Building scheme for SBS and SBT

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:

Hexagonal **SBS** and **SBT** can be built using the ***can*** cage with "handles" consisting of 24 T atoms (or six 4-rings) shown in Figure 1. The two-dimensional Periodic Building Unit (PerBU) is obtained when these cages are linked into the hexagonal layer depicted in Figure 2 through zigzag T-T bonds. 4-Rings and 8-rings are formed.

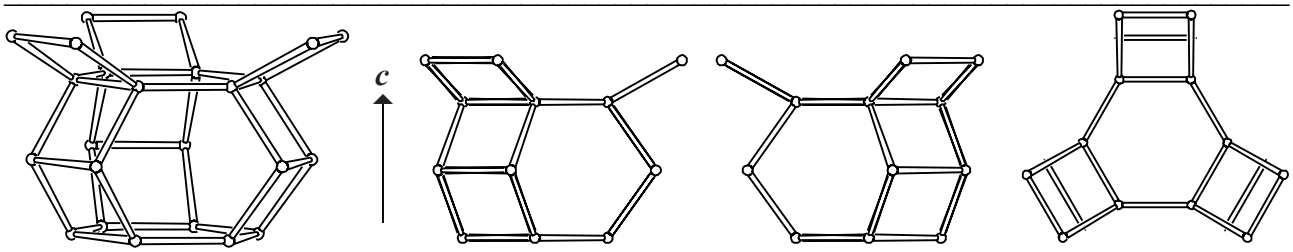


Figure 1. The ***can***-cage with "handles" (T24-unit). From left to right: perspective view perpendicular to ***c***; parallel projections perpendicular to ***c***, after rotation of +30º and -30º about ***c*** with respect to the most left drawing; and parallel projection down ***c***.

