

Building scheme for AFN



1. Periodic Building Unit – 2. Connection mode – 3. Parallel projections of the unit cell
4. Channels and/or cages – 5. Supplementary information

1. Periodic Building Unit:

AFN can be built using T8-units composed of three fused 4-rings (or, alternatively, of a not fully connected double 4-ring; both units in bold in Figure 1). T8-units, related by a rotation of 180° about b , are connected through (fused) 4-rings into chains along a . The Periodic Building Unit (PerBU) is obtained when neighboring chains, related by pure translations along c , are connected along c through single T-T bonds into the ac layer as depicted in Figure 1

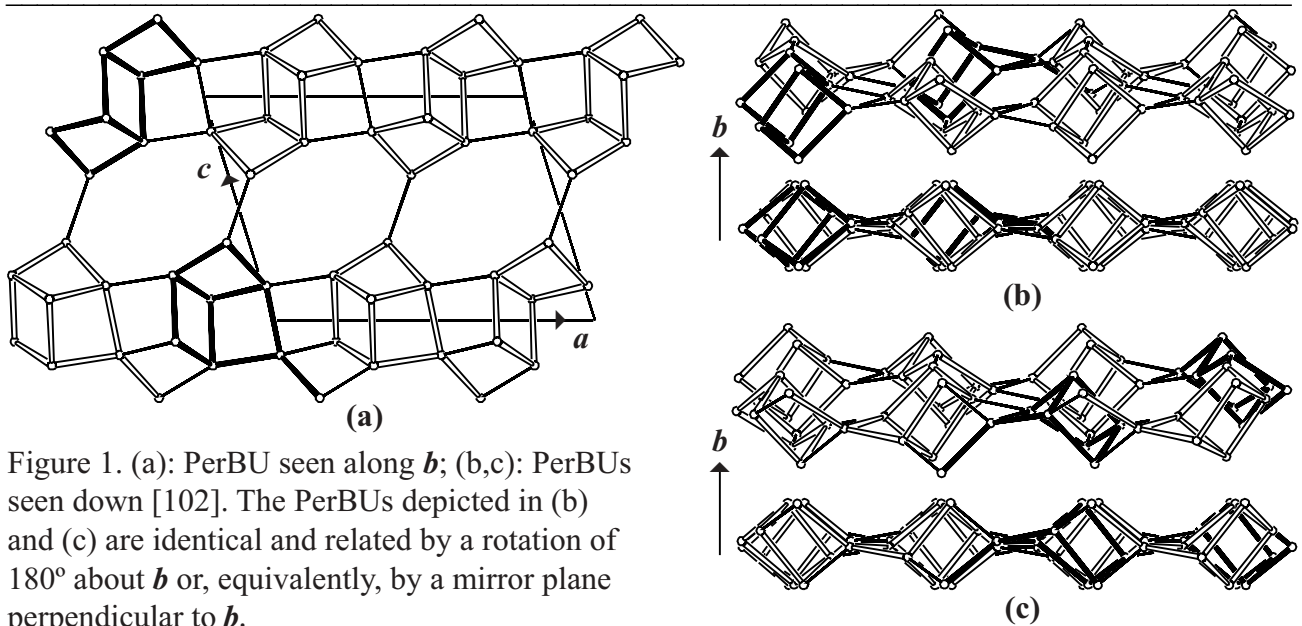


Figure 1. (a): PerBU seen along b ; (b,c): PerBUs seen down $[102]$. The PerBUs depicted in (b) and (c) are identical and related by a rotation of 180° about b or, equivalently, by a mirror plane perpendicular to b .

2. Connection mode:

Neighboring PerBUs, related by a rotation of 180° about b , are connected along b through (fused) 4- and 6-rings as shown in Figure 2. AFN can also be built from 8-rings that are formed.

