

# Building scheme for BRE



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 Periodic Building Unit (PerBU) in **BRE** is the double 4-ring (D4R) layer depicted in Figure 1. 2-Fold (1,3)-connected D4Rs (in bold) are linked in the *ac* layer after pure translations along *a* and *c* through (fused) 5-rings and 4-rings, respectively.

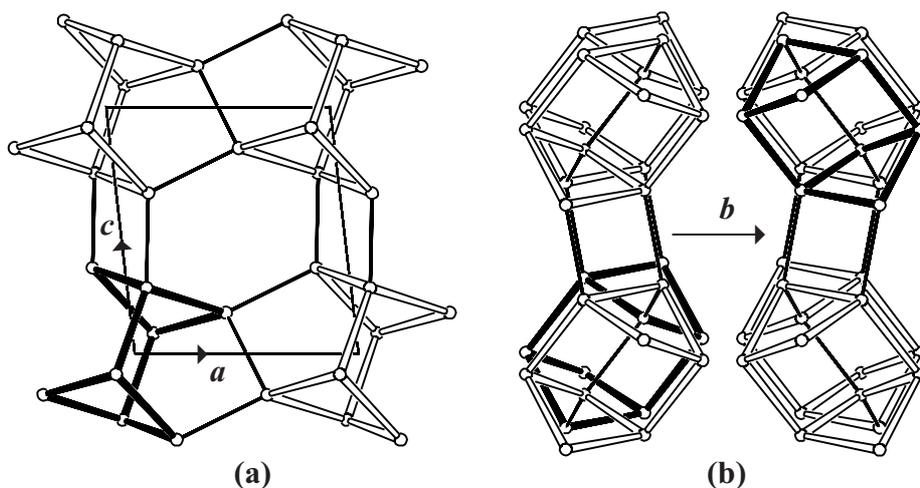


Figure 1.  
(a): PerBU constructed from 2-fold (1,3)-connected D4Rs viewed along *b*;  
(b): PerBUs, seen along *a*, are related by a rotation of 180° about *b*.



## 2. Connection mode:

Neighboring PerBUs, related by a rotation of 180° about *b*, connected along *b* through single T-T bonds as shown in Figure 2. 8-Ring windows perpendicular to *a* and *b* are formed.

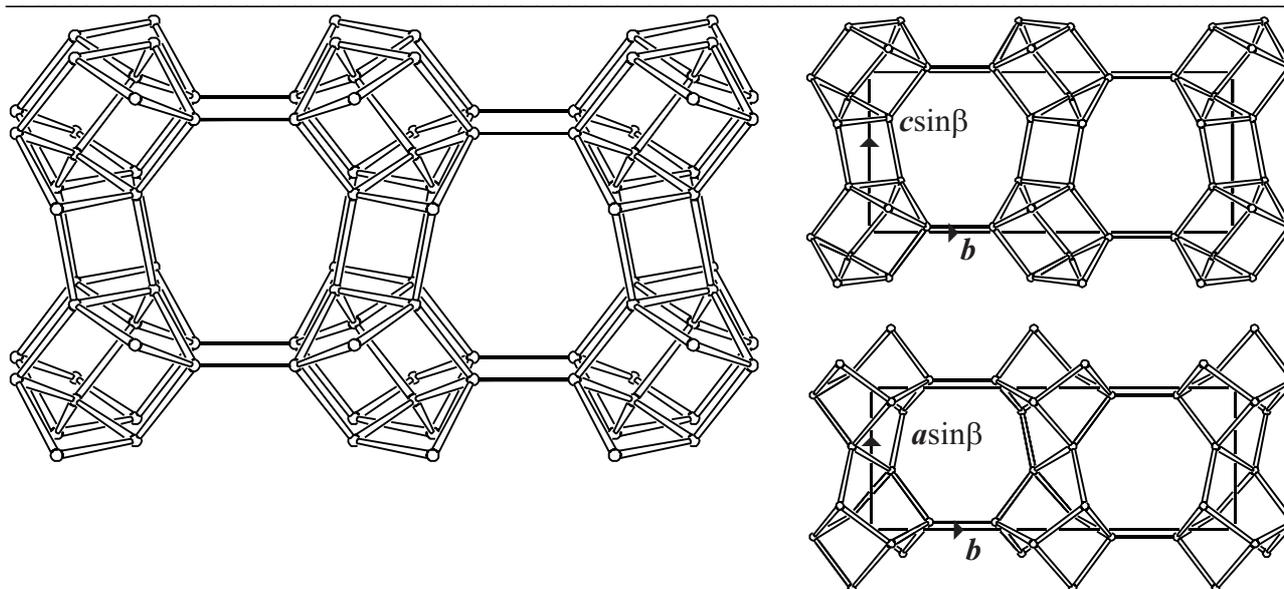


Figure 2. Connection mode viewed along *a* (left) and parallel projection of the unit cell content along *a* (top right), and along *c* (bottom right).



