

Building scheme for TUN



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:

TUN can be built using left- and right-handed units of 24 T atoms (one bold in Figure 1). The T24-unit consists of four 5-1 units, or four “finite” zigzag chains (each containing 4 T atoms) and four dimers. Left- and right-handed T24-units form left- and right-handed columns parallel to c , respectively. The T24-units in the column are related by a rotation of 180° about b . Left- and right-handed columns are connected into the two dimensional PerBU. The PerBU equals the bc layer shown in Figure 1 on next page.

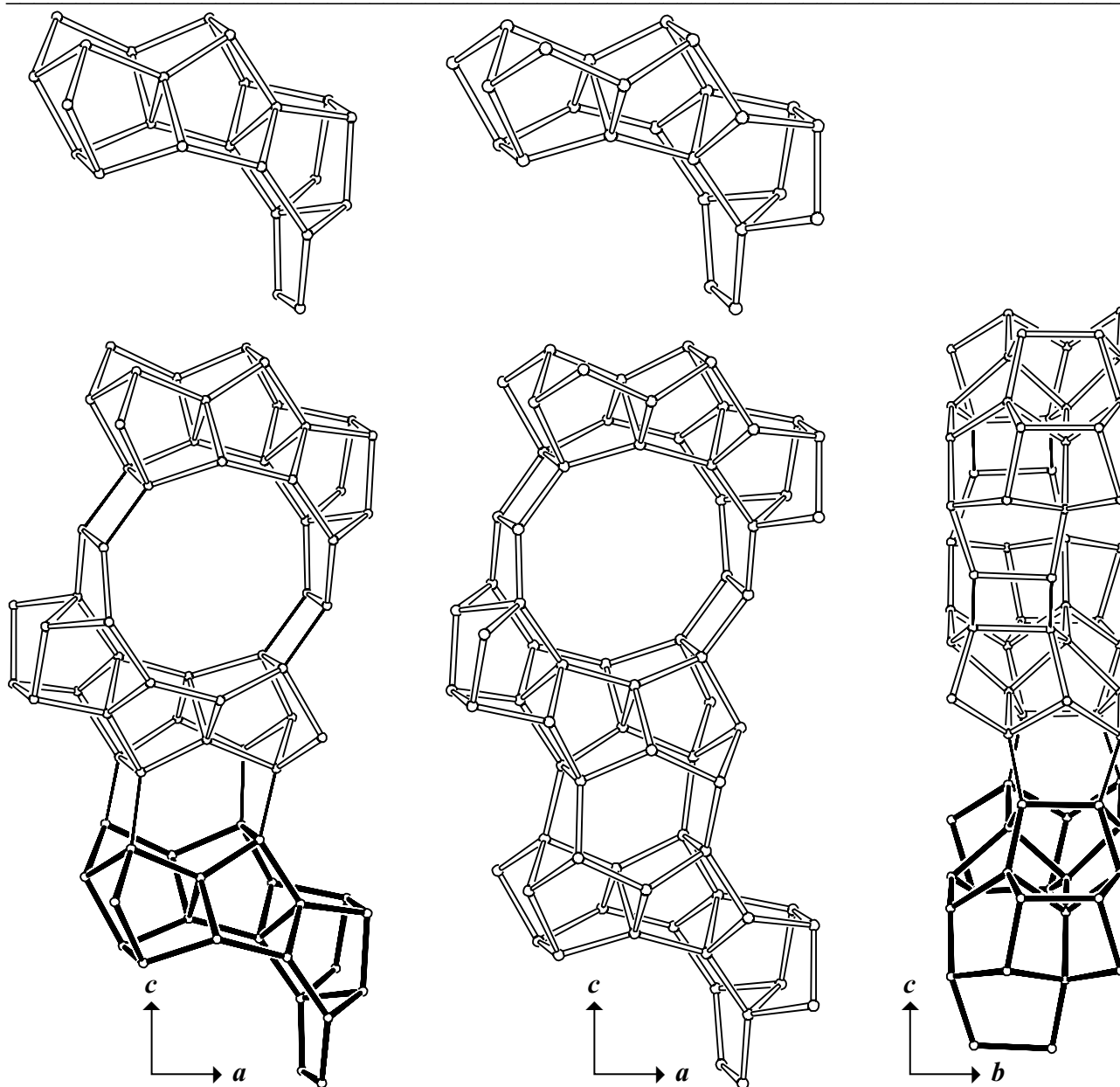


Figure 1(a). Left- and right-handed T24-units (top) and the polar columns obtained (bottom). Columns viewed along b (left and middle), and one column viewed along a (right). One T24-unit in bold. [Figure 1 is continued on next page]

