# **Building scheme for ATT**



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:

**ATT** can be built using the 4-ring and the crankshaft chain (bold in Fig.1 (left)) or using saw chains (see Figure 2). 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 two crankshaft chains and two T-T dimers (or 4-2 units) are connected in such a way that a tube with a 6-ring aperture is formed. The repeat unit of the PerBU consists of a 3-fold (1,2,3)-connected double 6-ring (D6R) and contains 12T atoms (bold in Fig.1 (right)). [The connection in the D6R is different from the connection in the D6R in AFI, ATV, AWO and UEI]



#### 2. Connection mode:

Neighboring PerBUs, related along b and c by pure translations, are connected along b through double crankshaft chains and along c through single crankshaft chains as shown in Figure 2. [The Figure also shows that **ATT** can as well be built using double saw chains (or 4-2 units)]





Figure 2. Connection mode and parallel projection of the unit cell content along a(left and middle) and parallel projection along b (top right). For clarity, only 1½ repeat units of the PerBUs along a are drawn. In the perspective drawing, one saw chain is indicated in bold (see Alternative description)

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



### 4. Channels and/or cages:

In **ATT** interconnecting channels are parallel to *a* and *b*. The channel intersection is depicted in Figure 3. The **pore descriptor** as added. The fusion of these cavities in the *bc* and *ac* plane is illustrated in Figure 4.



Figure 4. Fused intersections viewed along a (left), and along b (right). Interconnecting channels along a and b are formed.

# 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 ATT using saw chains

In several framework types at least one of the unit cell dimensions is ~ n\*7.5 Å (with n = 1,2..etc.). In many cases this indicates the presence of saw chains. **ATT** can be built using saw chains that are parallel to **b** (see Figure 2). The unit cell dimension along the saw chain axis is ~ 7.5 Å. In the **INTRO** pages links are given to descriptions of other framework types containing (twisted) saw chains (choose: **Saw 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 2**).

## Other framework types using (modified) double 6-rings (D6Rs)

Several framework types, like **ATT**, can be built using (modified) D6Rs (see Figure 1). 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**).