Building scheme for KFI and SAV

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 **KFI** and **SAV** is the double 6-ring layer depicted in Figure 1. Double 6-rings (D6Rs; one in bold, built from two 6-rings, three 4-rings or two 4-2 units), related by rotations of 180º about **x** and **y**, are connected into the **xy** layer through 4-rings (see also **alternative description** of PerBU in **SAV**).

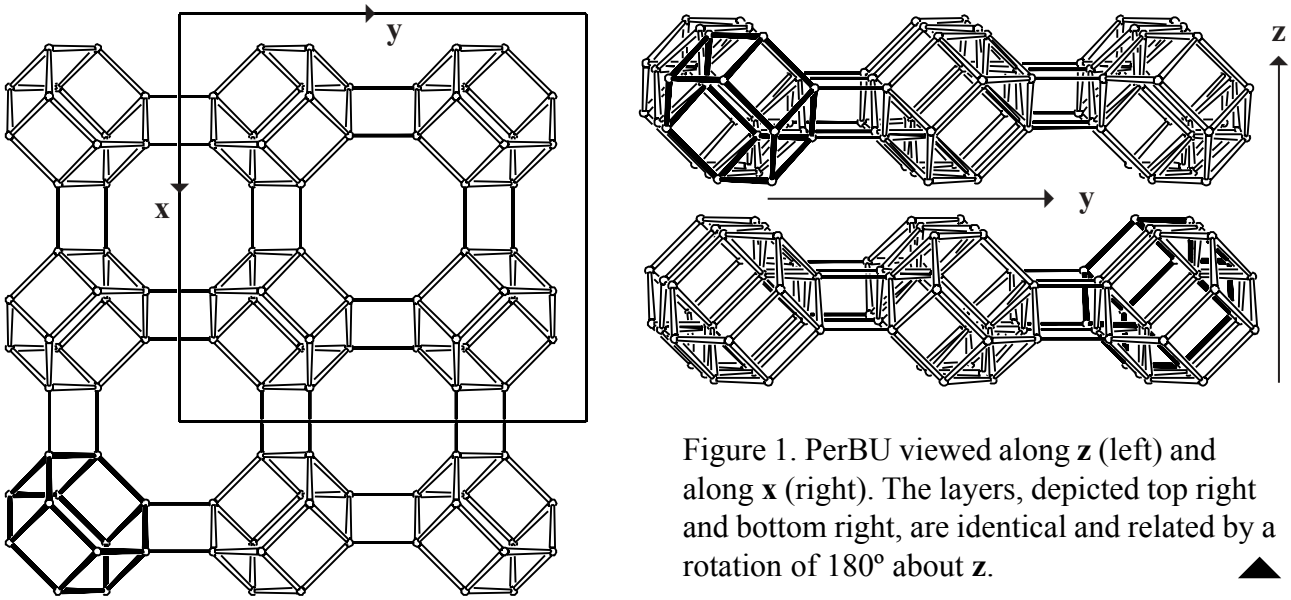


Figure 1. PerBU viewed along **z** (left) and along **x** (right). The layers, depicted top right and bottom right, are identical and related by a rotation of 180º about **z**.

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.

