

# Building scheme for TER



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:

The one-dimensional Periodic Building Unit (PerBU) is composed of units of 20 T atoms: two double 4-rings and four additional T atoms (or four 4-1 units; bold in Figure 1; compare BRE). The PerBU equals the strip, extending infinitely along  $c$ , shown in Figure 1. Neighboring T20-units in the strip, related by a rotation of  $180^\circ$  about  $c$ , are connected along  $c$  by (fused) 6-rings and 10-rings.

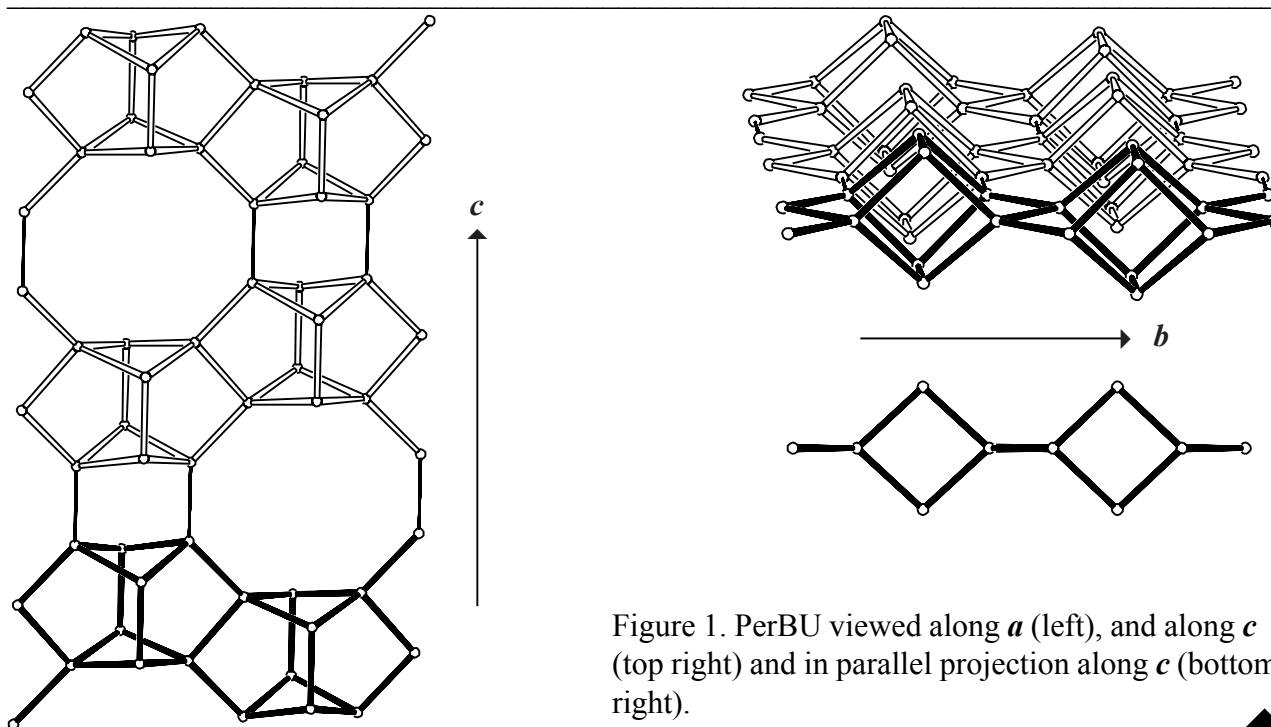


Figure 1. PerBU viewed along  $a$  (left), and along  $c$  (top right) and in parallel projection along  $c$  (bottom right). ▲

## 2. Connection mode:

Neighboring PerBUs, related by a shift of  $\frac{1}{2}(a + b)$ , are connected through 6-rings as shown in Figure 2. 10-Ring channels parallel to  $a$  are formed.

