Building scheme for ITW

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

1. Periodic Building Unit:

Finite building units of 12 T atoms are composed of one (finite) zigzag chain and a double 4-ring (Figure 1(a)). The two-dimensional Periodic Building Unit (PerBU) is obtained when these T12-units, related by pure translations along ***a***, and ***c***, are connected into a layer with an oblique repeat unit (Figure 1(b)). The repeat distance along the infinite zigzag chains formed is about 2x5.2 Å. A sheet of zigzag chains connecting double 4-rings is generated (Figure 1(c)).

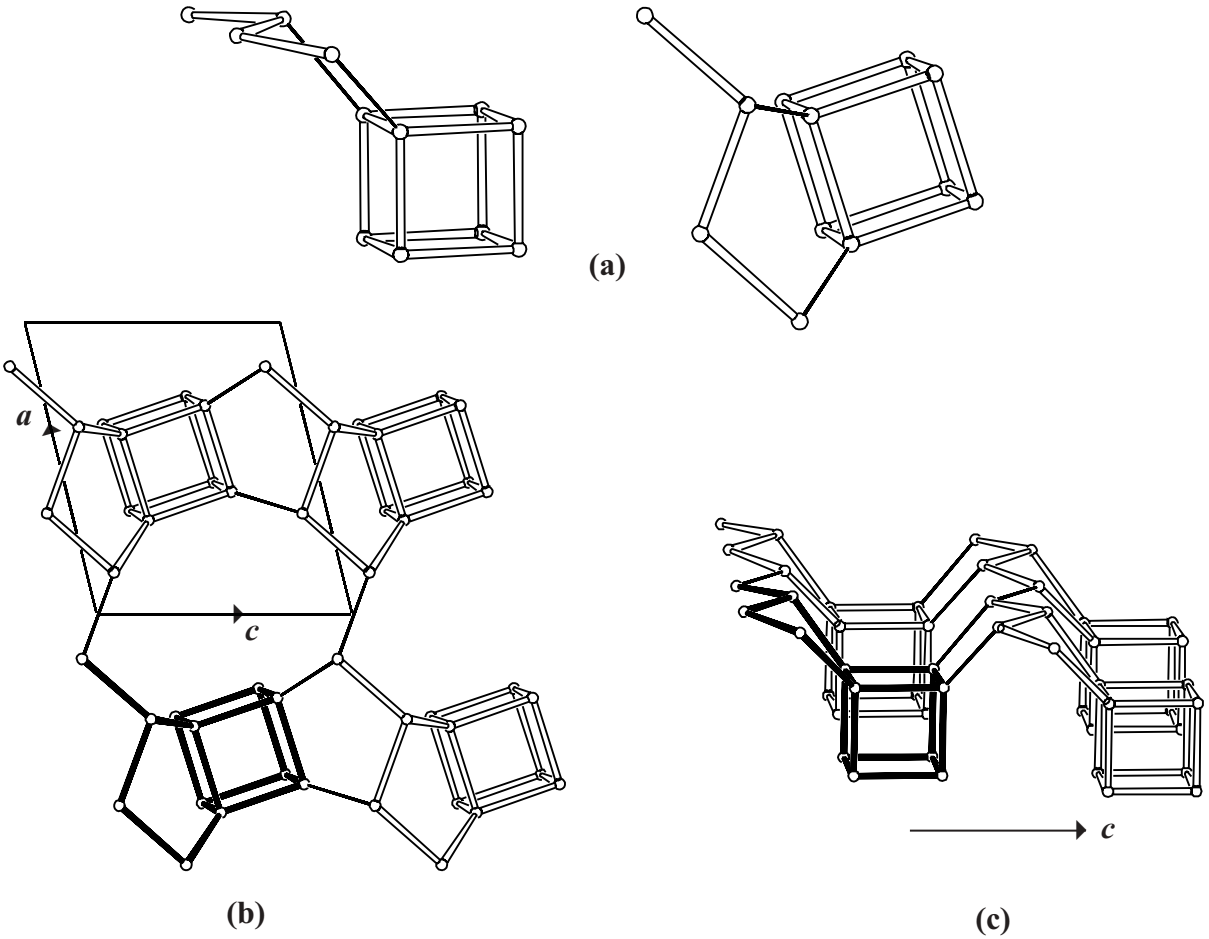

Figure 1. (a): T12-unit composed of one (finite) zigzag chain and a double 4-ring seen along ***a*** (left) and along ***b*** (right); (b): Perspective view of the PerBU along ***b***. (c): Perspective view of the PerBU along ***a*** illustrating the sheet composed of zigzag chains and double 4-rings.

