Building scheme for -LIT



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:

-LIT can be built using units of 12 T atoms. The T12-unit consists of a 3-fold (1,2,3)-connected double 6-ring (D6R; bold in Figure 1(left)). A one-dimensional Periodic Building Unit (PerBU) is obtained when T12-units, related by pure translations along **b**, are connected in such a way that two crankshafts chains and additional (fused) 4-rings are formed (bold in Figure 1 (right). Each crankshaft chain bears two independent terminal oxygen atoms. The repeat distance along a crankshaft chain varies between 8.4-9.9 Å. [Compare the connection of the D6R in **-LIT** with those in **AFI**, **ATT**, **ATV**, **AWO**, and **UEI**; The PerBU can also be built using 4-[1,1], or 4-2 units]

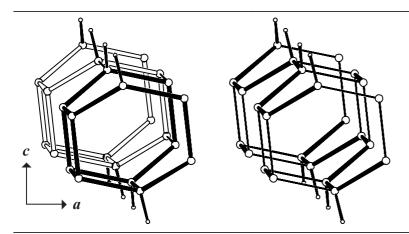
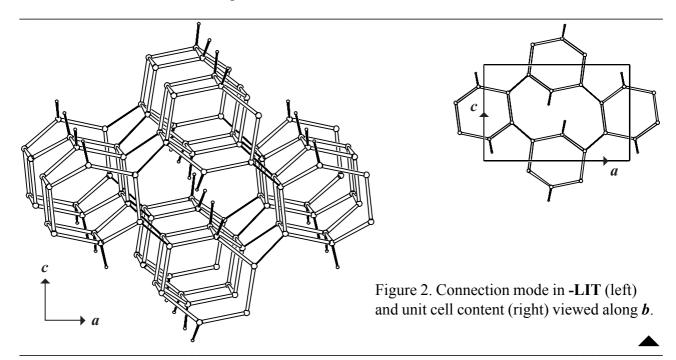


Figure 1. PerBU constructed from 3-fold connected double 6-rings (left) or from two crankshaft chains and dimers (right; see **Alternative description**). Terminal oxygen atoms are indicated by bold bonded small circles.

2. Connection mode:

Neighboring PerBUs, related by a rotation of 180° about \boldsymbol{a} and a shift of $\frac{1}{2}\boldsymbol{c}$, are connected through crankshaft chains as shown in Figure 2.



3. Projections of the unit cell content: See Figure 2.

4. Channels and/or cages:

One of the non-interconnecting 10-ring channels in **-LIT**, parallel to **b**, is shown in Figure 4. The **pore descriptor** is added in the Figure.

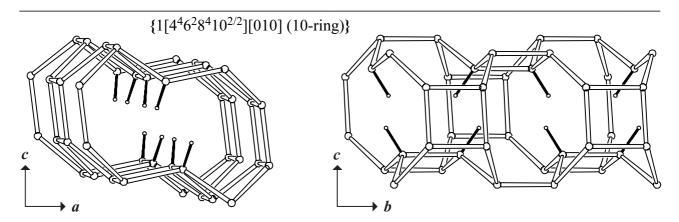


Figure 3. 10-Ring channel in **–LIT.** The terminal oxygen atoms (bold bonded small circles) seriously hamper the diffusion through the channel.

5. Supplementary information:

Other framework types containing (modified) double 6-rings (D6Rs)

Several framework types, like **-LIT**, can be built using (modified) D6Rs (see Figure 1). In the **INTRO** pages links are given to descriptions of other framework types containing (modified) D6Rs (choose: **Double 6-rings**). There is also a link provided to a summary of the Periodic Building Units used in the building schemes of these framework types (choose: **Appendix**; **Figure 7**).

Alternative description of -LIT using crankshaft chains

In several framework types, like in **-LIT**, at least one of the unit cell dimensions is between 8.4 and 9.9 Å. In many cases this indicates the presence of crankshaft chains.

In the **INTRO** pages links are given to detailed descriptions of these framework types (choose: **Crankshaft chains**). There is also a link provided to a summary of the Periodic Building Units used in the building schemes of these framework types (choose: **Appendix**; **Figure 3**).