

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:

IHW can be built using centrosymmetrical units composed of 28 T atoms: two 5-1 units and two 5-3 units that form two  $[4^{15}8]$  cages (sharing the 4-ring) with two additional T atoms (Figure 1(a)); one 5-1 and one 5-3 unit in bold). [An alternative building unit is shown in Figure 1(b): six finite zigzag chains connected through a 4-ring; compare this building unit with those in **CFI** and **EUO**]. A two-dimensional Periodic Building Unit (PerBU) is obtained when T28-units, related by a shift of  $\frac{1}{2}(a + b)$ , are connected as shown in Figure 2.

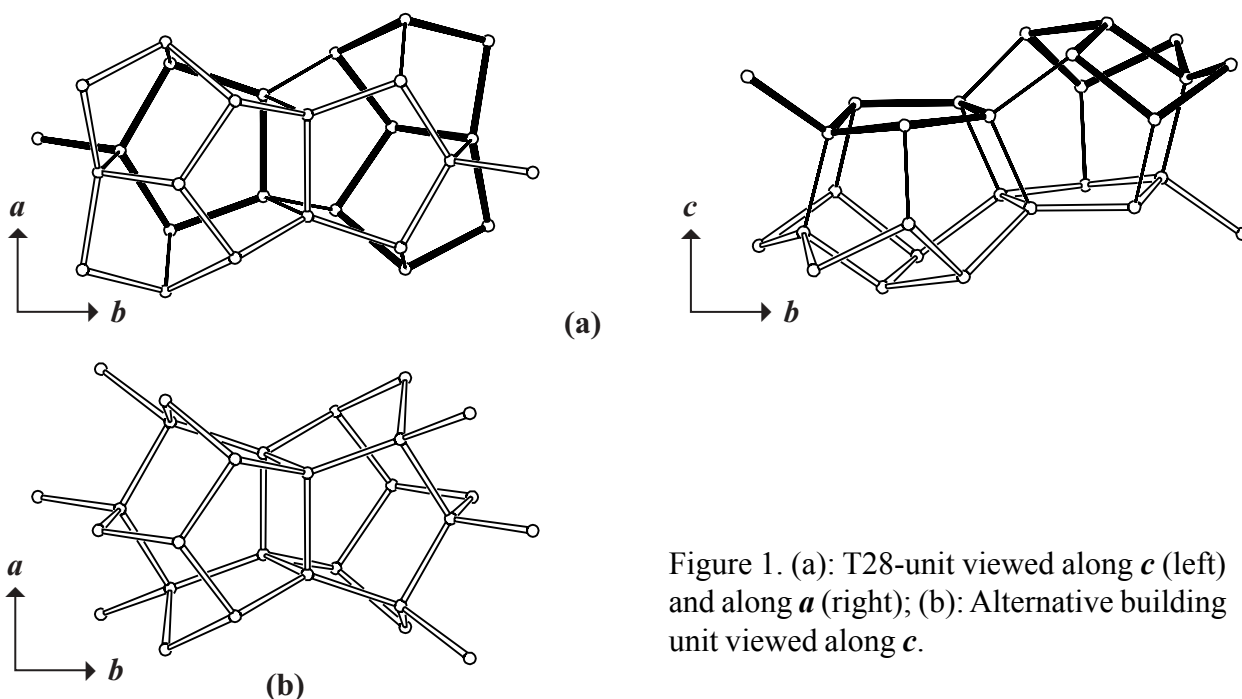


Figure 1. (a): T28-unit viewed along *c* (left) and along *a* (right); (b): Alternative building unit viewed along *c*.

