

Building scheme for STW



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- 4. Composite Building Units – 5. Supplementary information

1. Periodic Building Unit

Hexagonal STW can be built using units of 10 T atoms: a double 4-ring with two “dangling” T atoms (or two 4-1 units; bold in Figure 1). The D4Rs of the T10-units are connected along $(a + b)$ through the “dangling” T atoms into a chain along $(a + b)$. Non-connected chains, related along a (or b), by pure translations along a (or b) form the two-dimensional PerBU shown in Figure 1.

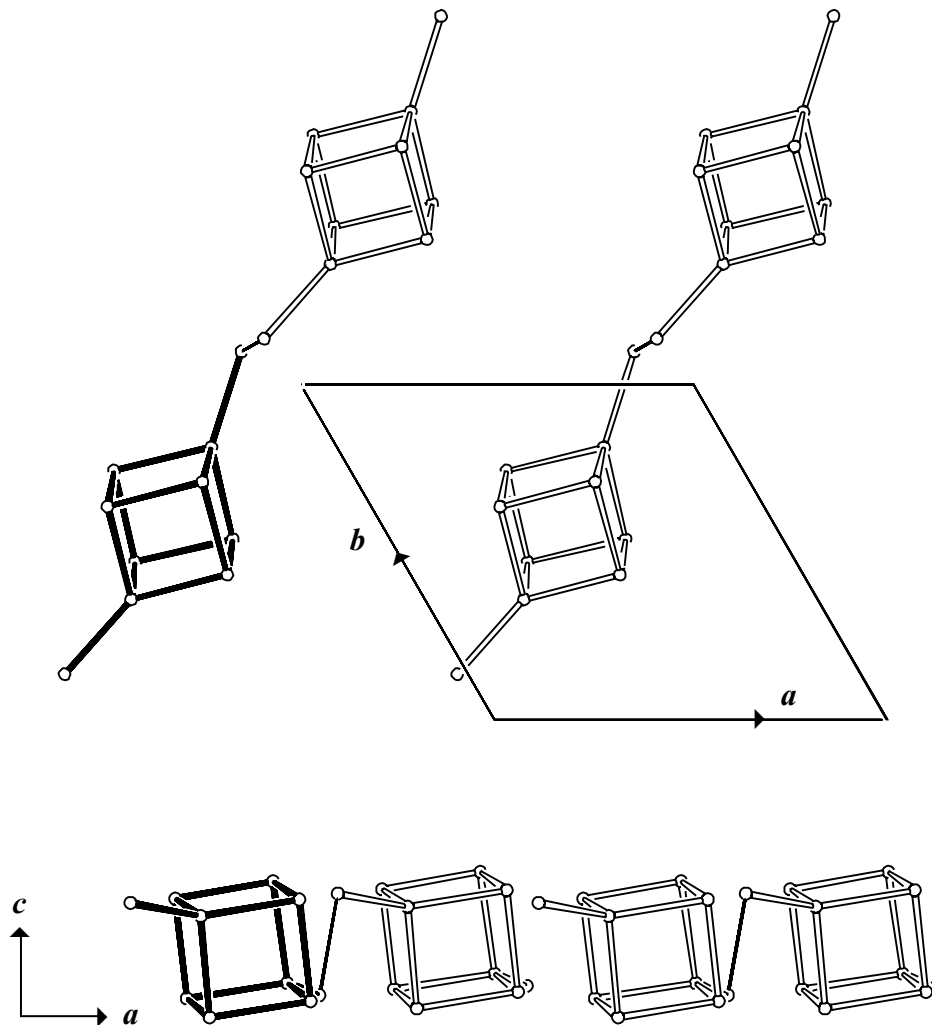


Figure 1. PerBU constructed from T10-units viewed along c (top) and along $[210]$ (bottom). ▲

2. Connection mode

Neighboring PerBUs, related by a rotation of 60° about c , are connected along c through 5-rings as shown in Figure 2 on next page.

