Building scheme for LTN

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1. Periodic Building Unit:

In cubic LTN two types of building units can be distinguished. The first Building Unit (BU1) consists of 120 T atoms. BU1 (Fig.1 (a); bottom) is obtained when the 6-rings in the α-cavity (Fig.1(a); top) are replaced by four cancrinite (can) cages (Fig.1 (c)) and four double 6-rings. The second Building Unit (BU2) consists of 72 T atoms. BU2 (Fig.1 (b); bottom) is obtained by replacing four 6-rings in the β-cage (or sodalite (sod) cage; Fig.1 (b); top) for four can cages. Both building units exhibit 4-fold inversion symmetry and can be built using 4-2 or 6 units. Neighboring BU1s, related by a translation over a ½(plane diagonal), form cube faces (Fig.1 (d), next page). The Periodic Building Unit (PerBU) is obtained when the empty spaces in the BU1 cubic face are filled with BU2 units. BU1 and BU2, related by a shift of ±½a (or ±½b), are connected through 6- and 4-rings as shown in Figure 1(e) on next page.

Figure 1. (a): α-cavity (top), and BU1 constructed from four can cages and four D6Rs (bottom; α-cavity in bold); (b): sod cage (top), and BU2 built from four can cages (bottom), and BU2 with sod-cage in bold); (c): can cage; [Figure 1 is continued on next page]
Figure 1(Cont’d), (d): Cube face built from BU1s. Cages from different BU1s are connected through 4-rings into a cube face with empty spaces; (e1): PerBU in LTN viewed along c. BU2s (in bold) fill the empty spaces in the ab plane. [Figure 1 is continued on next page]
2. Connection mode:

Neighboring $ab$ planes, related by a shift of $1/2b$ (or $1/2a$), are connected along $c$ to form the 3-dimensional structure shown in Figure 2. The connection modes in the $ac$- and $bc$-planes are equivalent to those shown in Figure 1 for the $ab$ plane.
3. Projections of the unit cell content: See Figure 2.

4. Channels and/or cages:

Cavities and cages are shown in Figure 1(a). Apertures are formed by 6-rings only. The pore descriptors are added in Figure 1(a).

5. Supplementary information:

Other framework types containing (modified) cavities
Several other framework types 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).