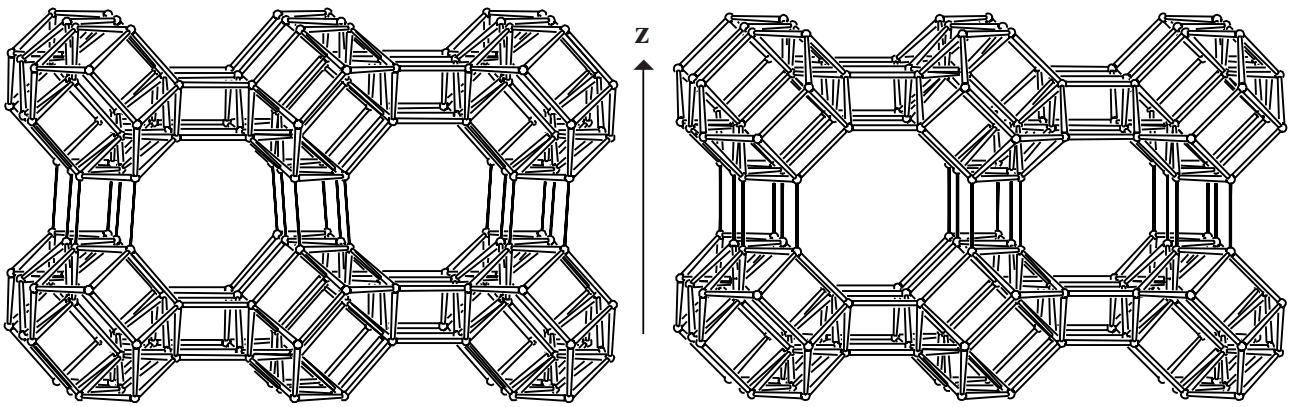


Figure 2. Connection mode **(1)** in **SAV** (left) and connection mode **(2)** in **KFI** viewed along **x**.

3. Projections of the unit cell content:

Pure **SAV** and **KFI** 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.

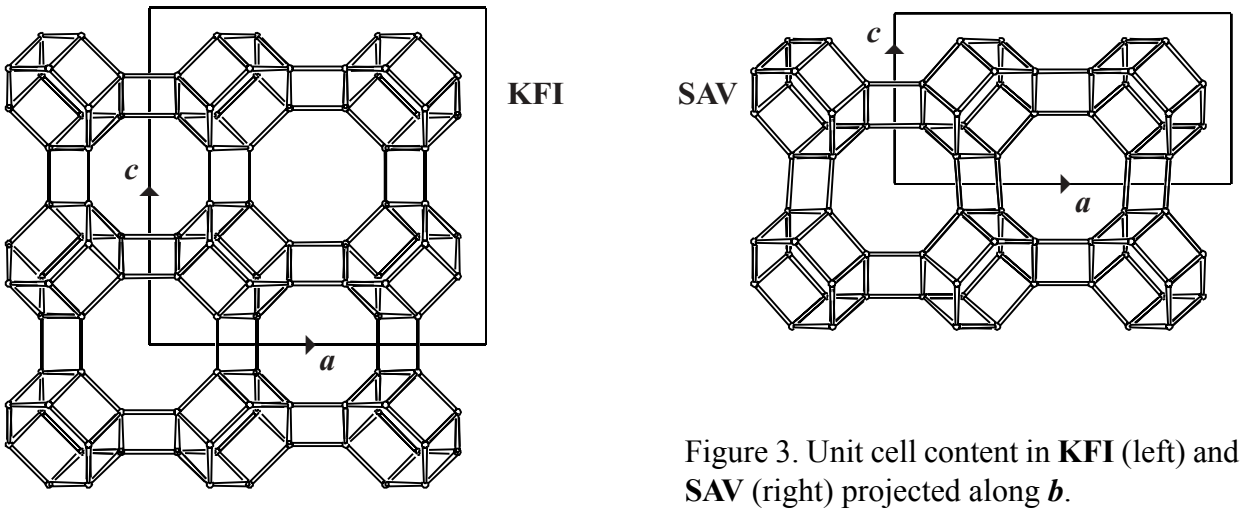
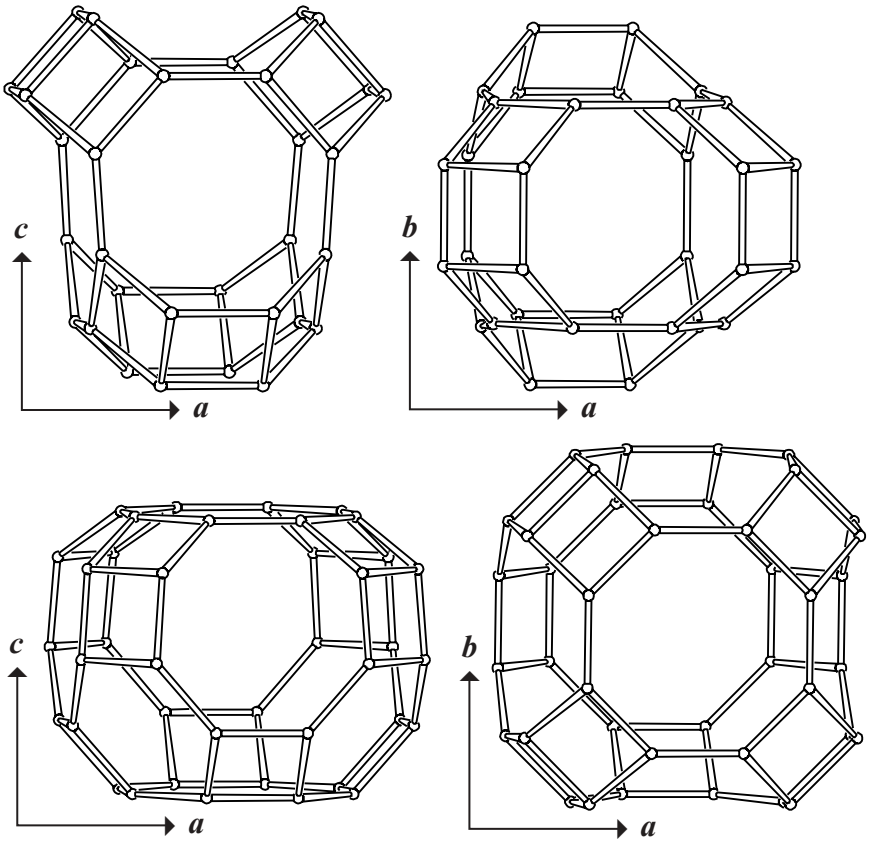


