Building scheme for IWS

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

1. Periodic Building Unit

IWS can be built using two building units: a $[4^6 6^{12}]$ cage with inserted 4-ring (36 T atoms; 4/mmm symmetry) and a "double" $[4^2 5^4 6^2]$ 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.

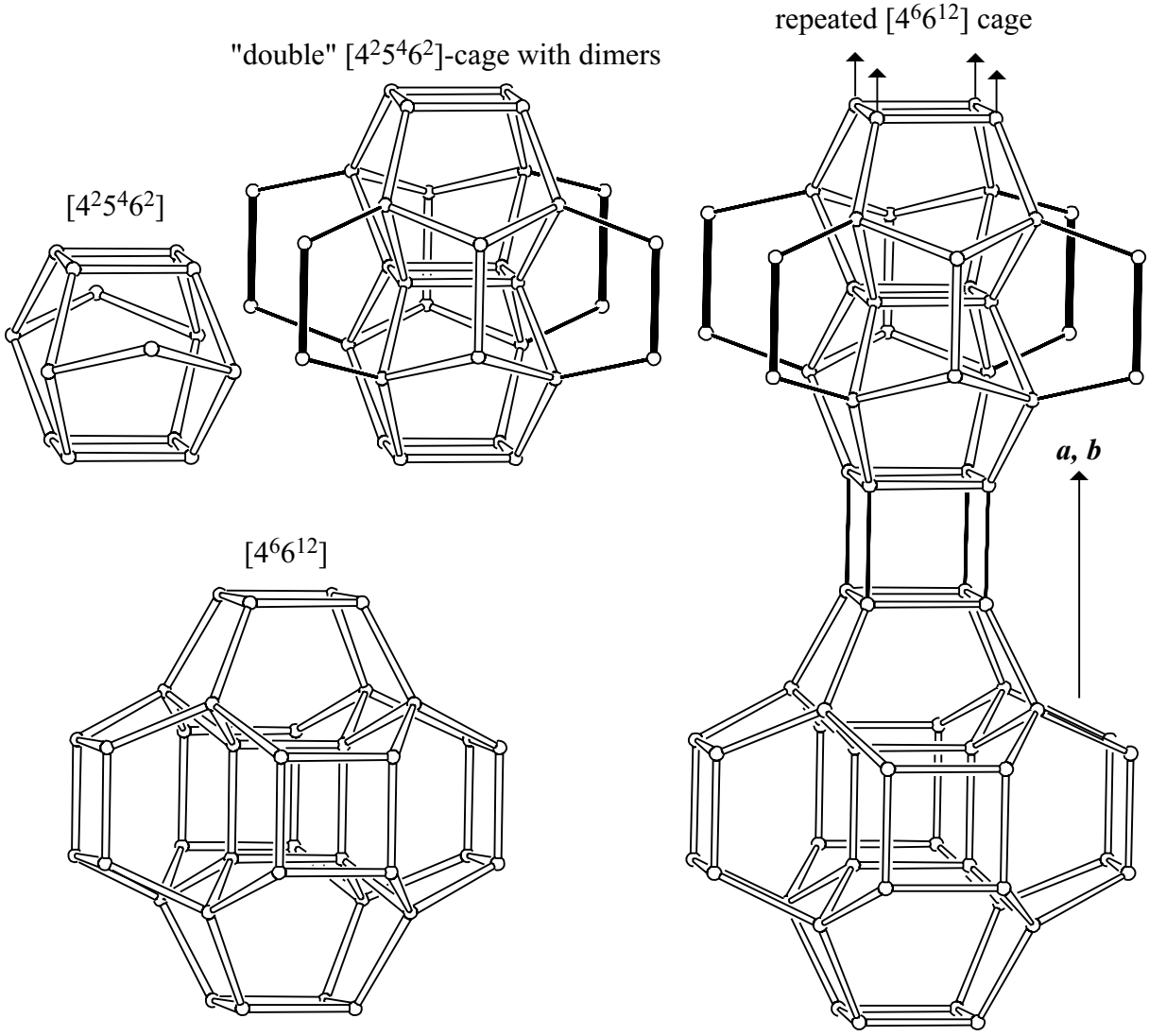


Figure 1. $[4^2 5^4 6^2]$ Cage (top left), "double" $[4^2 5^4 6^2]$ cage with one 4-ring in common and four additional dimers (top middle), $[4^6 6^{12}]$ cage with inserted 4-ring (bottom left) and PerBU (right) viewed nearly along ***c***. The four additional dimers are in bold.

