

The AEI/SAV family

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

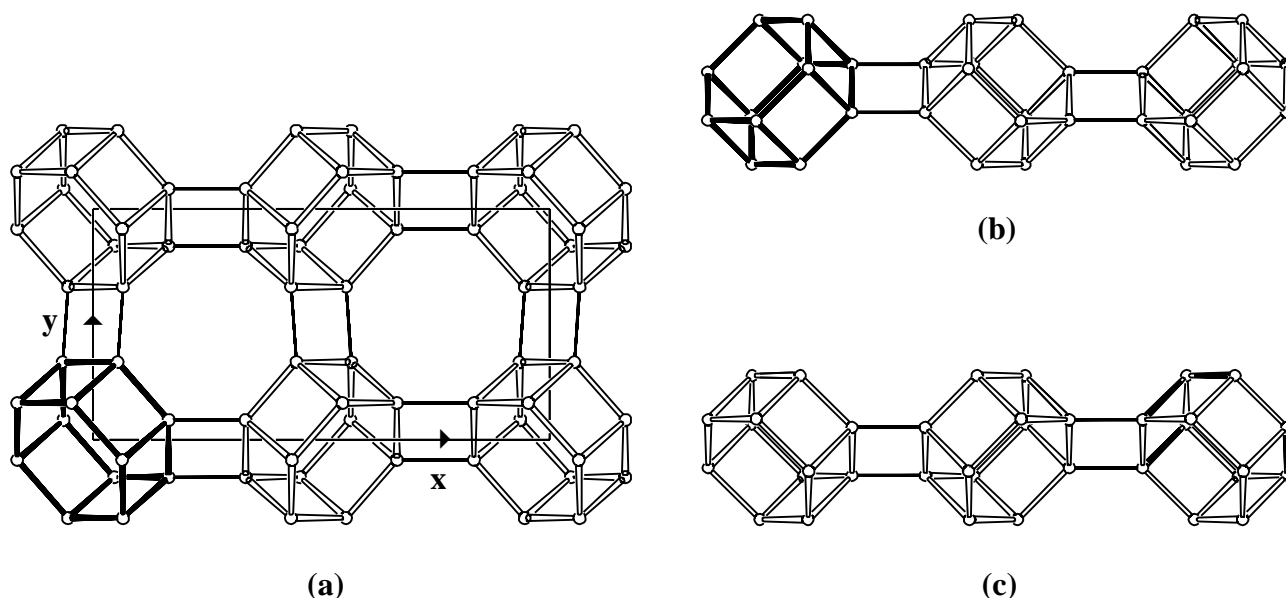


Figure 1: The PerBU of the AEI/SAV family of zeolite frameworks shown parallel to the plane normal z (a) and perpendicular to the plane normal z (b and c)

The PerBU of the AEI/SAV family of framework types is composed of double T6-rings (D6R's; Fig.1 in bold). Neighbouring D6R's, related by a rotation of 180° about x (or by a mirror plane perpendicular to x) and by a pure translation along y , are connected through T4-rings as shown in Figure 1. Projections of the PerBU along the plane normal z (Fig.1a), and along y (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 z or by a mirror operation perpendicular to z . [Compare this xy layer with the D6R layers in the AEI/CHA and KFI/SAV families].