Figure 3. Unit cell content in **KFI** (left) and in **SAV** (right) projected along ***b***.

4. Channels and/or cages:

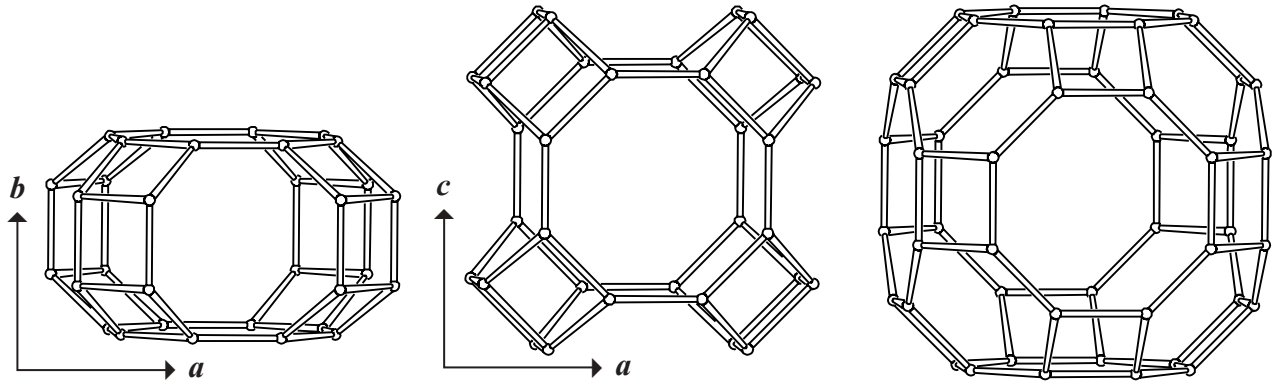
There are 8-ring channels parallel to the cell axes. The channel intersections, the ***merl***- and α-cavities in **KFI** and the type 1 and type 2 cavities in **SAV**, are depicted in Figure 4. A three-dimensional channel system is obtained by connecting the cavities through common 8-rings, double 6-rings and 4-rings as illustrated in Figure 5.



***Intersection* 1** in **SAV**:
Pore descriptor
{3 [$4^{12}8^6$] <100> (8-ring), [001] (8-ring)}

***intersection* 2 in SAV**:
Pore descriptor
{3 [$4^{12}6^48^6$] <100> (8-ring), [001] (8-ring)}

Figure 4. Two types of intersections of channels in **SAV** viewed along ***c*** (left) and along ***b*** (right). The **pore descriptor** is added.
[Figure 4 is continued on next page]



Pore descriptor ***merl*** cavity in **KFI**:
{3 [$4^{12}8^6$] <100> (8-ring)}

Pore descriptor α–cavity in **KFI**:
{3 [$4^{12}6^88^6$] <100> (8-ring)}

Figure 4 [Cont'd]. Intersection of channels in cubic **KFI**. ***merl***-Cavity viewed along ***c*** (left) and along ***b*** (right) and α-cavity (composed of six 8-rings) viewed along ***c***.