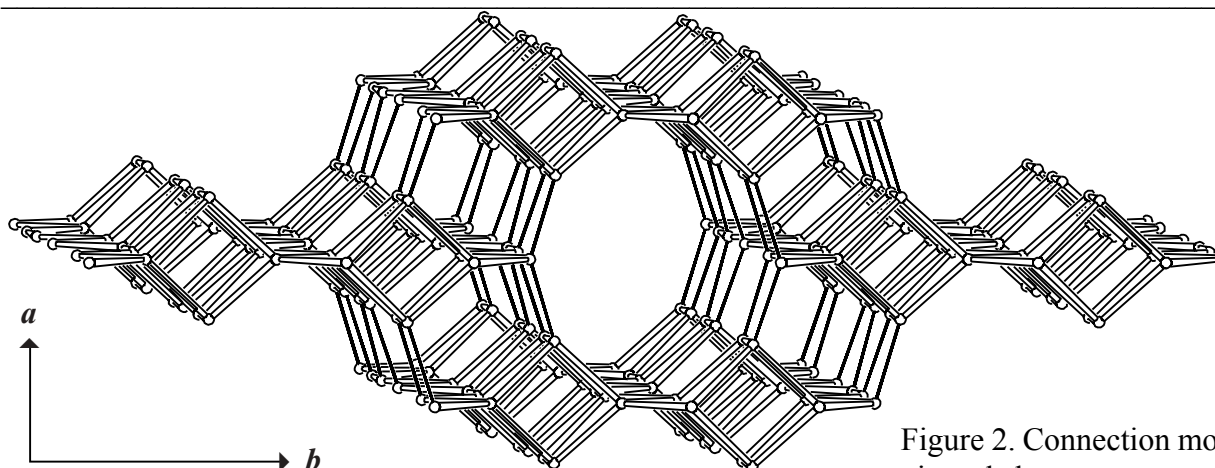
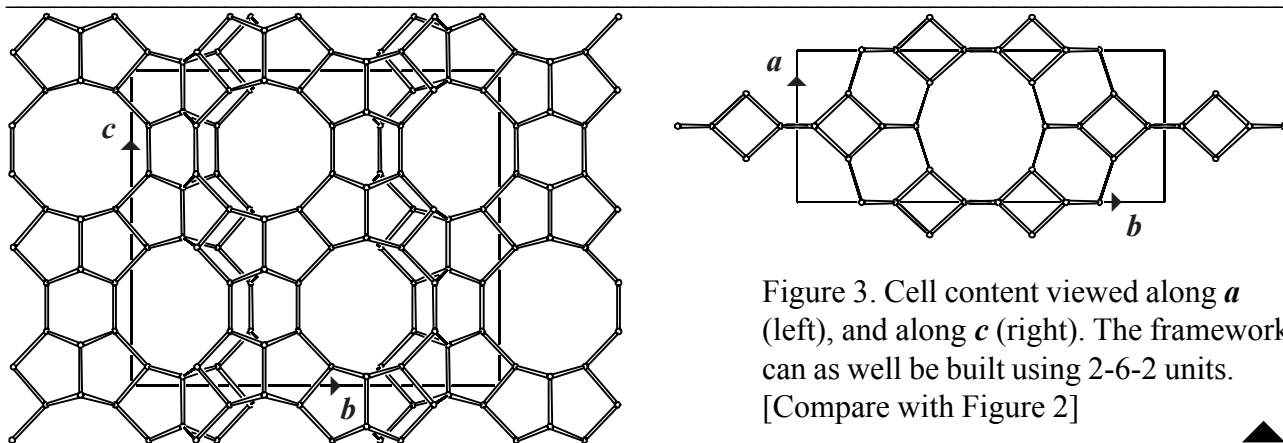


Figure 2. Connection mode viewed along  $c$ . ▲

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



### 4. Channels and/or cages:

There are intersecting 10-ring channels parallel to *a* and *c*. The channel intersection is shown in Figure 4(a) together with the **pore descriptor**. Channel intersections are linked into 10-ring channels parallel to *c* and to *a* as illustrated in Figure 4(b).

