Building scheme for AFS and BPH

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:

AFS and **BPH** can be built using units of 14 T atoms (bold in Figure 1(a)). The T14-unit consists of two double 4-rings each missing one T atom or two 6*1 units. The two-dimensional Periodic Building Unit (PerBU) equals the hexagonal layer obtained by connecting T14-units through 4-rings around a 6-fold inversion axis as shown in Figure 1(b-d).

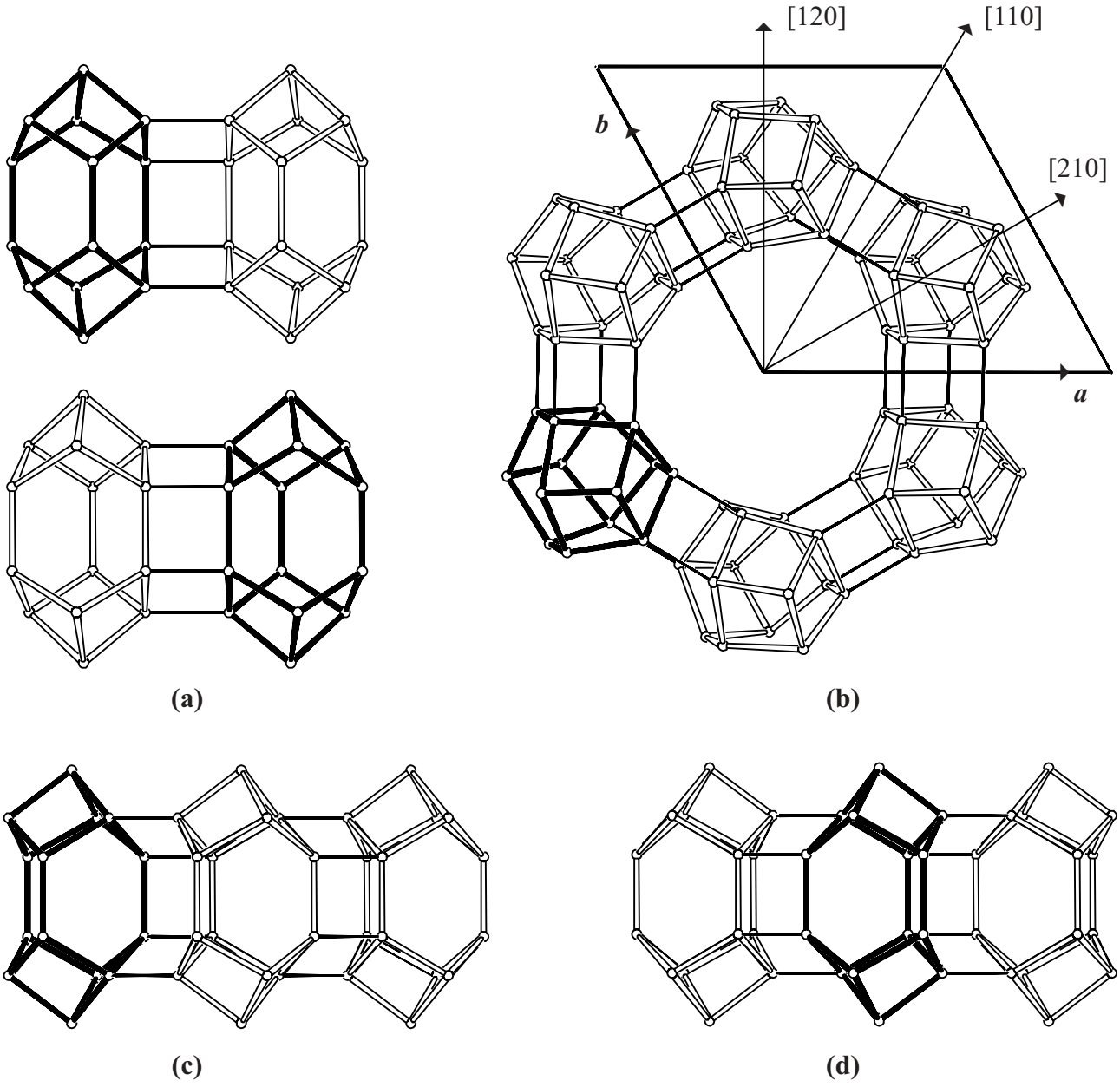


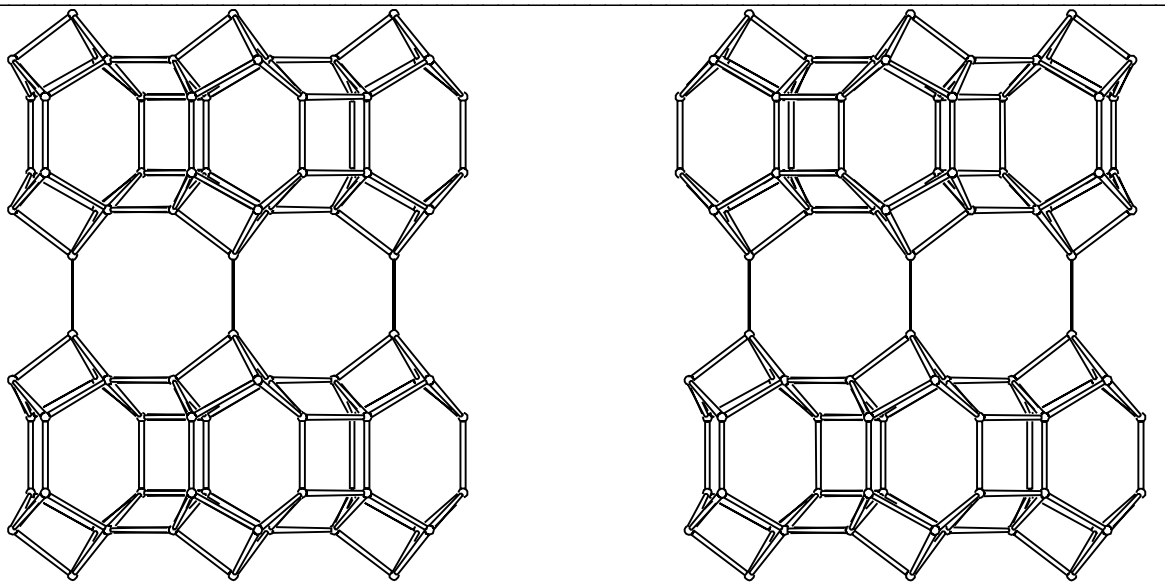
Figure 1. (a): Linkage between T14-units within the PerBU in **AFS** and **BPH** seen along [110] (top) and along [100] (bottom); (b): PerBU seen along ***c***, (c): Idem along [120] and (d): Idem along [210]. The layers depicted in Figure 1(c and d) are identical and related by a 60° rotation about the hexagonal plane normal ***c***.

2. Connection mode:

Neighboring layers can be connected along the PerBU plane normal parallel to ***c*** through 8-rings in two different ways:

(1): the lateral shift of the top layer along ***a*** and ***b*** is zero before connecting it to the bottom layer.

(2): the top layer is rotated over 60° about ***c*** before connecting it to the bottom layer.



(1) **(2)**

Figure 2. Connection modes **1** (left) and **2** (right) seen along [120].

