Building scheme for AFI



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:

AFI can be built using the crankshaft chain (bold in Figure 1 (left)) running parallel to *c*. The repeat distance along a crankshaft chain varies between 8.4-9.9 Å. The repeat unit consists of 4 T atoms. A one-dimensional Periodic Building Unit (PerBU) is obtained when six crankshaft chains are connected into a channel with a 12-ring aperture. The channel wall consists of fused 6-rings. The repeat unit of the PerBU is a cylindrical 6-ring band of 24 T atoms (bold in Figure 1 (right)).



2. Connection mode:

Neighboring PerBUs, related by pure translations along *a* and *b*, are connected through double crankshaft chains as shown in Figure 2. [In CAN the crankshaft chains are replaced by zigzag chains]



A double crankshaft chain (consisting of 2-fold (1,3)-connected double 4-rings), and 3-fold (1,3,5)-connected double 6-rings (like in **ATV**) are indicated in bold (see **Alternative descriptions**).

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



4. Channels and/or cages:

One of the non-interconnecting one-dimensional channels in AFI, parallel to c, is depicted in Figure 3. The **pore descriptor** is added.



5. Supplementary information:

Other framework types containing crankshaft chains

In several framework types at least one of the unit cell dimensions is between 8.4 and 9.9 Å. In many cases this indicates the presence of crankshaft chains.

In the **INTRO** pages links are given to detailed descriptions of these framework types (choose: **Crankshaft chains**). There is also a link provided to a summary of the Periodic Building Units used in the building schemes of these framework types (choose: **Appendix**; **Figure 3**).

Alternative description of AFI using (modified) double 4-rings (D4Rs)

Several framework types, like **AFI**, can be built using double crankshaft chains of the narsarsukite type consisting of 2-fold (1,3)-connected D4Rs (see Figure 2).

In the **INTRO** pages links are given to descriptions of other framework types containing (modified) D4Rs (choose: **Double 4-rings**). There is also a link provided to a summary of the Periodic Building Units used in the building schemes of these framework types (choose: **Appendix**; **Figure 5**).

Alternative description of AFI using (modified) double 6-rings (D6Rs)

Several framework types, like **AFI**, can be built using (modified) D6Rs (see Figure 2). In the **INTRO** pages links are given to descriptions of other framework types containing (modified) D6Rs (choose: **Double 6-rings**). There is also a link provided to a summary of the Periodic Building Units used in the building schemes of these framework types (choose: **Appendix**; **Figure 7**).