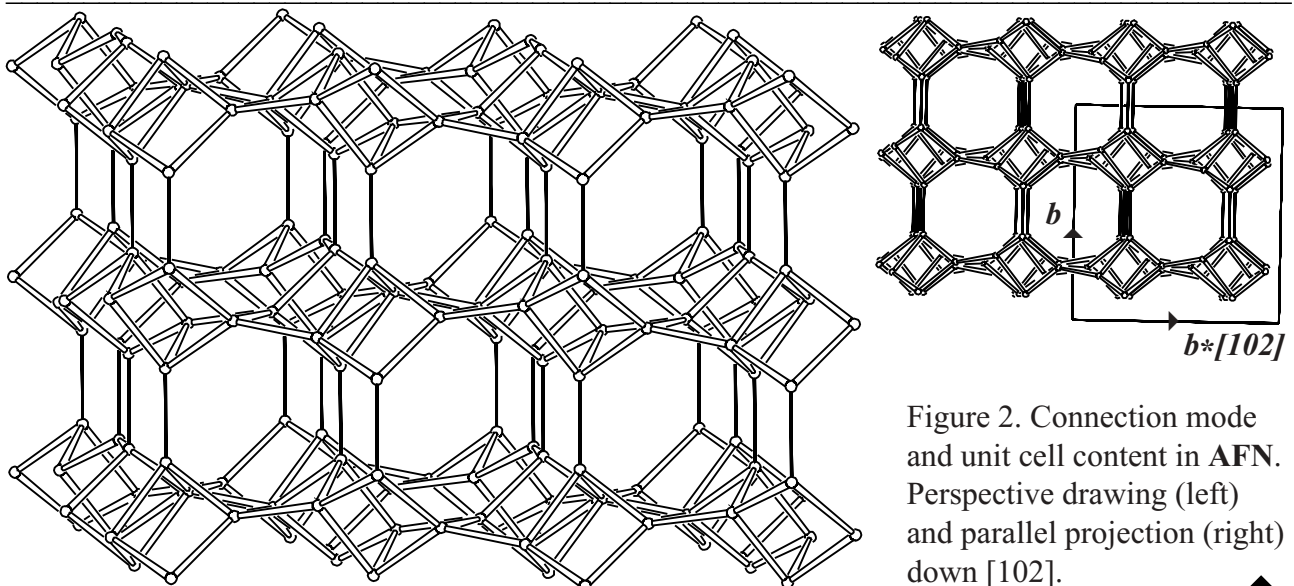


Figure 2. Connection mode and unit cell content in AFN. Perspective drawing (left) and parallel projection (right) down $[102]$.

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



4. Channels and/or cages:

Large cavities (the channel intersections), related by 2-fold screw axes parallel to b and by pure translations along a and c , are connected into 8-ring channels along $[010]$, $[102]$ and $[110]$ (and $[-110]$) as illustrated in Figure 3. The **pore descriptor** is added.

