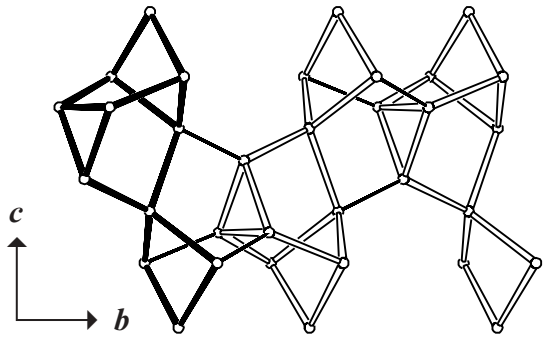
Building scheme for VNI

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:

Tetragonal **VNI** can be built using two periodic building units (PerBUs). The first PerBU (PerBU1) consists of chains of units of 11 T atoms parallel to [-110] (Figure 1). Each T11-unit is composed of two 4-rings and one 3-ring (one in bold). Neighboring T11-units in the chain, are related by a rotation of 180º about the chain axis. Neighboring chains, related by pure translations along ***a*** (or ***b***), are connected along [110] through single T-T bonds into the ***ab*** layer (PerBU1) depicted in Figure 2. The second PerBU (PerBU2), which is parallel to PerBU1, consists of 4-rings connected through single T-T bonds into the ***ab*** layer shown in Figure 3.



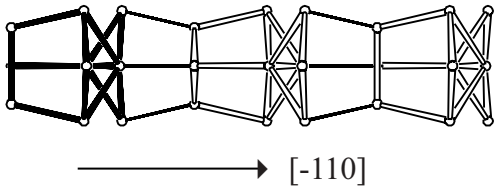
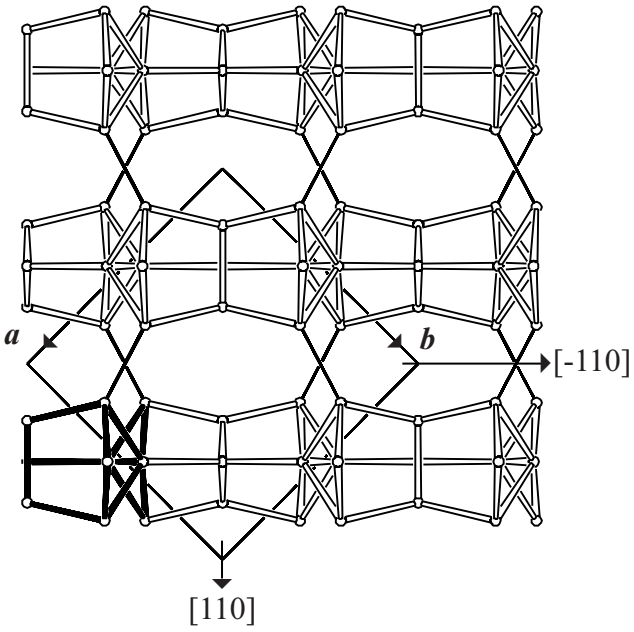


Figure 1. Chain of T11-units viewed along ***a*** (left), and down ***c*** (right).



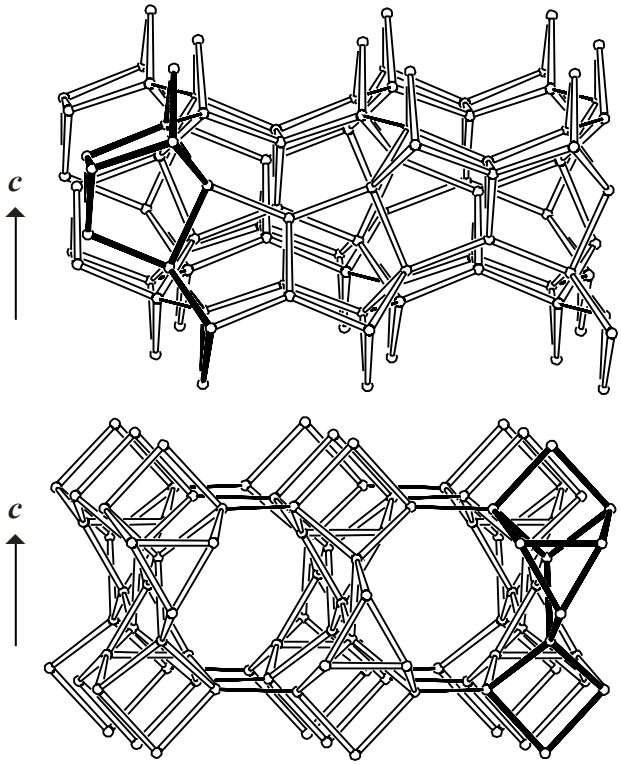


Figure 2. PerBU1 viewed along ***c*** (left), along [110] (top right) and along [-110](bottom right). The PerBUs, depicted at the right, are identical and related by a rotation of 90º about ***c***. [Figure 3 is on next page]