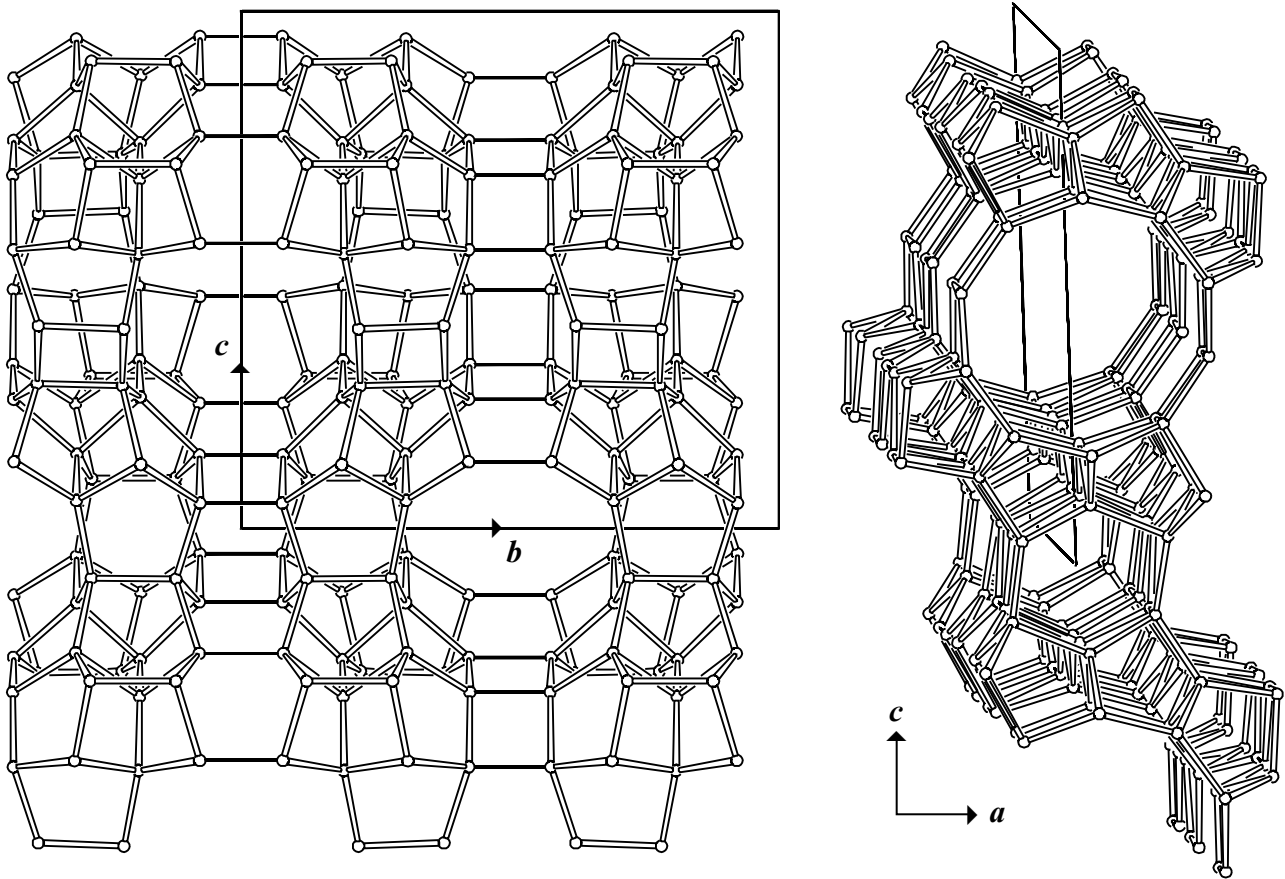


Figure 1(b). Left- and right-handed columns are connected along b through 4- and 6-rings into the PerBU viewed along a (left) and along b (right).