### 3. Projections of the unit cell content: See Figure 2.



### 4. Channels and/or cages:

8-Ring channels parallel to  $a$  and  $c$  intersect. The channel intersection is shown in Figure 3 together with the **pore descriptor**. The fusion of intersections is also illustrated.

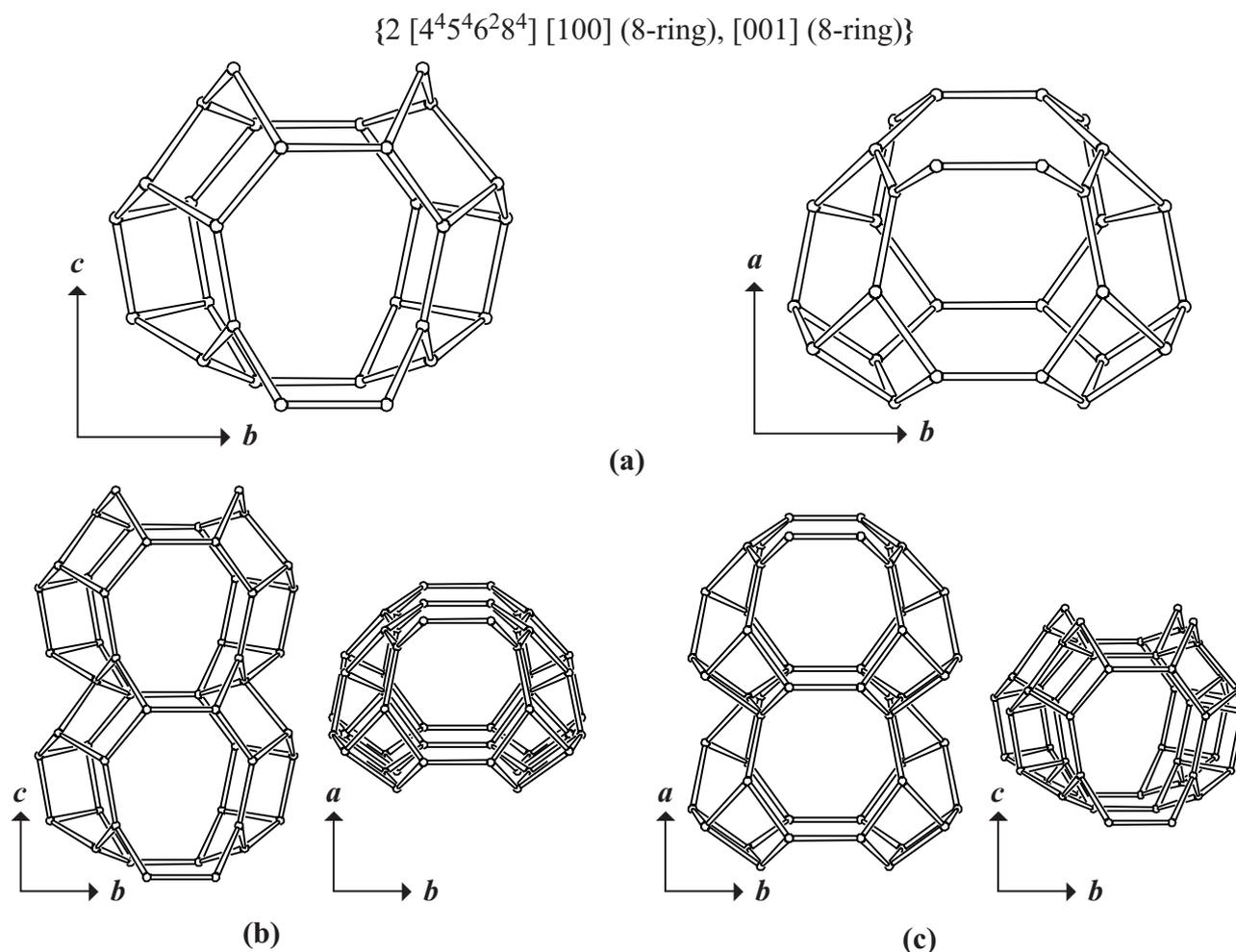


Figure 3. (a): Intersection of channels viewed along  $a$  (left), and along  $c$  (right); (b): Fused intersections along  $c$  viewed along  $a$  (left), and along  $c$  (right); (c): Fused intersections along  $a$  viewed along  $c$  (left), and along  $a$  (right).



### 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**).