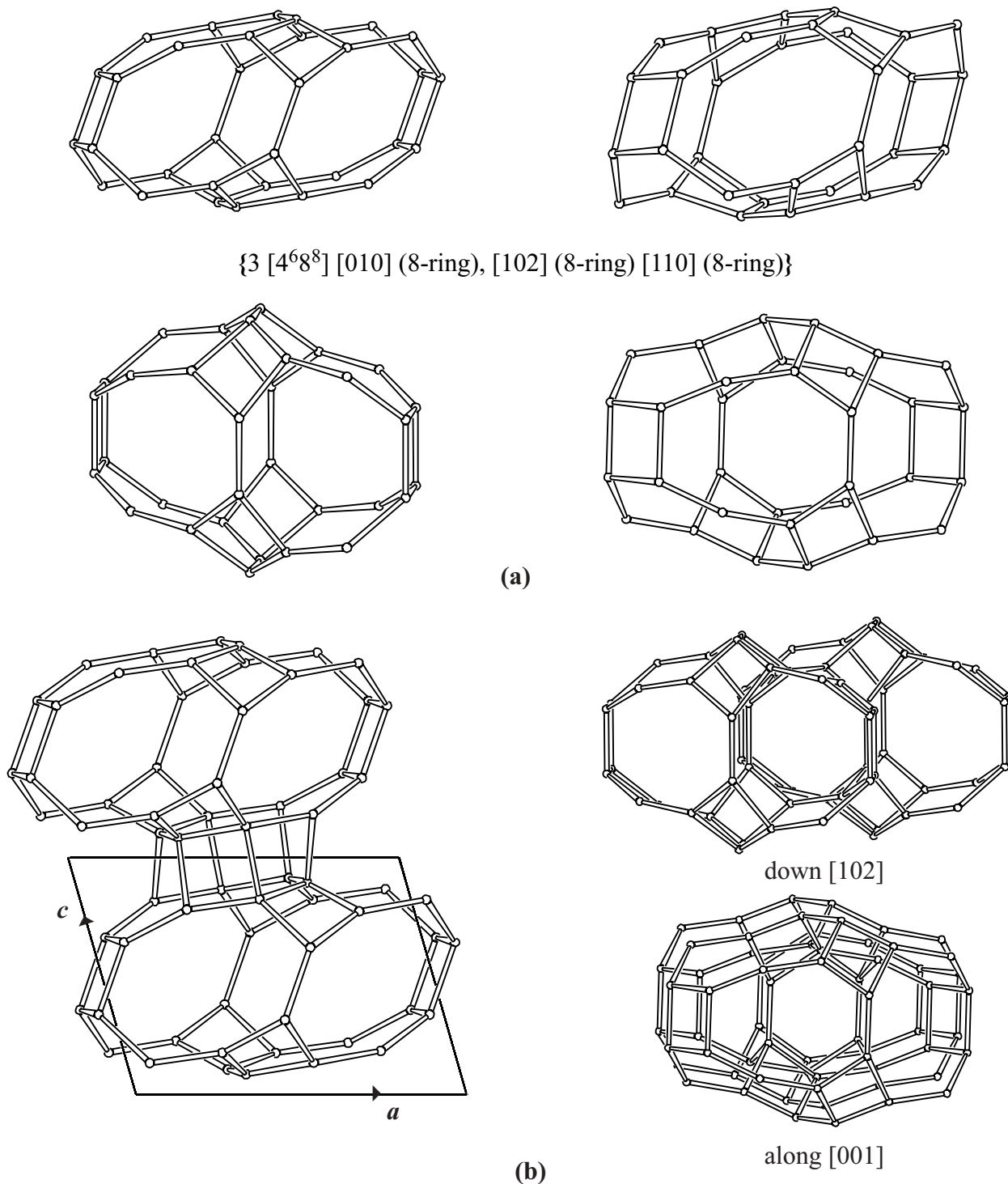


Figure 3. (a): Channel intersection in AFN in perspective view along $[010]$ (top left), along $[110]$ (top right), along $[102]$ (bottom left) and along $[001]$ (bottom right); (b): Connection of channel intersections parallel to $[001]$ seen along $[010]$ (left), along $[102]$ (top right) and along $[001]$ (bottom right); [Figure 3 is continued on next page].

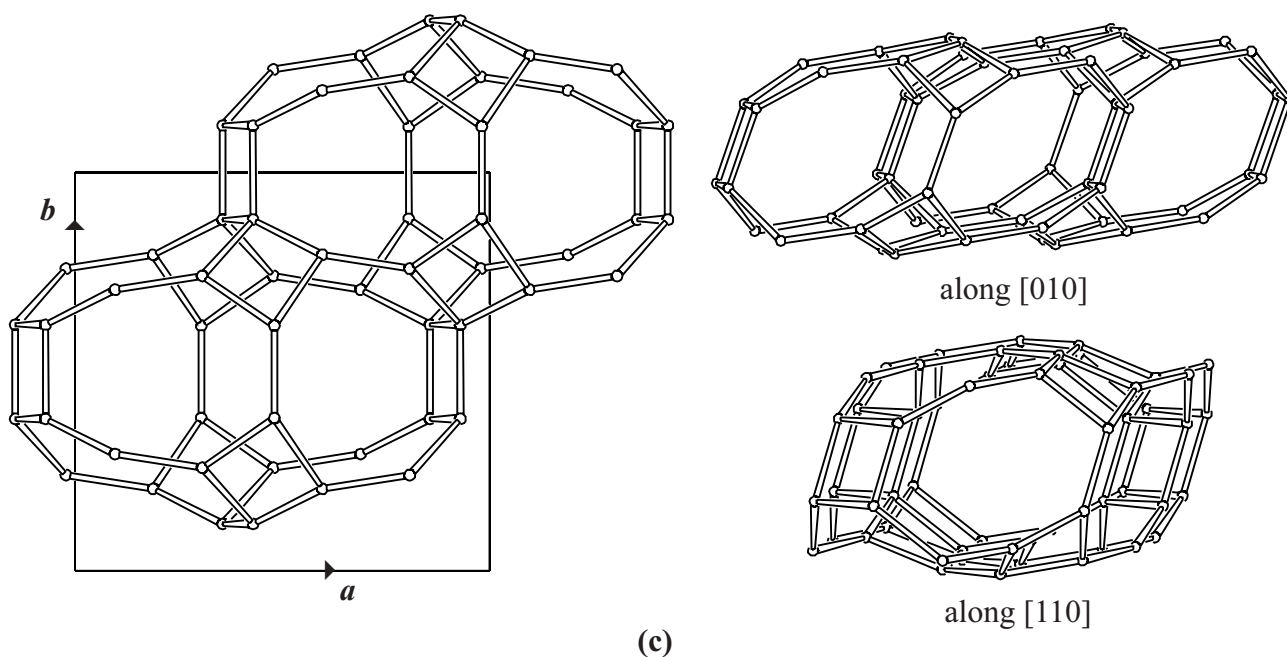


Figure 3 [Cont'd]. (c): Connection of channel intersections parallel to $[110]$ seen perpendicular to the ab plane (left), along $[010]$ (top right) and along $[110]$ (bottom right). ▲

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**). ▲