2. Connection mode:

Neighboring PerBUs, related along a by a shift of $1/2(a + b)$, are connected along a through 5-rings as depicted in Figure 2 on next page.

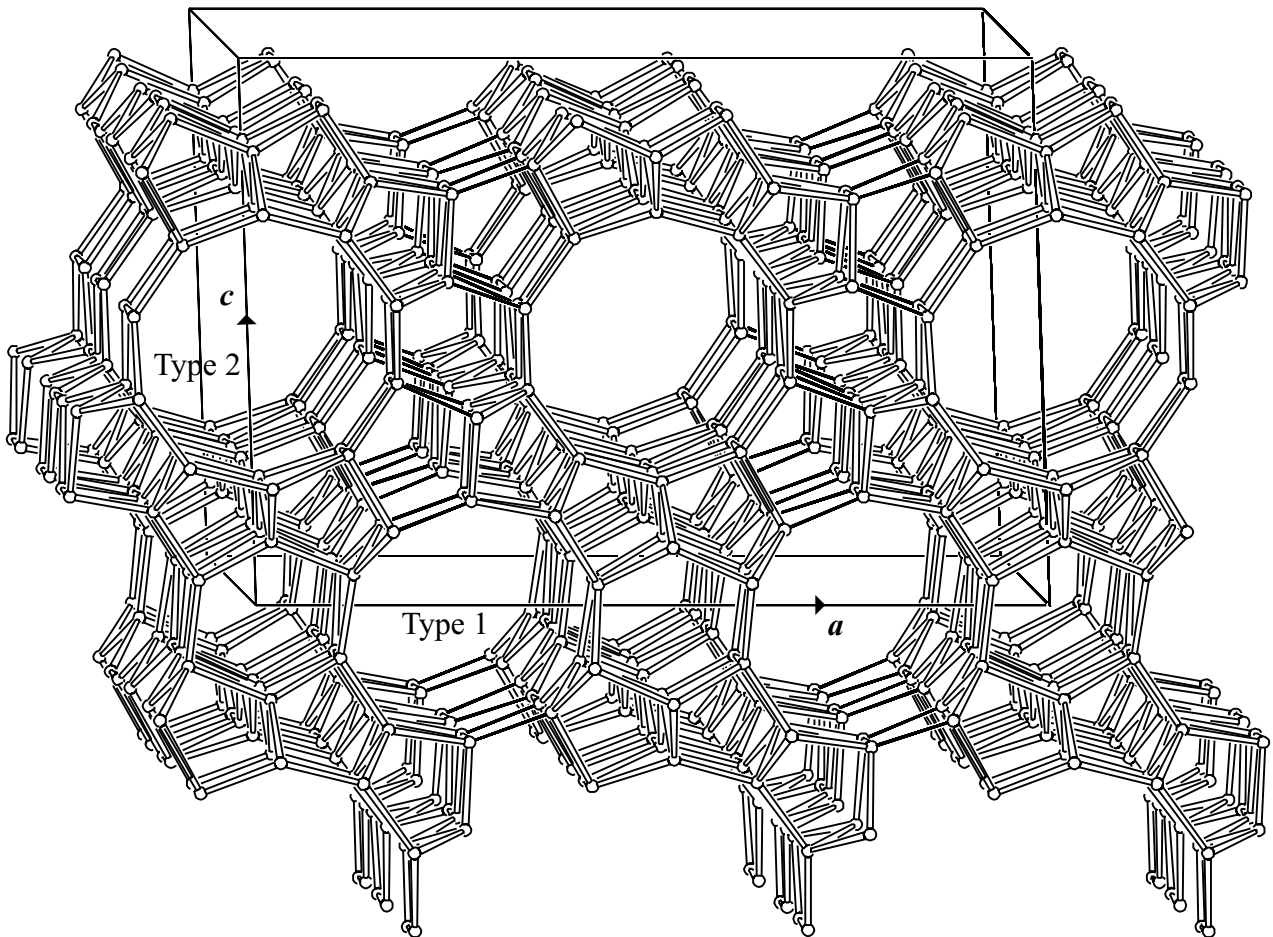


Figure 2. Connection mode (and unit cell content) viewed along b .