2. Connection mode:

Neighboring PerBUs, related by a lateral shift of ½(***a*** + ***b***), are connected along ***b*** as shown in Figure 2 on next page. Arrays of double 4-rings are connected through zigzag chains (in bold).

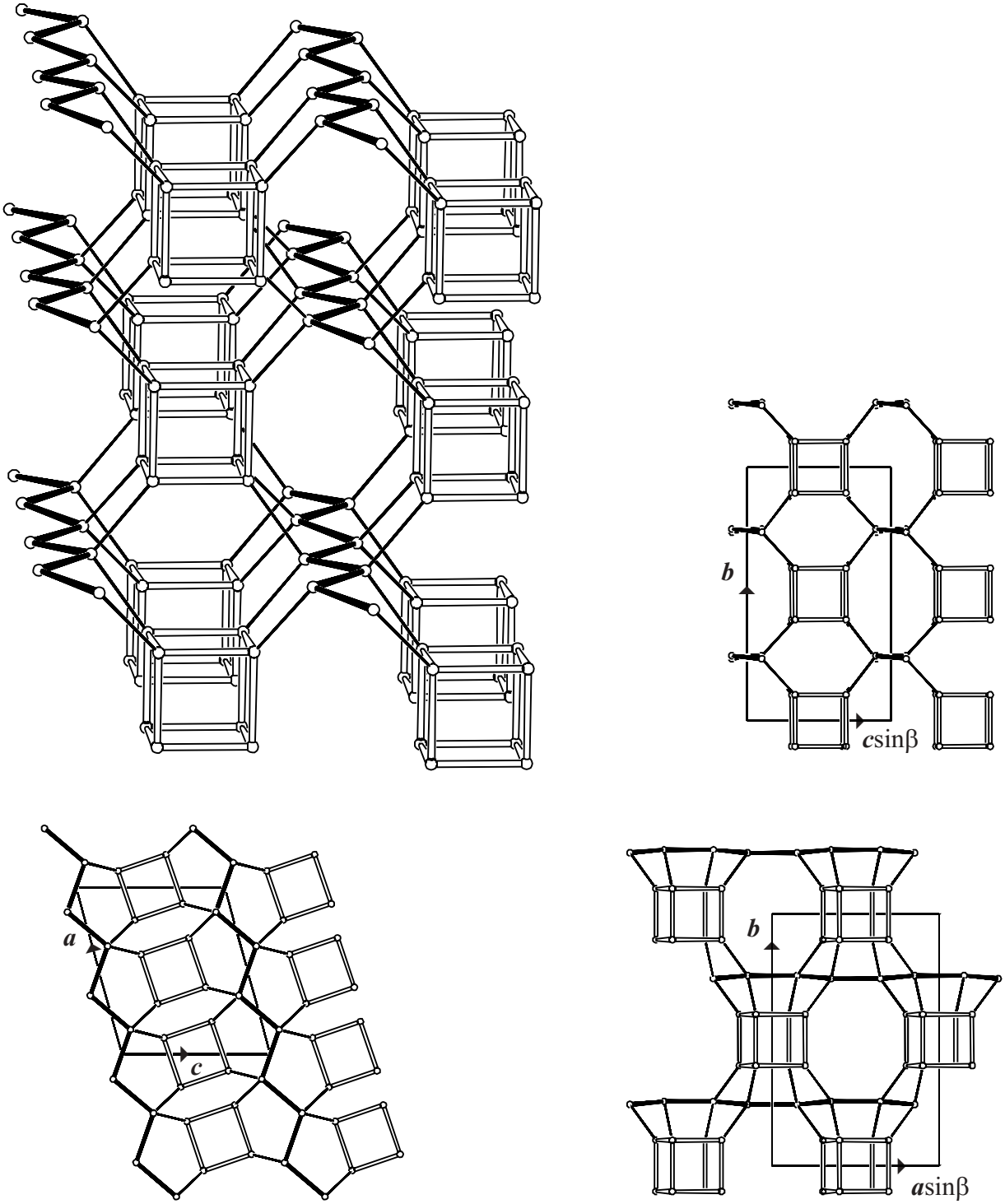

Figure 2. Connection mode in **ITW** viewed along ***a*** (top left), and unit cell content projected along ***a*** (top right), along ***b*** (bottom left) and along ***c*** (bottom right). **ITW** can as well be built using 1-4-1 or 4-[1,1] units as can be seen from the perspective drawing (top left).

---

3. Projections of the unit cell content: See Figure 2.

4. Channels and/or cages:

Interconnecting one-dimensional 8-ring channels are parallel to ***a***, and ***c***. The intersection of channels is illustrated in Figure 3 on next page. The **pore descriptor** is added.