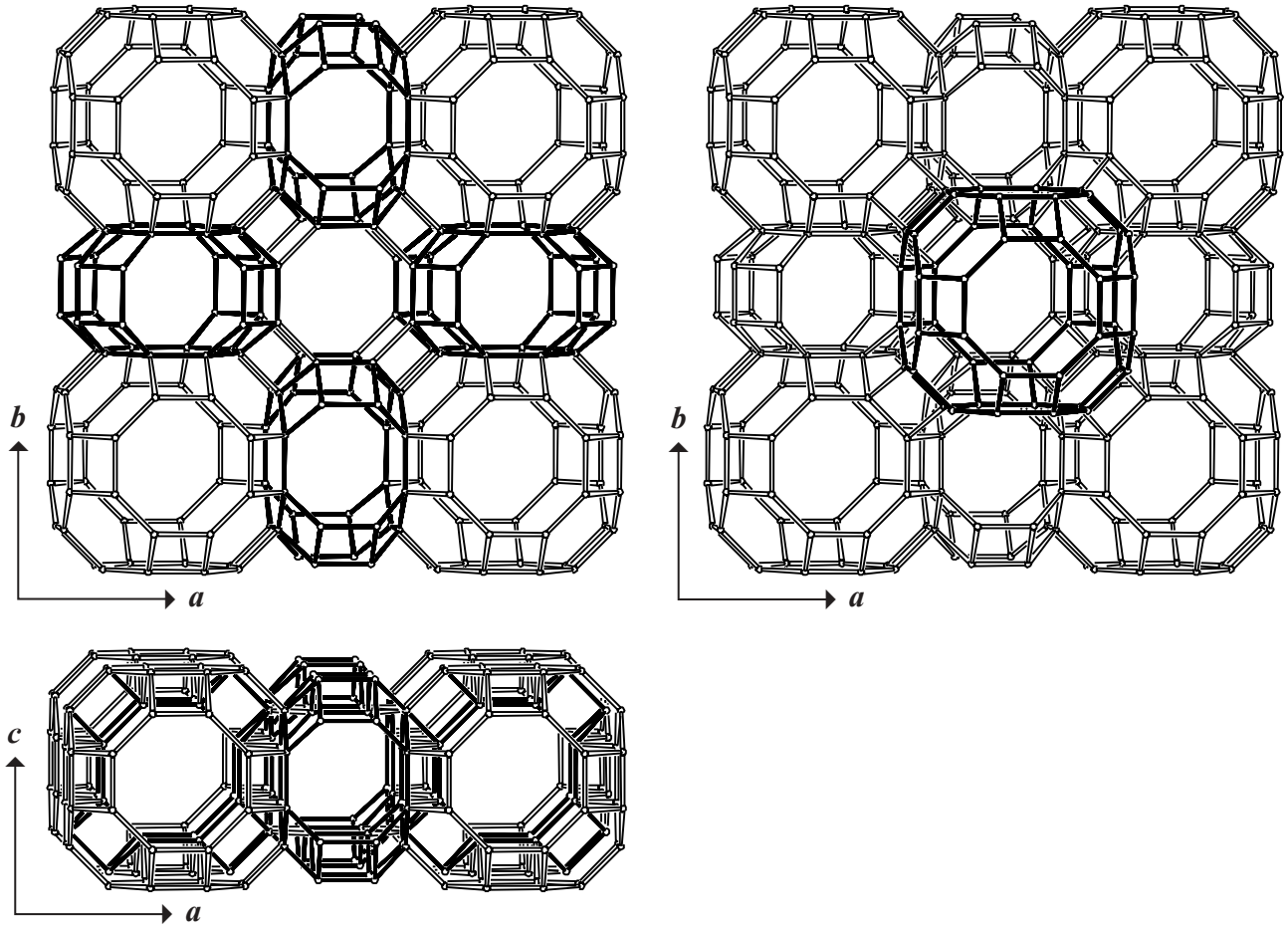


Figure5. Fusion of cavities in cubic **KFI**. The ***ab*** plane (top left); 8-ring channel(s) viewed along ***b*** (bottom left); and fusion of α-cavities along ***c*** viewed along ***c***; ***merl*** cavities are formed (top right). From this drawing it can be seen that **KFI** can as well be built using complete α-cavities (See **Alternative description** of **KFI**) or (more difficult to see) using 6-2 units. [Figure 5 is continued on next page]