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

3. The Layer Symmetry: the plane space group of the PerBU is $P2_1/m1$ (1). ▲

4. Connectivity Pattern of the PerBU:

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

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

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

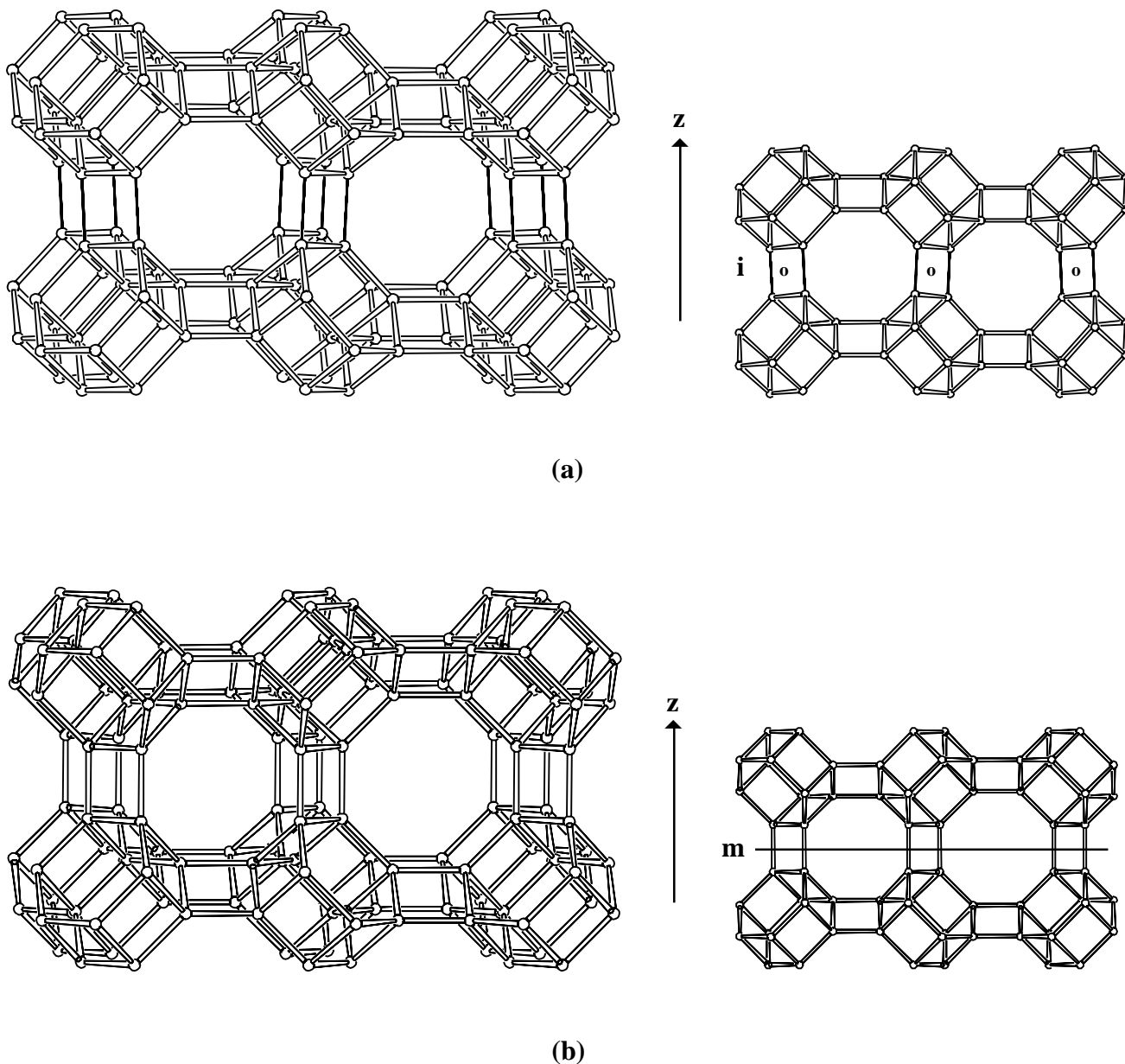


Figure 2: Perspective view (left) and parallel projection (right) along y of the connection modes (a) and (b) in the AEI/SAV family of zeolite frameworks

Once the distribution of the symmetry elements i and m between the layers stacked along z is known, the 3-dimensional structure is defined. ▲

