# **Building scheme for UFI**



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:

UFI can be built using units of 32 T atoms. This T32-unit is composed of two, mirror related, "halfcages". A half-cage consists of four (fused) 6-rings (or a 12-ring and a 4-ring) and exhibits 4-fold symmetry (Figure 1(a)). The T32-units (one in bold in Figure 1(b)), related by pure translations along a, and b, are connected into the Periodic Building Unit (PerBU) through 4-rings. The PerBU is equal to a layer of  $\alpha$ -cages connected along a, and b through common 8-rings. The PerBU can as well be built using 4-2 units and 4-rings in a ratio 2:1 (see Figure 1(b) and Alternative description).



Figure 1. (a): T32-unit viewed perpendicular to the 4-fold *c*-axis (top), and along the 4-fold axis (bottom); (b): PerBU viewed along *c* (top), and along *b* (or *a*; bottom).

#### 2. Connection mode:

Neighboring PerBUs, related by a shift of  $\frac{1}{2}(a+b)$ , are connected along *c* as shown in Figure 2 on next page: 8-rings of the  $\alpha$ -cages, parallel to the plane of the PerBU, are connected to the 12-rings of half-cages in neighboring PerBUs.



Figure 2. Connection mode in UFI viewed along *b* (or *a*).







### 4. Channels and/or cages:

8-Ring channels parallel to a, and b intersect. The channel intersection, equal to the  $\alpha$ -cavity, is depicted in Figure 4(a). Two "side-pockets" close the 8-ring windows of the  $\alpha$ -cavity that are perpendicular to c. The **pore descriptor** is added in Figure 4. The fusion of intersections is illustrated in Figure 4(b).



Figure 4. (a): Channel intersection and "side-pockets" in **UFI** viewed along b (or a); (b): Fusion of cavities and cages along a (or b) viewed along b (or a) (left), and along the 8-ring channel axis parallel to a (or b) (right).

## 5. Supplementary information:

### Other miscellaneous framework types

In the **INTRO** pages links are given to detailed descriptions of these framework types (choose: **Miscellaneous**). There is also a link to a summary of the Periodic Building Units used in the building schemes of these framework types (choose: **Appendix**; **Figure 12**).

### Alternative description of UFI using (modified) single 3- and/or 4-rings

Several framework types, like **UFI**, can be constructed using (modified) single 3- and/or 4-rings. In several cases additional T atoms are needed to build the framework.

In the **INTRO**-pages links are given to a detailed description of a sub-set of framework types that contain (modified) single 3- and/or 4-rings (choose: **Single 3- and/or 4-rings**). There is also a link to a summary of the Periodic Building Units used in the building schemes of these framework types (choose: **Appendix**; **Figure 4**).