Building scheme for CAS

1. Periodic Building Unit – 2. Connection mode – 3. Projections of the unit cell content
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1. Periodic Building Unit:

CAS can be built using the zigzag (zz) chain (bold in Fig. 1) running parallel to \( \mathbf{a} \). The repeat distance along the zigzag chain is about 5.2 Å. The repeat unit consists of 2 T atoms. Three zz chains are connected to an infinite building unit. A two-dimensional Periodic Building Unit (PerBU) is obtained when infinite building units, related by a 2-fold axis parallel to the plane of the paper (pointing from top to bottom) are connected along \( \mathbf{c} \) into a layer of (fused) 6-ring chairs and 6-ring boats decorated with additional zz chains as shown in Figure 1. [Compare this PerBU with those in BIK and NSI]

![Figure 1. Infinite building unit constructed from three zz chains (left) and from 5-1-units (middle; see also: Alternative description) seen along the chain axis \( \mathbf{a} \). Right: PerBU in CAS.](image)

2. Connection mode:

Neighboring PerBUs, related by a shift of \( \frac{1}{2} \mathbf{a} \), are connected along \( \mathbf{b} \) through 5-rings. Two zz chains of the infinite building unit are involved in the (fused) 6-ring layer and the third zz chain (in bold) connects the 6-ring layers. [Compare this connection mode with those in BIK and JBW]

![Figure 2. Connection mode in CAS viewed along \( \mathbf{a} \).](image)
3. Projections of the unit cell content:

Figure 3. Perspective view of the unit cell content along \(a\) (top left) and parallel projections of the unit cell content along \(a\) (top right), along \(b\) (bottom right), and along \(c\) (bottom left).

4. Channels and/or cages:

The 8-ring channel in CAS, depicted in Figure 4, is parallel to \(a\).

Figure 4. Channel in perspective view along \(a\) (left), and along \(c\) (right). The pore descriptor is added.
5. Supplementary information:

*Other framework types containing zigzag chains*
In several framework types at least one of the unit cell dimensions is about n*5.2 Å (where n = 1, 2, 3, etc.). In many cases this indicates the presence of zigzag chains.
In the **INTRO** pages links are given to detailed descriptions of these framework types (choose: **Zigzag chains**). There is also a link to a summary of the Periodic Building Units used in the building schemes of these framework types (choose: **Appendix; Figure 1**).

*Alternative description using (modified) 5-rings*
Several framework types, like **CAS**, can be constructed using (modified) 5-rings.
In the **INTRO** pages links are given to detailed descriptions of these framework types (choose: **5-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 6**).