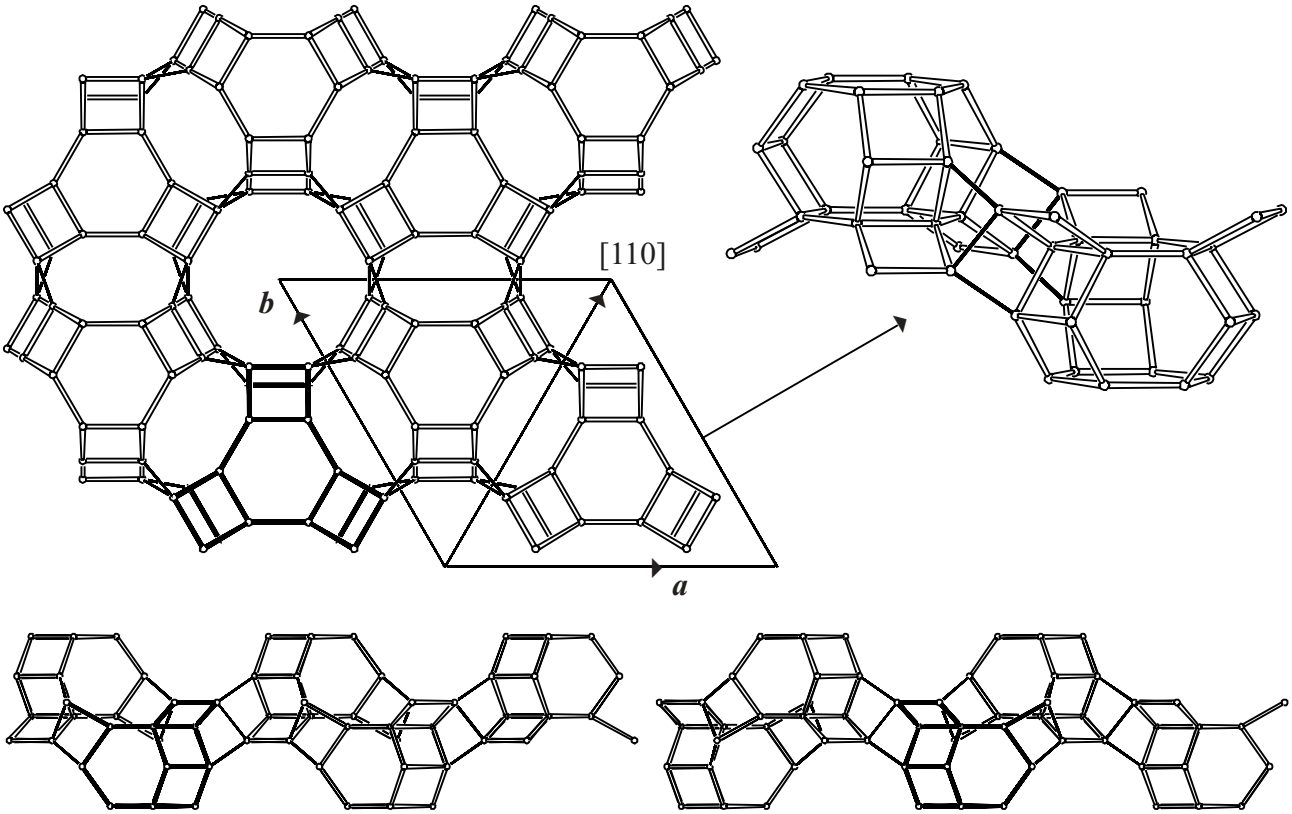


Figure 2. PerBU built from T24-units (one in bold) viewed along ***c*** (top), along ***b*** (bottom left) and along [110] (bottom right). The layers, depicted at the bottom at a different scale, are identical and related by a rotation of 60º about ***c*** or by a mirror operation perpendicular to ***c***. The inset (top right) gives the linkage through 4-rings of T24-units within the PerBU viewed nearly along [120].

2. Connection mode:

Neighboring PerBUs can be connected along [001] through double 6-rings in two different ways:
(1): the top layer is shifted over 1/3(-***a*** + ***b***) before connecting it to the bottom layer. The resulting connectivity exhibits inversion symmetry between successive layers.
(2): the top layer is rotated over 60º about [001], followed by a shift of 1/3(-***a*** + ***b***), before connecting it to the bottom layer. The connectivity shows mirror symmetry between successive layers (compare Figure 2).
N.B. The connection sequences of the PerBUs along ***c*** in **SBS** and **SBT** are equivalent to those in **EMT** and **FAU**, respectively.

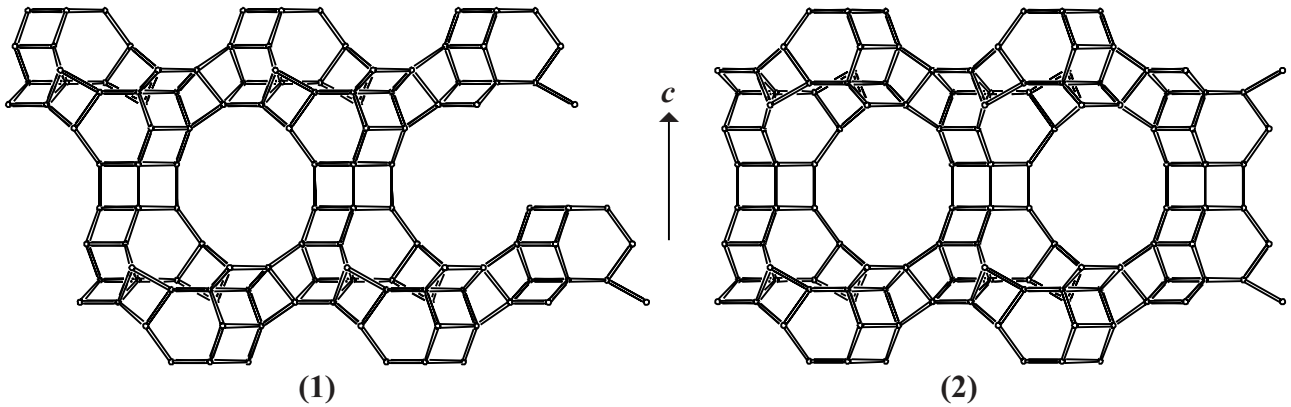


Figure 3. Connection mode (**1**) in **SBT** (left) and connection mode (**2**) in **SBS** viewed along ***b***.

