# The AEI/CHA Family



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

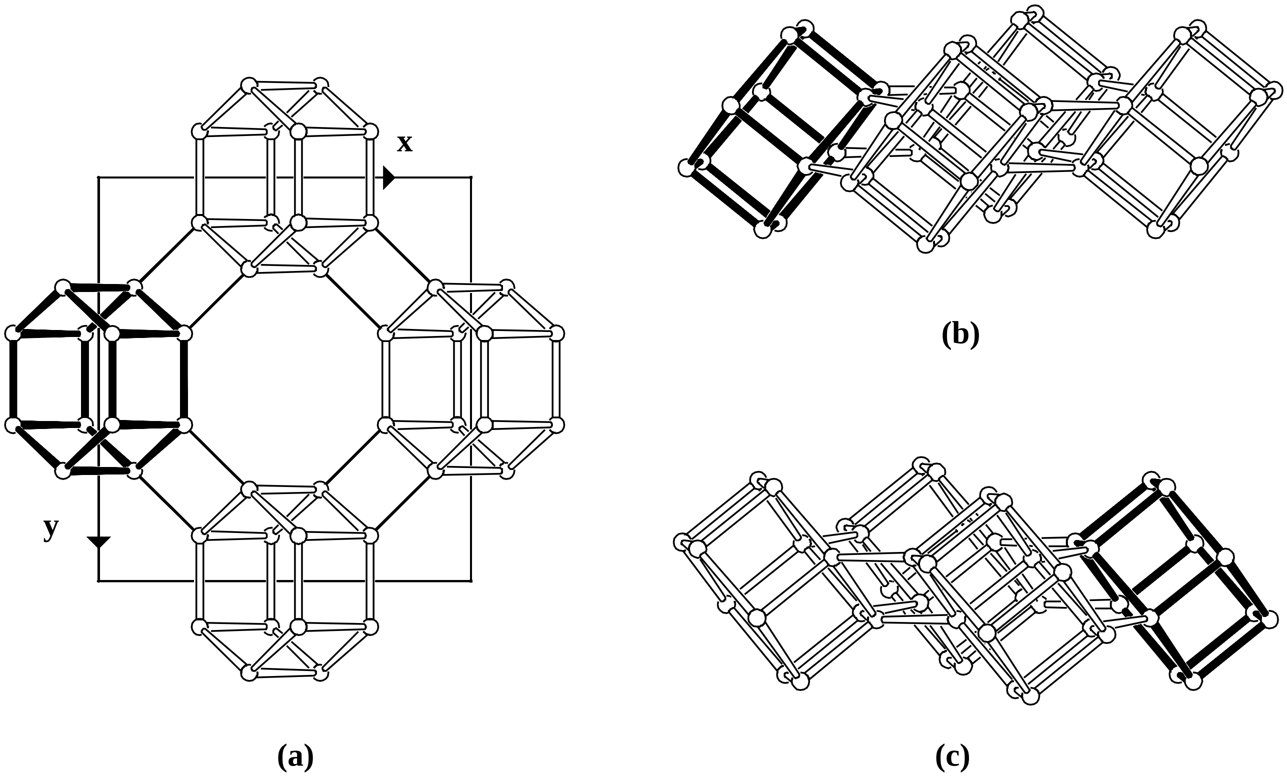



Figure 1: The PerBU in the AEI/CHA family of zeolite frameworks seen along the plane normal **z** (a) and along **y** (b,c).

The PerBU is composed of double T6-rings (D6R's; Fig.1 in bold) connected along the diagonals in the **xy** plane. The layers, depicted in Figure 1b and 1c in perspective view along **y**, are identical and related by a 180° rotation about the plane normal or by a mirror operation perpendicular to the plane normal. [Compare this **xy** layer with the D6R layers in the AEI/SAV 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 C 1 m (1).

## 4. Connectivity Pattern of the PerBU:

Neighbouring PerBU's can be connected along **z** via O-bridges in two different ways:
**(a)**: the lateral shift of the top layer along **x** and **y** is zero. The resulting connectivity exhibits inversion symmetry (**i**; o) between successive layers.
**(b)**: the top layer is rotated over 180° about **z** before connecting it to the bottom layer. The connectivity now shows mirror symmetry (**m**; |) between successive layers.

