

The KFI/SAV Family

1. The Periodic Building Unit (PerBU) -
2. Type of Faulting -
3. The Layer Symmetry
4. Connectivity Pattern of the PerBU -
5. The Simplest Ordered End-Members
6. Disordered Materials Synthesized to Date -
7. Supplementary Information -
8. References

1. The Periodic Building Unit (PerBU) equals the layer shown in Figure 1:

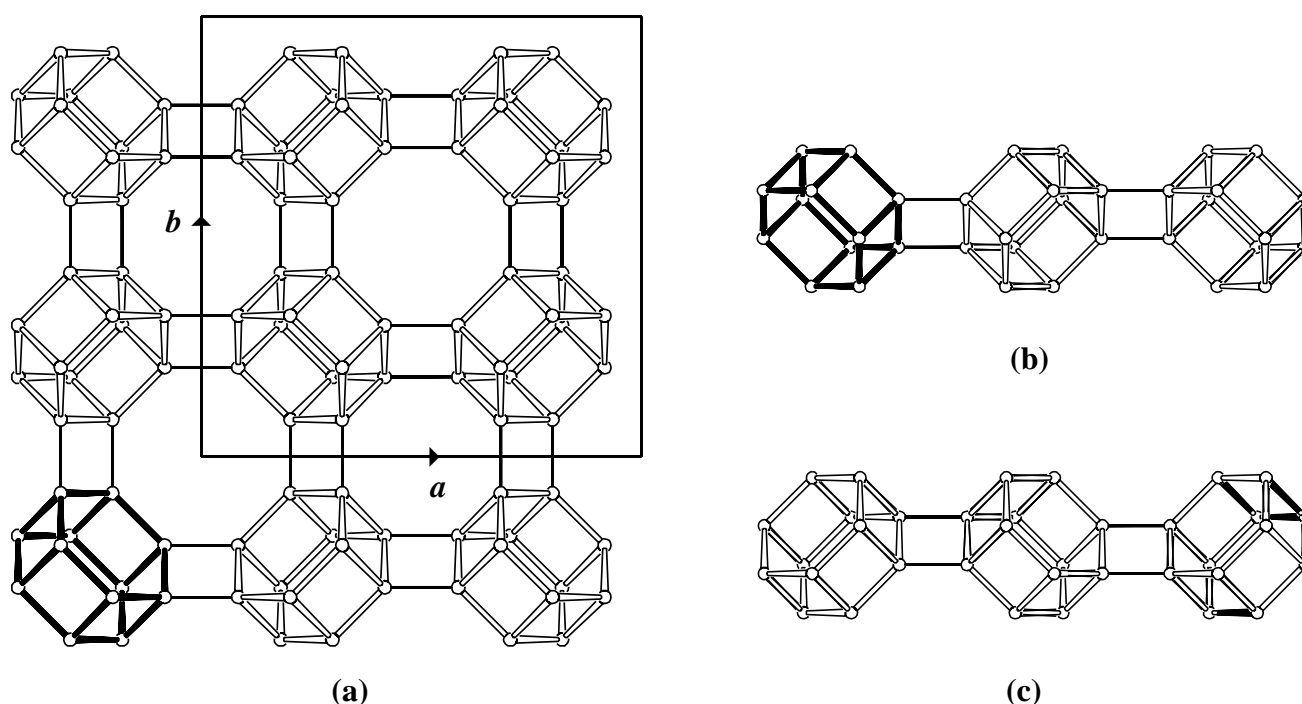


Figure 1: The PerBU of the KFI/SAV family of zeolite frameworks shown parallel to c (a) and perpendicular to c (b and c)

The PerBU of the KFI/SAV family of framework types, the tetragonal ab layer, is composed of double T6-rings (D6R's; Fig.1 in bold). D6R's, related by rotations of 180° about a and b (or by mirror planes perpendicular to a and b) are connected along a and b , respectively, through T4-rings as shown in Figure 1. Projections of the PerBU along $[001]$ (Fig.1a), $[010]$ (Fig.1b and 1c) are shown. The layers, depicted in Figure 1b and 1c are identical and related by a 180° rotation about the plane normal, c , or by a mirror operation perpendicular to c . [Compare this ab layer with the D6R layers in the AEI/CHA and AEI/SAV families].

2. **Type of Faulting:** 1-dimensional stacking disorder of the PerBU's along c . ▲

3. The Layer Symmetry: the plane space group of the PerBU is $P(4)mm$. ▲

4. Connectivity Pattern of the PerBU:

Neighbouring PerBU's are connected along c through T4-rings in two different ways:

(a): neighbouring PerBU's are related by pure translations along c . The resulting connectivity exhibits inversion symmetry (**i**:**o**) between successive layers.

