Building scheme for AEI and CHA

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 two-dimensional Periodic Building Unit (PerBU) in **AEI** and **CHA** is the double 6-ring layer depicted in Figure 1. Double 6-rings (one in bold; built from two 6-rings or two 4-2 units or three 4-rings), related by translations along the diagonals, are connected into the **xy** layer through 4-rings (see also **alternative description** of PerBU in **AEI**).

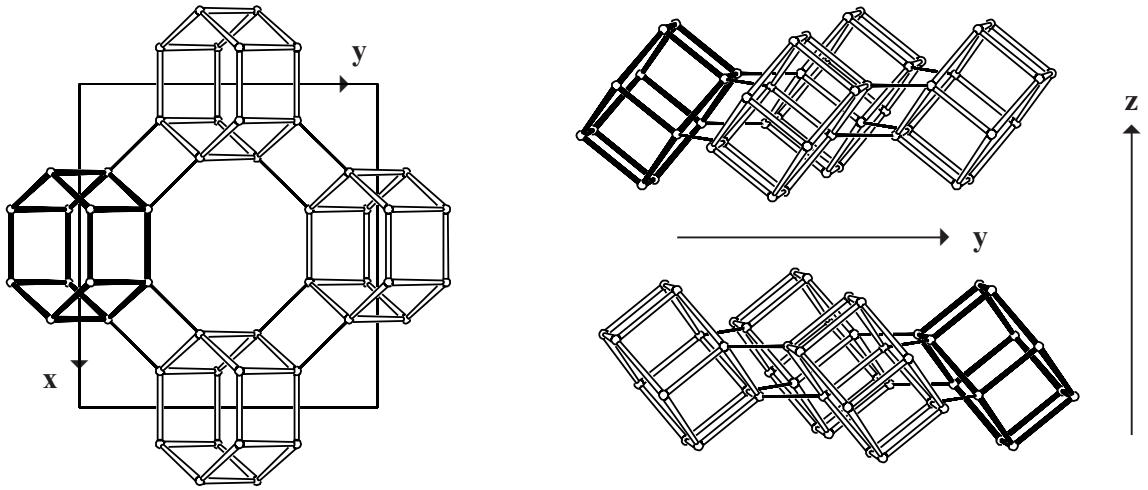

Figure 1. PerBU viewed along **z** (left) and along **x** (right). The layers, depicted top right and bottom right, are identical and related by a rotation of 180º about **z**.

2. Connection mode:

Neighboring PerBUs can be connected along the plane normal **z** through 4-rings in two different ways: (**1**): neighboring PerBUs are related by a pure translation along the plane normal;
(**2**): neighboring PerBUs are related by a rotation of 180º about the plane normal.