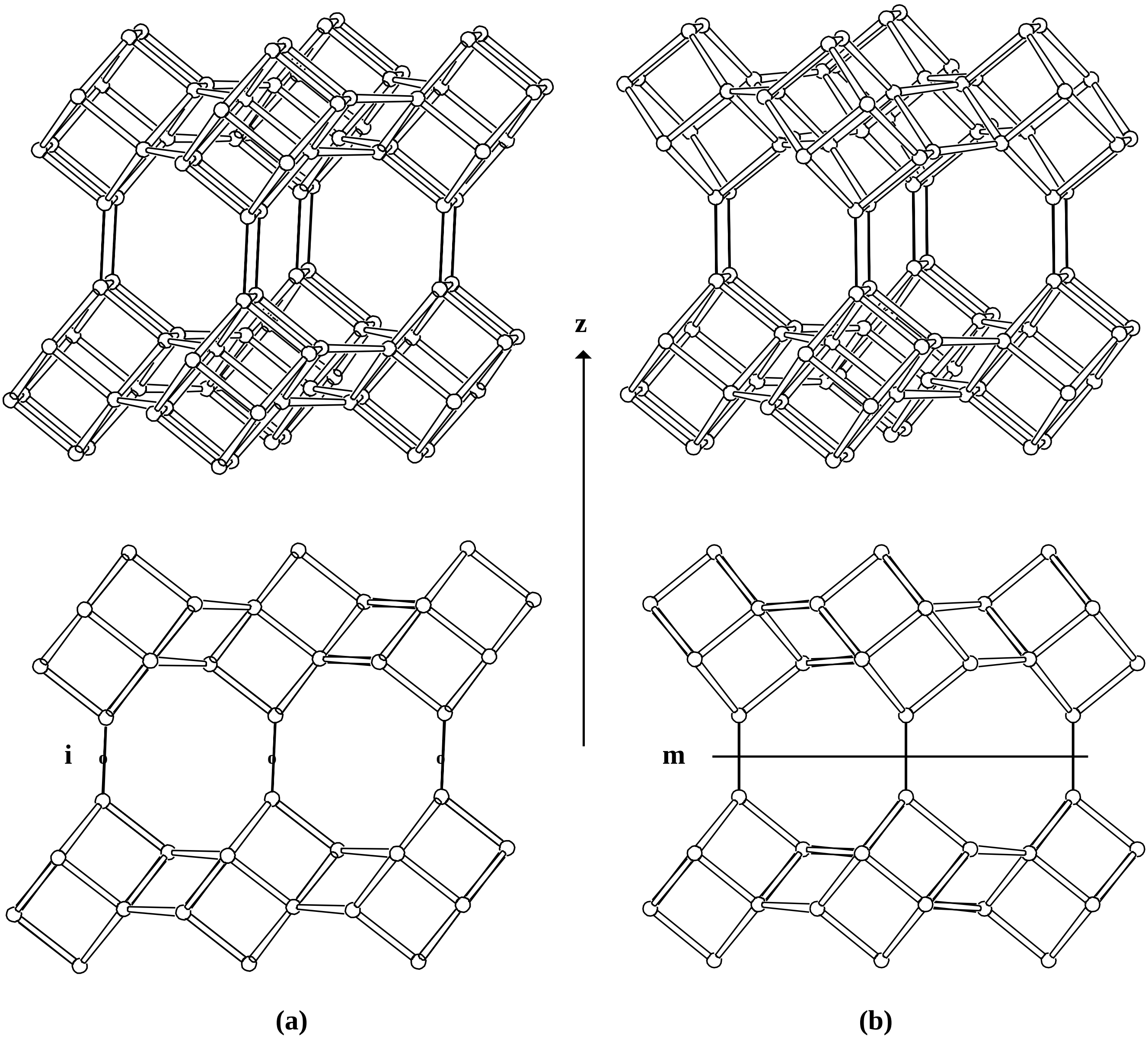



Figure 2: Perspective view (top) and parallel projection (bottom) along **y** of the connection modes **(a)** and **(b)** in the AEI/CHA family of zeolite frameworks

Once the distribution of the symmetry elements **i** and **m** between the PerBU's stacked along **z** is known, the 3-dimensional structure is defined.