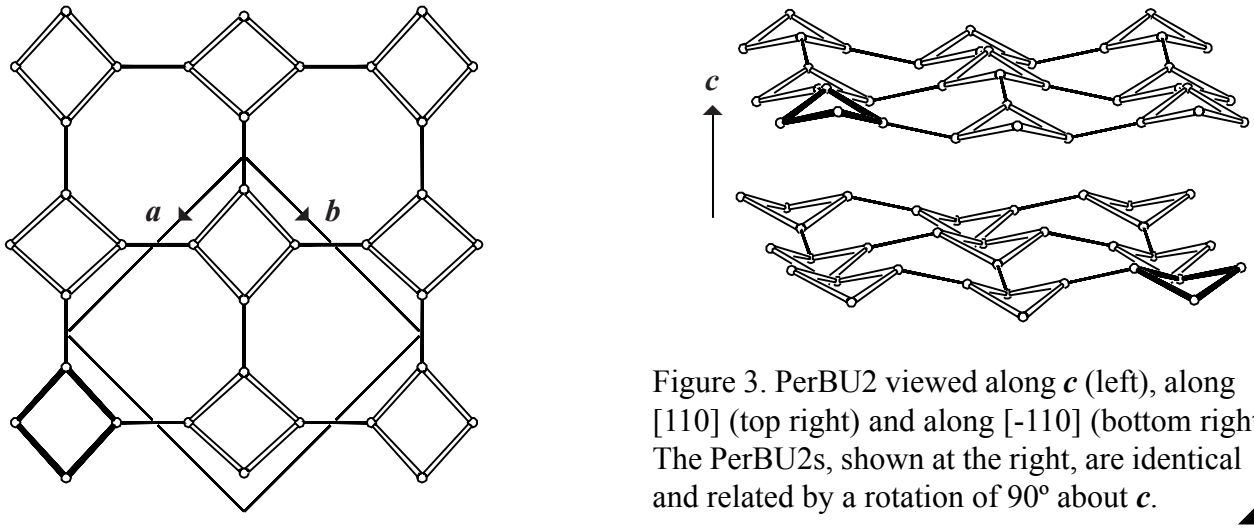


Figure 3. PerBU2 viewed along ***c*** (left), along [110] (top right) and along [-110] (bottom right). The PerBU2s, shown at the right, are identical and related by a rotation of 90º about ***c***.

2. Connection mode:

Two PerBU2s, related by a rotation of 90º about ***c*** and shifted with respect to each other over ½ ***c***, and one PerBU1 are connected along ***c*** through 3-rings as shown in Figure 4. Additional PerBU1s are connected through 3-rings to the 4-ring layers after a rotation of 90º about ***c*** (see Figure 5).