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.

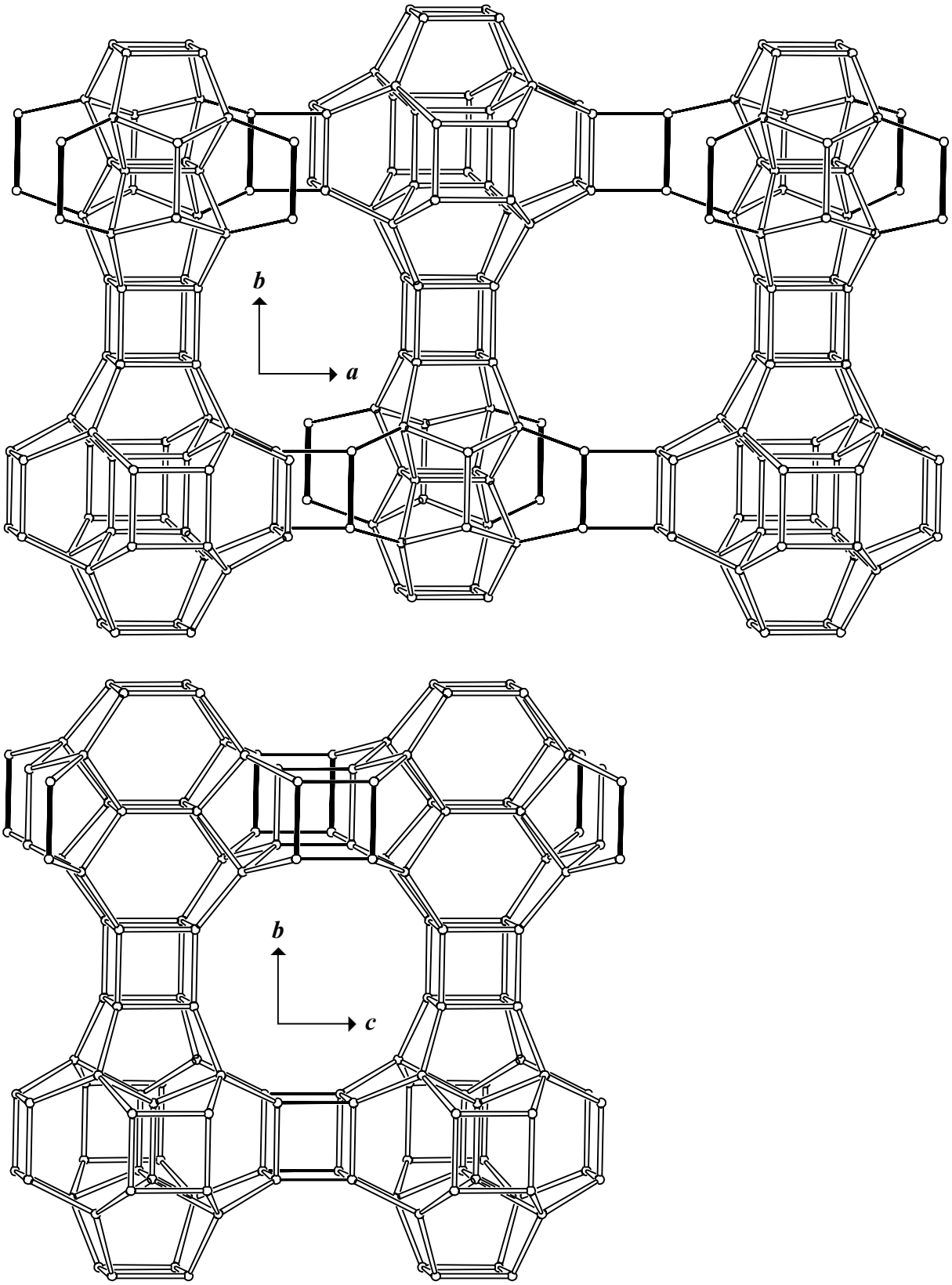


Figure 2a. Top: Connection mode through (double) 4-rings between PerBUs related by 1/2(***a*** + ***b*** + ***c***). Only one PerBU along ***c*** is shown for clarity. Bottom: Connection mode through (double) 4-rings between PerBUs related by pure translations along ***c***.

