Building scheme for CZP

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:

Hexagonal **CZP** can be built using units of 8 T atoms (three fused 4-rings: a double 4-ring with two disconnected edges; bold in Figure 1), related by a 3_1-axis along ***c***. The one-dimensional Periodic Building Unit (PerBU) is the helix depicted in Figure 1.

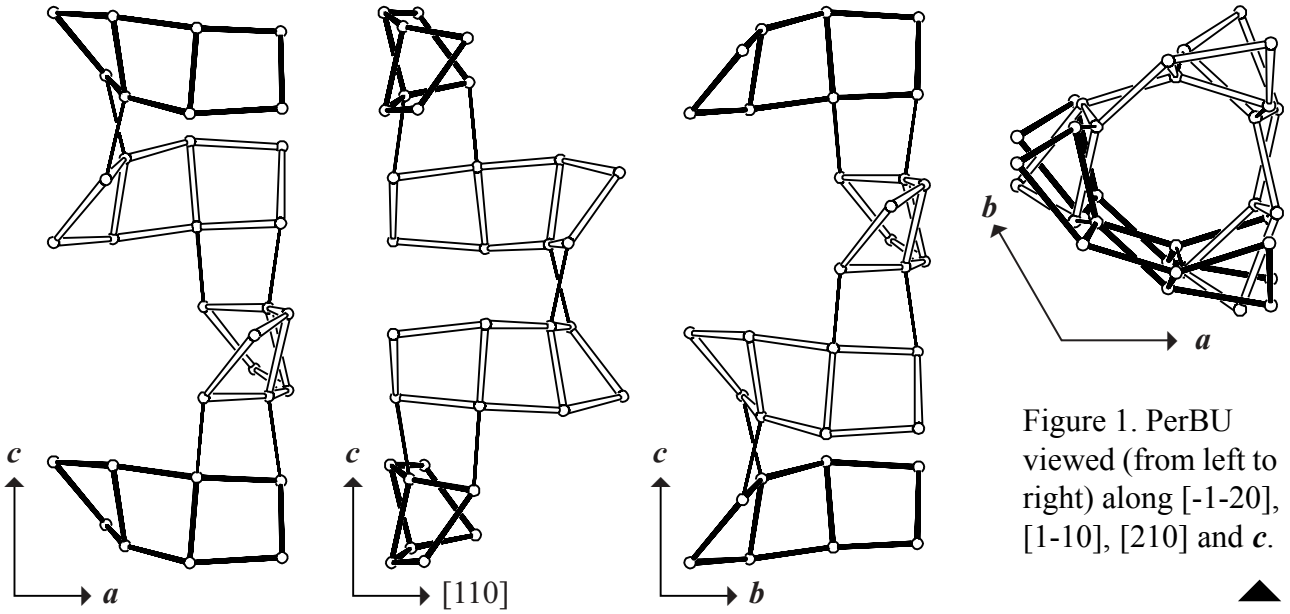

Figure 1. PerBU viewed (from left to right) along [-1-20], [1-10], [210] and ***c***.

2. Connection mode:

Neighboring PerBUs, related by pure translations along ***a*** and ***b***, are connected through 4-rings into the three-dimensional structure as shown in Figure 2.