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

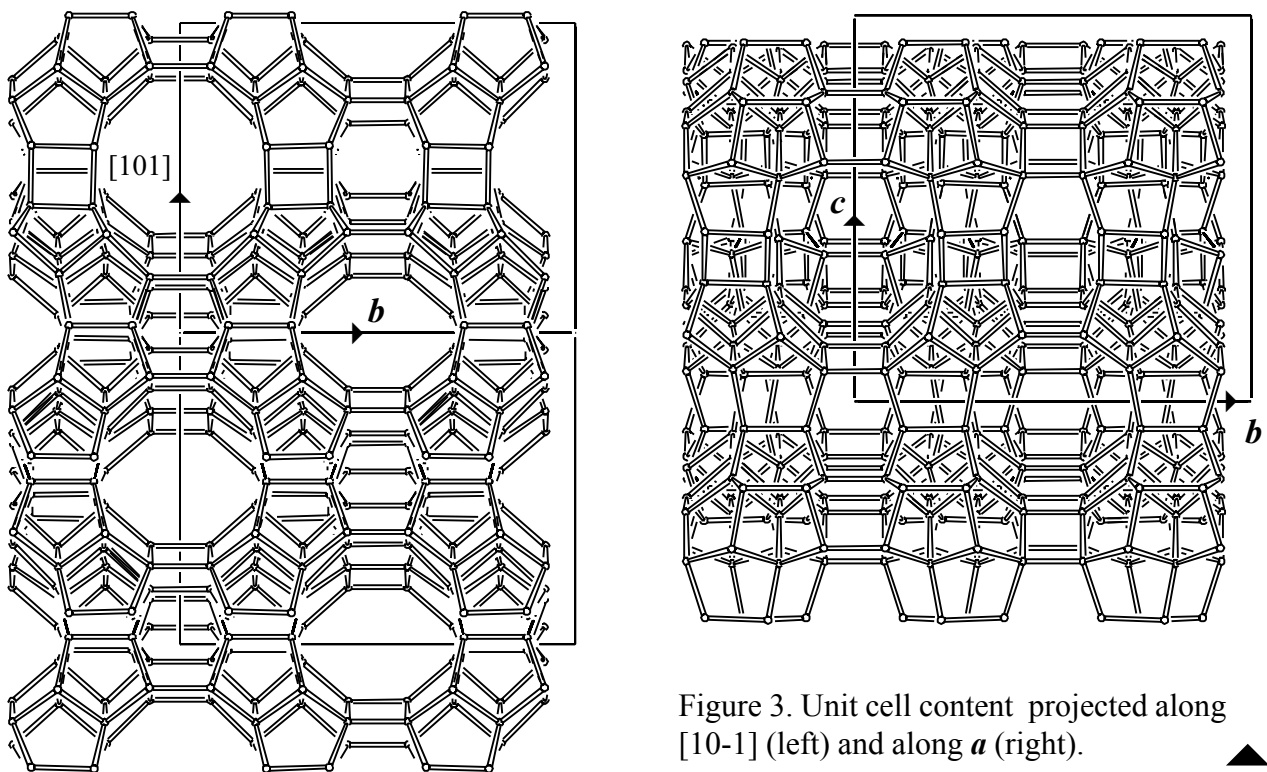


Figure 3. Unit cell content projected along $[10-1]$ (left) and along a (right).

4. Channels and/or cages:

Two types of 10-ring channels are parallel to b . The channels are interconnecting along $[-101]$. Pairs of channels of type 1 are interconnecting along a . Non-interconnecting sinusoidal 10-ring channels are perpendicular to b . The two types of channels and their interconnection are depicted in Figure 4. The **pore descriptors** are added. The interconnection between pairs of channels of type 1 along a can be seen in Figure 2.

