

Building scheme for ITR



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2. Connection mode
3. Channels and/or cages
4. Composite Building Units
5. Supplementary information

1. Periodic Building Unit

Orthorhombic **ITR** can be built using units of 28 T atoms (see Figure 1). T28-units, related along a by pure translations and along c by a 2-fold screw axis parallel c , are connected through 4-rings (and 6-rings) into the two-dimensional PerBU shown in Figure 1. [Compare with **ITH**]

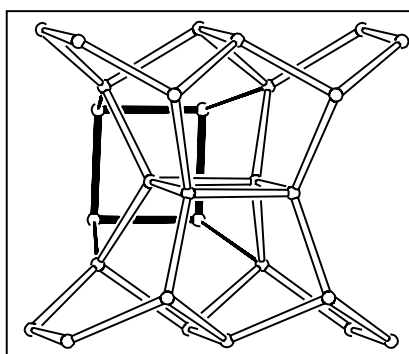
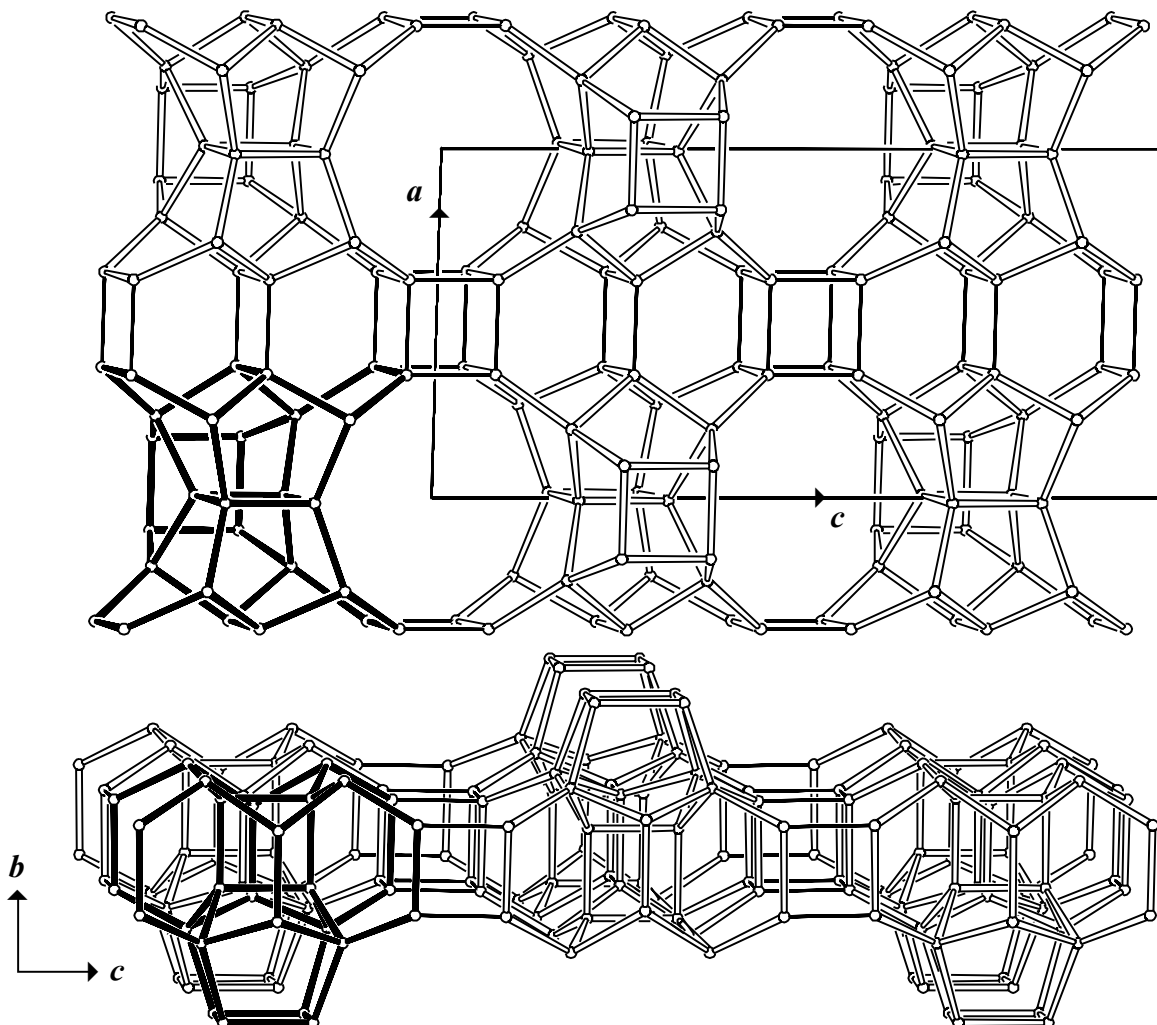


