Building scheme for PON


1. Periodic Building Unit:

PON can be built using units of 12 T atoms. The T12-unit (bold in Figure 1) consists of five fused 4-rings (or two 4-2 units). A two-dimensional Periodic Building Unit (PerBU) is obtained when T12-units, related by pure translations along \(a\) and \(b\), are connected into the \(ab\) layer shown in Figure 1.

Figure 1. PerBU viewed along \(c\) (left), and along \(b\) (right). The PerBUs, depicted at the right are identical and related by a rotation of 180° about the plane normal parallel to \(c\), or by a mirror operation perpendicular to the plane normal.

2. Connection mode:

Neighboring PerBUs, related by a rotation of 180° about \(c\), are connected along \(c\) through 6- and 10-rings as depicted in Figure 2.

Figure 2. Connection mode viewed along \(c\) (left) and projection of the cell content along \(a\) (right).
3. Projections of the unit cell content: See Figure 2.

4. Channels and/or cages:

The cavity in PON is shown in Figure 4(a). The pore descriptor is added. 10-Ring channels parallel to [100] are formed when cavities are linked along $a$ as illustrated in Figure 4(b).

Figure 4. (a): Cavity viewed along $b$ (left) and along $a$ (right); (b): Fusion of cavities along $a$ viewed perpendicular to the 10-ring channel axis parallel to $a$ (left) and along the 10-ring channel axis (right).

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).