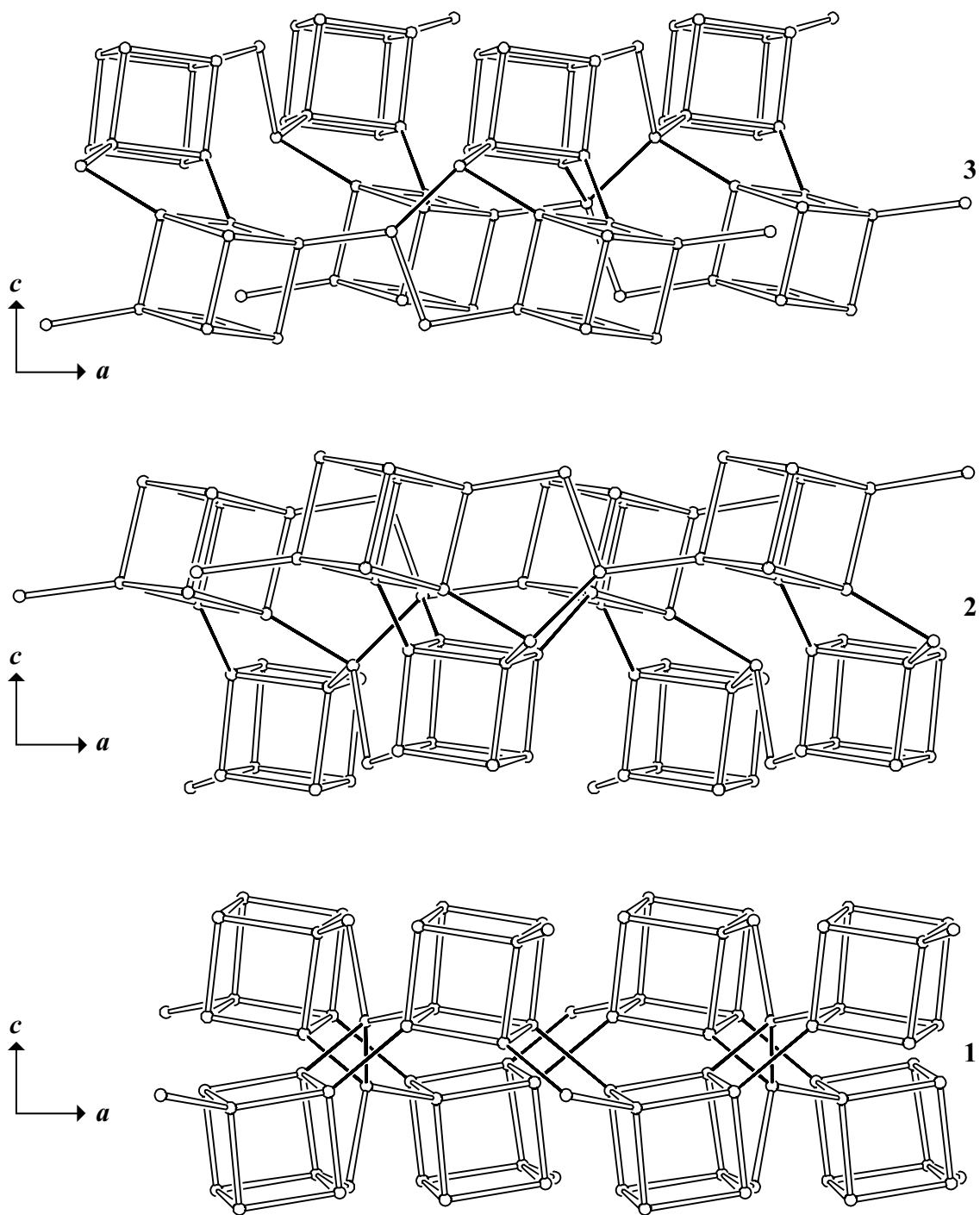


Figure 2a. Connection modes along c viewed (with little differences in order to illustrate the connection modes more clearly) approximately along $[120]$. Bottom: connection mode **1** between the first PerBU and the second one related by a rotation of 60° about c . Middle: connection mode **2** between the second PerBU and the third one. Top: connection mode **3** between the third PerBU and the fourth one. The first PerBU and the fourth one are related by a rotation of 180° about c and a translation of $1/2c$.

(Figure 2 is continued on next page.)