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

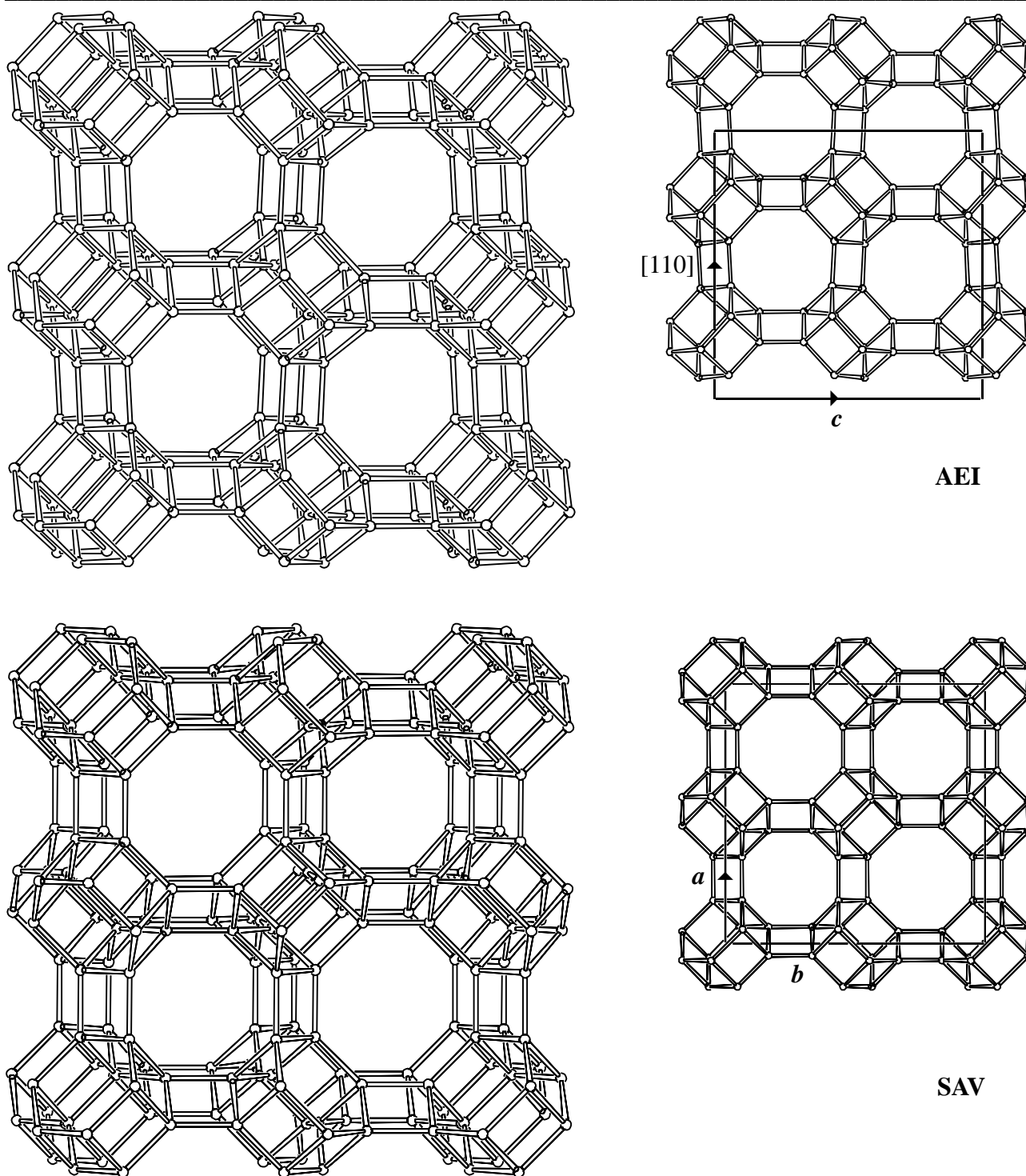


Figure 3: Cell content of AEI (top) and of SAV (bottom) seen along $[1-10]$ and $[001]$, respectively

Pure AEI (1) and SAV (2) are obtained when neighbouring PerBU's, stacked along the plane normal of the PerBU, are exclusively related by \mathbf{i} and \mathbf{m} , 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.