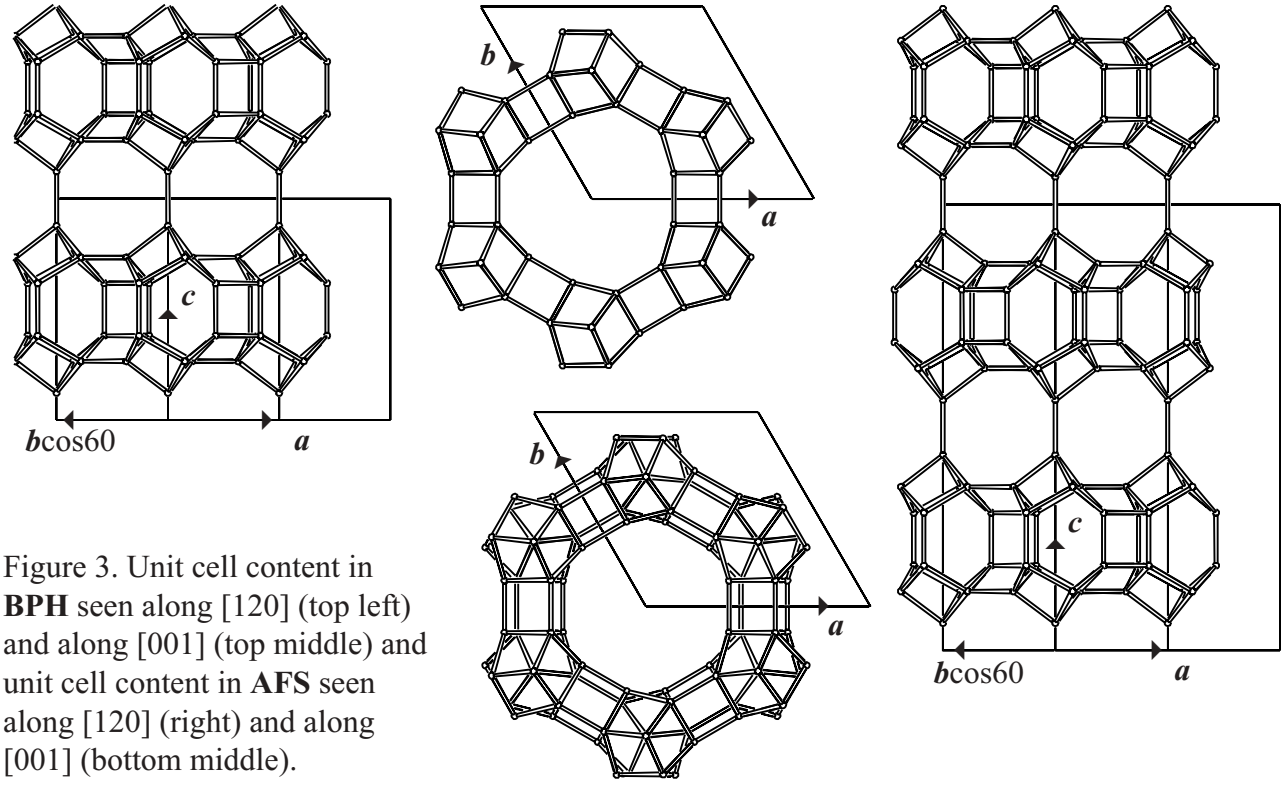


Figure 3. Unit cell content in **BPH** seen along [120] (top left) and along [001] (top middle) and unit cell content in **AFS** seen along [120] (right) and along [001] (bottom middle).

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

Pure **AFS** and **BPH** are obtained when neighboring PerBUs are exclusively related by translation along ***c*** or by a rotation of 60° about ***c***, respectively.

4. Channels and/or cages:

The channel intersection is depicted in Figure 4 together with the **pore descriptor**. The channel intersection is topologically equivalent to the intersection in **AFY**. Channel intersections are connected into channels along <100>, along <210> and along [001] as illustrated in Figure 5.

The intersections in both frameworkypes have the same pore descriptor:
{3 [$4^{18}8^{6}12^{2}$] <100> (8-ring), <210> (8-ring), [001] (12-ring)}