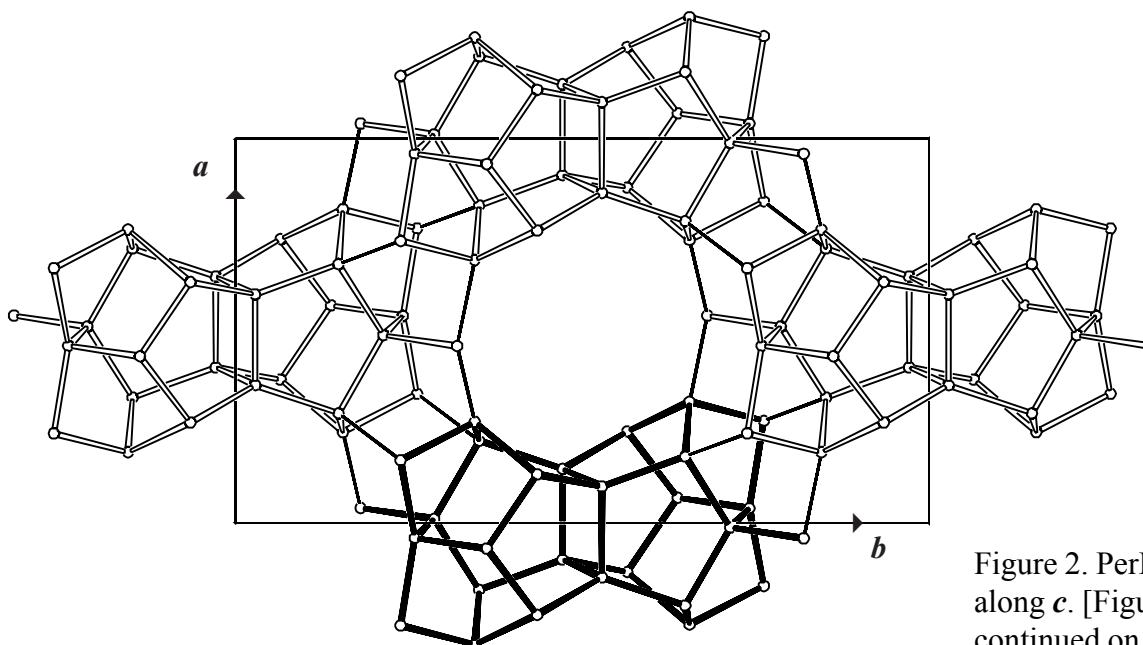


Figure 2. PerBU viewed along *c*. [Figure 2 is continued on next page]

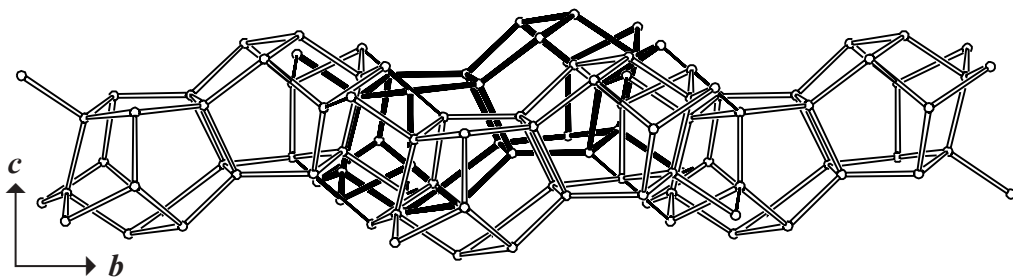


Figure 2 [Cont'd].  
PerBU viewed  
along *a*. ▲

## 2. Connection mode:

Neighboring PerBUs, related by a rotation of  $180^\circ$  about *b* and a shift of  $\frac{1}{2}b$ , are connected along *c* through (fused) 5-, 6- and 8-rings as shown in Figure 3.

