

The BEC/ISV family

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1. The Periodic Building Unit (PerBU) equals the **xy** layer shown in Figure 1. This layer is built from chains composed of T16 units shown in Figure 2.

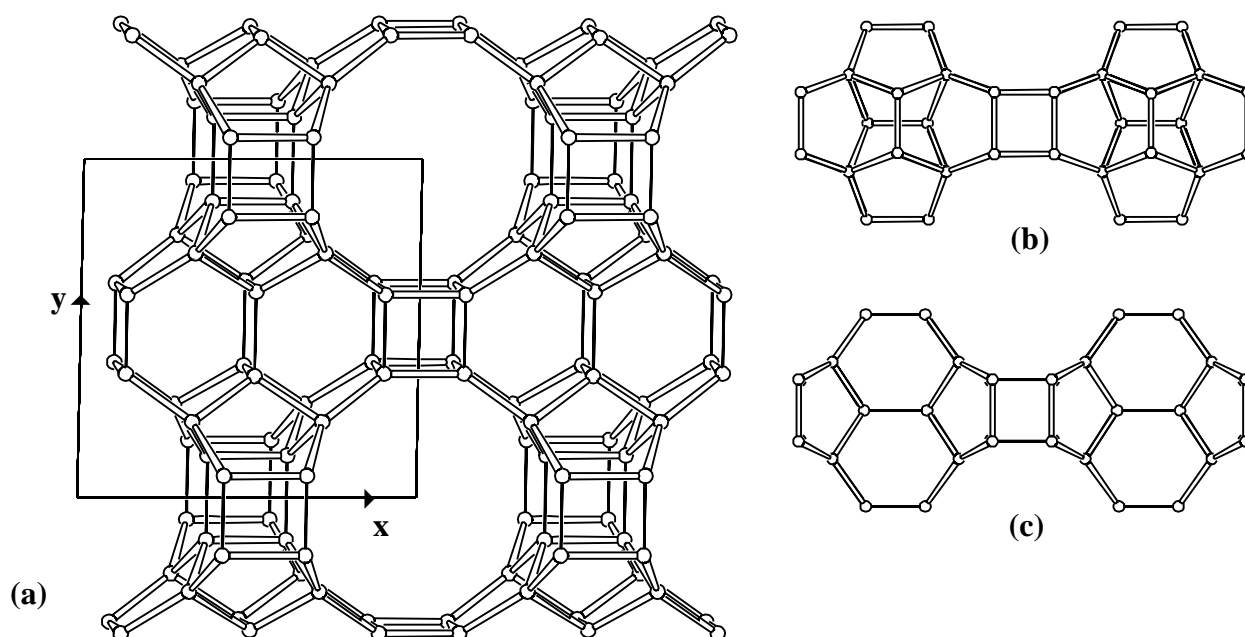


Figure 1: PerBU of the BEC/ISV family of zeolite frameworks shown in perspective view along the plane normal **z** (a) and in projection parallel to **y** (b) and parallel to **x** (c). The PerBU's, depicted in (b) and (c), are identical and related by a rotation of 90° about **z**

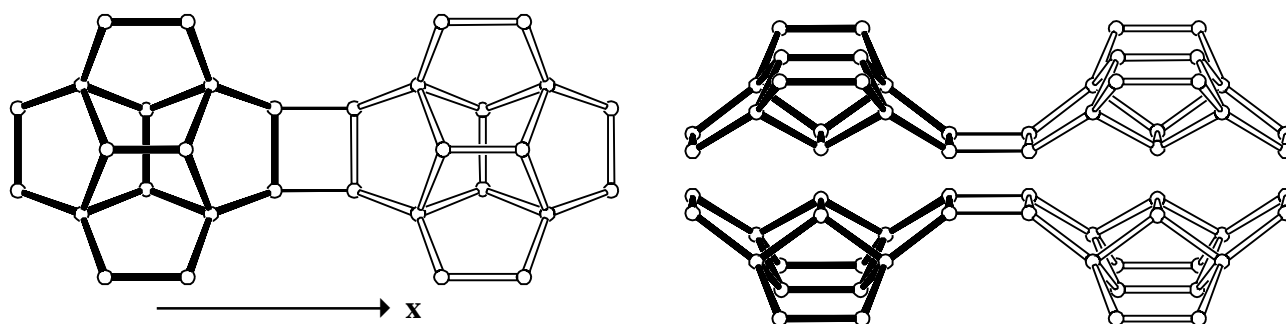


Figure 2: T16 units, related by pure translations along **x** are connected into chains along **x**. Chain seen along **y** (left) and along **z** (right). The chains on the right differ by a rotation of 180° about **x** ▲

The PerBU of the BEC/ISV family is composed of chains of T16 units (bold in Fig.2). Neighbouring chains, related by a rotation of 180° about the chain axis, accompanied by a zero lateral shift along **x** (or by a mirror plane perpendicular to **y**), are connected along **y** through T4-rings as shown in Figure 1. [Compare this connection with the different connection of T16 chains in the Beta family]

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 $P 2/m 2/m (2/m)$. ▲

4. Connectivity Pattern of the PerBU:

Neighbouring PerBU's are connected along z in two different ways:

- (a): neighbouring PerBU's are related by a pure translation along z . The connectivity exhibits mirror symmetry between successive layers (double T4-rings are formed).
- (b): neighbouring PerBU's are related by a rotation of 90° about z . Successive layers are related by a 4_2 axis (double T4-rings are formed).