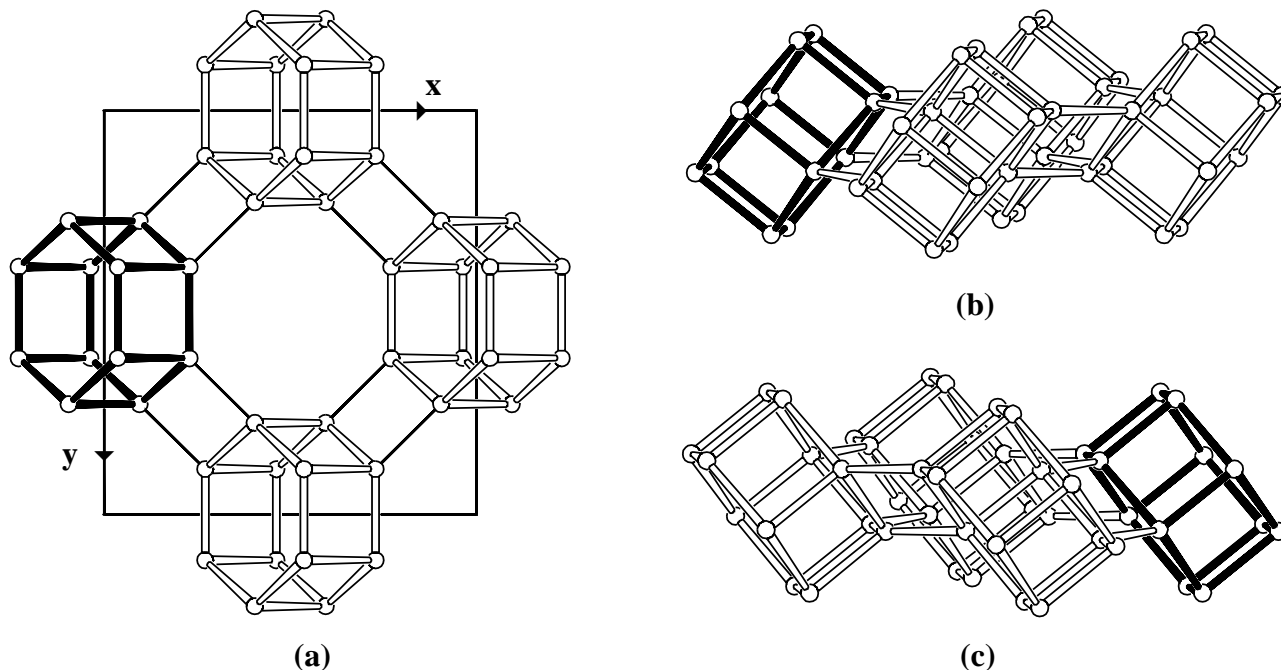


Figure 4: PerBU seen along the plane normal \mathbf{n} (a) and along \mathbf{y} (b,c). The layers, depicted in Figure 4b and 4c are identical and related by a rotation of 180° about the plane normal \mathbf{n} (or by a mirror operation perpendicular to \mathbf{n})