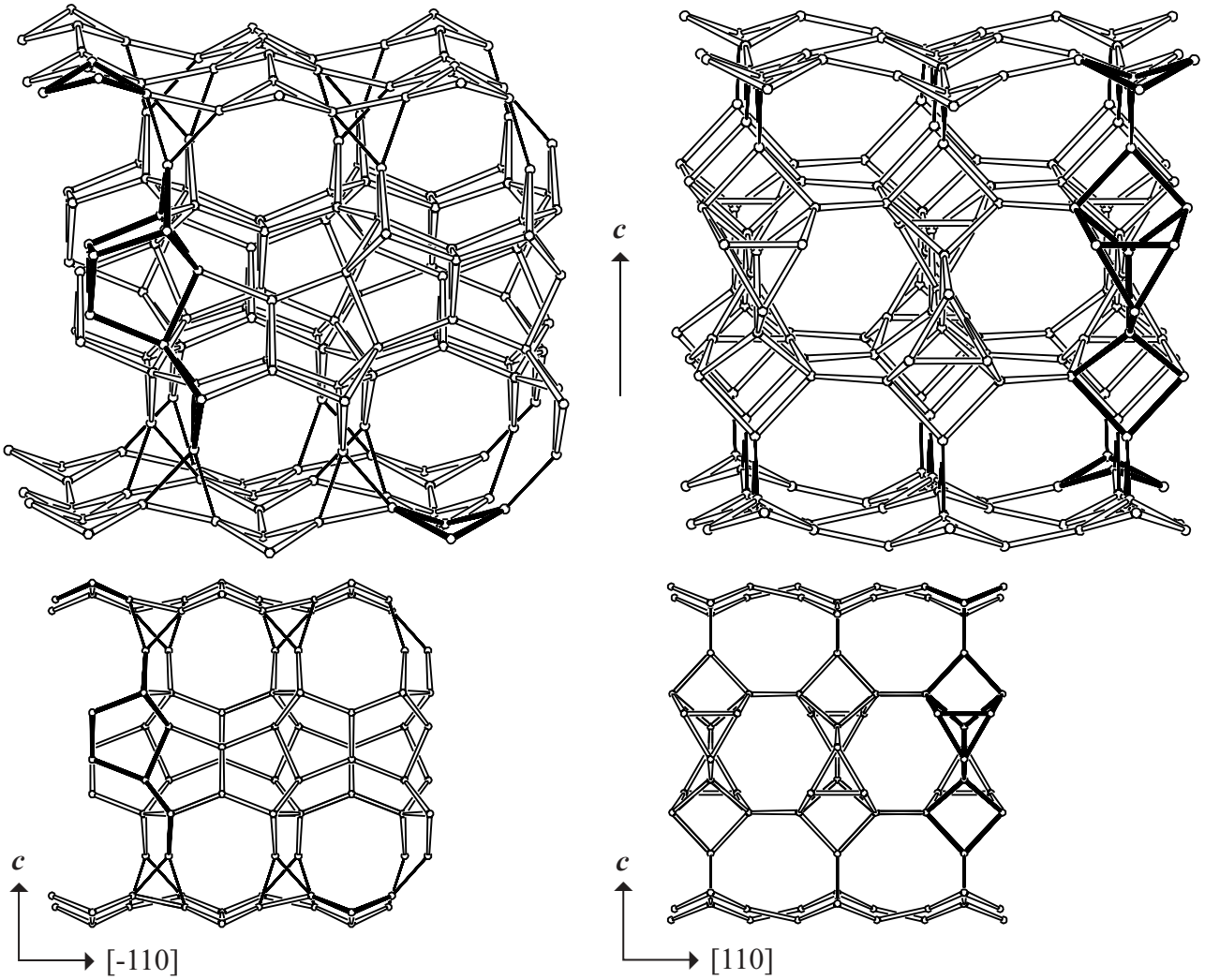


Figure 4. Connection mode in **VNI** viewed along [110] (left), and along [-110] (right). Perspective views (top) and parallel projections (on a different scale; bottom) are shown.