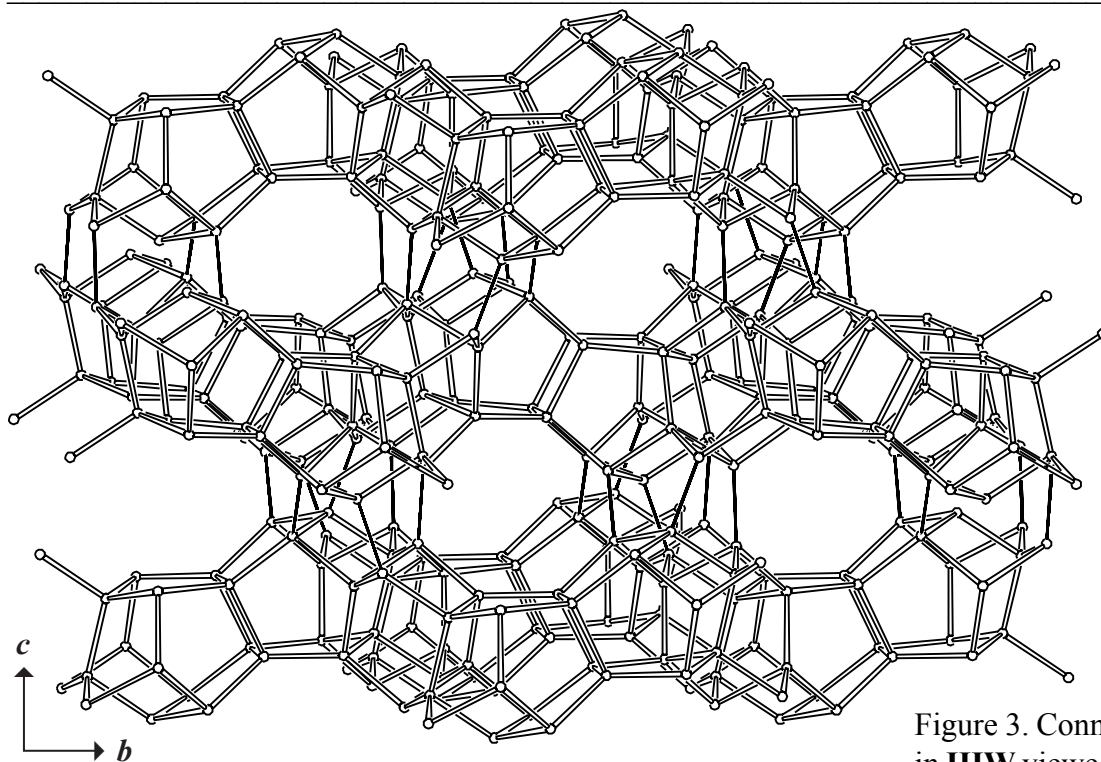


Figure 3. Connection mode  
in IHW viewed along *a*. ▲

## 3. Projections of the unit cell content:

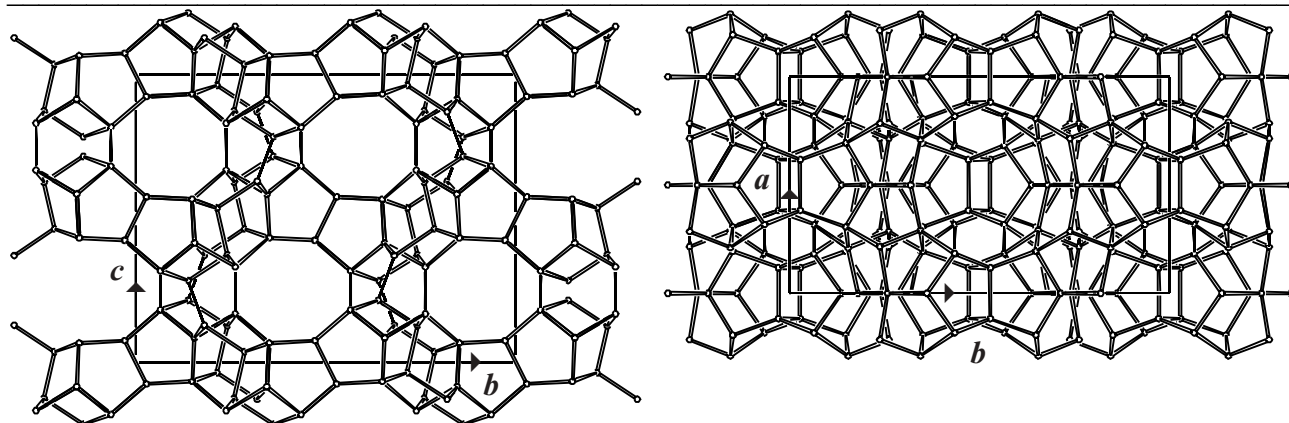


Figure 4. Projection of the unit cell content viewed along *a* (left), and along *c* (right). ▲

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

Two (equal) smaller cavities are connected through an interconnecting cavity into a large cavity shown in Figure 5. The **pore descriptors** are added. Large cavities form 8-ring channels parallel to *a*. The 8-ring channels are interconnected along *c* through 12-ring windows. The linkage of the large cavities is illustrated in Figure 6.

$$\{1 [5^6 6^2 8^2 12^1] [100] (8\text{-ring}) / 1 [5^4 6^4 12^2] [001] (12\text{-ring})\}$$