Figure 1. Top: T28-unit consisting of two $[4^1 5^2 6^4]$ -cages sharing the 4-ring, and an additional 4-ring (in bold). A $[4^1 5^6]$ -cage is formed. [The dimers in the T28-unit in **ITH**, are replaced in **ITR** by a 4-ring]. Middle: PerBU viewed along b and along a (bottom).



2. Connection mode

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

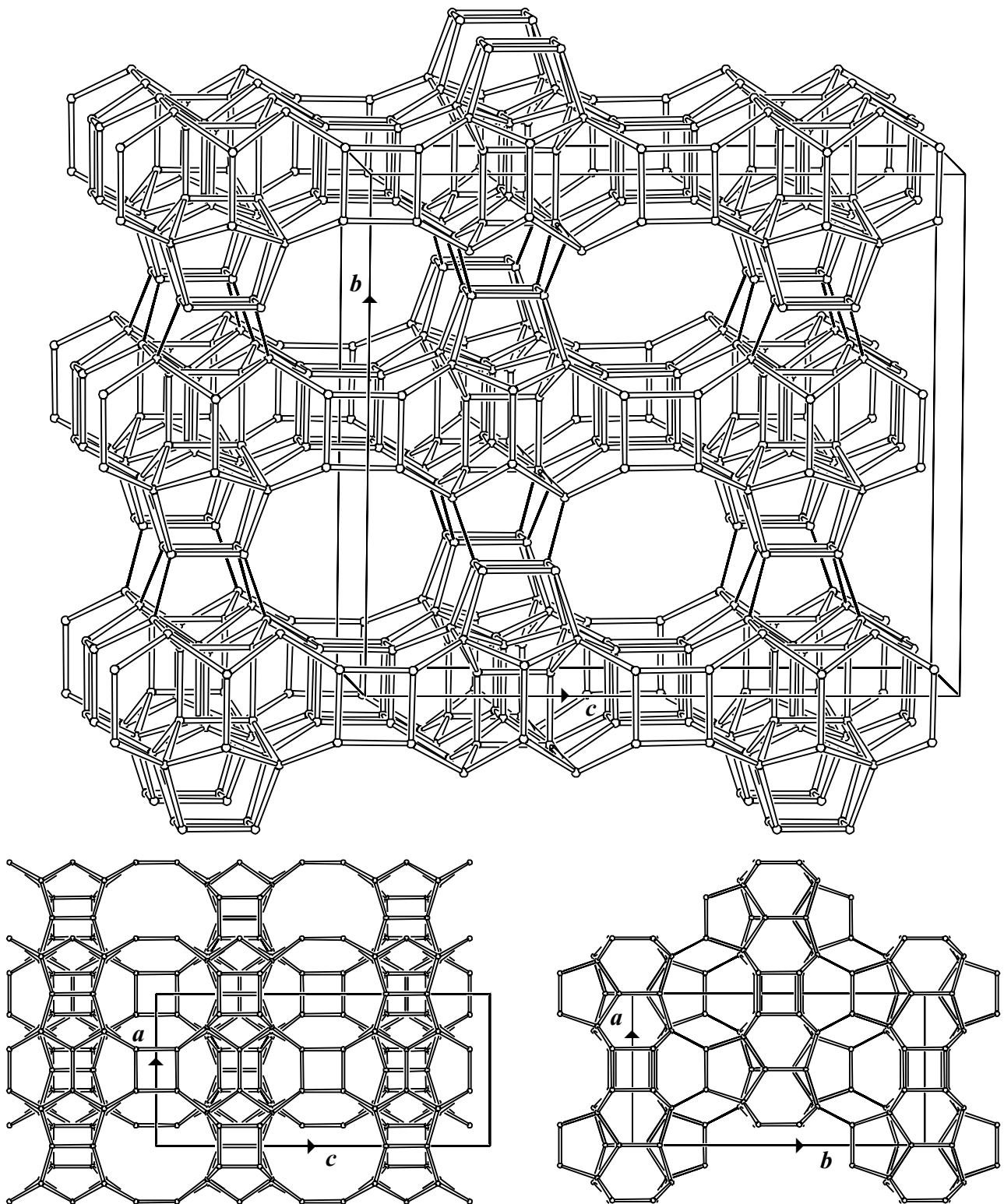