(b): neighbouring PerBU's are related by a mirror plane perpendicular to c (or by a rotation of 180° about c). The connectivity now shows mirror symmetry (**m**:**l**) between successive layers.

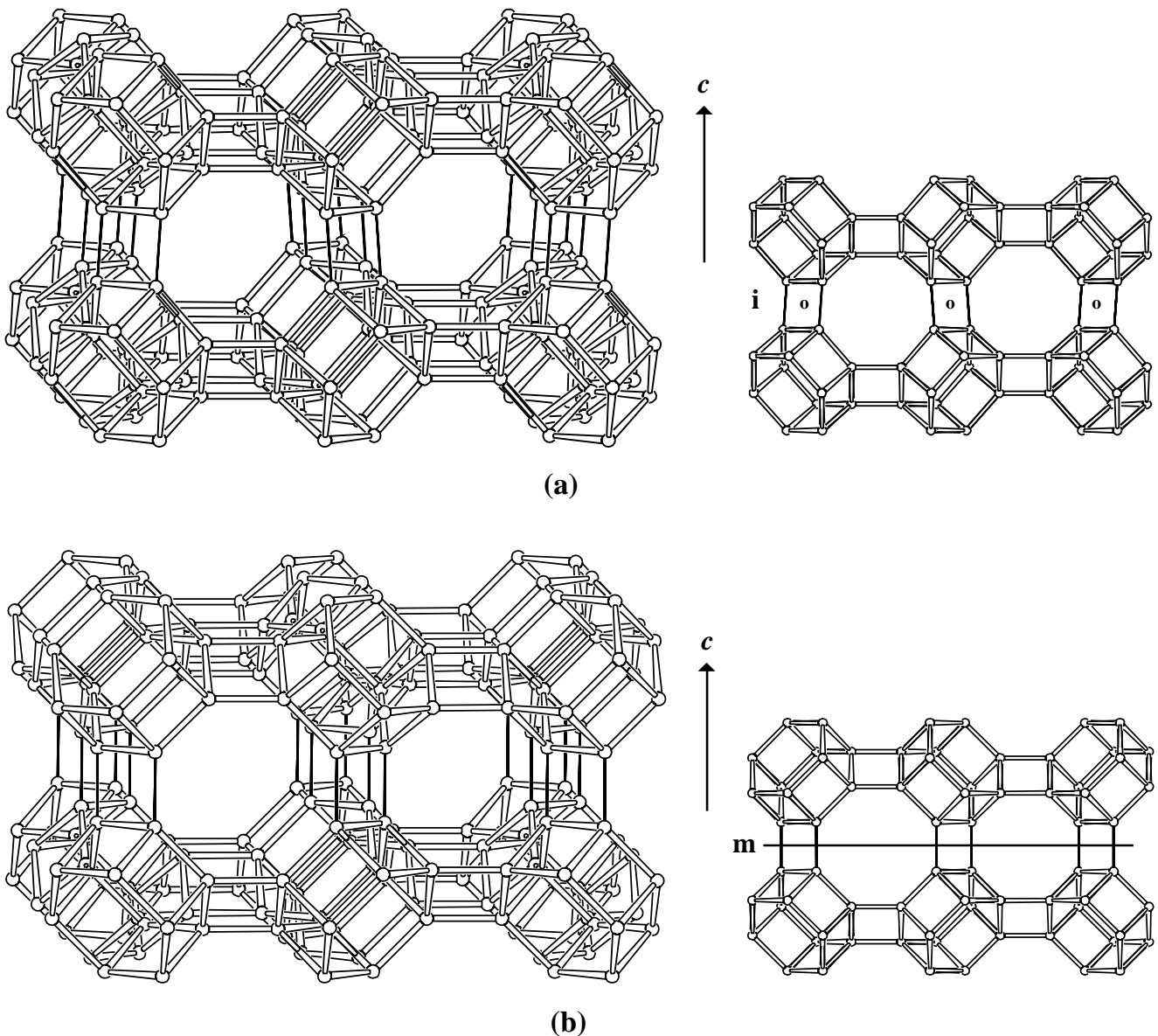


Figure 2: Perspective view (left) and parallel projection (right) along b of the connection modes **(a)** and **(b)** in the KFI/SAV family of zeolite frameworks

Once the distribution of the symmetry elements **i** and **m** between the layers stacked along $[001]$ is known, the 3-dimensional structure is defined. ▲