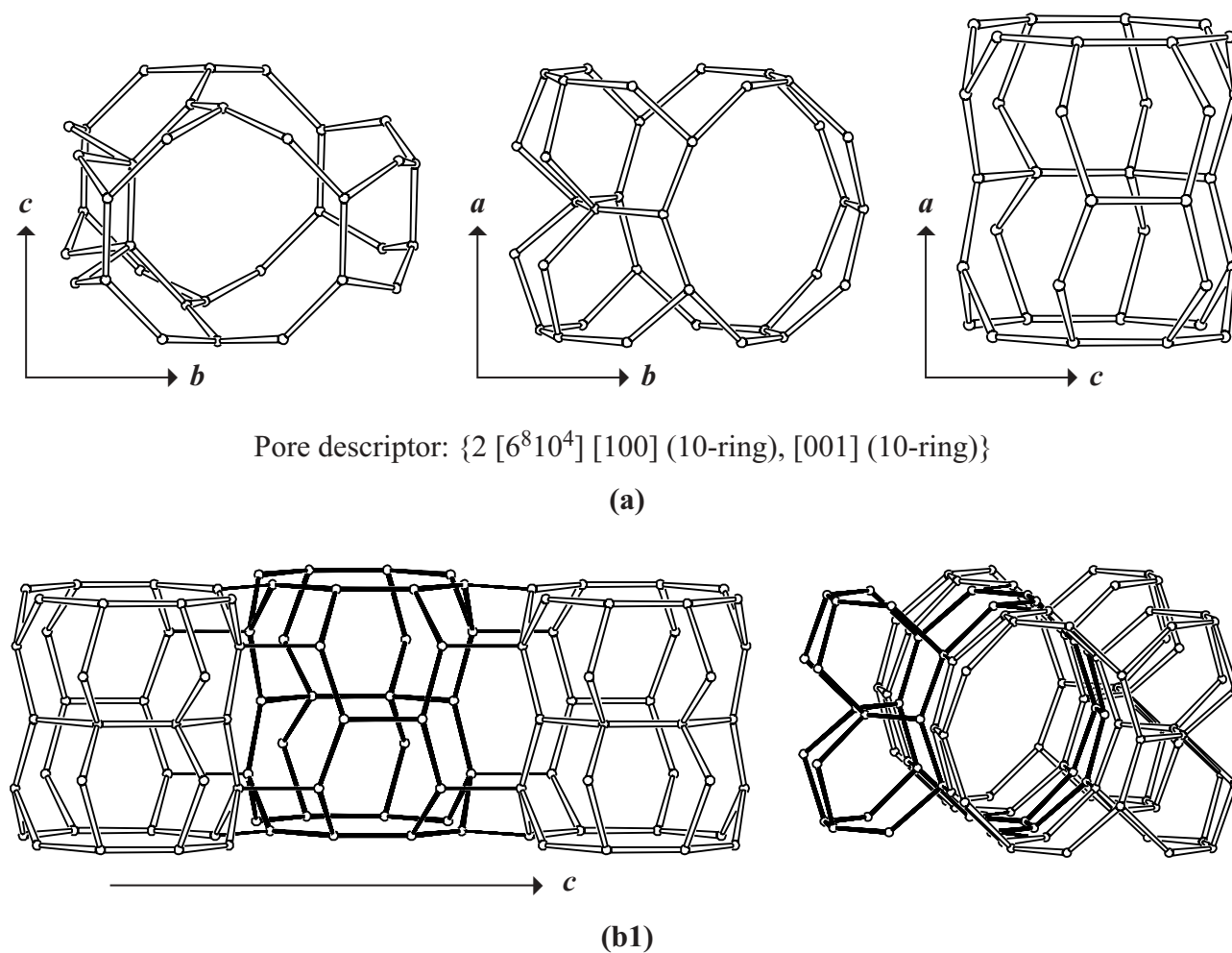


Figure 4. (a): Channel intersection, with pore descriptor, viewed (from left to right) along *a*, *c* and *b*; (b1): Linked channel intersections along *c* viewed along *b* (left), and viewed along the 10-ring channel axis parallel to *c* (right); [Figure 4 is continued on next page]

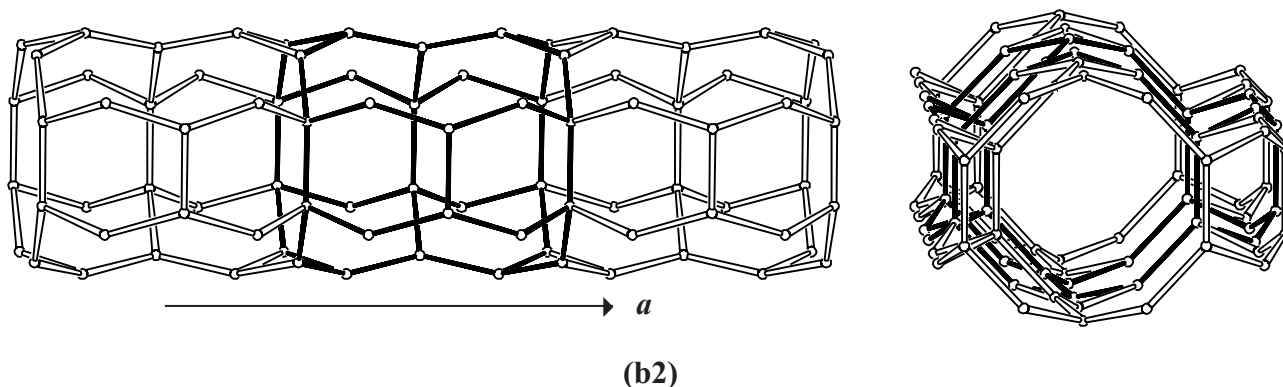


Figure 4 [Cont'd]. (b2): Fused channel intersections along  $a$  viewed along  $b$  (left), and along the 10-ring channel axis parallel to  $a$  (right).

---

## 5. Supplementary information:

### *Other framework types containing (modified) double 4-rings (D4Rs)*

Double 4-rings (D4Rs) can be connected in several other ways. In some cases the 4-rings of the D4Rs are not 4-fold connected and/or 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) D4Rs (choose **Double 4-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 5**).