

**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:

**MSO** can be built using units of 30 T atoms (Figure 1(a)). The T30-unit consists of two double 6-rings connected through 6 T atoms (or of three 2-6-2 units, or six 4-1 units). The Periodic Building Unit (PerBU) equals the hexagonal array of non-connected T30-units (Figure 1(b)). The T30-units, related by pure translations along  $a$ , and  $b$ , are centered at (0,0) in the  $ab$  layer. This position is usually called the A position.

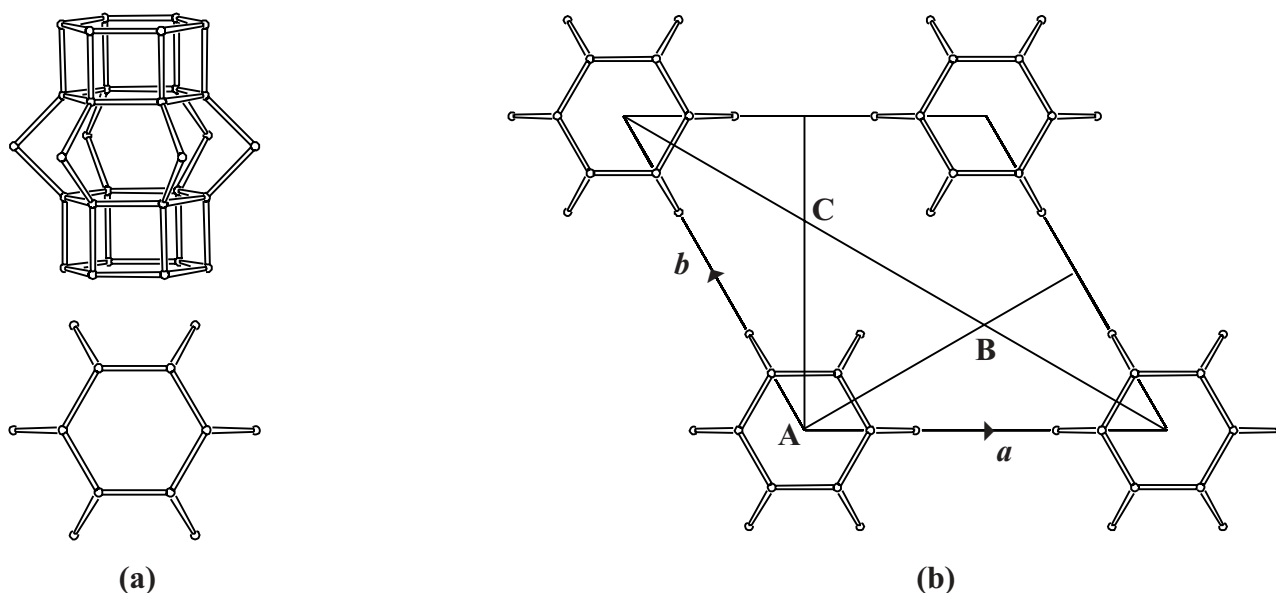


Figure 1. (a): Building Unit consisting of 30 T atoms viewed perpendicular to the hexagonal  $c$  axis (top) and down  $c$  (bottom); (b): PerBU of non-connected T30-units. The definition of the positions of the T30-units in neighboring PerBUs with respect to each other is indicated. ▲

## 2. Connection mode:

Neighboring PerBUs are connected along  $c$  through 6-rings in the following way: the next layer (second layer) is shifted by  $+(2/3a + 1/3b)$  before connecting it to the first layer. The T30-units in the second layer are centered at  $(2/3, 1/3)$ . This position is usually denoted as the B position as illustrated in Fig.1 (b). The same connection mode is repeated: a third PerBU is shifted with respect to the second layer by (again)  $+(2/3a + 1/3b)$ . The T30-units are now centered at  $(4/3, 2/3)$  [or, equivalently, at  $(1/3, 2/3)$ ]. This position is called the C position (See Fig. 1(b)). 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 T30-units is again obtained. The resulting stacking sequence is denoted as ABC(A) stacking (see Figure 2 on next page). [Compare this stacking sequence with the stacking sequence in **SOD**: when the single 6-rings in **SOD** are replaced by T30-units **MSO** is obtained]. ▲

