Building scheme for ITH



Periodic Building Unit – 2. Connection mode – 3. Parallel projections of the unit cell
4. Channels and/or cages – 5. Supplementary information

1. Periodic Building Unit:

ITH can be built using chains parallel to *a* constructed from 28 T atoms (bold in Figure 1). The T28units are related by pure translations along *a*. The chain resembles a "double" chain in **CON** with two additional "handles". The two-dimensional Periodic Building Unit (PerBU) is equal to the *ab* layer depicted in Figure 2. The PerBU is built from parallel chains related by pure translations along *b*. [Compare this chain and PerBU with those in the **Beta-like framework types**]



Figure 1. Chain of T28-units (one in bold) viewed perpendicular to the chain axis (left) and along the chain axis (right).



Figure 2. PerBU in **ITH** viewed along c (left) and along a (one T28-unit in bold). The connecting T-T bonds in the fused 4-6-6 ring sequences formed are drawn as single lines.

2. Connection mode:

Neighboring PerBUs, related by a shift of $\frac{1}{2}(b+c)$, are connected through 9-rings as shown in Figure 3.



Figure 3. Connection mode viewed along *a*. Only one T28-unit along *a* is drawn for clarity.

3. Projections of the unit cell content: See Figure 4.



Figure 4. Unit cell content in ITH viewed along (from left to right) *b*, *c* and *a*.

4. Channels and/or cages:

Interconnecting straight 9- and 10-ring channels are parallel to a, and b, respectively. A sinusoidal 10-ring channel is parallel to c. The channels are depicted in Figure 5 on next page together with their **pore descriptor**. The fusion of channels is illustrated in Figure 6. Diffusion through the (sinusoidal) 12-ring channel parallel to c is obstructed as can be seen from Figures 4, 5 and 6.



Pore descriptor 9-ring channel parallel to *a*:

{2 [4¹5²6⁴9^{2/2}10³] [100] (9-ring), [010] (10-ring)}









{3 [4²5²6²9²10²10²/²] [100] (9-ring), [010] (10-ring), [100] (10-ring)}





Figure 5. Straight 9-ring channel (top) viewed along a (left), along c (top right) and along b (bottom right) and straight 10-ring channel (bottom) viewed along b (left), along a (top right) and along c (bottom right)

[Figure 6 is on next page]



5. Supplementary information:

Beta-like framework types

Beta-like framework types can be constructed using chains that resemble the chain in the **BEA** framework type.

In the **INTRO**-pages links are given to a description of the framework types that contain these chains (choose: **Beta-family**). There is also a link provided to a summary of the chains and PerBUs used in the building schemes of the framework types (choose: **Appendix**; **Figure 9**).