Building scheme for AFN


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](image1.png)

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](image2.png)

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 \( \text{AFN} \) 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**).