

# Building scheme for SFH and SFN



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:

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](#)]

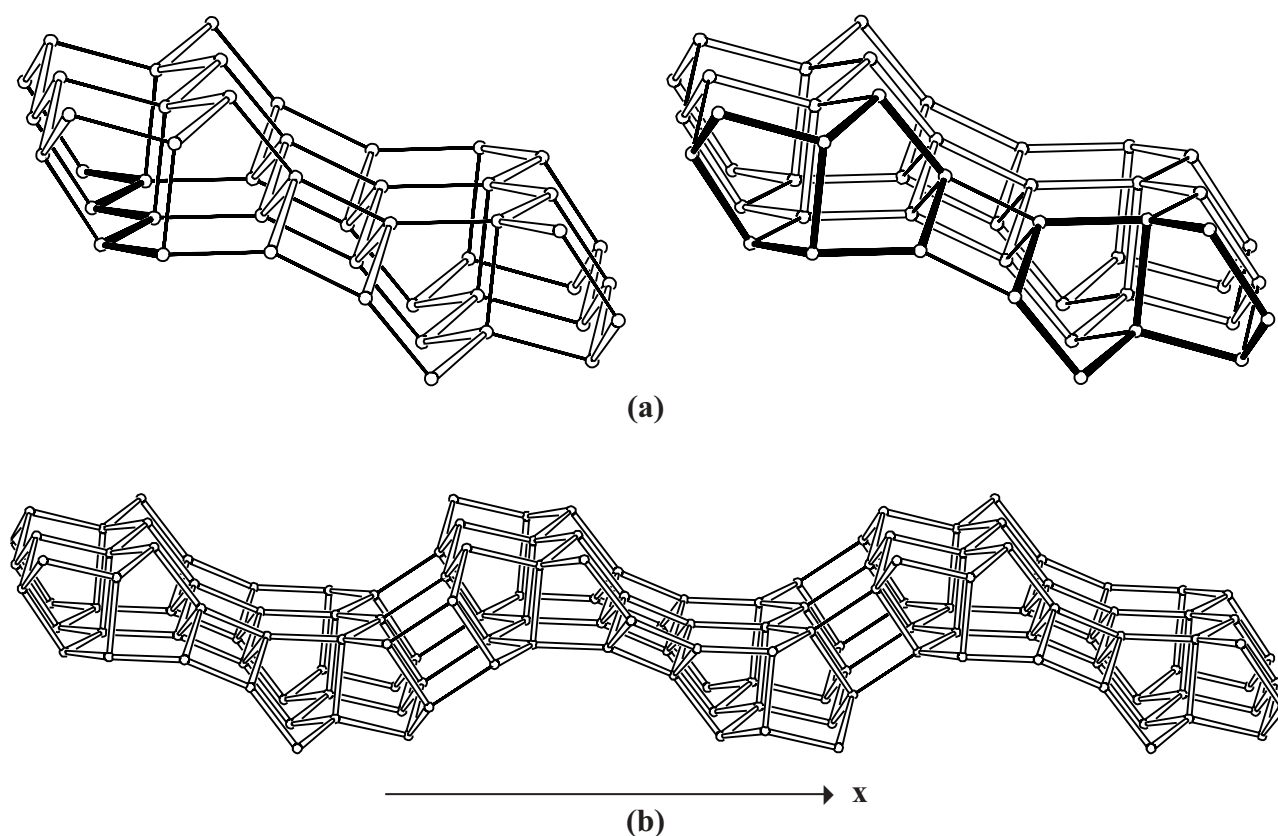


Figure 1. (a): Infinite building unit constructed from eight zigzag chains (left) and from T16-units (right); (b): PerBU obtained when infinite building units are connected along  $x$ .



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  $180^\circ$  about  $y$ .