3. Projections of the unit cell content: See Figure 5.

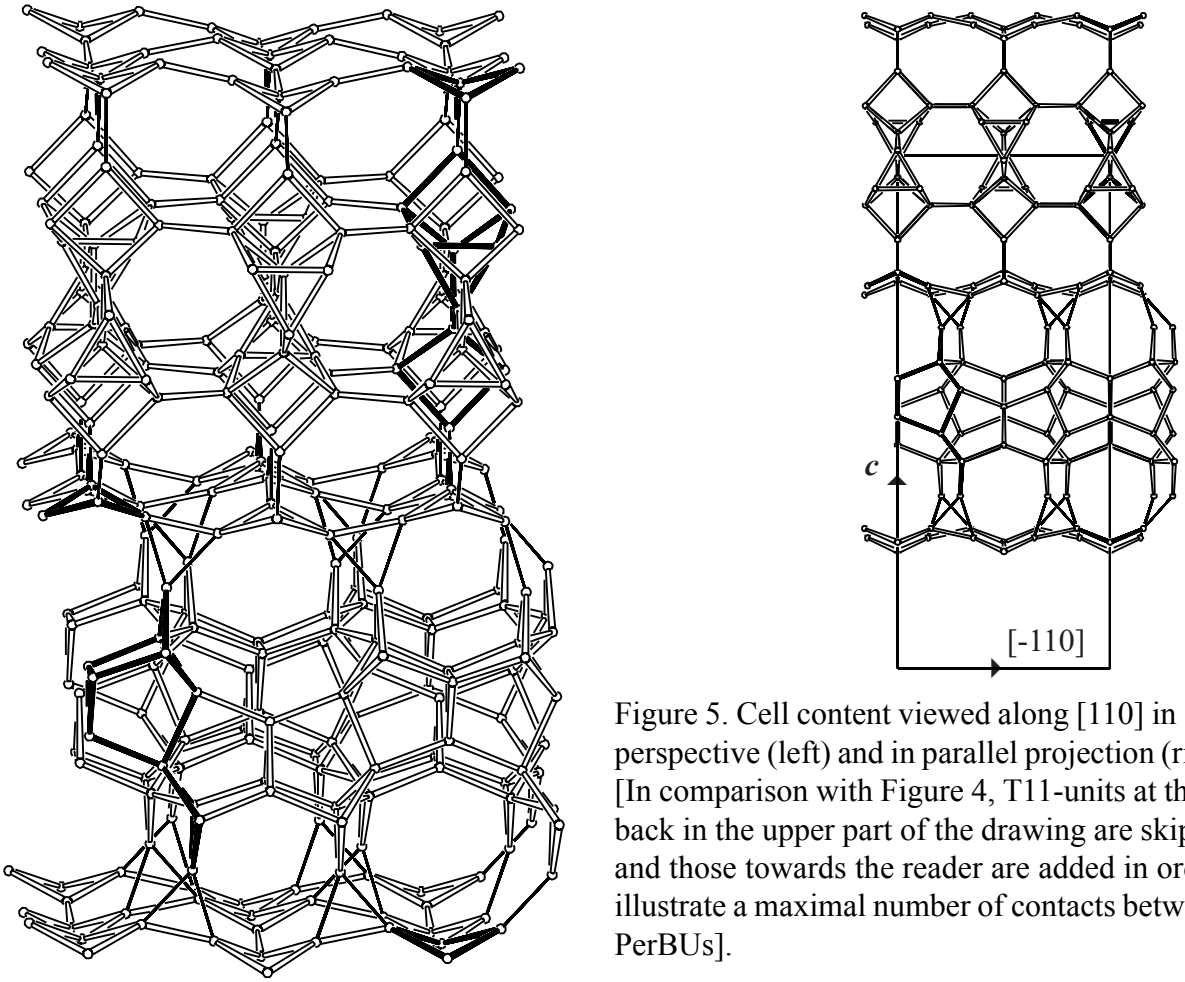
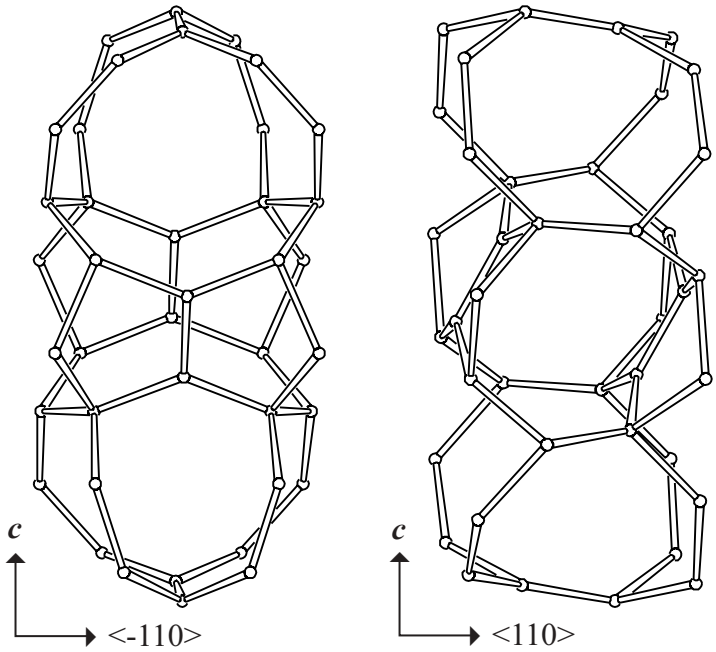


Figure 5. Cell content viewed along [110] in perspective (left) and in parallel projection (right). [In comparison with Figure 4, T11-units at the very back in the upper part of the drawing are skipped and those towards the reader are added in order to illustrate a maximal number of contacts between the PerBUs].

4. Channels and/or cages:

There are three types of 8-ring channels parallel to <110>. Two types intersect; the third type interconnects the other two along ***c***. Two intersecting cavities and one interconnecting cavity is shown in Figure 4. The **pore descriptors** are added. The fusion of cavities is illustrated in Figure 5.