5. The Simplest Ordered End-Members in the KFI/SAV family are shown in Figure 3:

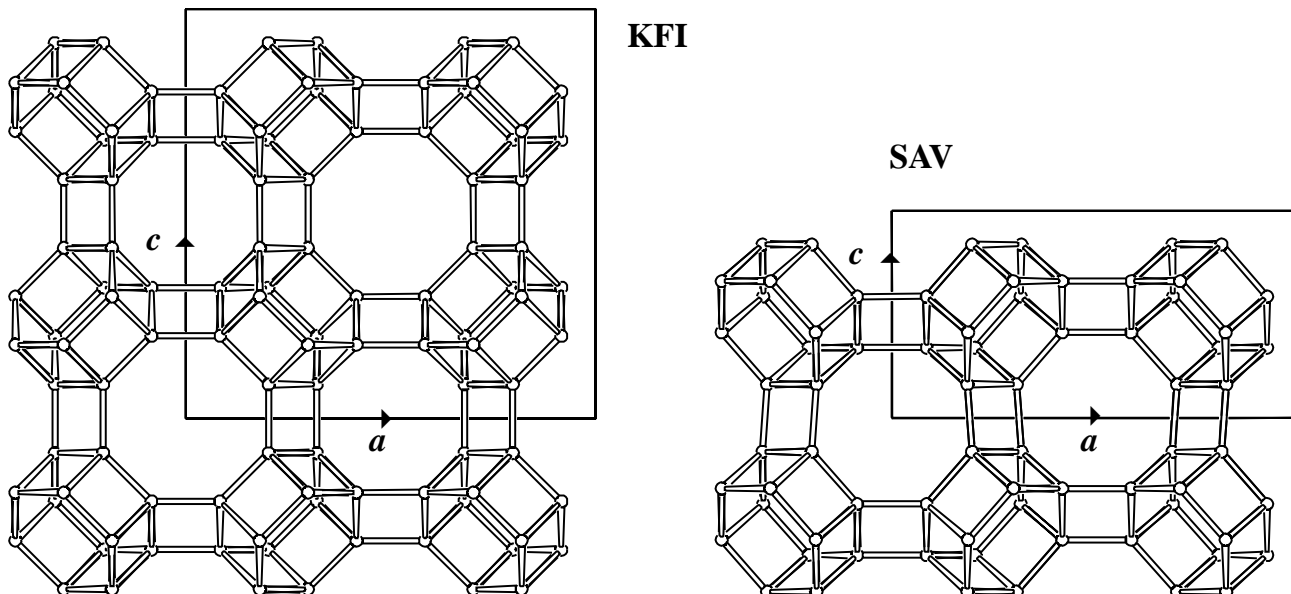


Figure 3: Projection of the unit cell content along b of the two simplest ordered end-members in the KFI/SAV family: KFI (left) and SAV (right)

Pure KFI (1) and SAV (2) are obtained when neighbouring PerBU's, stacked along c , are exclusively related by \mathbf{m} and \mathbf{i} , respectively. ▲

6. Disordered Materials Synthesized and Characterized to Date:

No disordered materials known to date.

7. Supplementary Information

7.1 Comparison with the AEI/CHA family:

The PerBU in the AEI/CHA family is composed of D6R's, related by pure translations along the diagonals in the xy plane as shown in Figure 4.