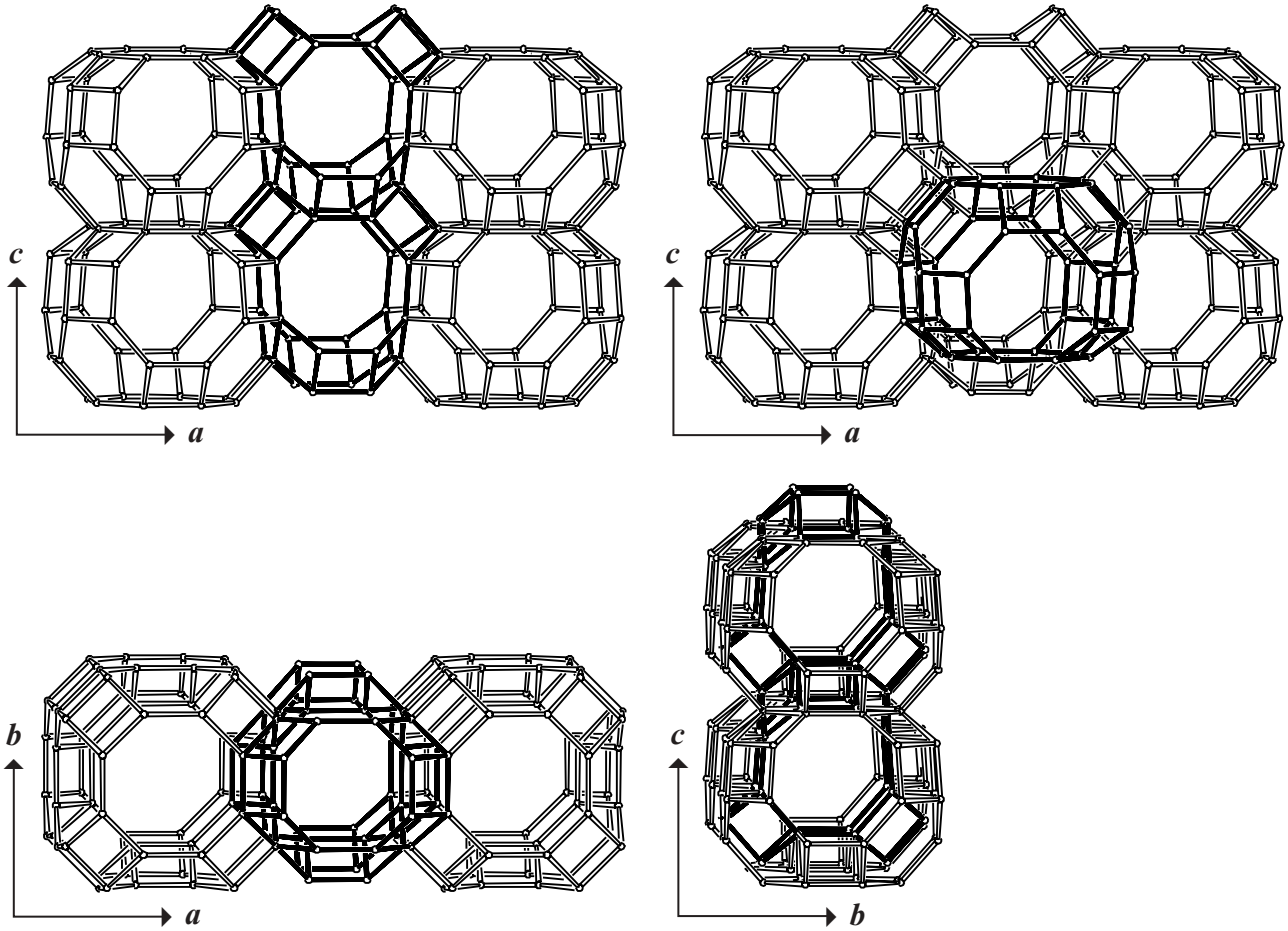


Figure5 [Cont'd]. Fusion of cavities in tetragonal **SAV**: the ***ac*** plane (top left); two types of 8-ring channels viewed along ***c*** (bottom left); 8-ring channels viewed along ***a*** (bottom right), and fusion of cavities along ***b*** viewed along ***b*** (top right).