**5. The Simplest Ordered End-Members** in the AEI/CHA family are given below.

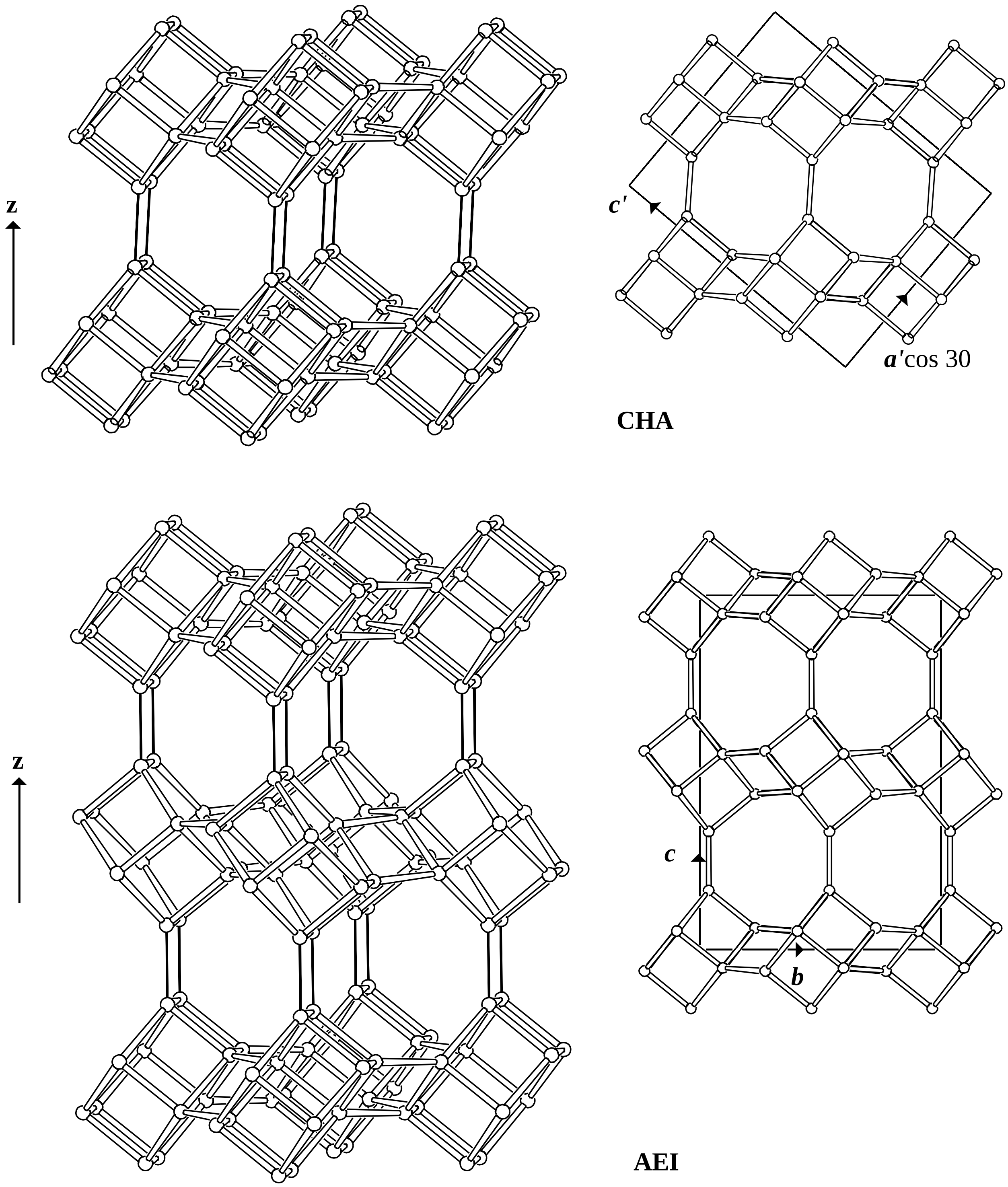



Figure 3: Perspective drawing (left) and parallel projection along **y** of the unit cell content (right) of the two simplest ordered end-members in the AEI/CHA family: CHA (top) and AEI (bottom).
[***a′*** and ***c′*** are the unit cell constants used in the hexagonal description of the structure of CHA]

Pure CHA(1,2) and AEI(3) are obtained when neighbouring PerBU’s along **z** are exclusively related by **i** and **m**, respectively.

## 6. Disordered Materials Synthesized and Characterized to Date:

to be added

## 7. Supplementery Information

### 7.1 *Comparison with the AEI/SAV family:*

The PerBU in the AEI/SAV family is composed of D6R’s, related by rotations of 180° about **x** and by pure translations along **y** as shown in Figure 4.