3. Projections of the unit cell content:

Pure **SBS** and **SBT** are obtained when neighboring PerBUs are related along the hexagonal ***c*** axis by reflection and inversion, respectively (Figure 4).

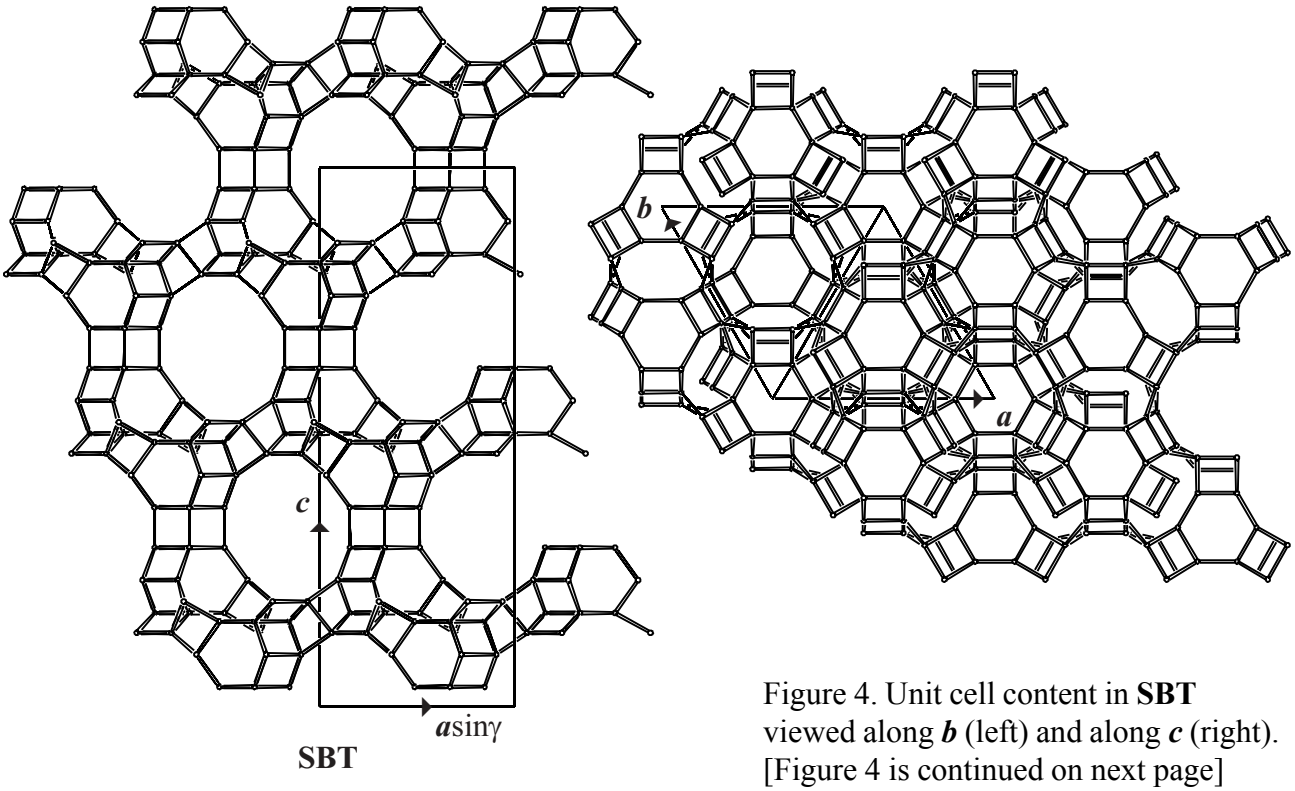
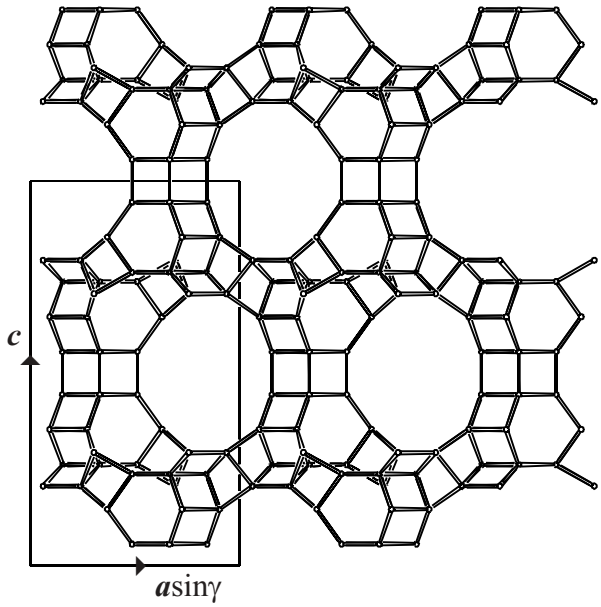