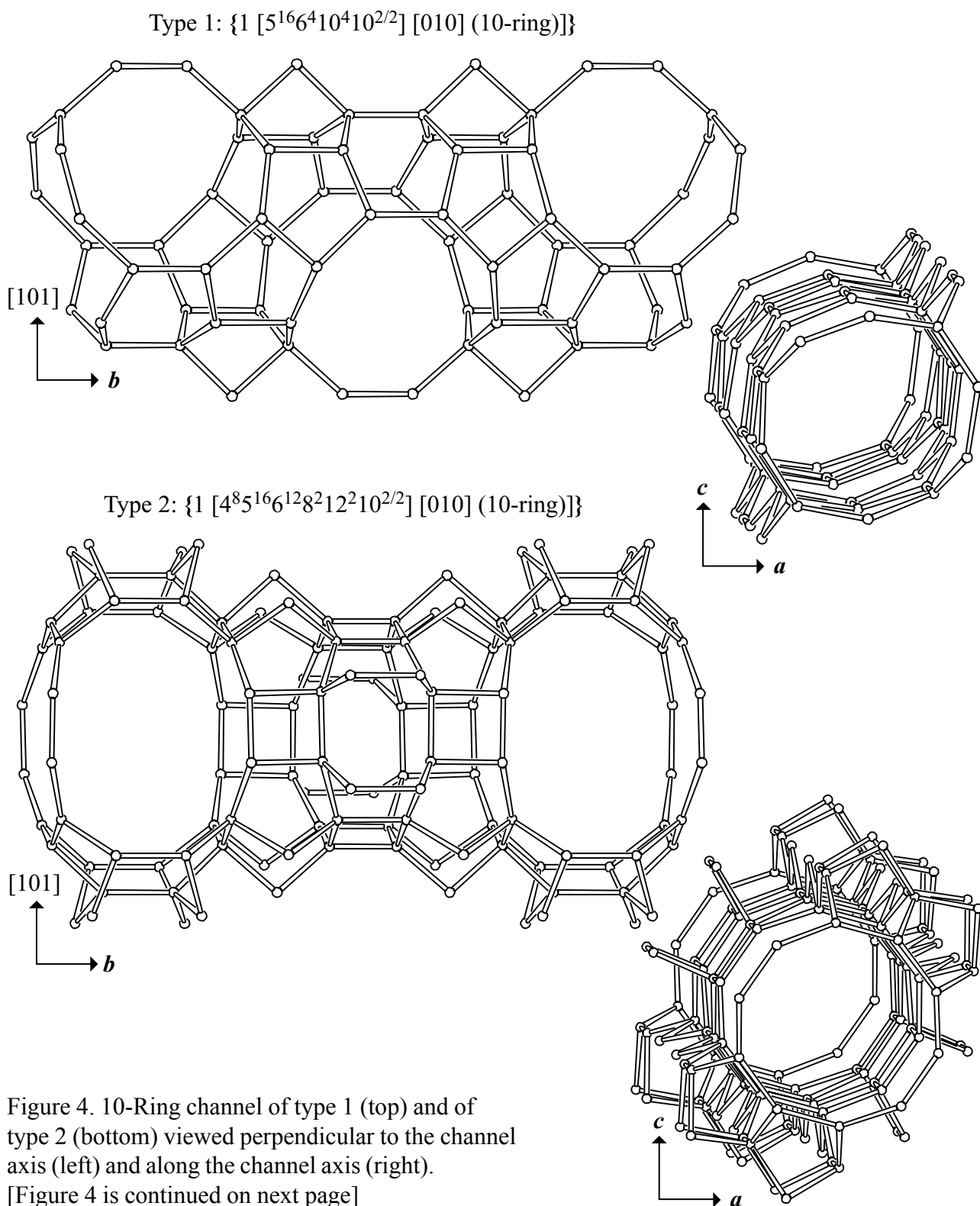


Figure 4. 10-Ring channel of type 1 (top) and of type 2 (bottom) viewed perpendicular to the channel axis (left) and along the channel axis (right).
[Figure 4 is continued on next page]

