Building scheme for AFY

1. Periodic Building Unit:

AFO can be built using the double 4-ring (D4R) drawn bold in Figure 1. The Periodic Building Unit (PerBU) equals the hexagonal layer obtained by connecting D4Rs through 4-rings around a 3-fold inversion axis as shown in Figure 1.

Figure 1. Perspective views of the PerBU in **AFY** along **c** (left) and along [120] (top right) and parallel projection along [120] (bottom right).

▲
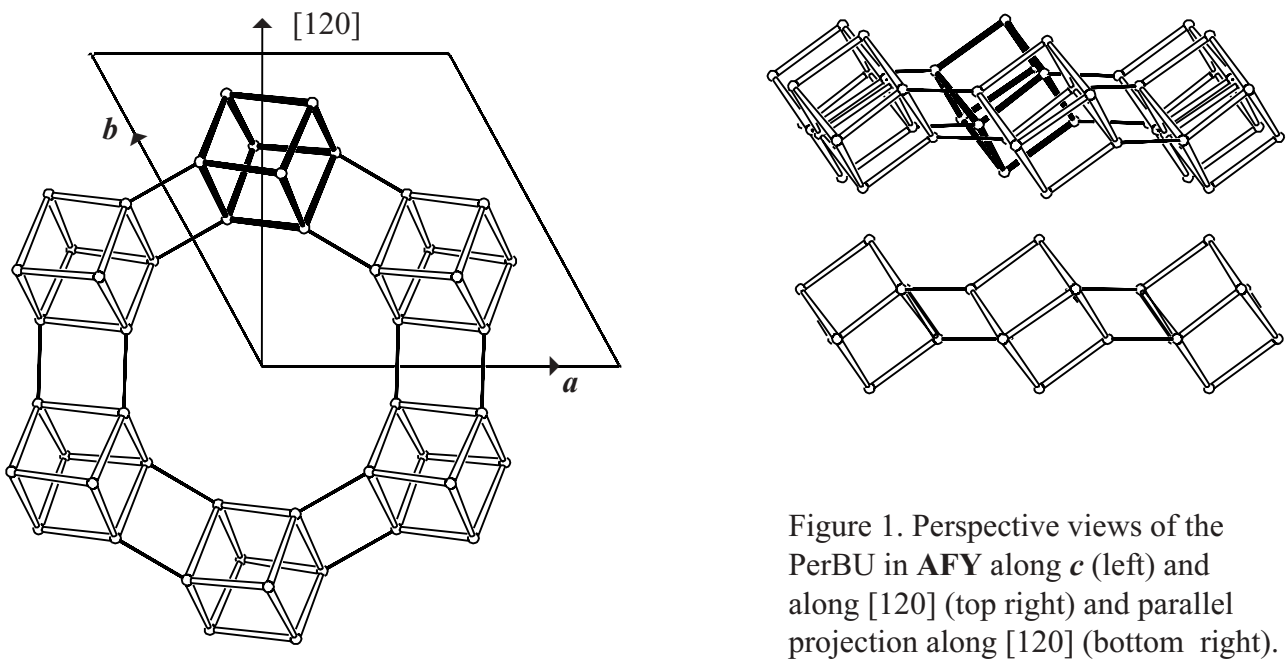
2. Connection mode:

Neighboring PerBUs, related by pure translations along **c**, are connected along **c** through single T-T bonds. 8-Rings are formed.

Figure 2. Connection mode along **c** and unit cell content in **AFY** viewed along [120].