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

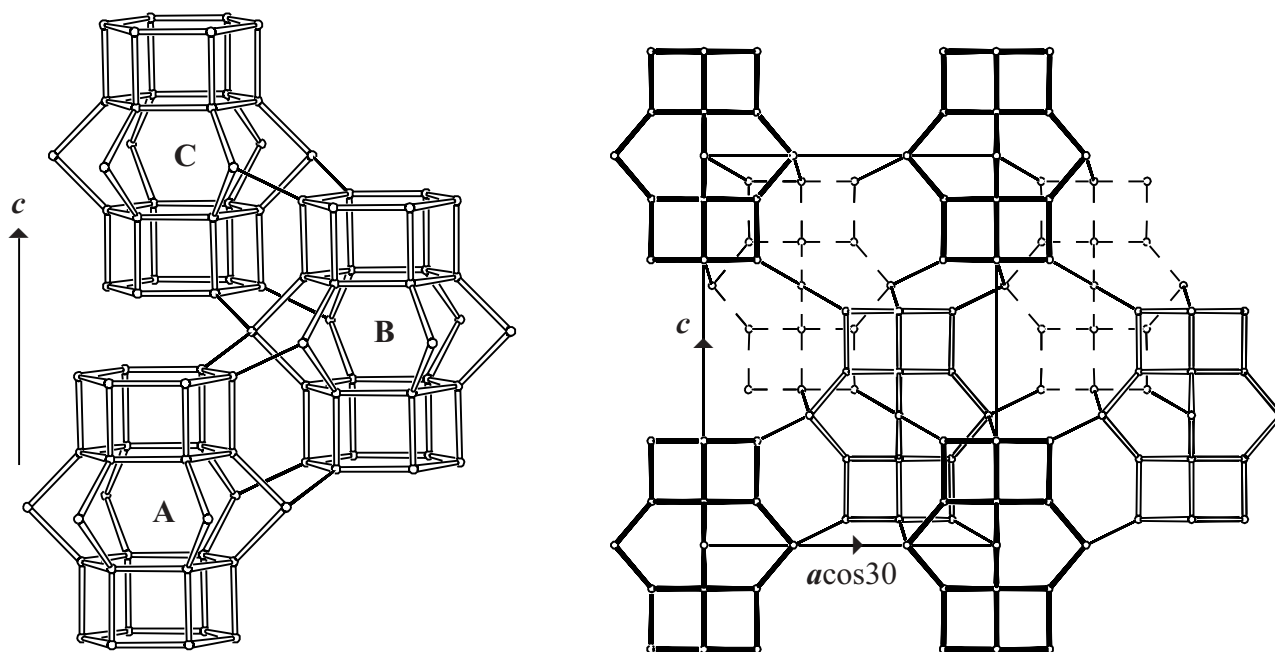


Figure 2. Left: ABC(A) stacking in **MSO** viewed perpendicular to  $c$ . Each PerBU is represented by one T30-unit. Right: Parallel projection of the unit cell along  $b$ . For clarity, T30-units at A positions are drawn in heavy bold, at B positions with open bonds and at C positions with broken lines. ▲

### 4. Channels and/or cages:

The two types of cages in **MSO** are depicted in Figure 3. Cages are connected through (common) 4- and 6-rings as shown in Figure 4. Apertures are formed by 6-rings only.