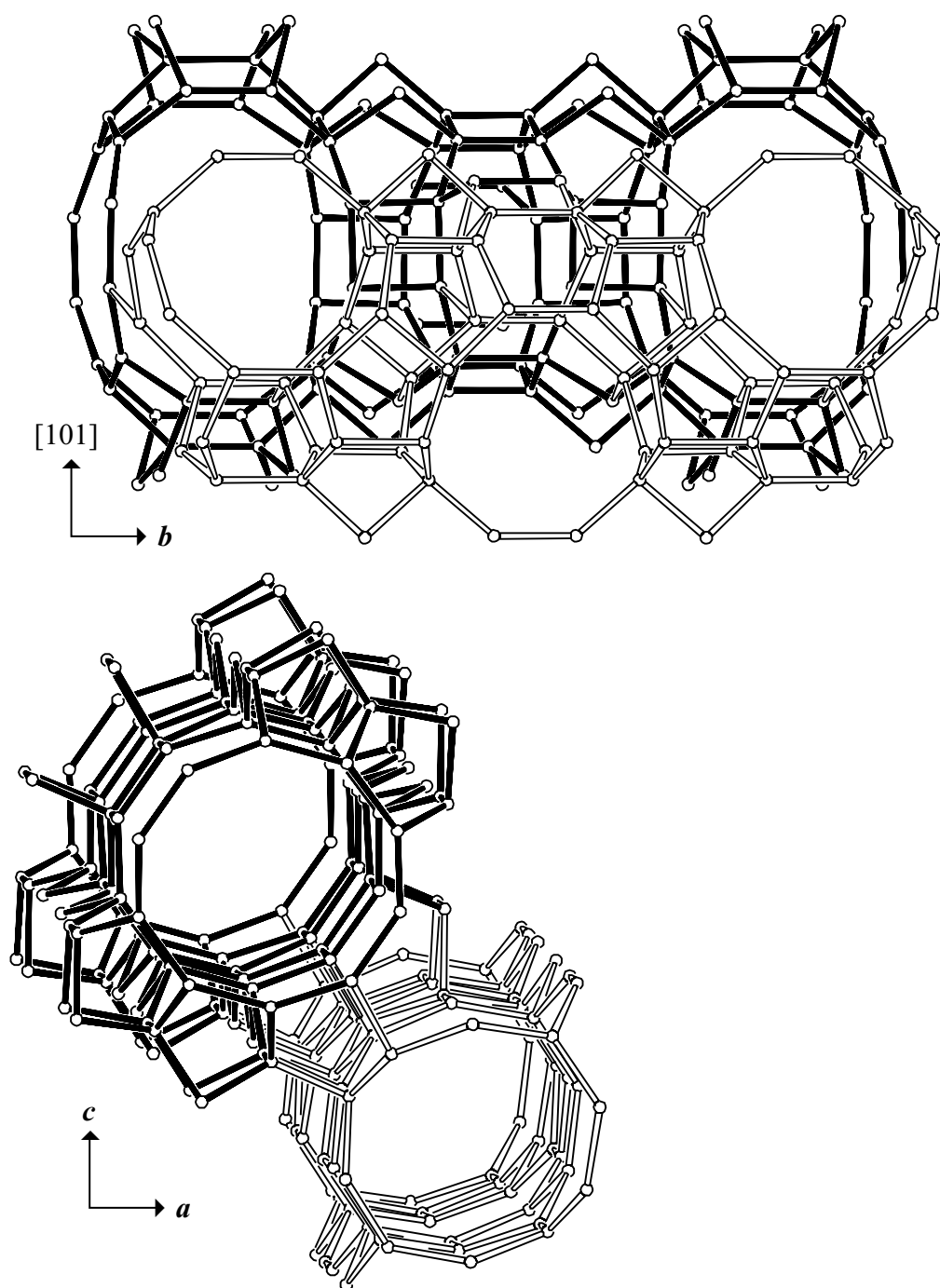


Figure 4 [Cont'd]. Interconnection of channels (type 2 channel in bold). ▲

5. Supplementary information:

Other framework types containing (modified) 5-rings

5-Rings can be connected in several other ways. In all cases additional T atoms are needed to build the framework.

In the [INTRO](#)-pages links are given to a detailed description of a sub-set of framework types that contain (modified) 5-rings (choose: **5-Rings**). There is also a link provided to a summary of the PerBUs used in the building schemes of these framework types (choose: **Appendix; Figure 6**). ▲