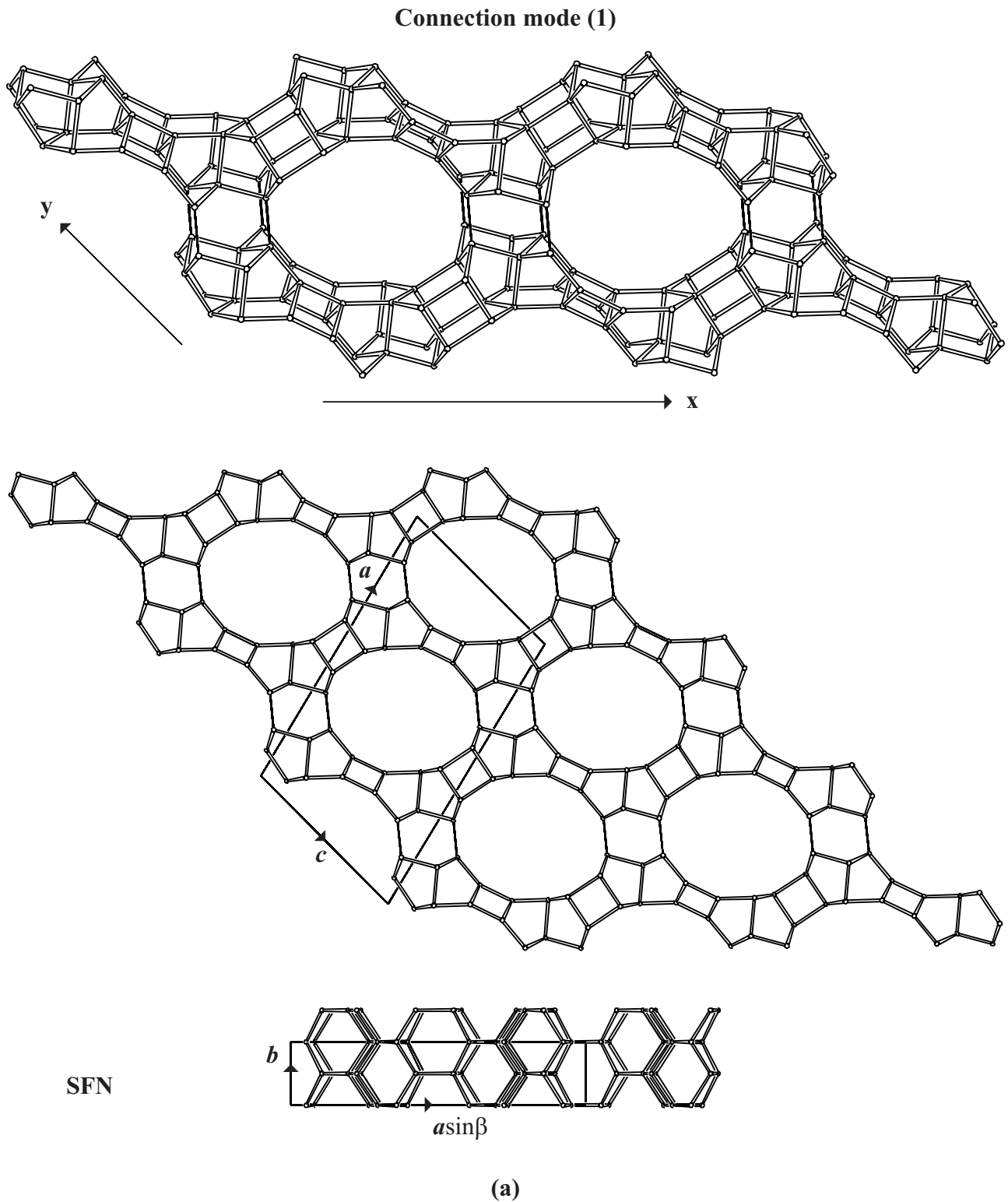


Figure 2. (a): Perspective view along  $z$  of the connection mode (1) in SFN (top) and parallel projection of the unit cell content along  $b$  and along  $c$  (middle and bottom). Only two repeat units of the PerBUs are drawn for clarity. [Figure 2 is continued on next page]