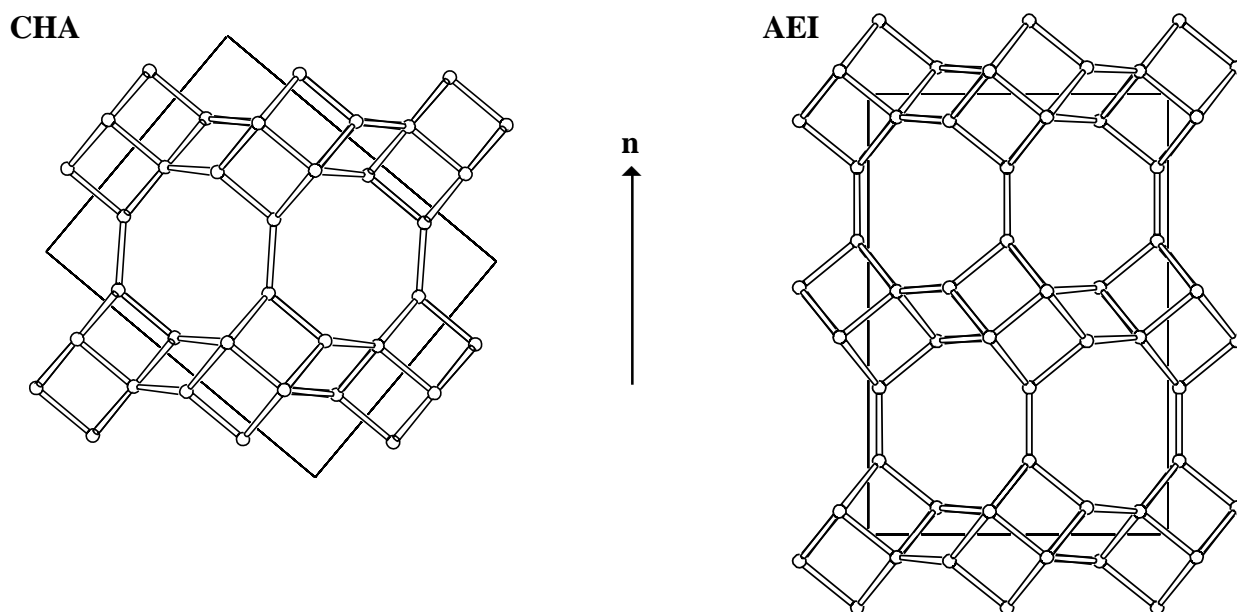


Figure 5: Unit cell content of the simplest ordered end-members in the AEI/CHA family: CHA (left) and AEI (right) seen perpendicular to the plane normal \mathbf{n} of the PerBU

7.2 Comparison with the KFI/SAV family:

The PerBU in the KFI/SAV family is the tetragonal layer composed of D6R's, related by rotations of 180° about x and y (or by mirror planes perpendicular to x and y) as shown in Figure 6.