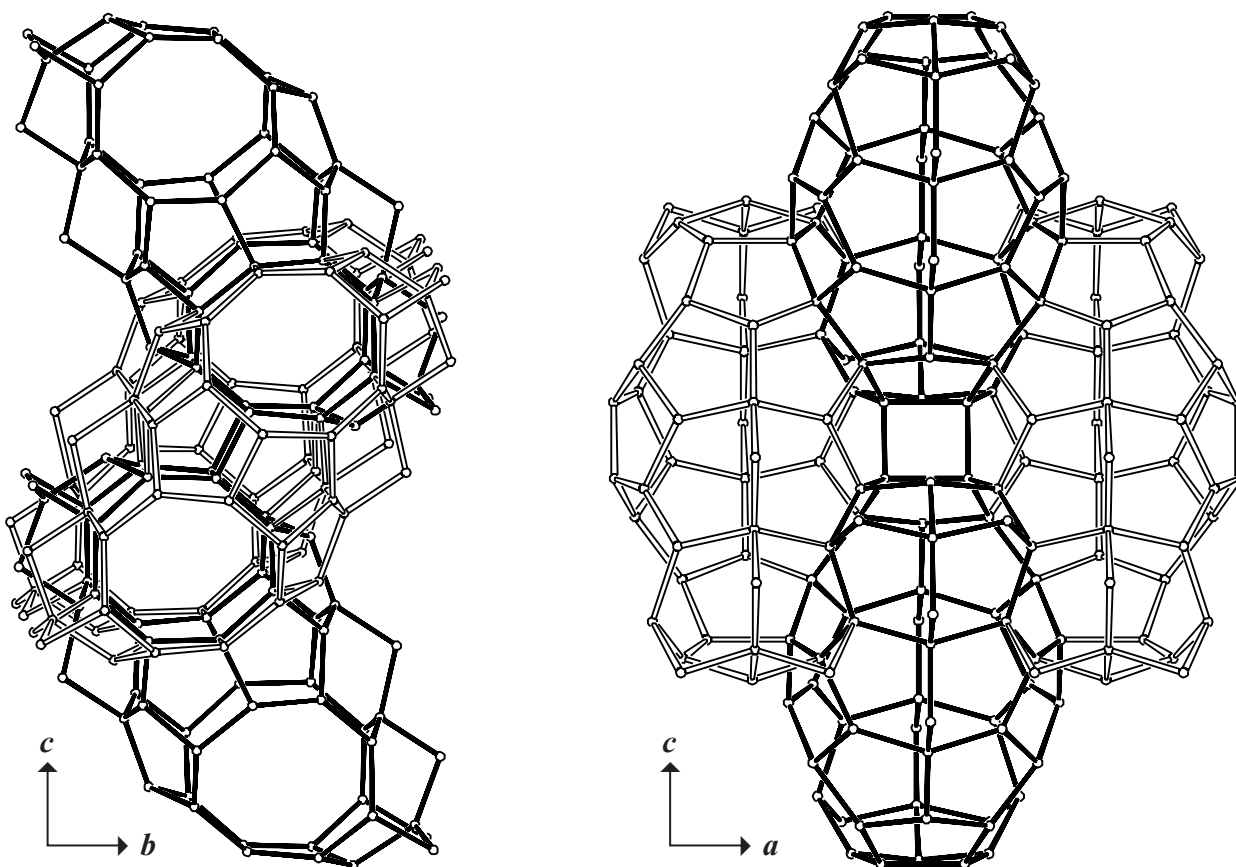
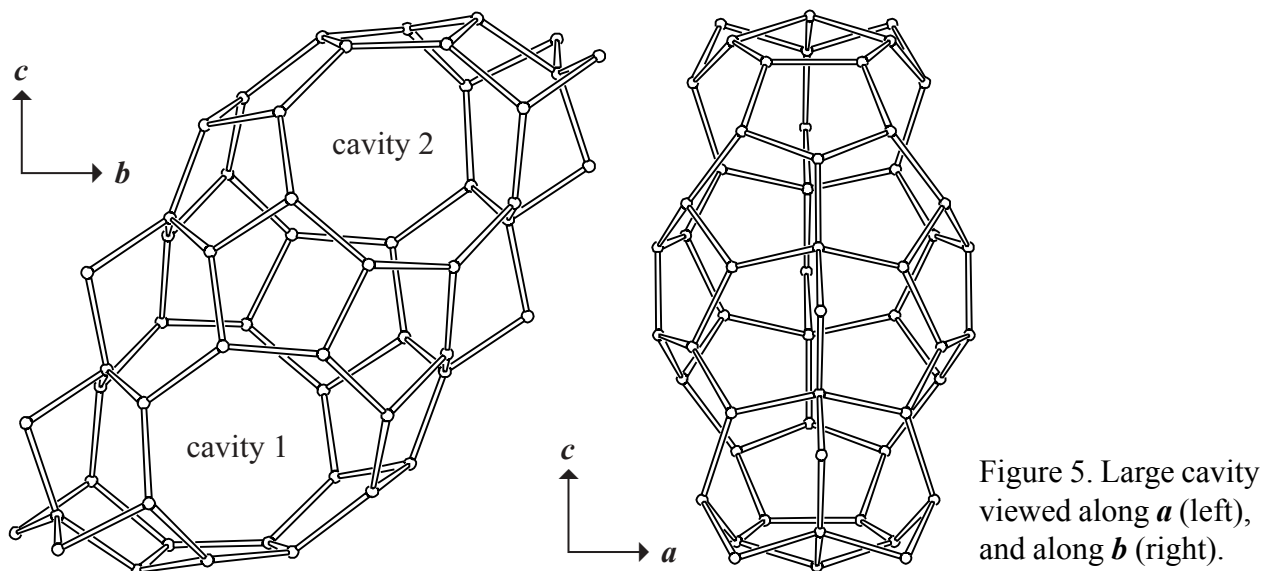


Figure 6. Linkage of large cavities along *a*, and *c* viewed along *a* (left), and along *b* (right). ▲

## 5. Supplementary information:

### *Other framework types containing (modified) 5-rings*

5-Rings can be connected in several other ways. In all 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) 5-rings (choose: **5-Rings**). There is also a link provided to a summary of the PerBUs used in the building schemes of these framework types (choose: **Appendix; Figure 6**).

