Building scheme for IWS


1. Periodic Building Unit

IWS can be built using two building units: a $[4^6_{12}]$ cage with inserted 4-ring (36 T atoms; 4/mmm symmetry) and a “double” $[4^25^46^2]$ cage with 4 additional dimers (32 T atoms; 2/mmm symmetry). The one-dimensional PerBU is obtained when the building units are connected along a (or b) through double 4-rings into a column as shown in Figure 1.

Figure 1. $[4^25^46^2]$ Cage (top left), “double” $[4^25^46^2]$ cage with one 4-ring in common and four additional dimers (top middle), $[4^6_{12}]$ cage with inserted 4-ring (bottom left) and PerBU (right) viewed nearly along c. The four additional dimers are in bold.

2. Connection mode

Neighboring PerBUs, related by a shift of $1/2(a + b + c)$ and by pure translation along c, are
connected through (double) 4-rings as shown in Figure 2.

Figure 2a. Top: Connection mode through (double) 4-rings between PerBUs related by $1/2(a + b + c)$. Only one PerBU along $c$ is shown for clarity. Bottom: Connection mode through (double) 4-rings between PerBUs related by pure translations along $c$. 
3. Channels and/or cages

Straight 12-ring- and sinusoidal 12-ring-channels are parallel to \( c \) and \(<011>\), respectively (Figure 3).
4. Composite Building Units

**Figure 3b.** Connection of channels along \(a\) and \(b\) viewed along \(c\) (left) and along [011] (right).

**Figure 4.** Composite Building Units. The pore descriptors are given.

- **d4r: \([4^6]\)**
  - 8
  - ACO, AFY, AST, ASV, BEC, -CLO, DFO, ISV, ITH, ITW, IWR, IWS, IWW, LTA, UFI, UOZ, UTL

- \([4^15^26^4]\)
  - 10
  - CON, DON, ITH, IWR, IWS, IWW, MEL, MFI, *MRE, MWW, SFG, SSF, *STO
  - See also 30

- \([4^25^46^2]\) -b
  - 17
  - *BEA, BEC, GON, ISV, IWS, MSE, MTW, SFH, SFN, SSF

- \([4^26^4]\)-a
  - 19
  - ASV, BCT, IWS, IWW, -RON, SAO, UOZ
  - See also 17 and 22

- \([4^612]\)
  - \([4^6]\)
  - IWS
  - See also 68 and 69

- \([5^4]\)
  - 55
  - *BEA, BEC, ISV, IWS, IWW, MEL, MFI, MFS, MSE, RWR, TUN
  - See also 68 and 69
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).

The secondary building units in IWS are 4 and 4-[1,1] and 5-1.