Figure 4. Unit cell content in **SBT** viewed along ***b*** (left) and along ***c*** (right).
[Figure 4 is continued on next page]



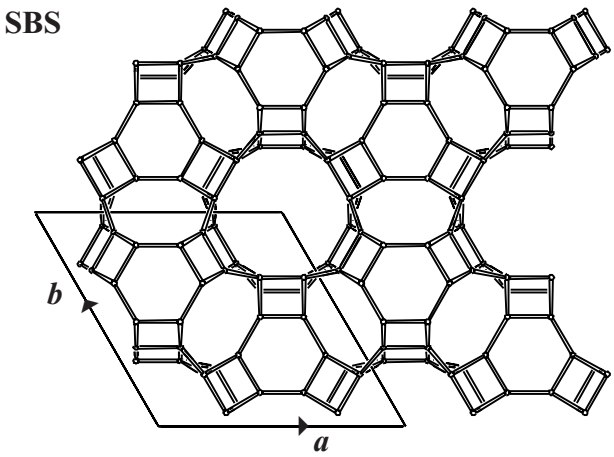


Figure 4 [Cont'd]. Unit cell content in **SBS** viewed along ***b*** (left) and along ***c*** (right).

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4. Channels and/or cages:

In **SBS** and **SBT** 12-ring channels are parallel to <010>. In **SBS** there are also 12-ring channels parallel to [001]. Channel, cages and channel intersections (or cavities) are depicted in Figure 5. For each type of cavity the **pore descriptor** is added in Figure 5. The fusion of channel, cages and cavities is illustrated in Figure 6.

