2) between the PerBUs are observed.

3. Projections of the unit cell content:

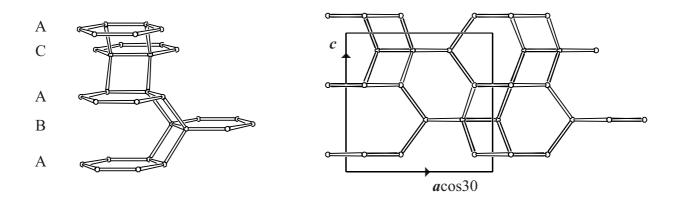


Figure 3. Perspective drawing (left) and projection of the unit cell content (right) along **b**. The stacking sequence is given. In the perspective drawing each PerBU is represented by one 6-ring.

4. Channels and/or cages:

The two types of cages in **LOS** are depicted in Figure 4. The **pore descriptor** is added. Cages are connected through common 4- and 6-rings. Apertures are formed by 6-rings only.

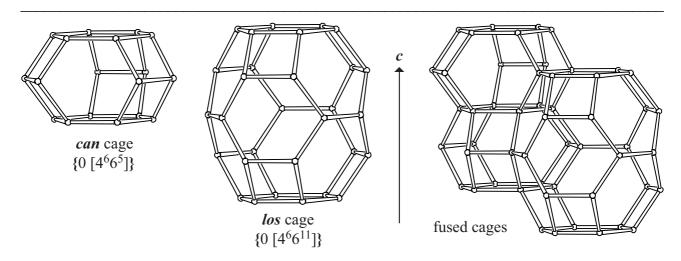


Figure 4. *can* Cage (or ε-cage; top left) and *los* cage (middle) and fused cages (right) viewed perpendicular to *c*. [**LOS** can also be built from 4-rings or 6-2 units as can be seen from the Figure]

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**).