Building scheme for ATV

1. Periodic Building Unit:

ATV can be built using the crankshaft chain (bold in Fig.1 (left)) running parallel to *a* or using saw chains parallel to *b* (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 three crankshaft chains are connected in such a way that a tube with a 6-ring aperture is formed. The tube wall consists solely of 6-rings. The repeat unit of the PerBU consists of a 3-fold (1,3,5)-connected double 6-ring (D6R) and contains 12T atoms (bold in Fig.1 (right)). [The connection in the D6R in **ATV** is equal to the connection in the D6R in **AFI** and is different from the connection in the D6R in **ATT**, **AWO** and **UEI**]
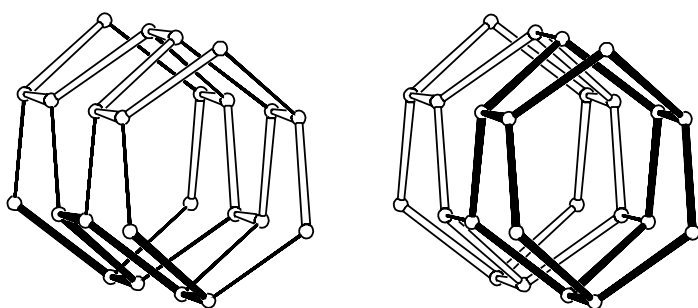

Figure 1. PerBU constructed from crankshaft chains (left) and PerBU constructed from 3-fold connected double 6-rings (see **Alternative description**).

2. Connection mode:

Neighboring PerBUs, related along *b* by a shift of ½*a* and along *c* by a pure translation, are connected along *b* through double crankshaft chains and along *c* through single crankshaft chains as shown in Figure 2.
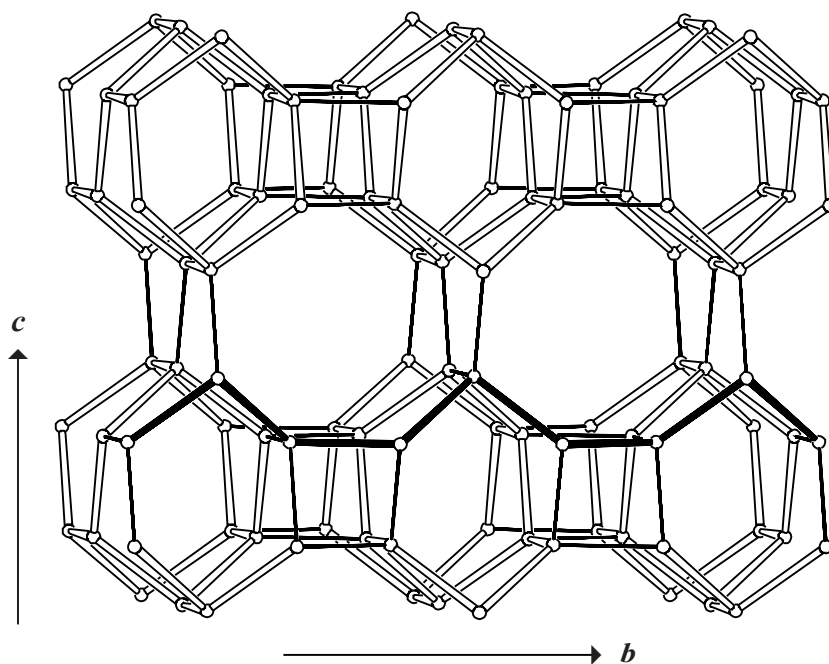

Figure 2. Connection mode viewed along *a*. For clarity, only 1½ repeat units of the PerBUs along *a* are drawn. One saw chain is indicated in bold (see **Alternative description**).

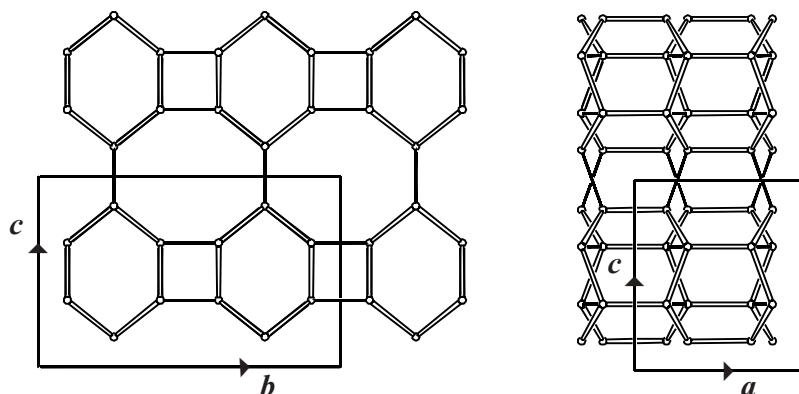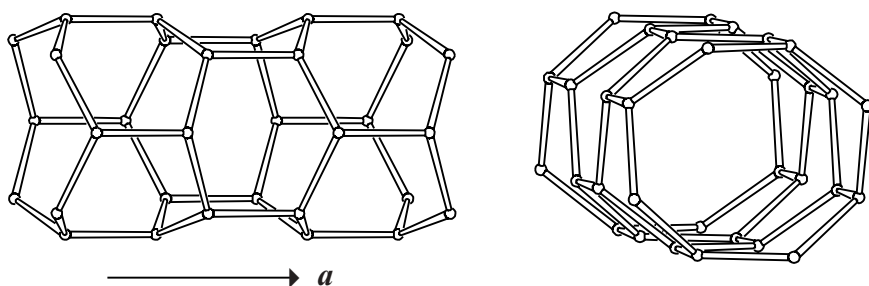## 3. Projections of the unit cell content: See Figure 3.

Figure 3. Parallel projection of the unit cell content along *a* (left), and along *b* (right).

4. Channels and/or cages:

PerBUs form non-interconnecting channels with an 8-ring aperture parallel to *a*. The channel wall consists of fused 6-rings as shown in Figure 4. The **pore descriptor** is added.

$\{1\ [6^8 8^{2/2}]\ [100]\ (8\text{-ring})\}$

Figure 4. 8-Ring channel viewed along *a* (left), and perpendicular to *a* (right).

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 ATV *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. **ATV** can be built using (twisted) saw chains that are parallel to *b* (see Figure 2). The unit cell dimension along the saw chain axis is ~ 2*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**).

Alternative description of ATV *using (modified) double 6-rings (D6Rs)*
Several framework types, like **ATV**, 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**).