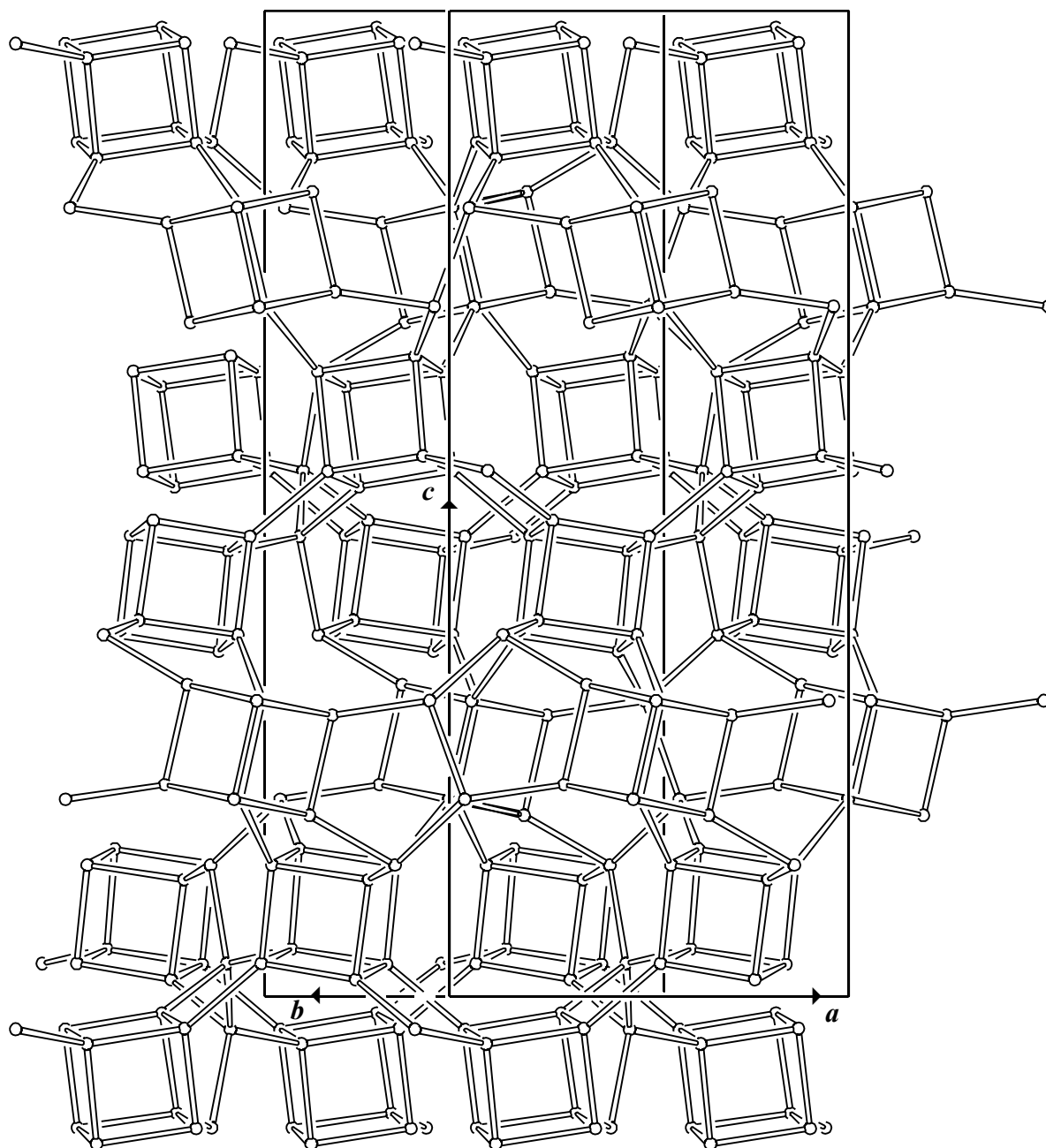


Figure 2b. Cell content viewed along $[120]$.



3. Channels and/or cages

Cavity and channels are illustrated in Figure 3 on next page. The **pore descriptor** is added. 8-Ring channels are parallel to $\langle 100 \rangle$. Chiral 10-ring channels, in which diffusion will be difficult, are parallel to c .