Fig. 2. Connection mode and unit cell content viewed along a (top) and projected along b (bottom left) and along c (bottom right).



3. Channels and/or cages

10-Ring channels are parallel to a . The 10-ring channels are interconnected along b through 10-rings in neighboring channels and along c through 9-rings in neighboring channels as is shown in Figure 3. The **pore descriptor** is added.

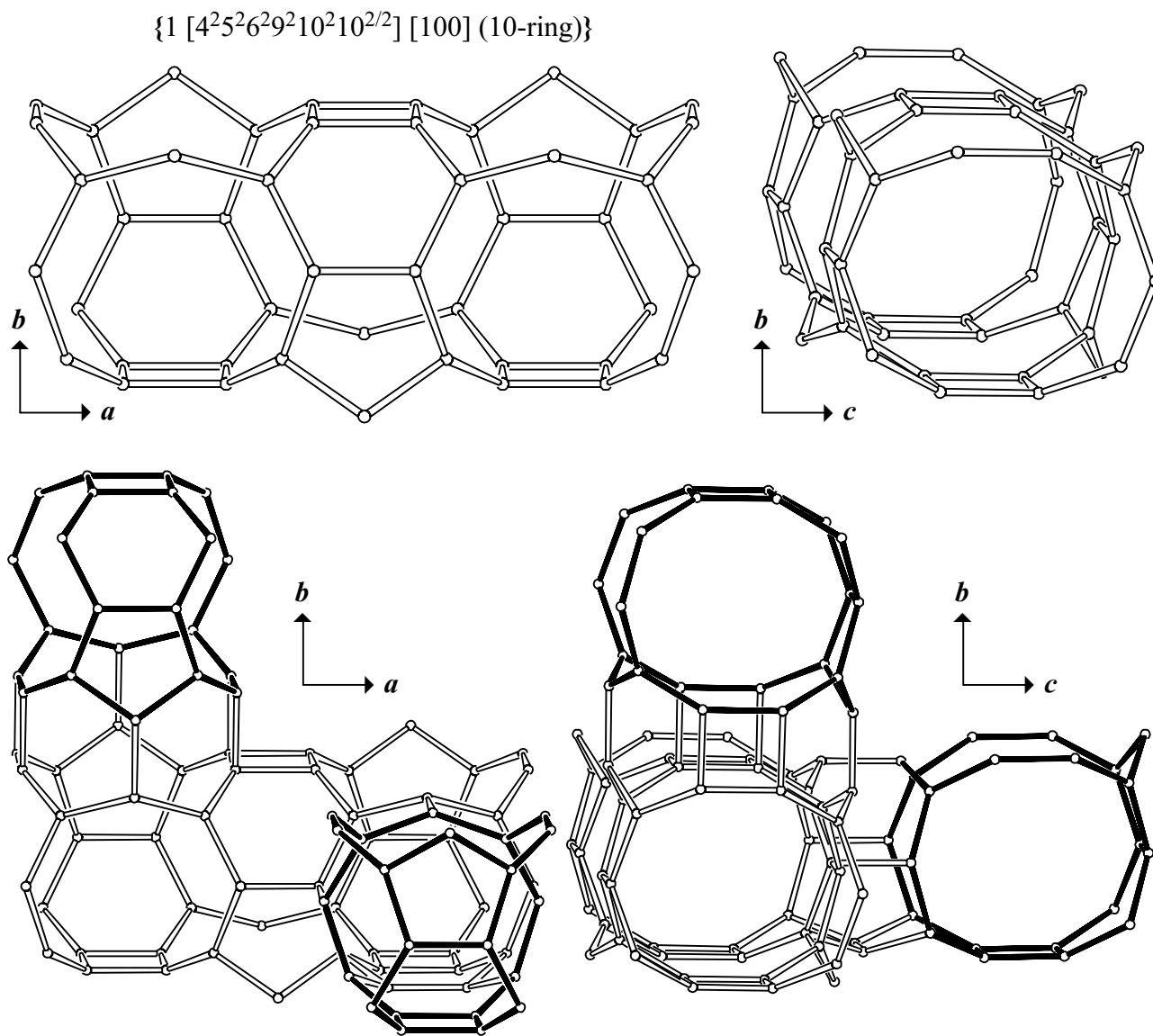
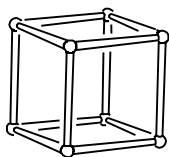


