Building scheme for -CHI

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:

The interrupted framework of **-CHI** can be built using the zigzag chain (bold in Figure 1) running parallel to ***a*** and 8 additional T atoms. The repeat distance along the zigzag chain is about 5.2 Å. The one-dimensional Periodic Building Unit (PerBU) is obtained when three zigzag chains (connected into distorted 4-rings) are linked to trimers and pentamers that form 5-rings and 9-rings as shown in Figure 1. Terminal oxygen atoms are bonded to two T atoms in each 5-ring and in each 9-ring. An alternative PerBU consists of 5-[1,1] units (bold in Fig.1 (right)). [See **Alternative description**]

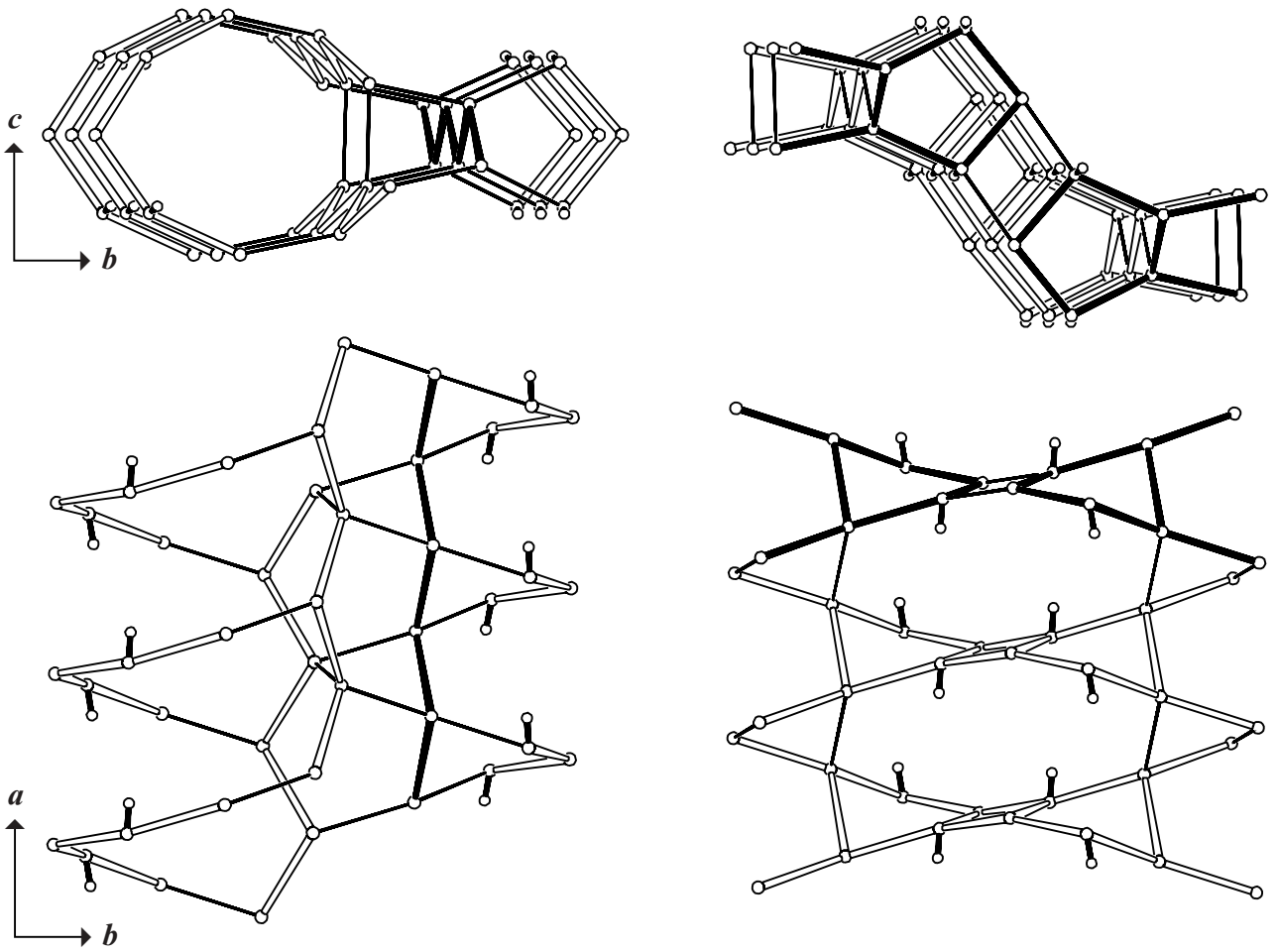


Figure 1. PerBU in **-CHI**, built from zigzag chains, pentamers and trimers (left) or from 5-[1,1] units (right), viewed along ***a*** (top), and along ***c*** (bottom). Terminal oxygen atoms are indicated.

2. Connection mode:

Neighboring PerBUs, related by a pure translation along ***c*** and by a rotation of 180º about ***c*** and a shift of ½***c***, are connected along ***c*** through additional zigzag chains and 4-rings and along ***b*** (and ***c***) through 4-rings. A backbone of 4-rings having one T atom in common parallel to ***c*** is formed.

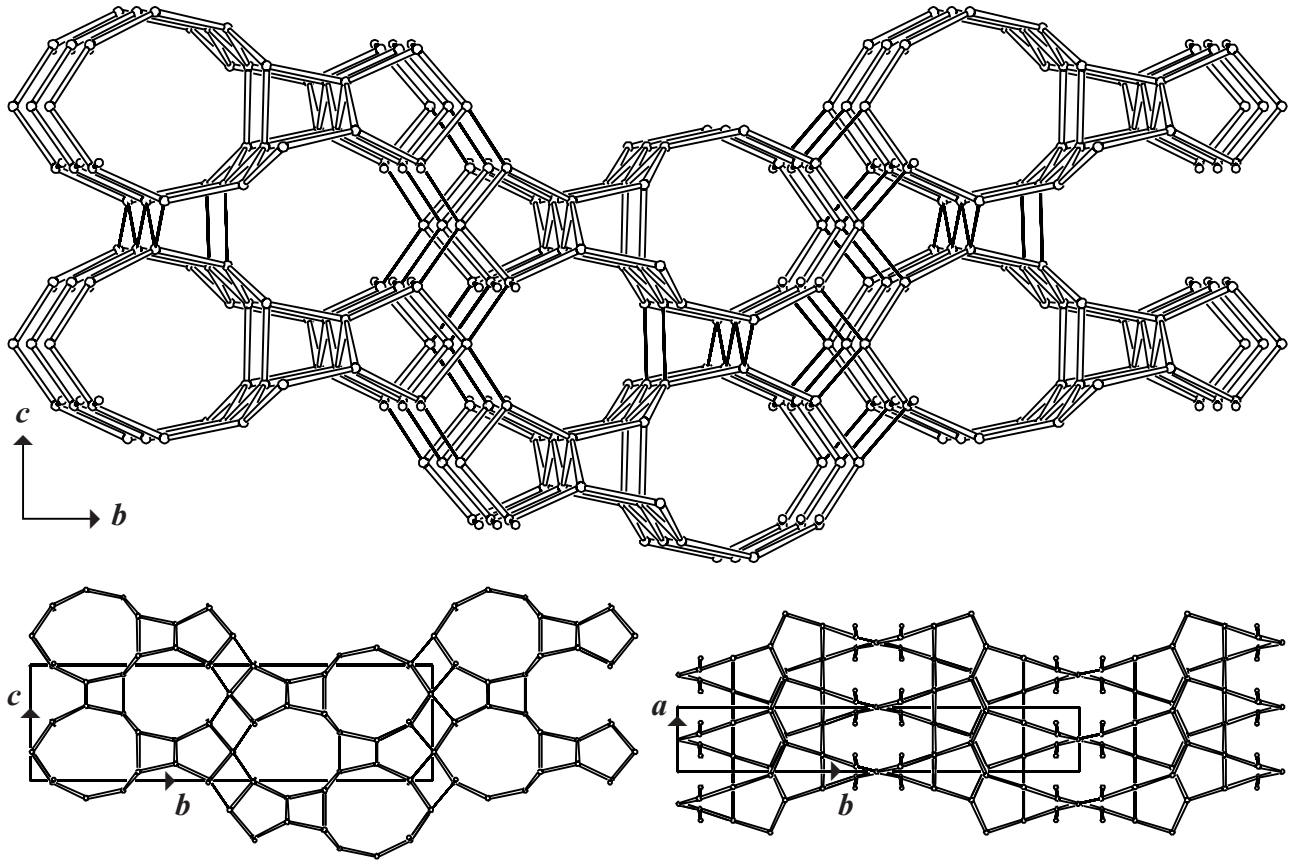
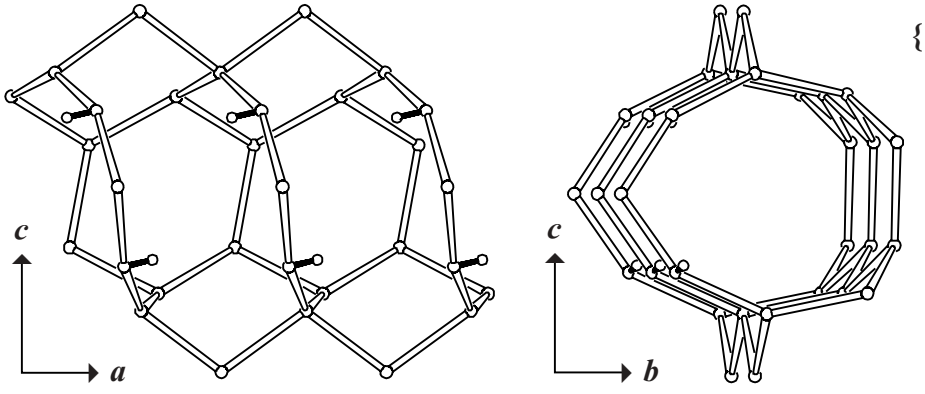