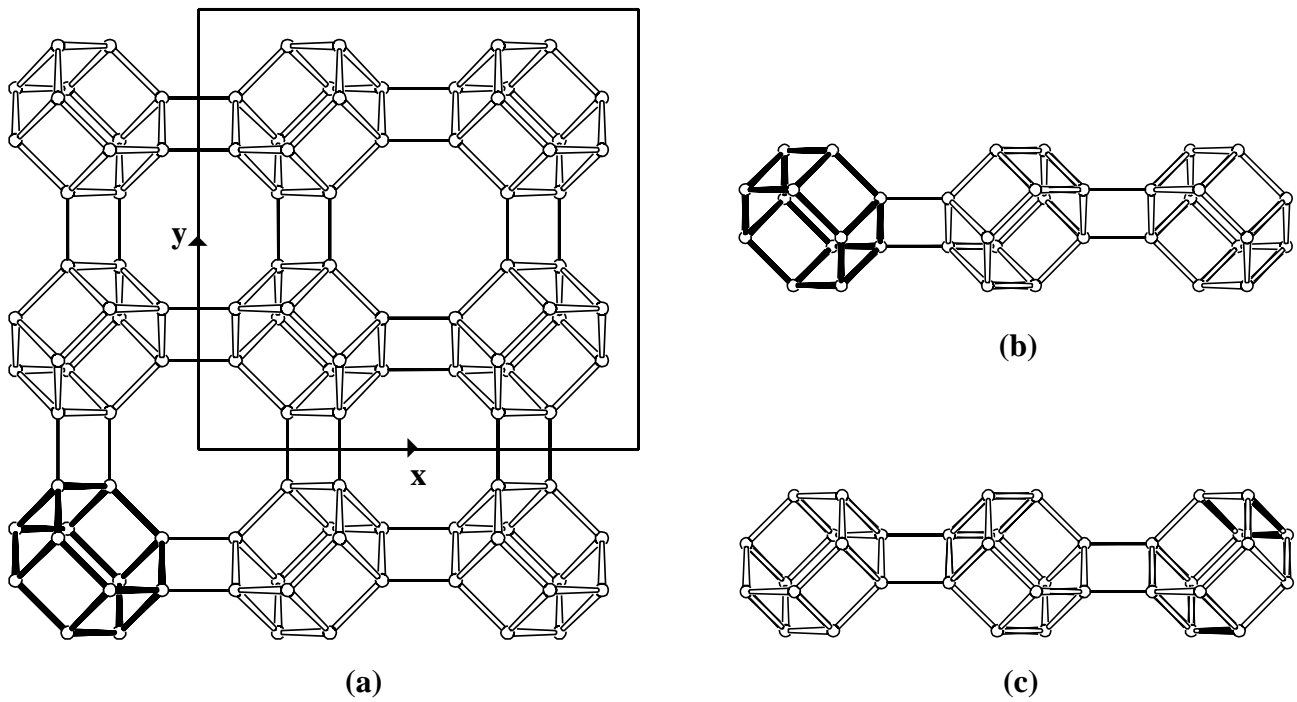


Figure 6: PerBU seen along the plane normal \mathbf{n} (a) and along y (b,c). The layers, depicted in Figure 6b and 6c are identical and related by a rotation of 180° about \mathbf{n} (or by a mirror operation perpendicular to \mathbf{n})

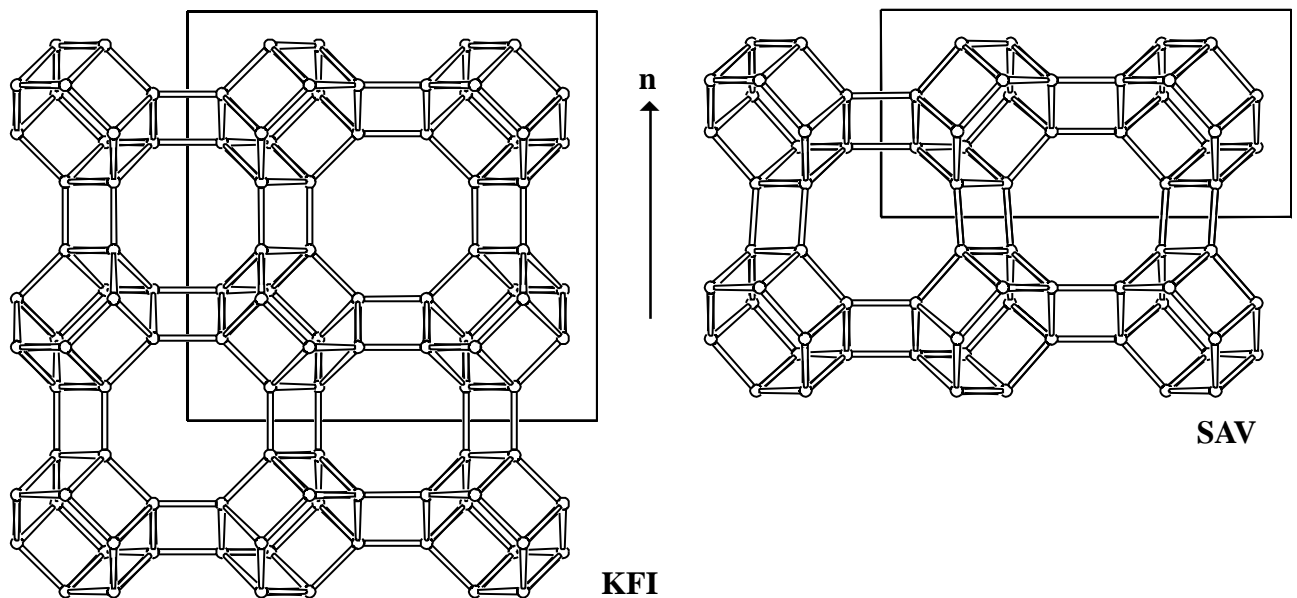


Figure 7: Unit cell content of the simplest ordered end-members in the KFI/SAV family: KFI (left) and SAV (right) seen perpendicular to the plane normal \mathbf{n}



8. References

- (1) A.Simmen, L.B. McCusker, Ch. Baerlocher and W. M. Meier, *Zeolites* **11**, 654 (1991).
- (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).