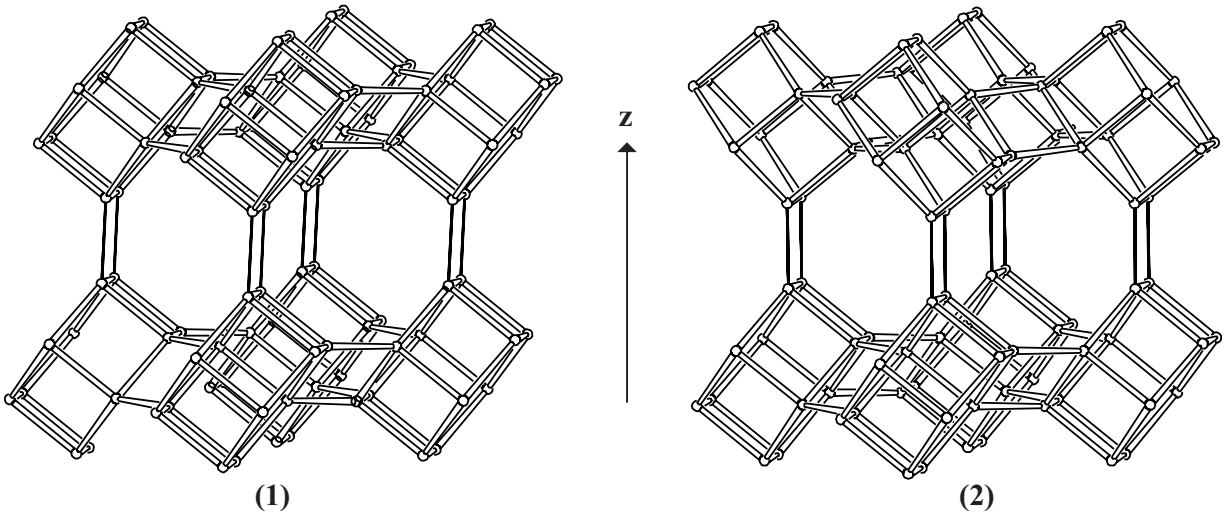

Figure 2. Connection mode **(1)** in **CHA** (left) and connection mode **(2)** in **AEI** viewed along **x**.

3. Projections of the unit cell content:

Pure **CHA** and **AEI** are obtained when neighboring PerBUs are exclusively related along the plane normal **z** by translation or by a rotation (over 180º), respectively. The projections of the unit cell content are shown in Figure 3.

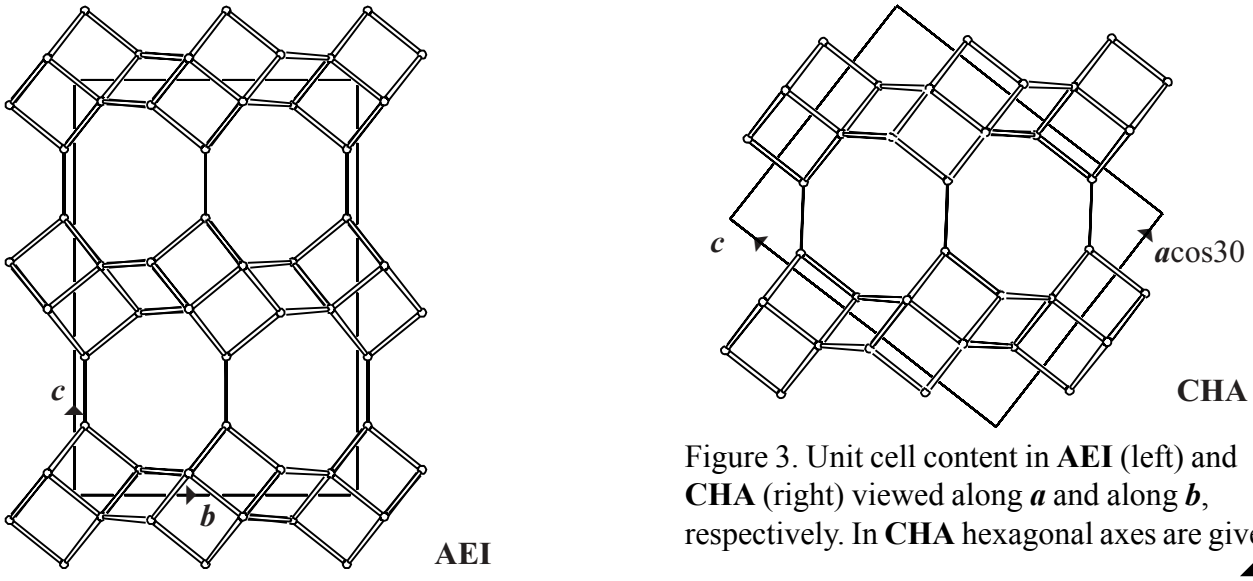

Figure 3. Unit cell content in **AEI** (left) and **CHA** (right) viewed along ***a*** and along ***b***, respectively. In **CHA** hexagonal axes are given.

4. Channels and/or cages:

There are channels parallel to [001] and [100] and [110]. The channel intersections, or the ***chab***- and ***aei***-cavities, are depicted in Figure 4. The three-dimensional channel system is obtained by connecting the cavities through common 8-rings and double 6-rings as illustrated in Figure 5 for **AEI** and in Figure 4 of the alternative building scheme for **CHA** (see also **Alternative description**).