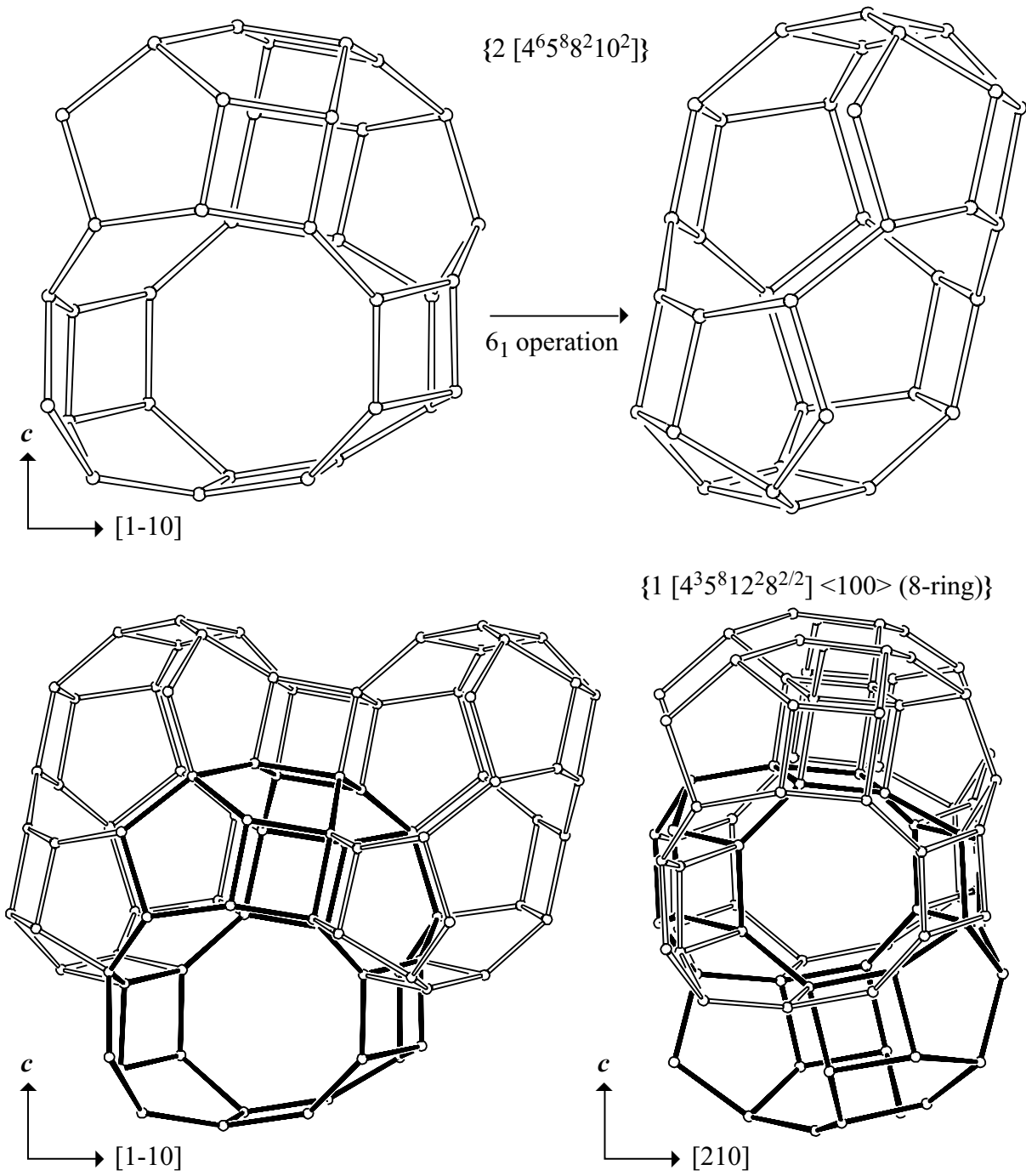
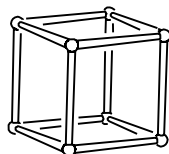


Figure 3. Cavity viewed along [110] (top left) and after a rotation of 60° about c (top right). The cavities, related by a rotation of 60° about c and related by a rotation of 60° about c followed by a pure translation along a (or b), are connected through common 10-rings and common 8-rings, respectively (bottom left). Bottom right: view along the 8-ring channel parallel to b . ▲

4. Composite Building Units

$d4r: [4^6]$



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

Figure 4. Composite Building Unit. ▲

5. Supplementary information

Other framework types containing (modified) double 4-rings (D4Rs)

Double 4-rings (D4Rs) can be connected in several other ways. In some cases the 4-rings of the D4Rs are not 4-fold connected and/or 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) D4Rs (choose: **Double 4-rings**). There is also a link provided to a summary of the PerBUs used in the building schemes of these framework types (choose: **Appendix; Figure 5**).

The secondary building unit in **STW** is 4-1.