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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* KFI *using (modified) cavities
Several framework types, like **KFI**, can be built using (modified) cavities (see Figure 4).
In the **INTRO** pages links are given to a detailed description of a sub-set of framework types that contain (modified) cavities (choose: **Cages**). There is also a link provided to a summary of the PerBUs used in the building schemes of these framework types (choose: **Appendix**; **Figure 11**).

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

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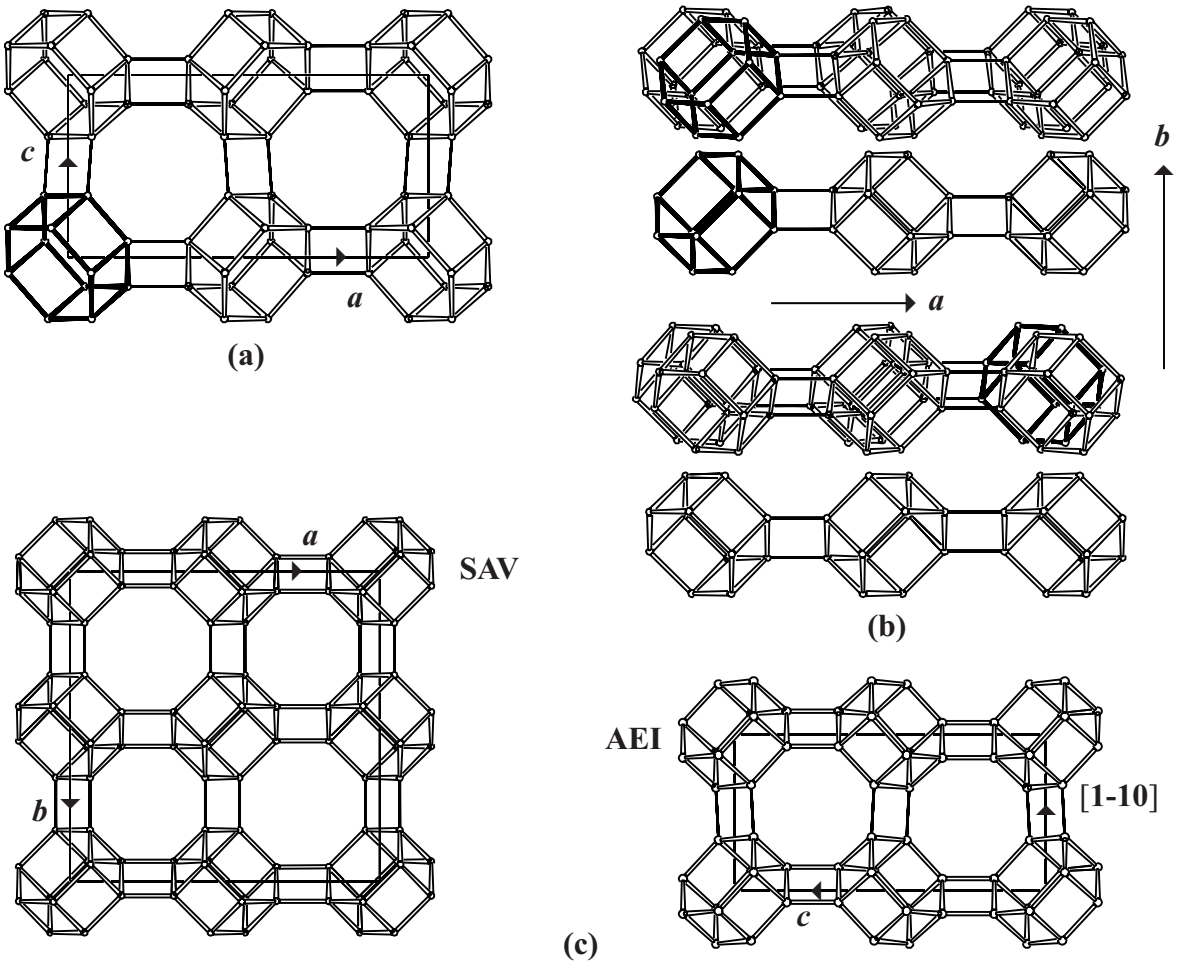

Figure 6. (a): PerBU in **AEI** and **SAV** seen along the plane normal ***b***; (b): The two PerBUs, viewed along ***c*** in perspective view (top) and in parallel projection (bottom), are identical and are related by a rotation of 180º about ***b***; (c): Projections of the cell content in **SAV**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