Building scheme for SFH and SFN

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

SFH and SFN can be built using the zigzag (zz) chain (bold in Fig. 1(a); left) running parallel to \( z \). The repeat distance along the zigzag chain is about 5.2 Å. The repeat unit consists of 2 T atoms. Eight zz chains are connected into an infinite building unit (Figure 1(a); left). The repeat unit of this building unit is composed of two 5-3 units (bold in Fig. 1(a), right; see Alternative description). A two-dimensional Periodic Building Unit (PerBU) is obtained when infinite building units, related by a translation of \( \frac{1}{2}(x + z) \), are connected along \( z \) through 4-rings as shown in Figure 1(b). [Compare this PerBU with the PerBUs in MTT, MTW, SFE, SSY and TON]

Figure 1. (a): Infinite building unit constructed from eight zigzag chains (left) and from T16-units (right); (b): PerBU obtained when infinite building units are connected along \( x \).

2. Connection mode: See next page.
2. Connection mode:

Neighboring PerBUs can be connected along $y$ through 6-rings in two different ways:
(1): neighboring PerBUs are related by pure translations along $y$;
(2): neighboring PerBUs are related by a rotation of 180° about $y$.

Figure 2. (a): Perspective view along $z$ of the connection mode (1) in SFN (top) and parallel projection of the unit cell content along $b$ and along $c$ (middle and bottom). Only two repeat units of the PerBUs are drawn for clarity. [Figure 2 is continued on next page]
3. Projections of the unit cell content:

Pure SFN and SFH are obtained when neighboring PerBUs are exclusively related by translations along \( c \) (in SFN) and by 2-fold rotations along \( b \) (in SFH), respectively, as shown in Figure 2.
4. Channels and/or cages:

The one-dimensional non-interconnecting 14-ring channels in SFN and SFH are depicted in Figure 3. The **pore descriptor**, equal for both cavities, is added.

\[ \{1[4^66^14^{2/2}]\ [010] \text{(14-ring)}\}\]

Figure 3. Channel in SFN in perspective view along \( b \) (top left) and along \( c \) (top right) and channel in SFH in perspective view along \( a \) (bottom left), and along \( c \) (bottom right).

\[ \{1[4^66^14^{2/2}]\ [100] \text{(14-ring)}\}\]

5. Supplementary information:

In several framework types at least one of the unit cell dimensions is about \( n \times 5.2 \, \text{Å} \) (where \( n = 1, 2, 3, \text{etc.} \)). In many cases this indicates the presence of zigzag chains.

In the **INTRO** pages links are given to detailed descriptions of framework types containing zigzag chains (choose: **Zigzag chains**). There is also a link to a summary of the PerBUs used in the building schemes of these framework types (choose: **Appendix; Figure 1**).

**Alternative description using (modified) 5-rings**

Several framework types, like SFH and SFN, 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**).