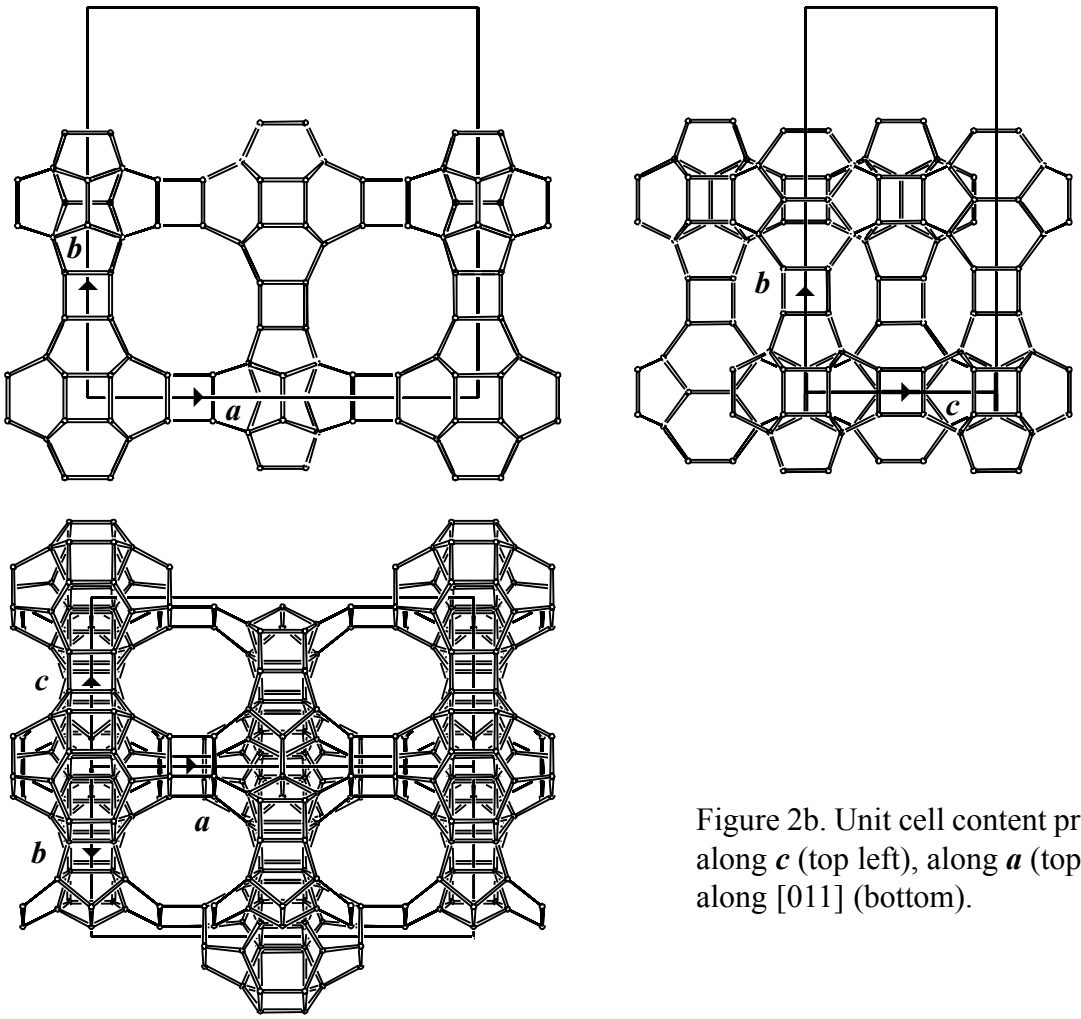


Figure 2b. Unit cell content projected along ***c*** (top left), along ***a*** (top right) and along [011] (bottom).

