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 180° 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 90° about c. [Figure 3 is on next page]
2. Connection mode:

Two PerBU2s, related by a rotation of 90° 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 90° about c (see Figure 5).

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 90° about c.

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.

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.

\[
\begin{align*}
\{2[8^{410}] & <110> \text{ (8-ring)}, <-110> \text{ (8-ring)} \\
/2[5^{8^4}] & <-110> \text{ (8-ring)}, [001] \text{ (8-ring)}
\end{align*}
\]

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].

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).

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**).