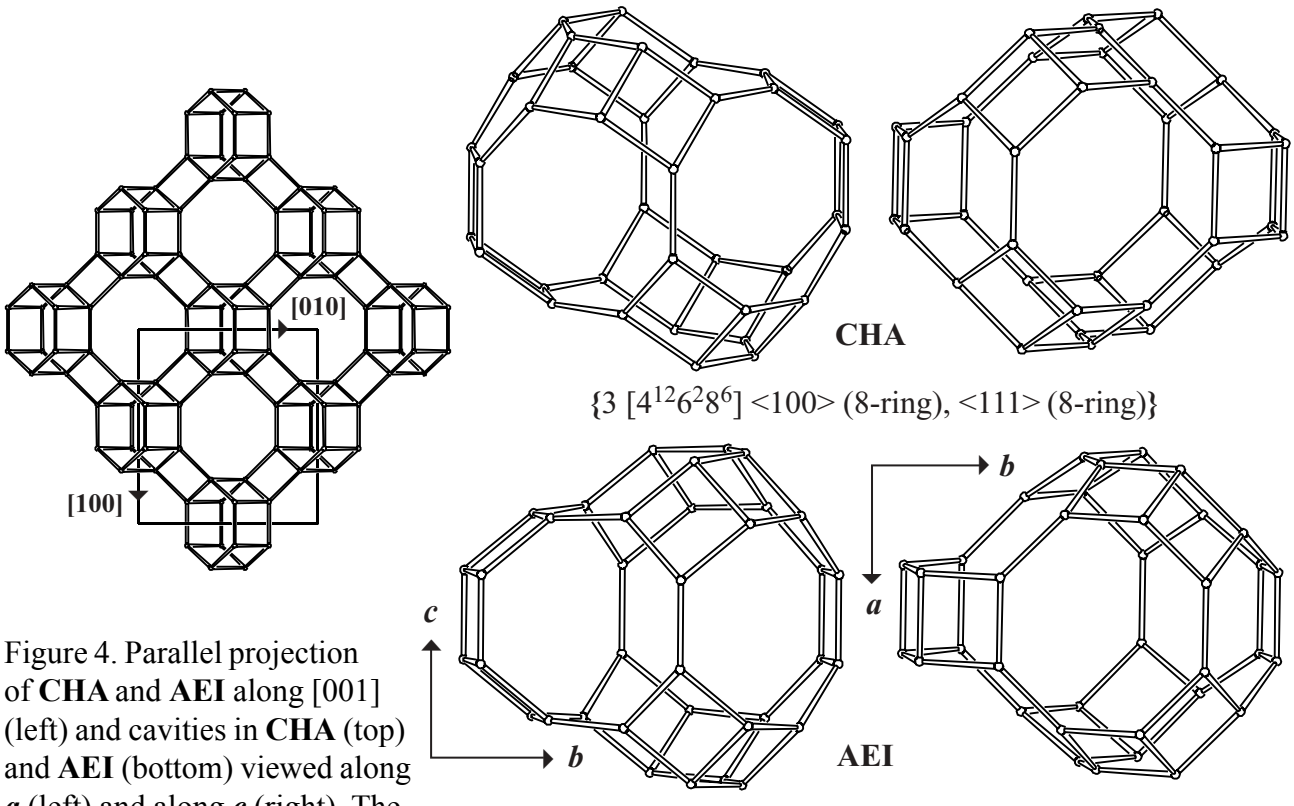

Figure 4. Parallel projection of **CHA** and **AEI** along [001] (left) and cavities in **CHA** (top) and **AEI** (bottom) viewed along ***a*** (left) and along ***c*** (right). The **pore descriptor** is added.