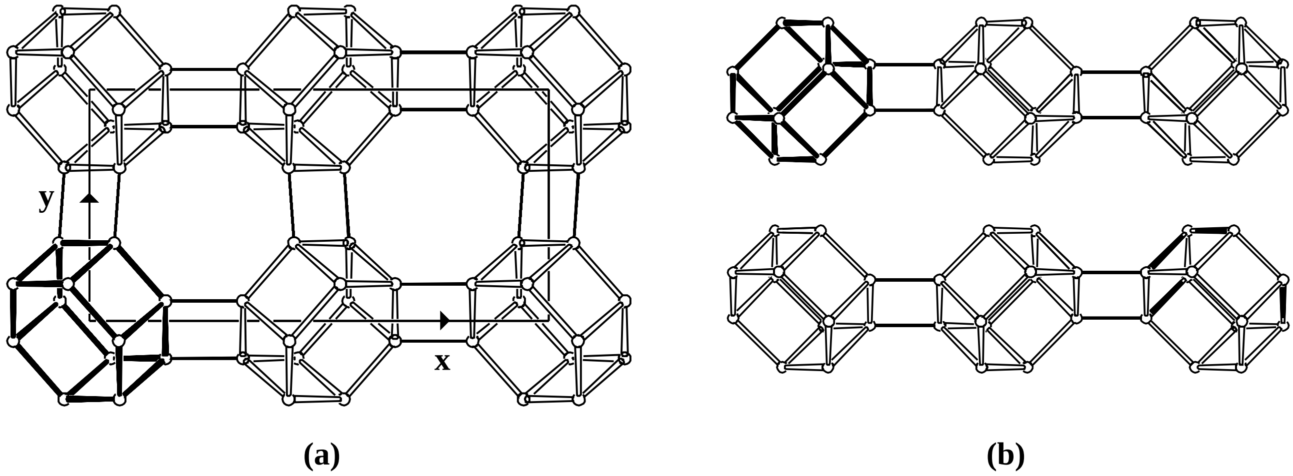



Figure 4: PerBU seen along the plane normal **n** (a) and along **y** (b). The layers in Figure 4b are identical and related by a rotation of 180° about the plane normal **n** or by a mirror operation perpendicular to **n**

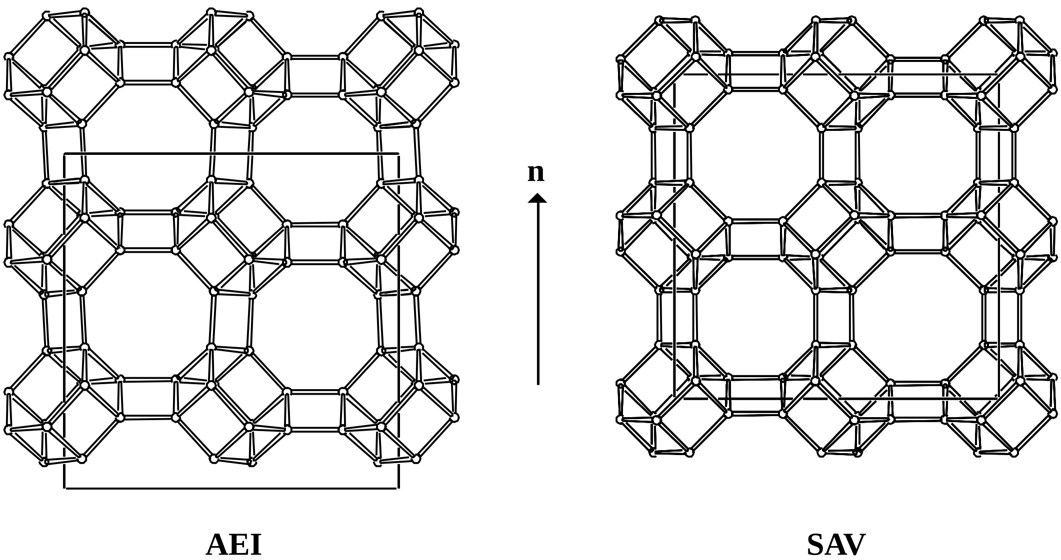
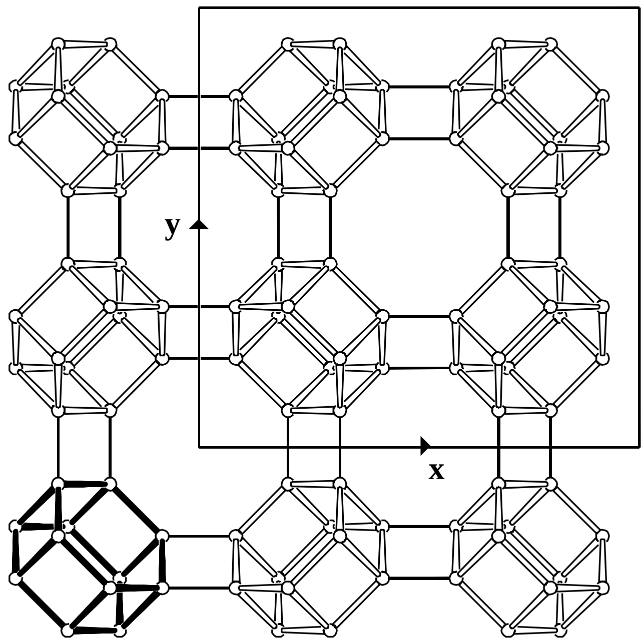