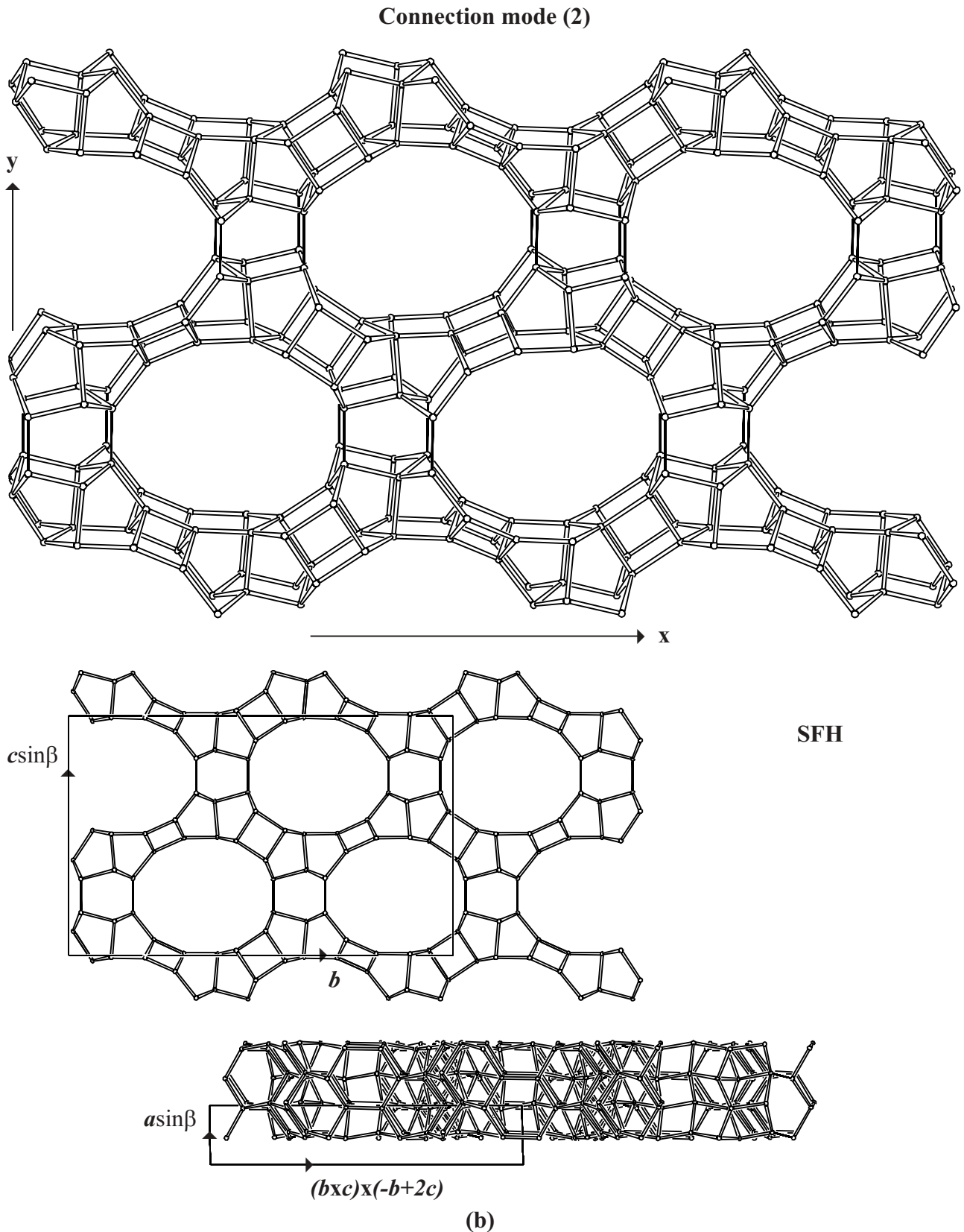


Figure 2 [Cont'd]. (b): connection mode (2) in SFH (top) and parallel projection of the unit cell content along  $a$  and along  $[0-12]$  (middle and bottom). Only two repeat units of the PerBUs are drawn for clarity. ▲