Pore descriptor:
{2 [$4^6 5^8 6^4 8^4$] [100] (8-ring),[001] (8-ring)}

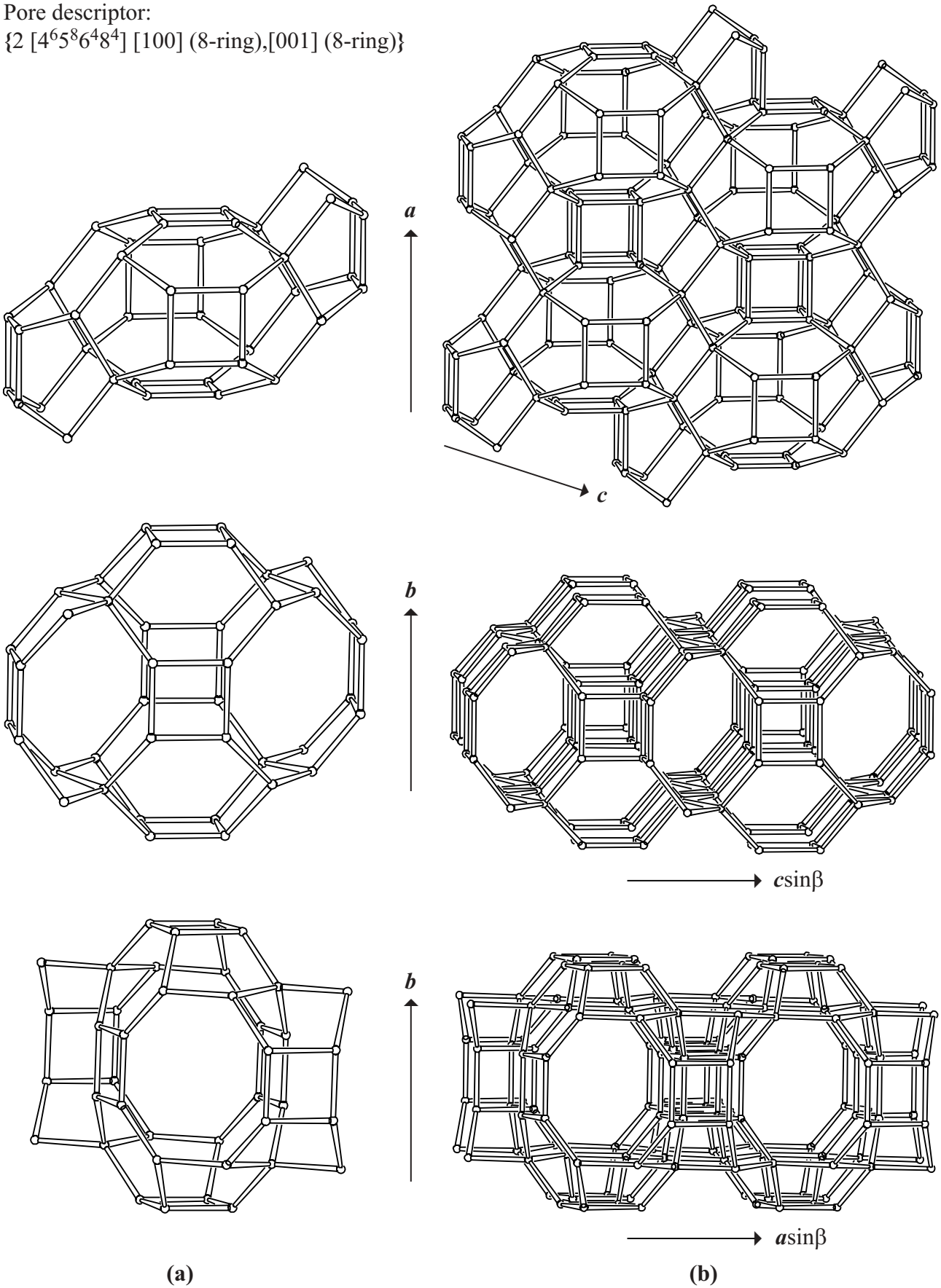

Figure 3. (a): View of the channel intersection along (from top to bottom) ***b***, ***a*** and ***c***.
(b): Fusion of channel intersections along ***a*** and ***c*** viewed along (from top to bottom) ***b***, ***a*** and ***c***.
Interconnected channels with 8-ring windows are parallel to ***a*** (middle), and parallel to ***c*** (bottom).

5. Supplementary information:

Other framework types containing zigzag chains

In several framework types at least one of the unit cell dimensions is about n*5.2 Å (where n = 1, 2, 3, etc.). In many cases this indicates the presence of zigzag chains.

In the **INTRO** pages links are given to detailed descriptions of these framework types (choose: **Zigzag chains**). 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 1**).

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**).