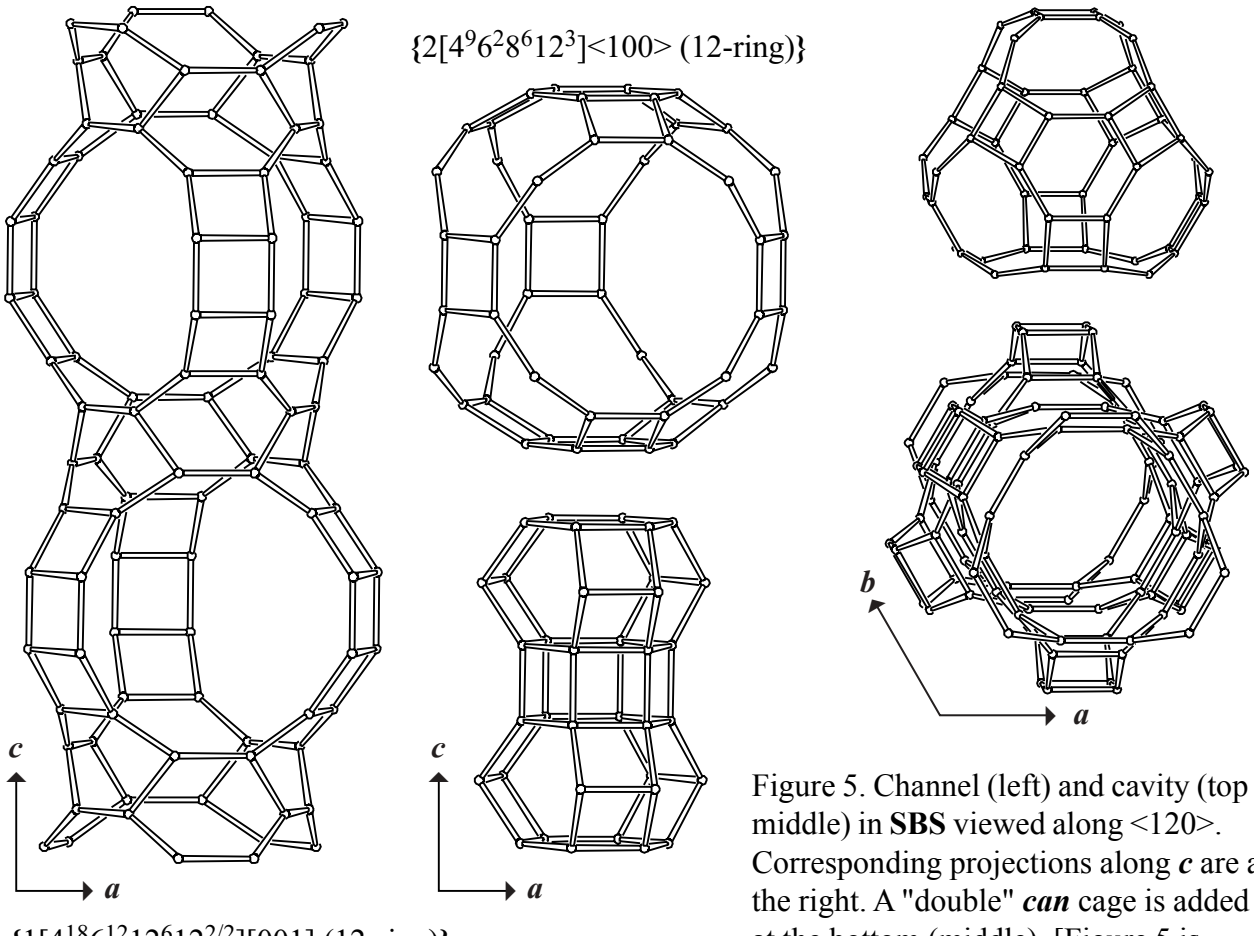


Figure 5. Channel (left) and cavity (top middle) in **SBS** viewed along <120>. Corresponding projections along ***c*** are at the right. A "double" ***can*** cage is added at the bottom (middle). [Figure 5 is continued on next page]