▲

---

3. Channels and/or cages

Straight 12-ring- and sinusoidal 12-ring-channels are parallel to ***c*** and <011>, respectively (Figure 3).

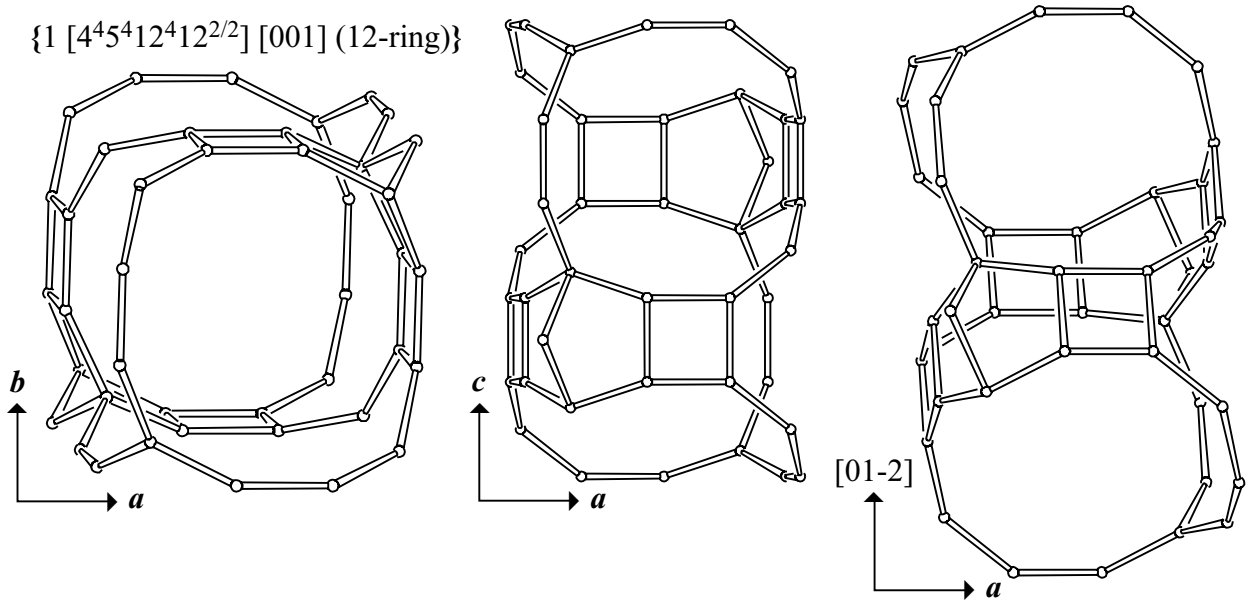


Figure 3a. Straight12-ring channel parallel to ***c*** viewed along ***c*** (left) and along ***b*** (middle). Right: sinusoidal channel viewed along [011].