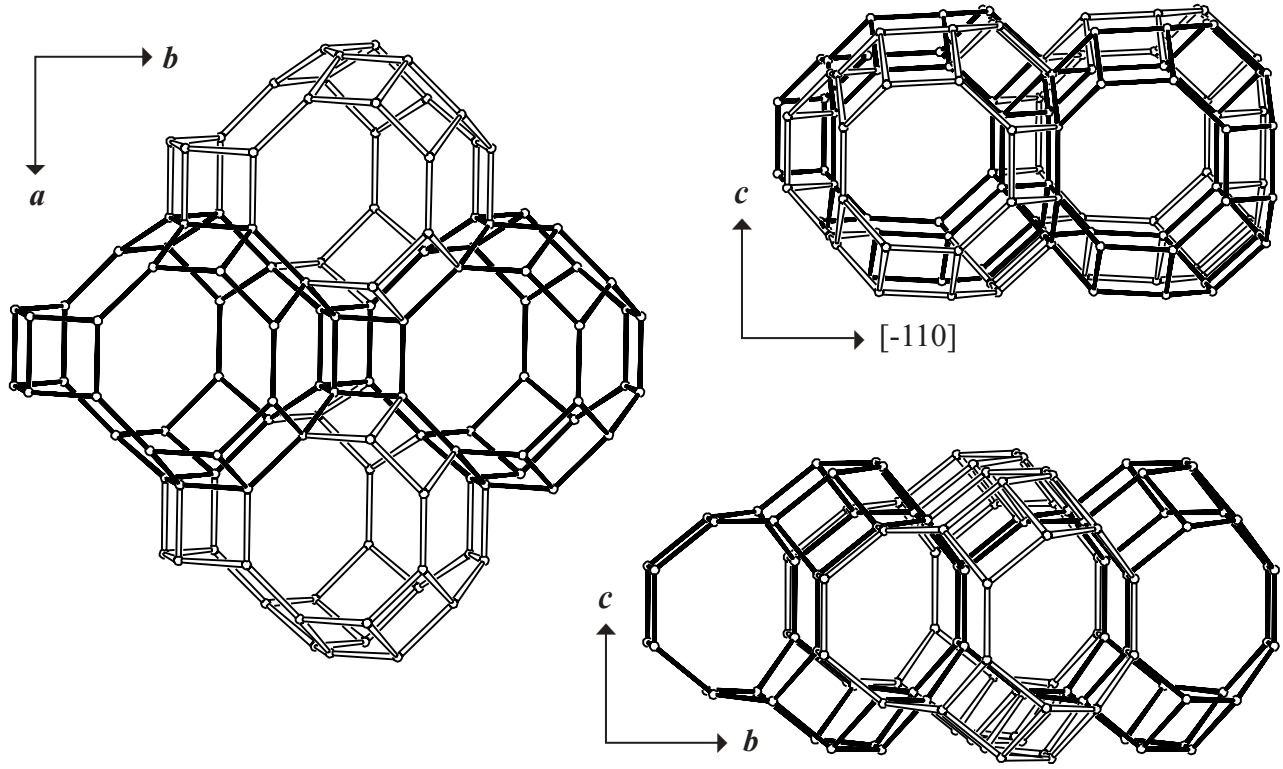

Figure5 (a): Fusion of cavities in **AEI** in the ***ab*** plane (left). 8-Ring channels viewed along [110] (top right) and along ***a*** (bottom right).