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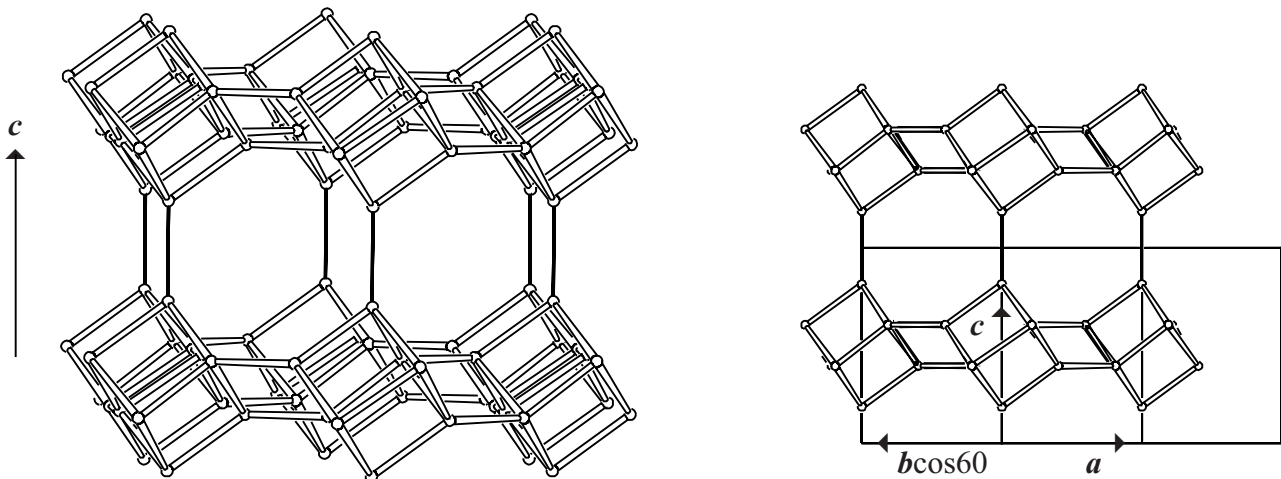
3. Projections of the unit cell content: See Figure 2.

4. Channels and/or cages:

The channel intersection is depicted in Figure 3 together with the **pore descriptor**. The channel intersection is topologically equivalent to the intersection in **AFS** and **BPH**. Channel intersections are connected into channels along <100>, along <210> and along [001] as illustrated in Figure 4.