{2[$8^4 10^1$] <110> (8-ring), <-110> (8-ring) / 2[$5^4 8^4$] <-110> (8-ring), [001] (8-ring)}

Figure 6. Intersecting cavities and interconnecting cavity viewed along <110> (left), and along <-110> (right). [Figure 7 is on next page]

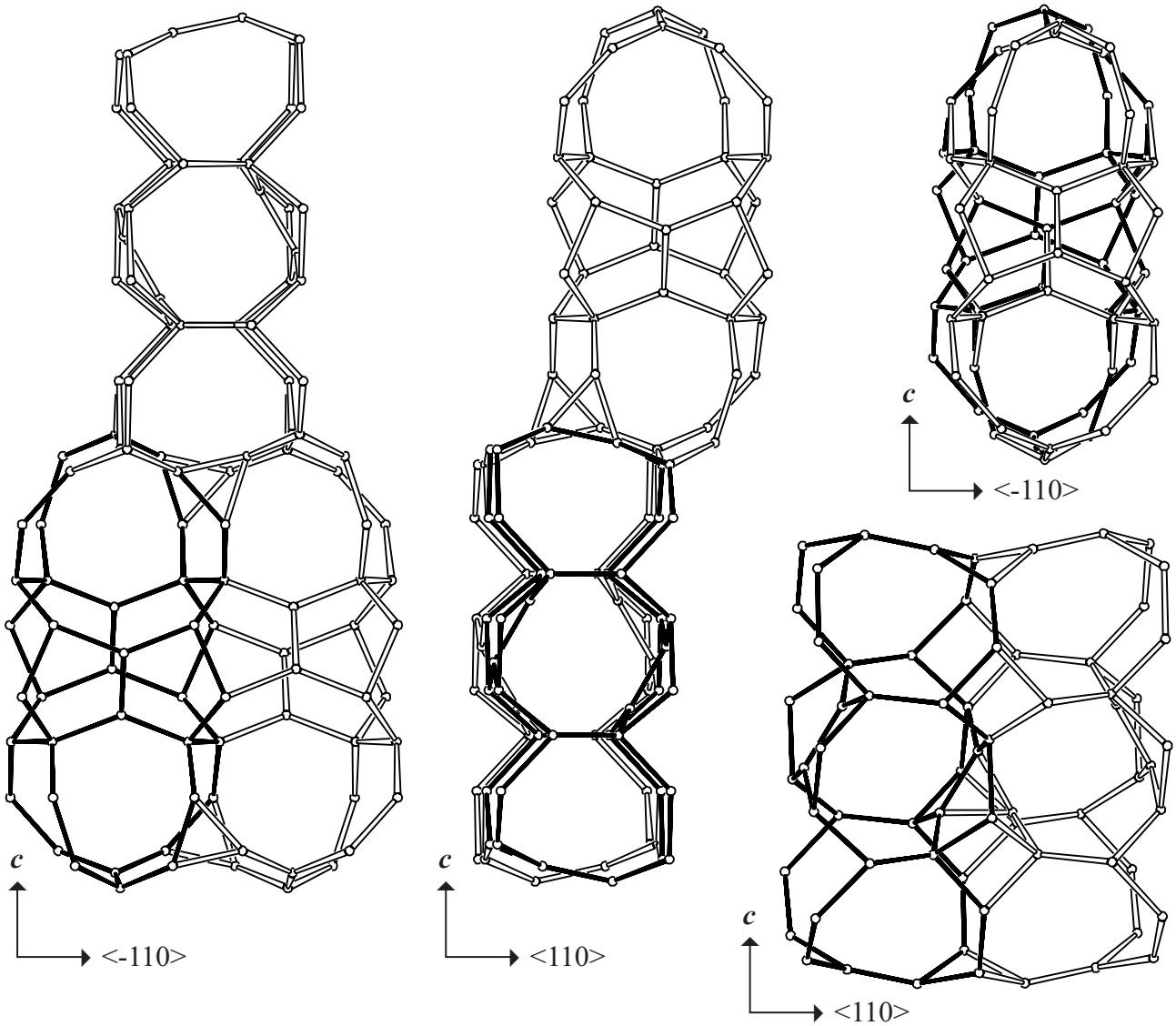


Figure 7. (a): Fusion of intersections along <-110> and [001] viewed along <110> (left), and along <-110> (right); (b): Fusion of intersections along <110> viewed along <-110> (bottom), and along <110> (top).

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5. Supplementary information:

Other framework types containing (modified) single 3- and/or 4-rings

Single 3- and/or 4-rings can be connected in several other ways. In several 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) single 3- and/or 4-rings (choose: **Single 3- and/or 4-rings**). 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 4**).