Fig. 3. Top: 10-Ring channel viewed along c (left) and along the channel axis parallel to a (right); Bottom: Interconnection between neighboring channels along b through 10-rings and along c through 9-rings. Only a part of the neighboring channels is shown (in bold). ▲

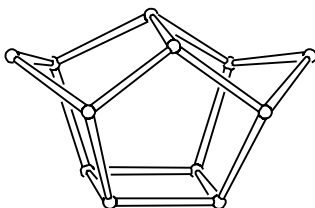
4. Composite Building Units

$[4^6]$ *d4r*



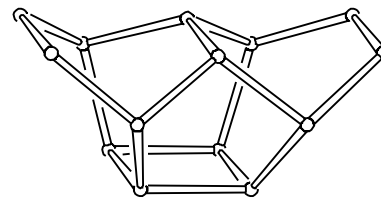
ACO, AFY, AST, ASV, BEC,
-CLO, DFO, ISV, ITH, ITR,
ITW, IWR, IWS, IWW, IXX,
LTA, SOF, STW, UFI, UOS,
UOZ, UTL

$[4^15^6]$ *stf*



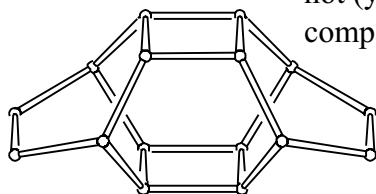
IME, ITR, IWW,
SFF, STF, TUN

$[4^15^26^4]$ *mel*



BOF, CON, DON, ITH,
ITR, IWR, IWS, IWW,
MEL, MFI, *MRE,
MWW, SFG, SFS, SSF,
*STO

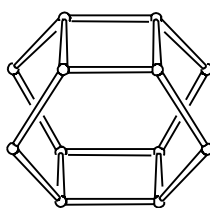
$[4^26^6]$



not (yet) in Atlas
compare with:

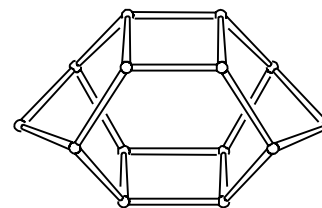
ATO, CON, DFO, EZT, IFR,
ITH, ITR, IWR, IWS, LAU,
MSO, OSI, TUN

$[4^26^4]$ *lau*



ASV, BCT, IWW,
-RON, SAO, UOZ

$[4^25^46^2]$ *mtw*



*BEA, BEC, GON, ISV,
IWS, MSE, MTW, SFH,
SFN, SSF, UOS

Fig. 4. Composite Building Units. [I suggest to call *lau* the CBU at the bottom left and to define a new name for *lau* in the middle (*asv*?).] ▲

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](#)).

Alternative description using (modified) 5-rings

Several other framework types can be constructed using (modified) 5-rings.

In the [INTRO](#) pages links are given to detailed descriptions of these framework types (choose: [5-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 6](#)). ▲