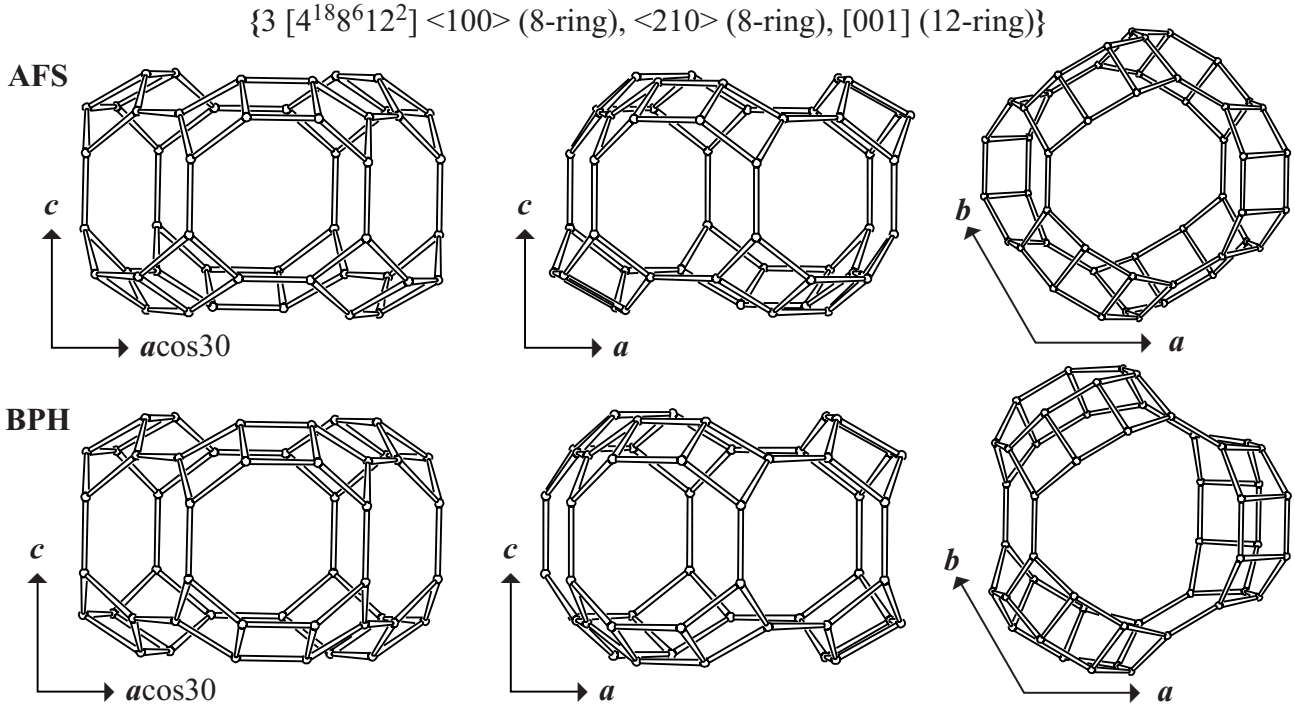


Figure 4. Channel intersections in **AFS** (top) and **BPH** (bottom) in perspective view along (from left to right) <100>, <210> and [001].