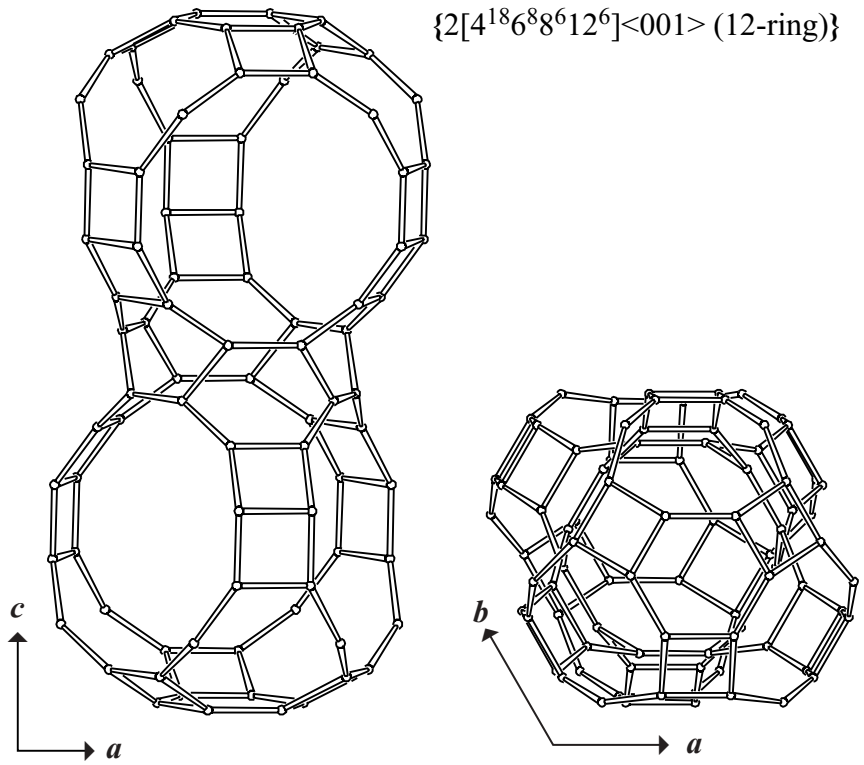
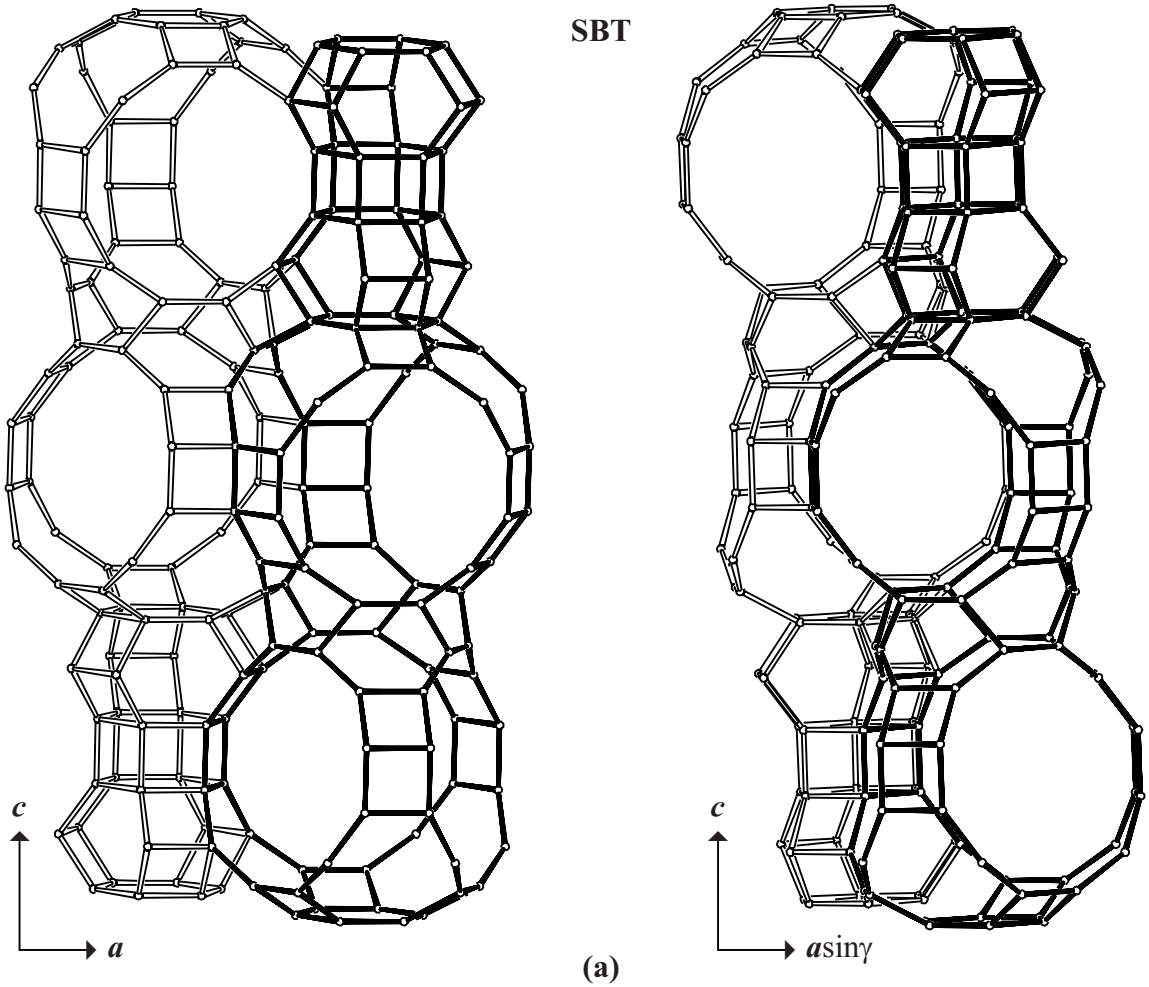