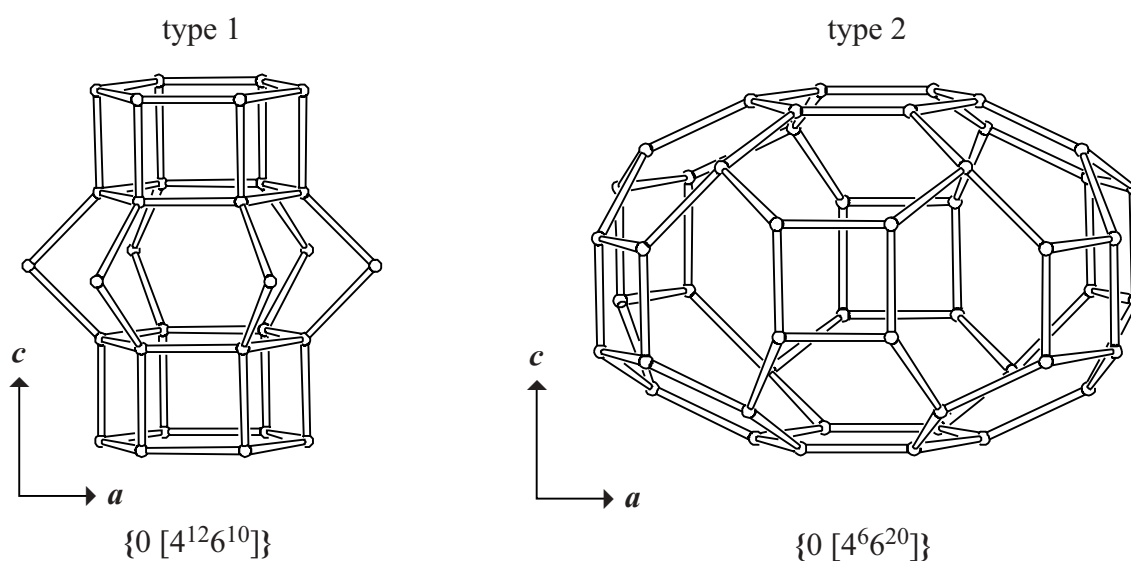


Figure 4. Cages viewed along  $\langle 120 \rangle$ . The "type 1" cage equals the T30 building-unit. The **pore descriptor** is added.

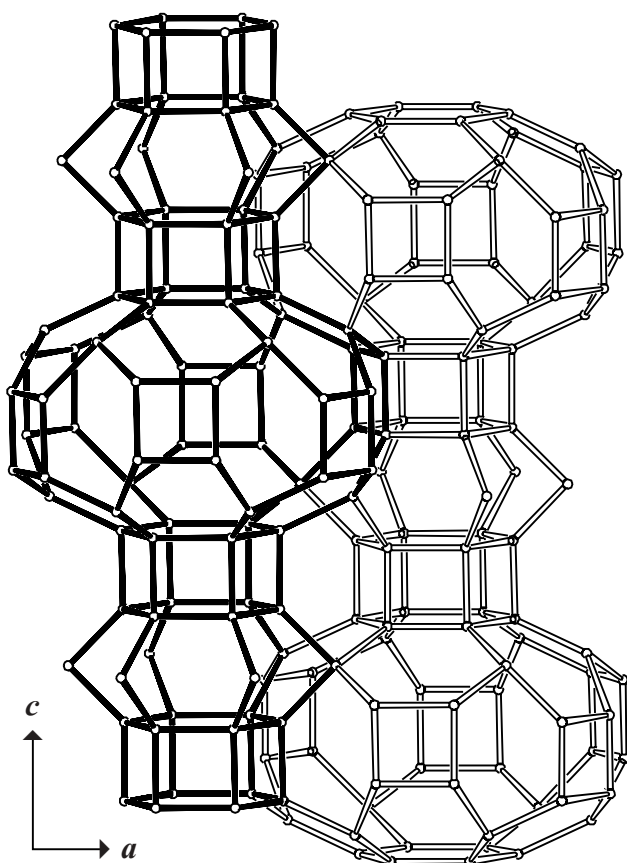


Figure 5 Connection of the cages viewed along  $\langle 120 \rangle$ .



## 5. Supplementary information:

### *Other framework types containing a hexagonal array of non-connected (double) 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  $\approx (n^*)2.55 \text{ \AA}$  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](#)).

### *Other framework types containing (modified) double 6-rings (D6Rs)*

Several other framework types 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](#)).