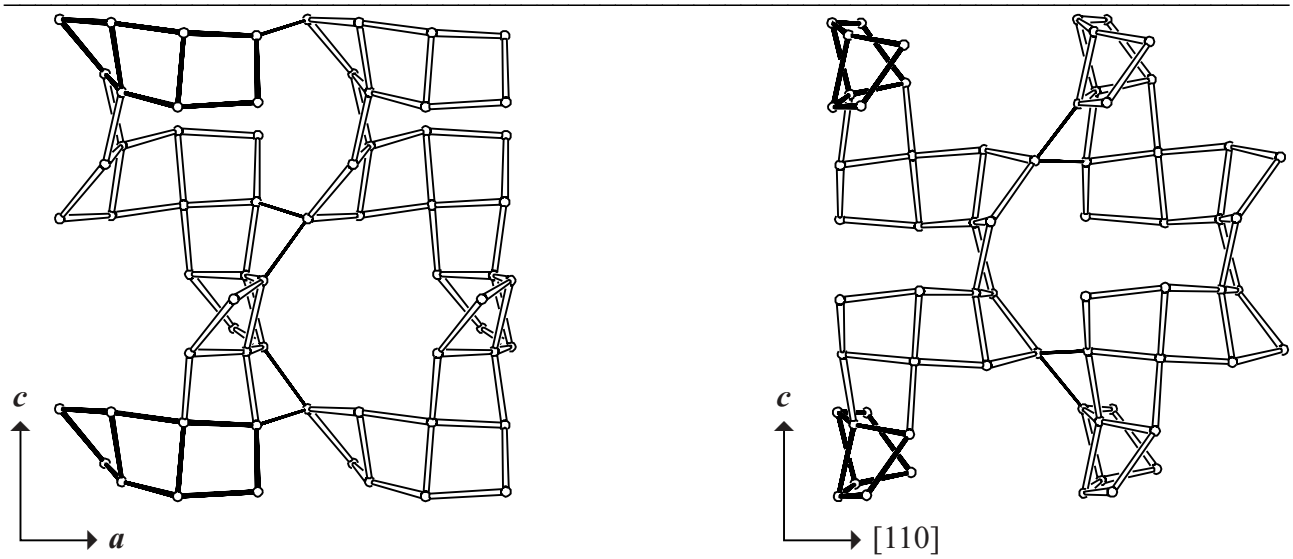

Figure 2. (Equal) connection modes along ***a*** viewed along [-1-20] (left), and along [110] viewed along [1-10] (right). [Figure 2 is continued on next page]

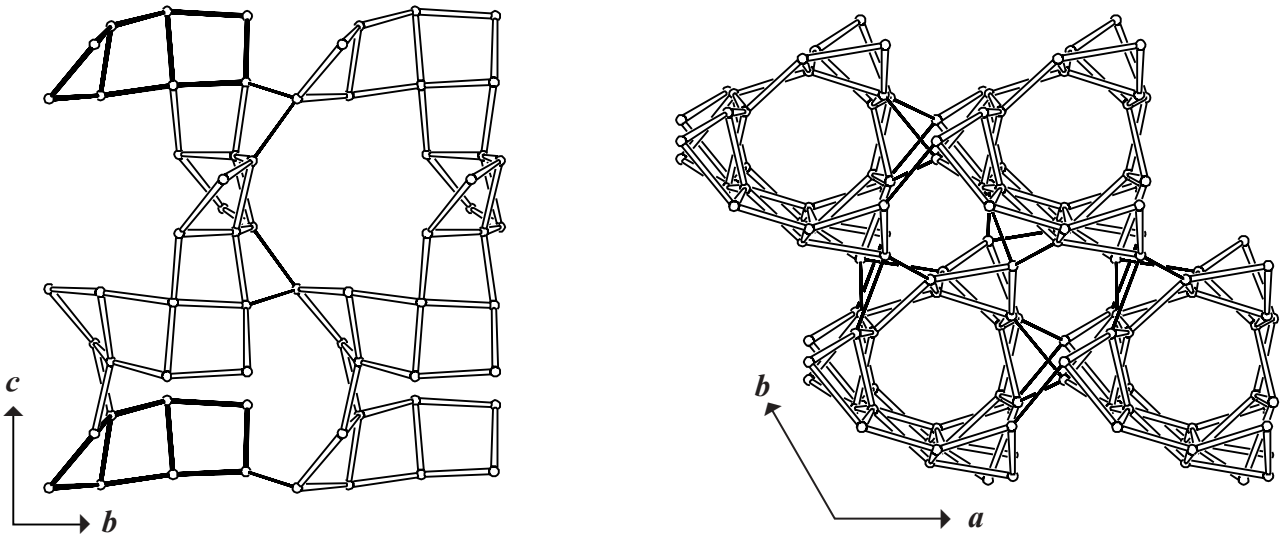

Figure 2 [Cont'd]. Same connection mode along ***b*** viewed along [210] (left), and the three (equal) modes viewed along ***c*** (right).

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3. Projections of the unit cell content:

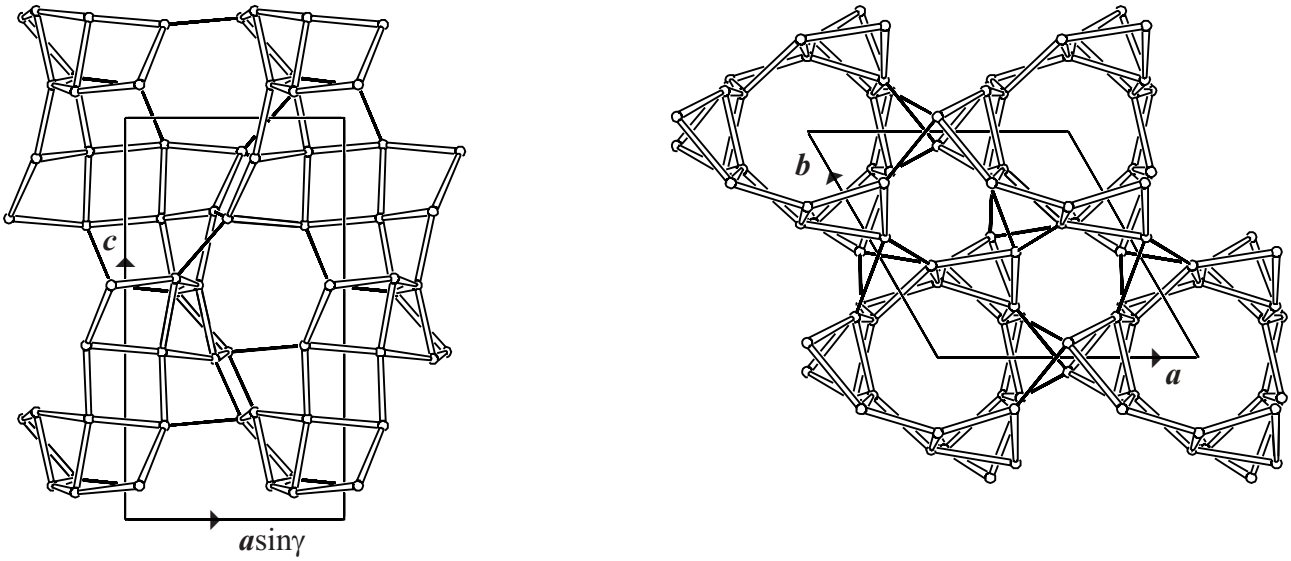

Figure 3. Unit cell content viewed along ***b*** (left), and along ***c*** (right).

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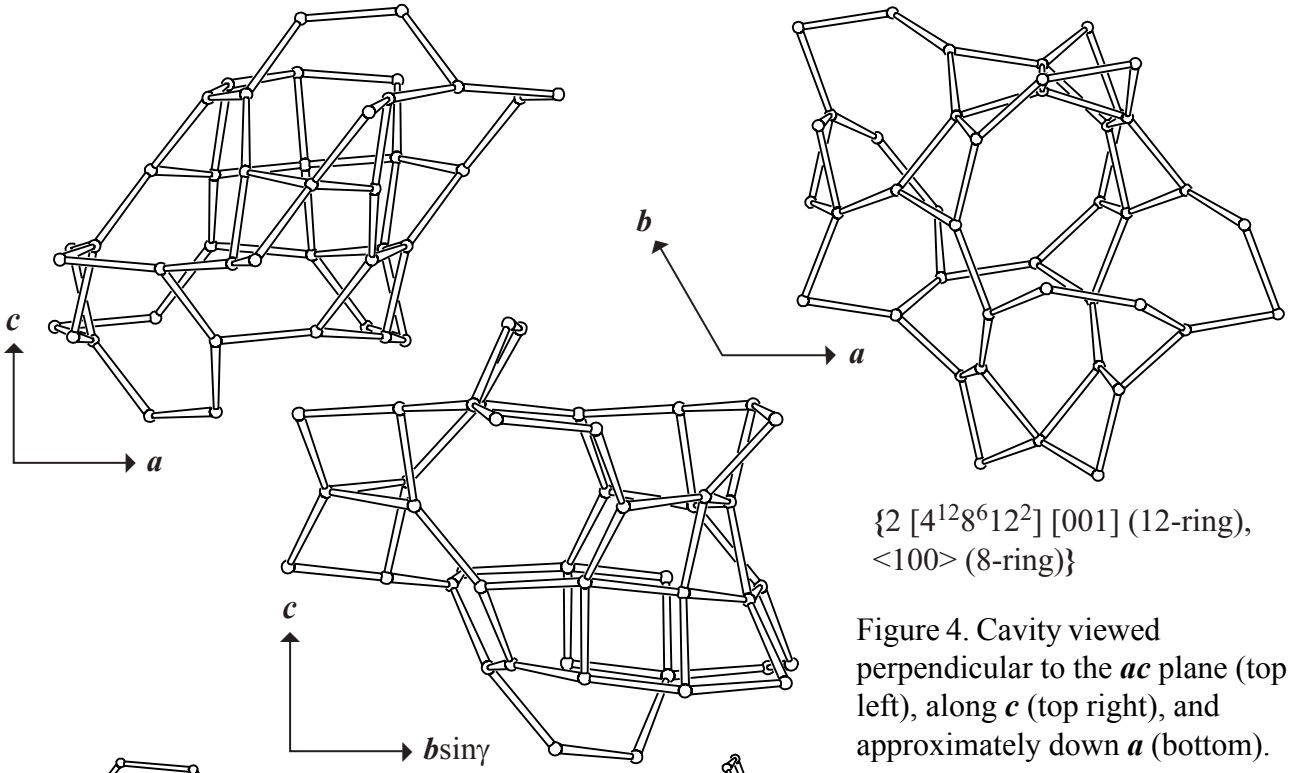
4. Channels and/or cages:

A rather complicated cavity can be constructed from (partly fused) 12-rings related by rotations of 30º about ***c***. Additional T atoms complete the cavity shown in Figure 4. The **pore descriptor** is added. Fusion of cavities, related by a 2-fold screw axis along ***c***, into a chiral channel along ***c*** is illustrated in Figure 5. Figure 4 and Figure 5 are on next page.



{2 [$4^{12}8^{6}12^{2}$] [001] (12-ring), <100> (8-ring)}

Figure 4. Cavity viewed perpendicular to the ***ac*** plane (top left), along ***c*** (top right), and approximately down ***a*** (bottom).

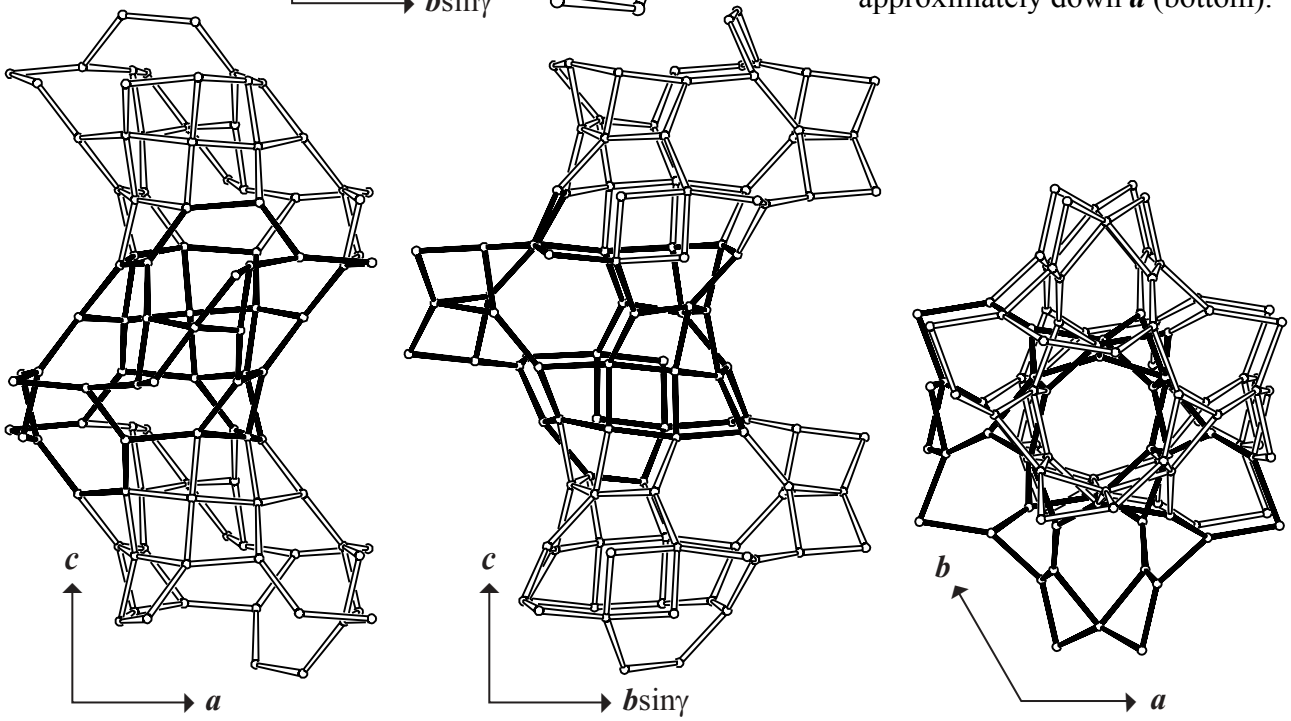


Figure 5. Fusion of cavities into a chiral channel of strongly distorted 12-rings and 8-rings along ***c***.

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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**).