Figure 5 [Cont'd]. Cavity in **SBT** viewed along <120> (left) and along ***c*** (middle). A "double" ***can*** cage is added at the top right.

SBT



(a)

Figure 6(a). Fusion of double ***can*** cages and cavities in **SBT** viewed along <120> (left) and along the 12-ring channel axis parallel to <010> (right). The framework of **SBT** can as well be constructed from double ***can*** cages with "handles" (see Figure 3: connection mode **(1)** and Figure 5). [Figure 6 is continued on next page]

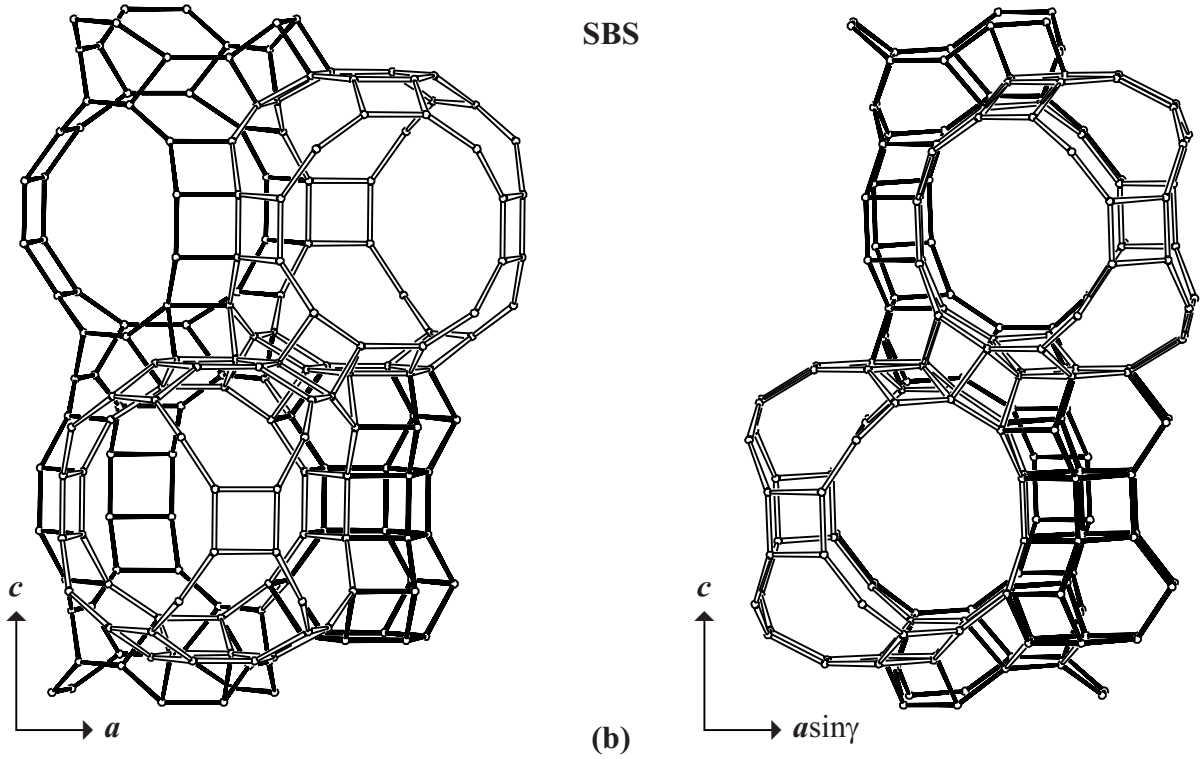


Figure 6(b). Fusion of channel, ***can*** cages and cavities in **SBS** viewed along <120> (left) and along the 12-ring channel axis parallel to <010> (right). The framework of **SBS** can as well be constructed from complete cavities (built from six 8-rings; see Figures 5 and 6(b)) as from double ***can*** cages with "handles" (see Figure 3: connection mode **(2)** and Figure 5). Compare the linkage of cavities with the linkage of cavities in **SBE**.

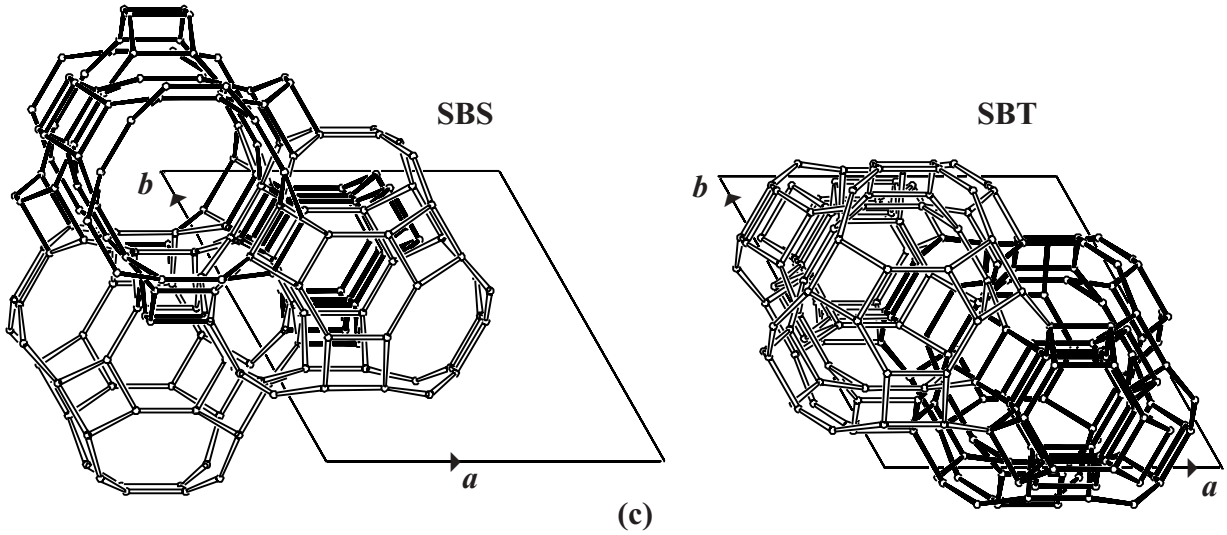


Figure 6(c). **SBS** (left), and **SBT** (right) viewed along ***c***. In **SBT** the free entrance to the 12-ring channel parallel to ***c*** is seriously hampered.

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5. Supplementary information:

Other framework types containing (modified) cavities

Several framework types, like **SBS** and **SBT**, can be built using (modified) cavities.
In the **INTRO** pages links are given to a detailed description of a sub-set of framework types that contain (modified) cavities (choose: **Cages**). There is also a link provided to a summary of the PerBUs used in the building schemes of these framework types (choose: **Appendix**; **Figure 11**).