$\{3 \ [4^{18}8^612^2] <100> \text{ (8-ring)}, <210> \text{ (8-ring)}, [001] \text{ (12-ring)}\}$
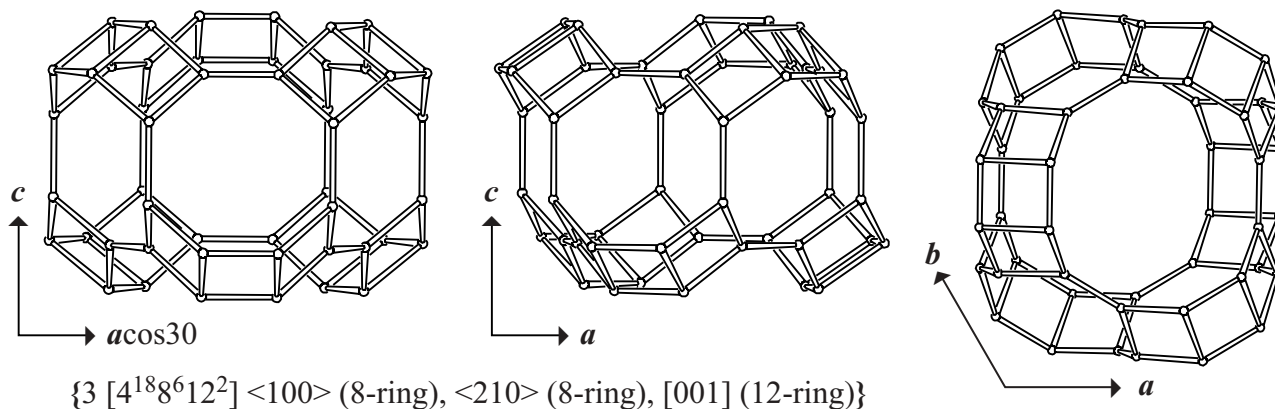
Figure 3. Channel intersections in **AFY** viewed along (from left to right) <100>, <210> and [001].
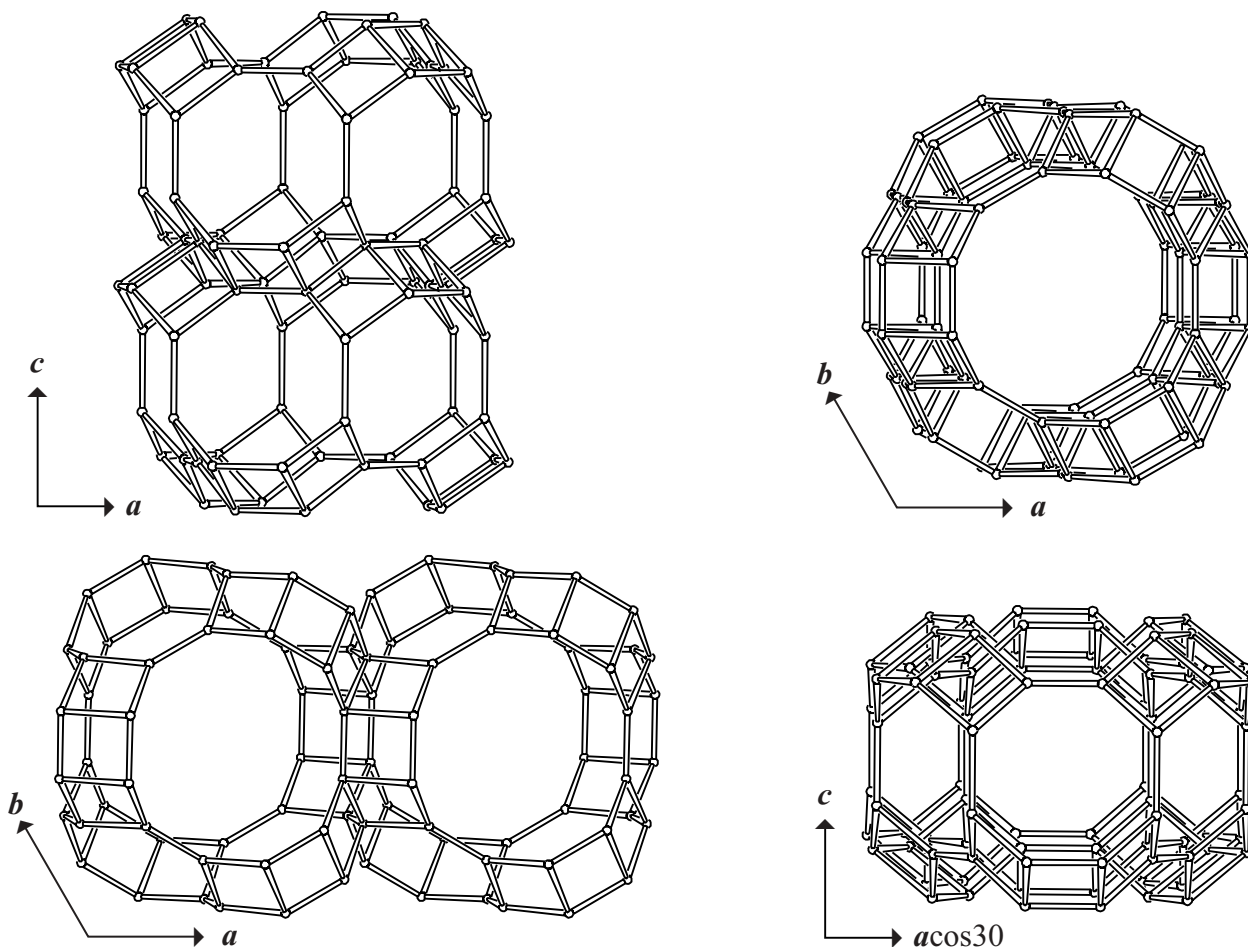

Figure 4. Connection of channel intersections parallel to [001] viewed along <210> (left) and along [001] (right); (c): Connection of channel intersections parallel to <100> viewed along [001] (left) and along <100> (right).

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**).

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