### 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.

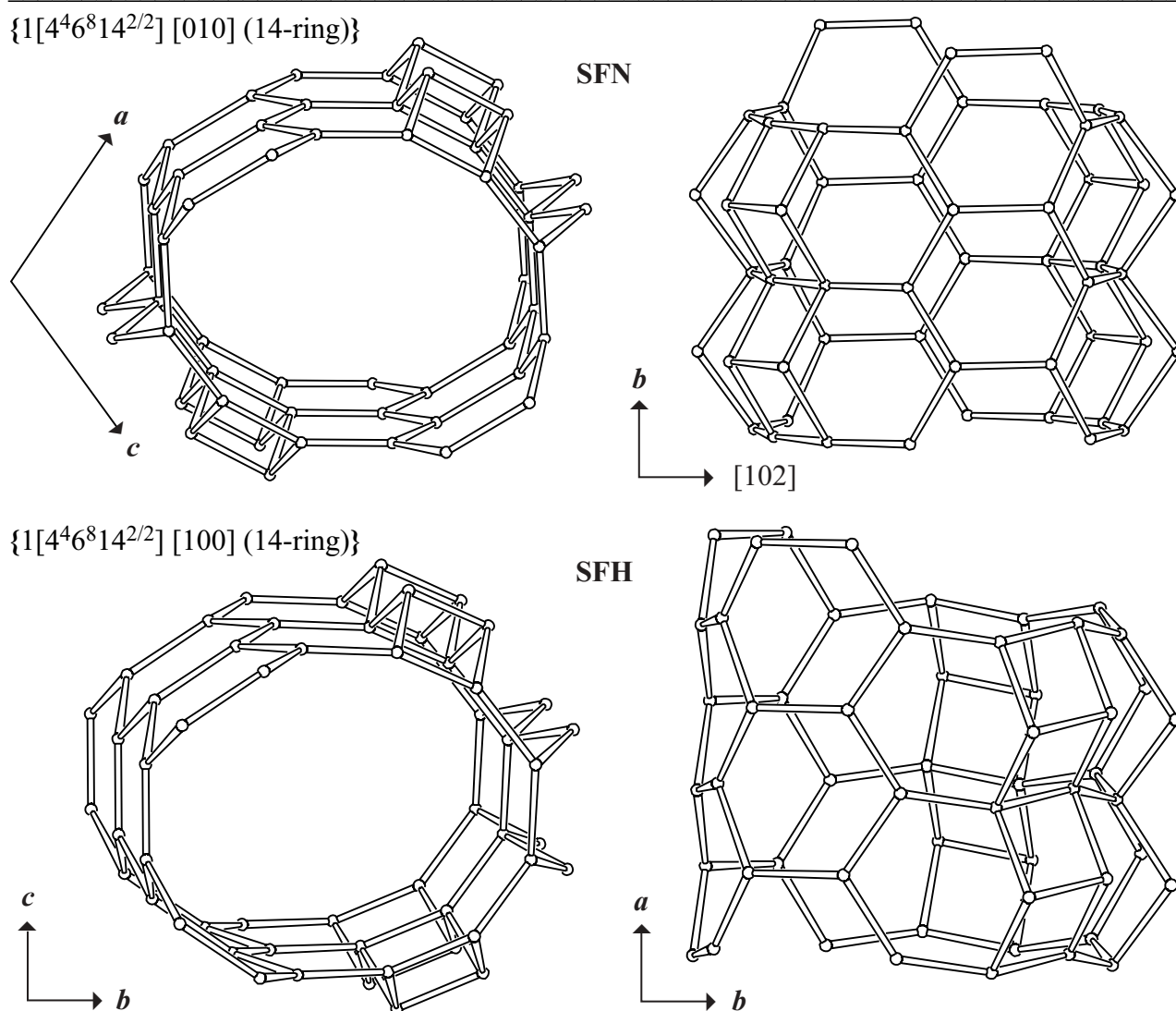


Figure 3. Channel in **SFN** in perspective view along **b** (top left) and along **c** (top right) and channel in **SFH** in perspective view along **a** (bottom left), and along **c** (bottom right). ▲

#### 5. Supplementary information:

In several framework types at least one of the unit cell dimensions is about  $n \cdot 5.2 \text{ \AA}$  (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**). ▲