Building scheme for CZP

1. Periodic Building Unit – 2. Connection mode – 3. Projections of the unit cell content
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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 $e$. The one-dimensional Periodic Building Unit (PerBU) is the helix depicted in Figure 1.

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

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).

3. Projections of the unit cell content:

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

4. Channels and/or cages:

A rather complicated cavity can be constructed from (partly fused) 12-rings related by rotations of 30° 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 \( e \), into a chiral channel along \( c \) is illustrated in Figure 5. Figure 4 and Figure 5 are on next page.
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**).