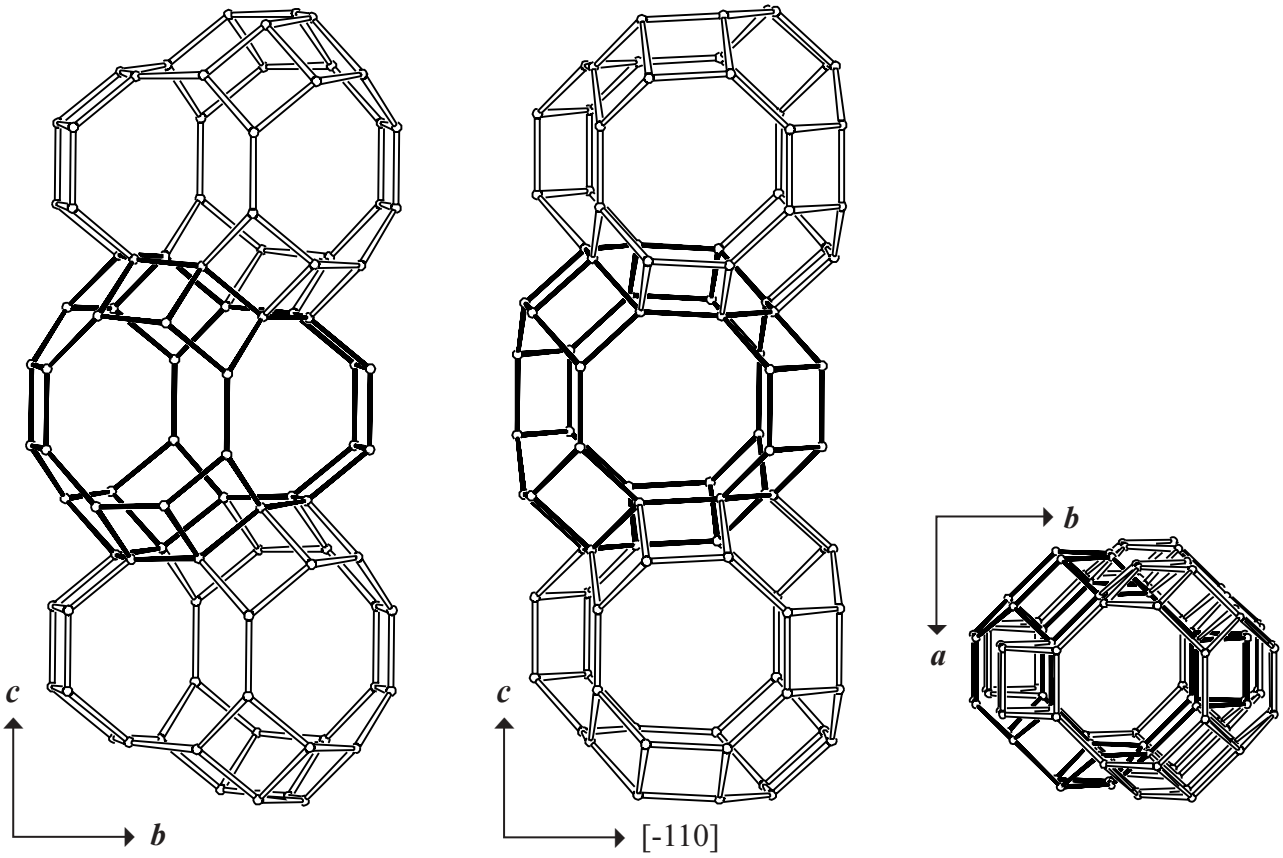

Figure5 (b): Fusion of cavities in **AEI** along ***c*** (left). 8-Ring channels viewed along [110] (middle) and along ***c*** (right).

5. Supplementary information:

Other framework types containing (modified) double 6-rings (D6Rs)
Several other framework types can be built using (modified) D6Rs.
In the **INTRO** pages links are given to descriptions of other framework types containing (modified) D6Rs (choose: **Double 6-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 7).**

Alternative description of* CHA *using a hexagonal array of non-connected 6-rings
A large number of framework types, like **CHA**, can be constructed using a hexagonal array of non-connected 6-rings as PerBU. They all belong to the ABC-6 family. In these framework types the unit cell dimension along the hexagonal axis is ≈(n*)2.55 Å where n is equal to the number of PerBUs that are connected along the hexagonal axis.
In the **INTRO** pages links are given to detailed descriptions of framework types belonging to the ABC-6 family (choose: **ABC-6 family**).

Alternative description of* AEI *using another PerBU of double 6-rings
The alternative PerBU (see Figure 6) is identical to a diagonal layer in the **AEI** framework. The D6Rs in the diagonal layer are related by a rotation of 180º about ***c*** and by pure translations along [110]. This PerBU is equal to the ***ac***-layer in **SAV**. The framework types **AEI** and **SAV** can be obtained when neighboring PerBUs are exclusively related by translation along the plane normal [1-10] (**AEI**) or by a rotation of 180º about this plane normal (**SAV**) as shown in Figure 6.