Figure 5: Unit cell content of the simplest ordered end-members in the AEI/SAV family: AEI (left) and SAV (right) seen perpendicular to the plane normal **n** of the PerBU

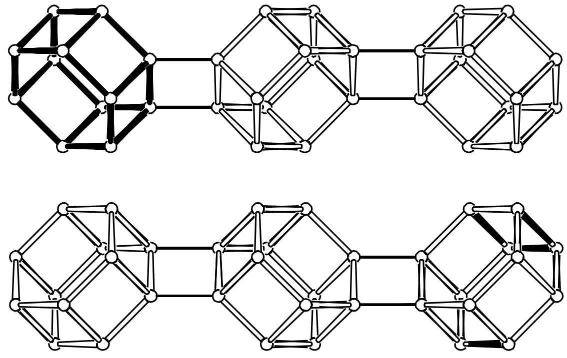
For more details: see the description of the AEI/SAV family in this 'Catalog'.

### 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 180º about **x** and **y** (or by mirror planes perpendicular to **x** and **y**) as shown in Figure 6.

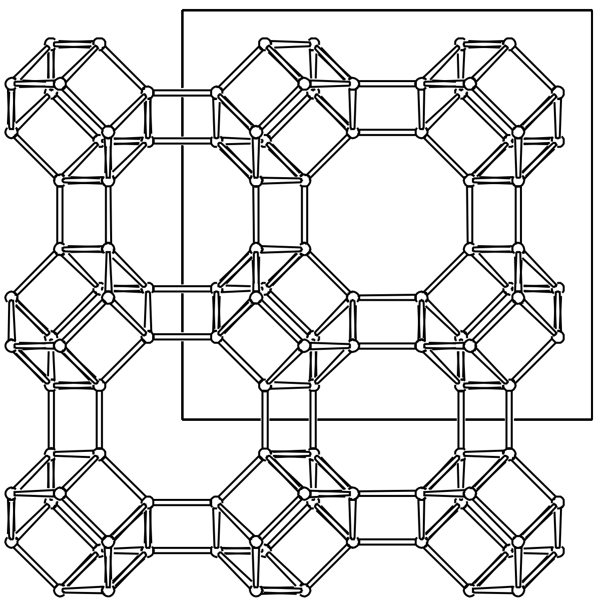



**(a)**

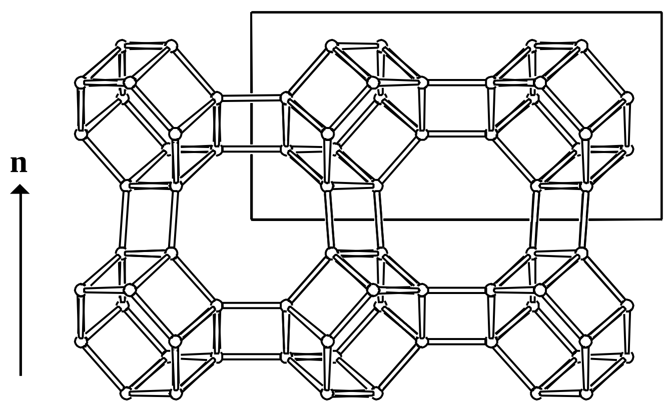


**(b)**

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



**KFI**




**SAV**

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 **n**

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

## 8. References


(1) a) L.S. Dent and J.V. Smith, Nature **181**, 1794 (1958).
b) J.V. Smith, R. Rinaldi and L.S. Dent, Acta Cryst. **16**, 45 (1963).

(2) K.P. Lillerud and D. Akporiaye. In: *Zeolites and Related Microporous Materials: State of the Art 1994.* Studies in Surface Science and Catalysis, Vol. 84. J. Weitkamp, H.G. Karge, H. Pfeifer and W. Hoelderich (Eds.). Elsevier Science B.V., 1994, p 543.

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