Figure 2. Connection mode in **-CHI** viewed along ***a*** (top), and parallel projection of the unit cell content along ***a*** (bottom left), and along ***c*** (bottom right).

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

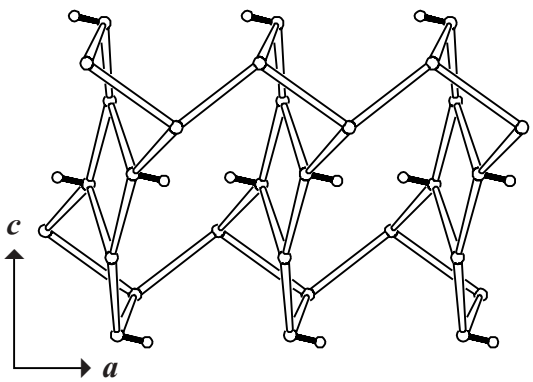
4. Channels and/or cages:

The 9- ring channel, parallel to ***a***, and a second cavity are depicted in Figure 3. The **pore descriptor** is added. Fusion of the cavities is illustrated in Figure 2.



{1 [$6^3 12^1 9^{2/2}$] [100] (9-ring)}

Figure 3. 9-Ring channel in **-CHI** viewed along ***b*** (left), and along ***a*** (right). [Figure 3 is continued on next page]



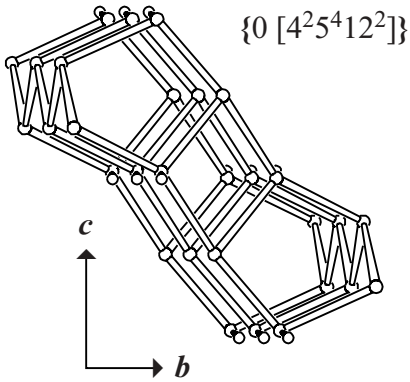


Figure 3 [Cont'd]. Second cavity viewed along ***b*** (left), and along ***a*** (right). The limiting 10-ring window is blocked by terminal oxygen atoms.

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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**).

Alternative description using (modified) 5-rings

Several framework types, like **-CHI**, 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**).