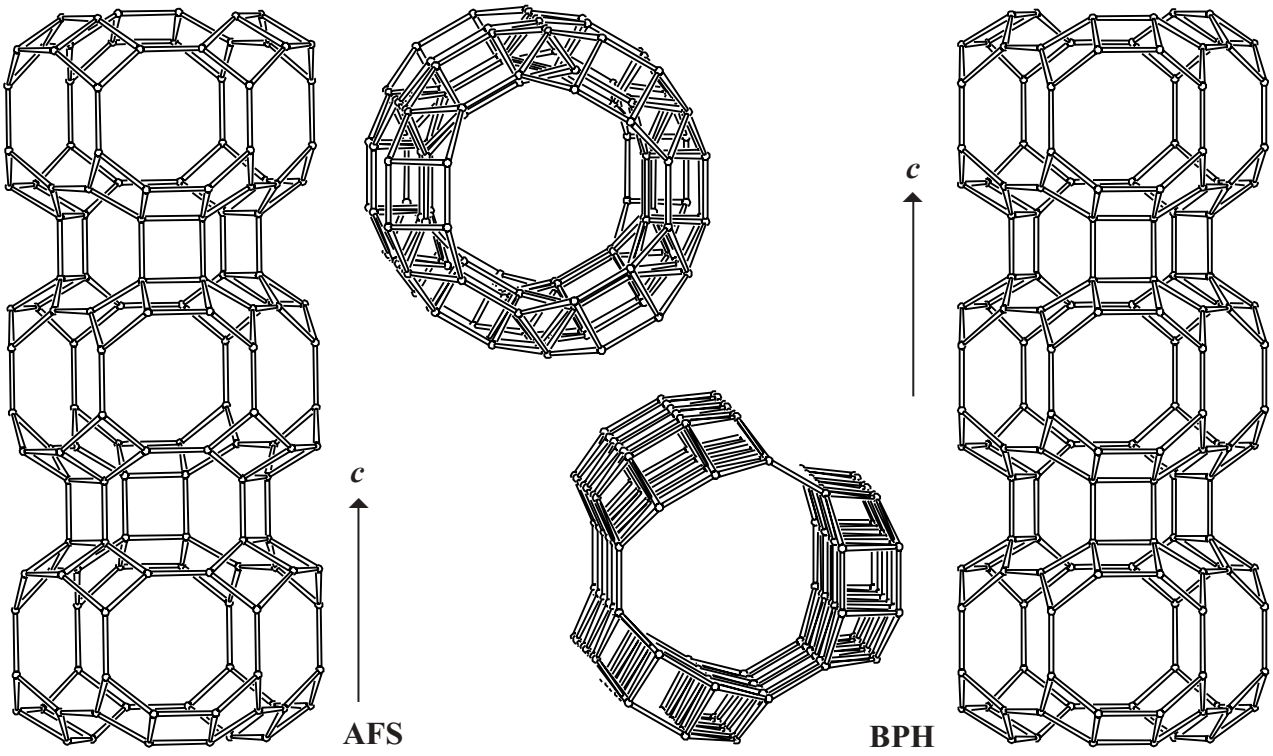


Figure 5. Connection of intersections parallel to [001] in **AFS** (left) and **BPH** (right) viewed along <100> (left and right) and along [001] (middle top and bottom). [Fig.5 is continued on next page]

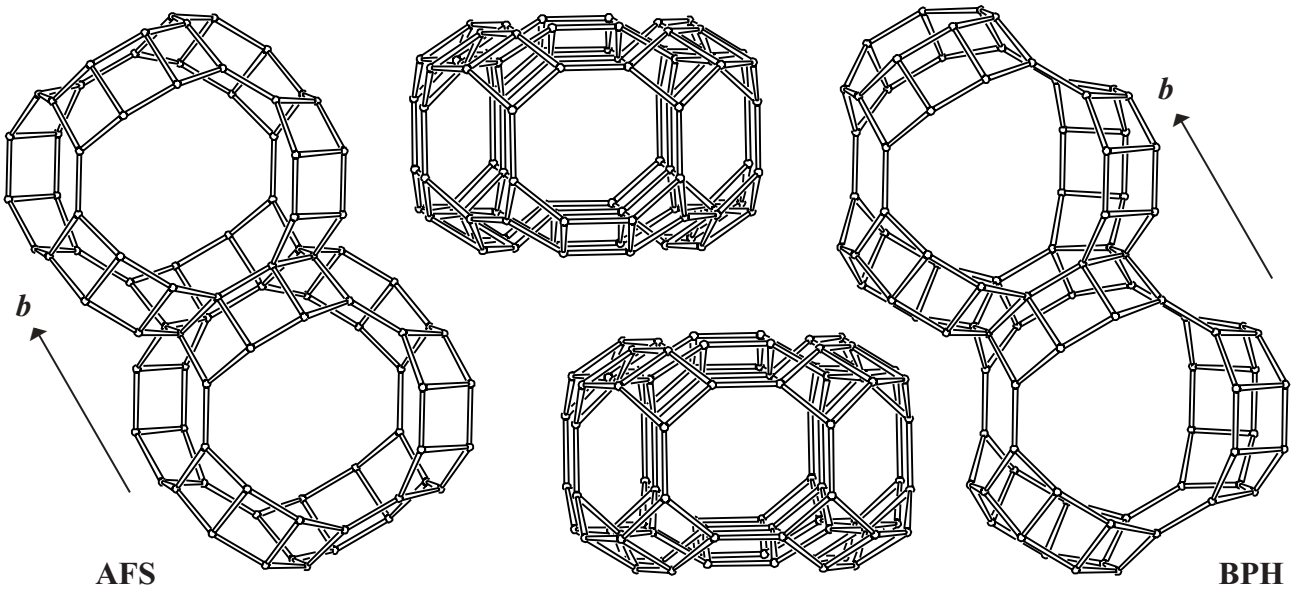


Figure 5 [Cont'd]. Connection of channel intersections parallel to <100> in **AFS** (left) and **BPH** (right) seen along [001] (left and right) and along <010> (middle top and bottom).

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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**).