▲

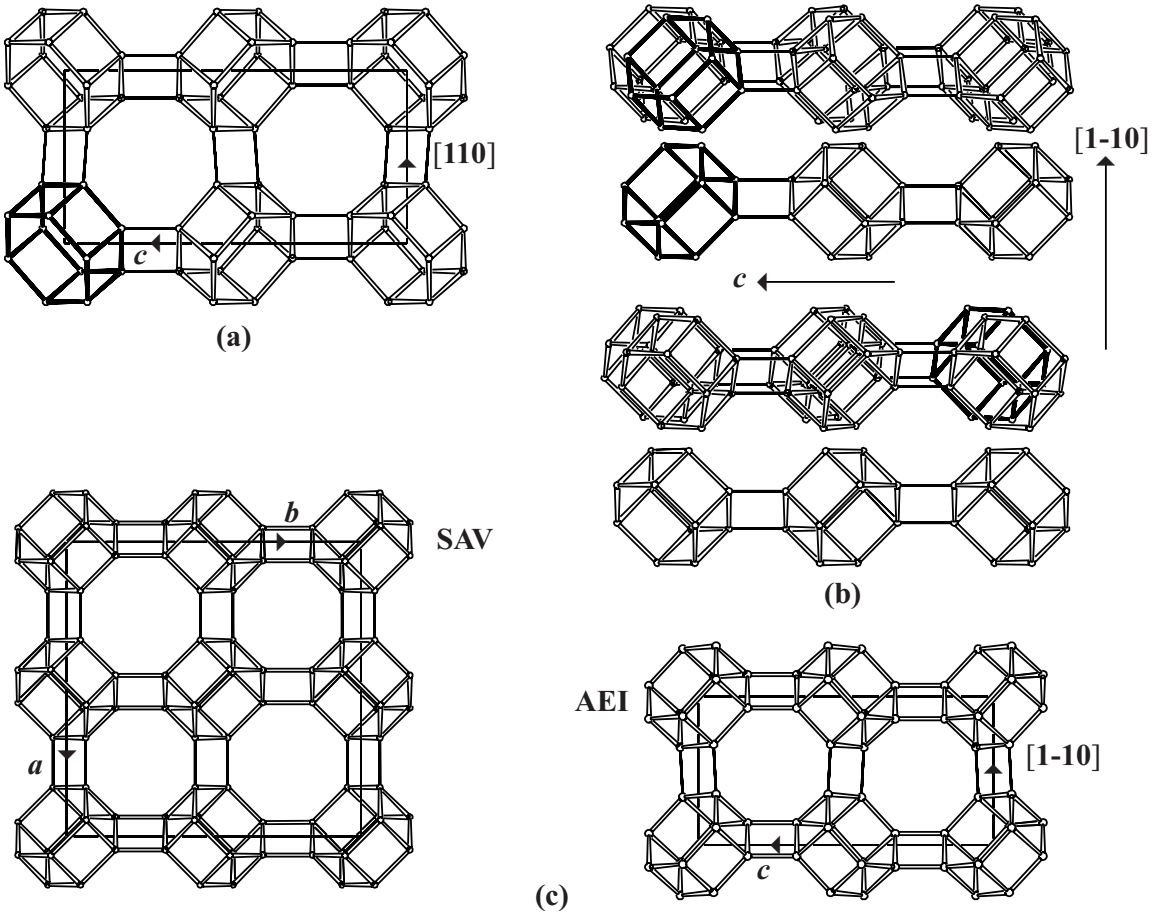

Figure 6. (a): PerBU in **AEI** and **SAV** seen along the plane normal [1-10]; (b): The two PerBUs, viewed along [110] in perspective view (top) and in parallel projection (bottom), are identical and are related by a rotation of 180º about [1-10]; (c): Projections of the cell content in **SAV** and **AEI**.