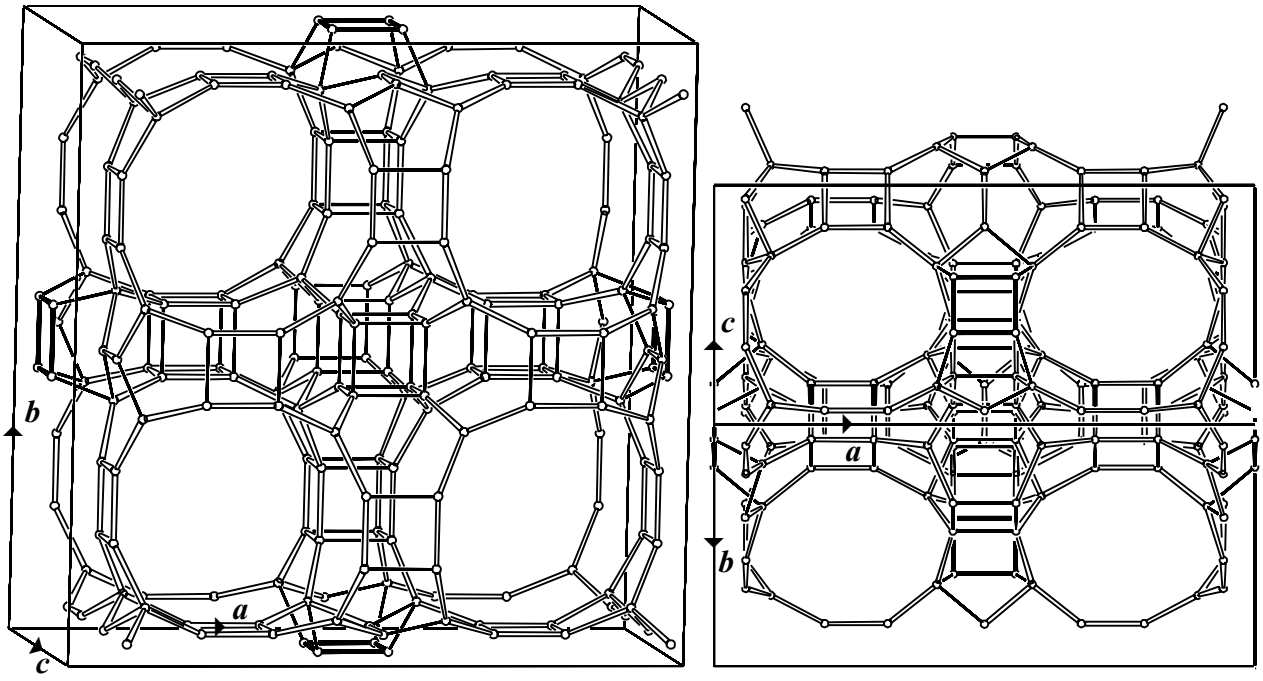
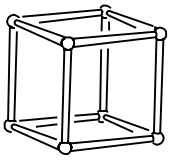


Figure 3b. Connection of channels along ***a*** and ***b*** viewed along ***c*** (left) and along [011] (right).

4. Composite Builing Units

d4r: $[4^6]$

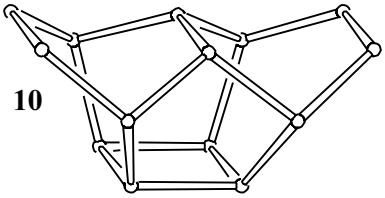
8



ACO, AFY, AST, ASV, BEC, -CLO, DFO, ISV, ITH, ITW, IWR, IWS, IWV, IWW, LTA, UFI, UOZ, UTL

$[4^15^26^4]$

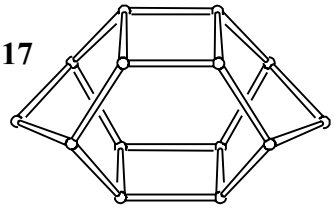
10



CON, DON, ITH, IWR, IWS, IWW, MEL, MFI, *MRE, MWW, SFG, SSF, *STO
see also **30**

$[4^25^46^2]$-b

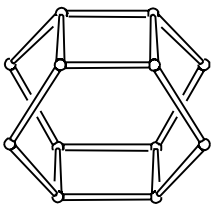
17



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

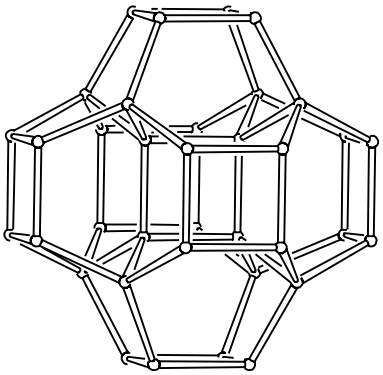
$[4^26^4]$-a

19



ASV, BCT, IWS, IWW, -RON, SAO, UOZ
see also **17** and **22**

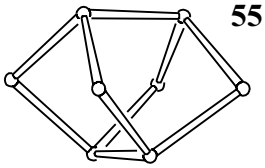
$[4^66^{12}]$



IWS

$[5^4]$

55



***BEA, BEC, ISV, IWS, IWW, MEL, MFI, MFS, MSE, RWR, TUN**
see also **68** and **69**

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

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.