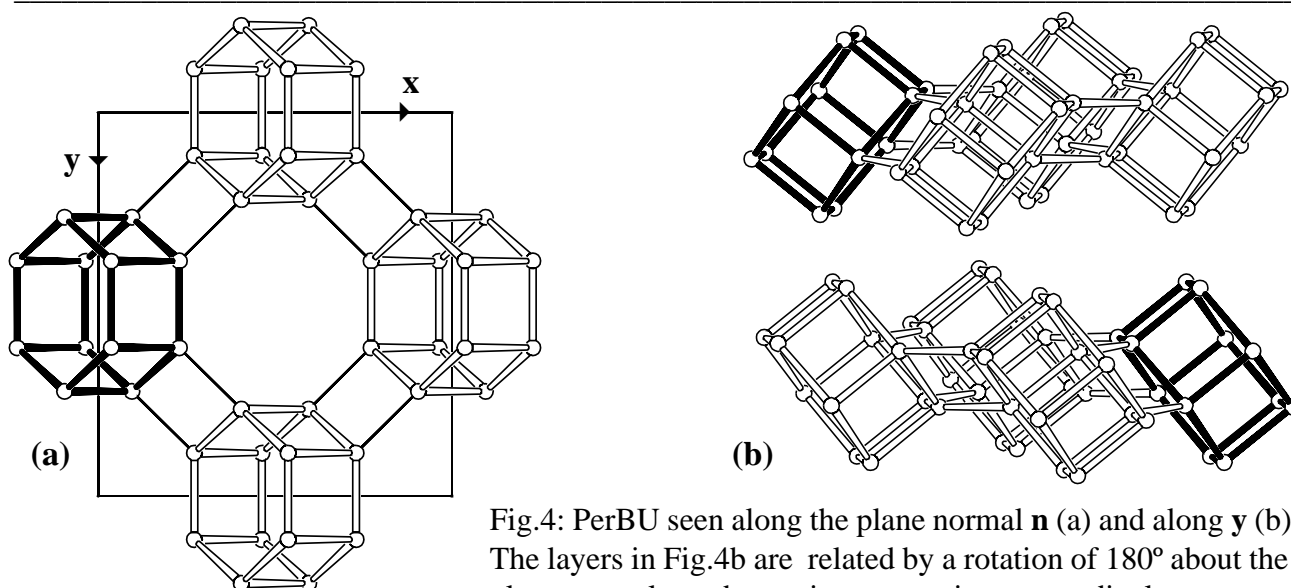


Fig.4: PerBU seen along the plane normal \mathbf{n} (a) and along y (b). The layers in Fig.4b are related by a rotation of 180° about the plane normal \mathbf{n} or by a mirror operation perpendicular to \mathbf{n}

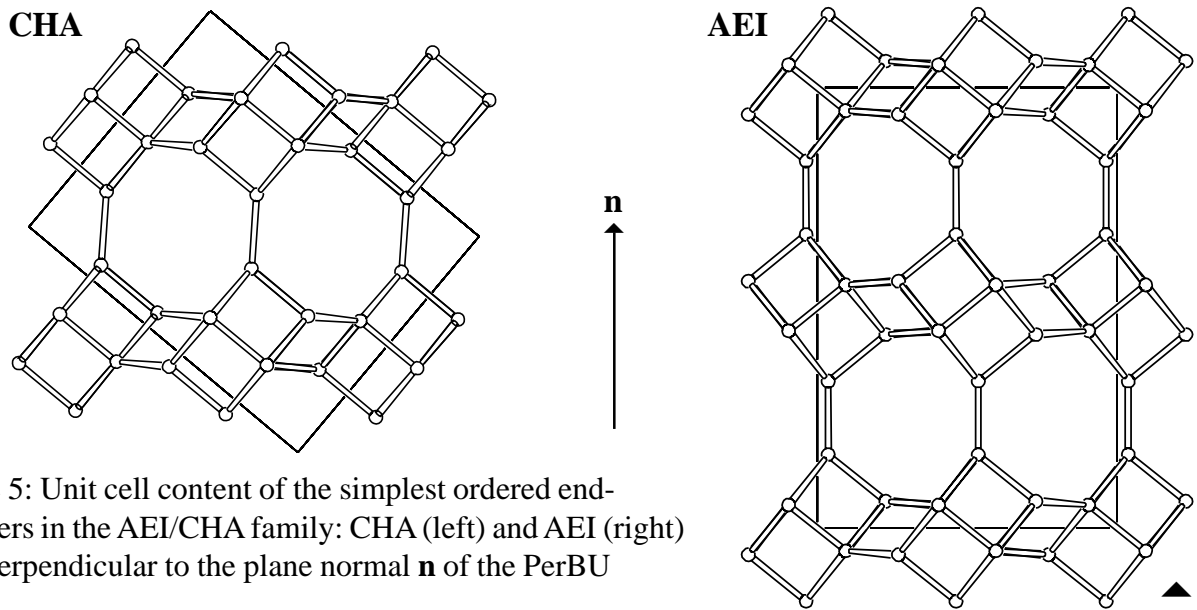


Figure 5: Unit cell content of the simplest ordered end-members in the AEI/CHA family: CHA (left) and AEI (right) seen perpendicular to the plane normal \mathbf{n} of the PerBU

For more details: see the description of the AEI/CHA family in this 'Catalog'.

7.2 Comparison with the AEI/SAV family:

The PerBU in the AEI/SAV family is composed of D6R's, related by rotations of 180° about \mathbf{x} and by pure translations along \mathbf{y} as shown in Figure 6.

