# **Building scheme for MEP**



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 (PerBU):

Cubic **MEP** belongs to the clathrasil family and can be built using the 12-ring double cups, shown in Figure 1. The 12-ring double cups consist of 30 T atoms. T30-units are connected into an orthogonal layer. The "empty" spaces between the T30-units are occupied by tetra-(1,1,4,4)-substituted 6-rings (bold in Figure 2(a)). The connection of T30-units through these substituted 6-rings generates [5<sup>12</sup>]- and [5<sup>12</sup>6<sup>2</sup>]-cages. The [5<sup>12</sup>6<sup>2</sup>]-cages form columns parallel to *c* by sharing the hexagon faces. The two-dimensional PerBU in **MEP** is obtained when 6-rings from an additional 6-ring layer (bold in Figure 2(b)) are stacked on top of the T30-units. This stacking generates another set of [5<sup>12</sup>6<sup>2</sup>]-cages. [Compare this PerBU with the PerBUs in **DDR**, **DOH** and **MTN**]

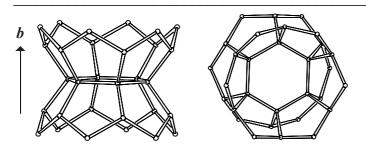


Figure 1. T30-unit in the clathrasil family viewed perpendicular to b (left) and along the cup-axis b (right). Two "zigzag" 12-rings are connected though a common 6-ring to form two half cages or a 12-ring double cup.

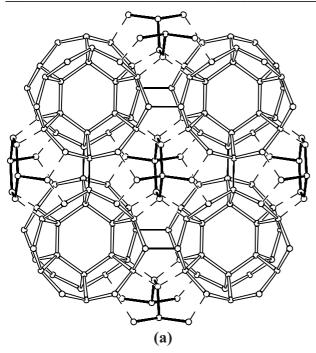
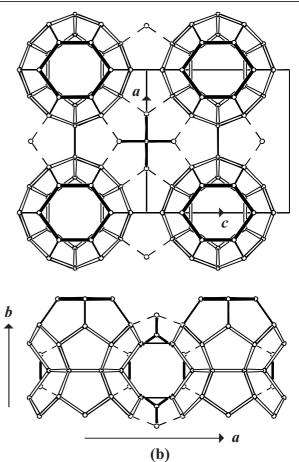


Figure 2. (a): Orthogonal layer viewed along b. Connections to the space filling substituted 6rings (in bold) are dashed. (b): PerBU in **MEP** viewed and along b (top) and along c (bottom). The additional 6-rings are in heavy bold. [Figure 2 is continued on next page]



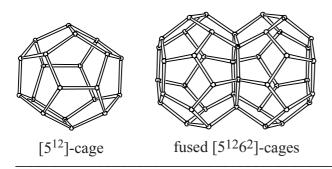


Figure 2 [Cont'd]. (c): Cages in the PerBU.

### 2. Connection mode:

Neighboring PerBUs, related by pure translations along  $\boldsymbol{b}$ , are connected through O-bridges along  $\boldsymbol{b}$ . [5<sup>12</sup>6<sup>2</sup>]-Cages and [5<sup>12</sup>]-cages are generated. The [5<sup>12</sup>6<sup>2</sup>]-cages form columns parallel to  $\boldsymbol{b}$  by sharing the hexagon faces as illustrated in Figure 3.

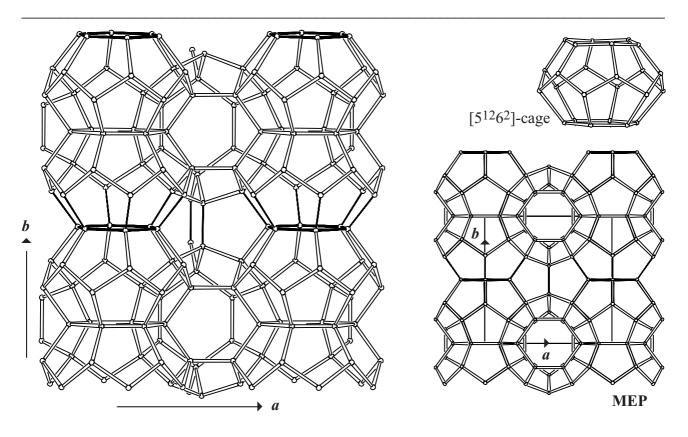


Figure 3. Connection mode in **MEP** viewed along *c* in perspective view (left) and in projection (bottom right). In the perspective drawing only one two T30-units and one tetra-substituted 6-ring in each PerBU is shown for clarity. The additional 6-rings are drawn in bold. The newly formed interlayer cage is shown at the top right.

## **3.** Projections of the unit cell content: See Figure 3.

#### 4. Channels and/or cages:

Cages are shown in Figure 2. The pore descriptor is added. Apertures are formed by 6-rings only.

# 5. Supplementary information:

# Other framework types containing a layer of (modified) T30-units

Three other framework types can be constructed using the (modified) PerBU described in Section 1. They belong to the clathrasil family.

In the **INTRO** pages links are given to detailed descriptions of these framework types (choose: **Clathrasils**). 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 10**).