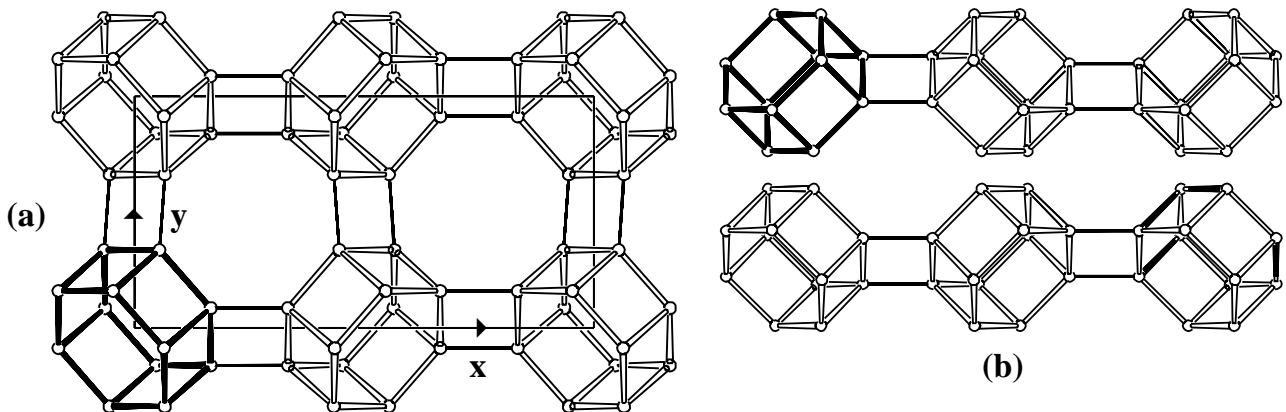


Figure 6: PerBU seen along the plane normal \mathbf{n} (a) and along \mathbf{y} (b). The layers in Figure 6b are related by a rotation of 180° about the plane normal \mathbf{n} or by a mirror operation perpendicular to \mathbf{n}

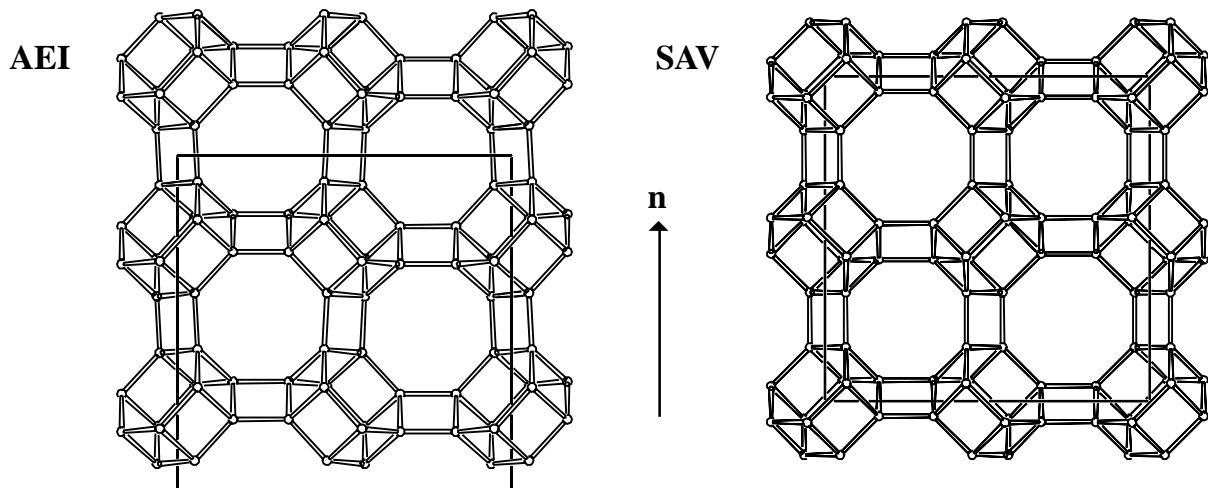


Figure 7: Unit cell content of the simplest ordered end-members in the AEI/SAV family: AEI (left) and SAV (right) seen perpendicular to the plane normal \mathbf{n} of the PerBU

For more details: see the description of the AEI/SAV family in this 'Catalog'.

8. References

- (1) W.M. Meier and G.T. Kokotailo, *Z. Kristallogr.* **121**, 211 (1965).
- (2) P.A. Wright, M.J. Maple, A.M.Z. Slawin, V. Patinec, R.A. Aitken, S. Welsh and P.A. Cox, *J. Chem. Soc., Dalton Trans.* **2000**, 1243 (2000). ▲