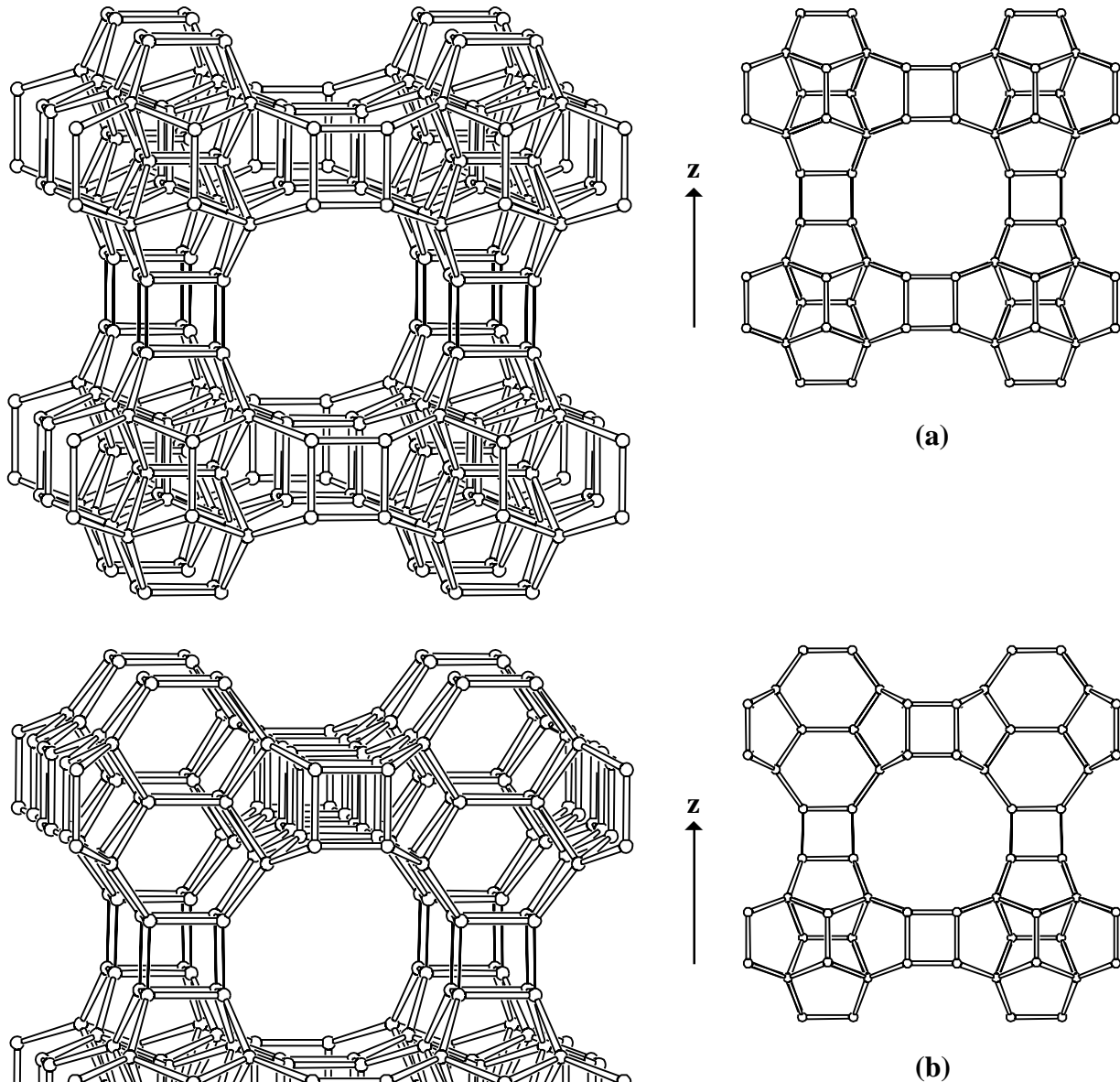


Figure 3: Perspective view (left) and parallel projection (right) along y of the connection modes (a) and (b) in the BEC/ISV family of zeolite frameworks

Once the distribution of the symmetry elements m and 4_2 between the layers stacked along z is known, the 3-dimensional structure is defined. ▲

5. The Simplest Ordered End-Members in the BEC/ISV family are shown in Figure 4:

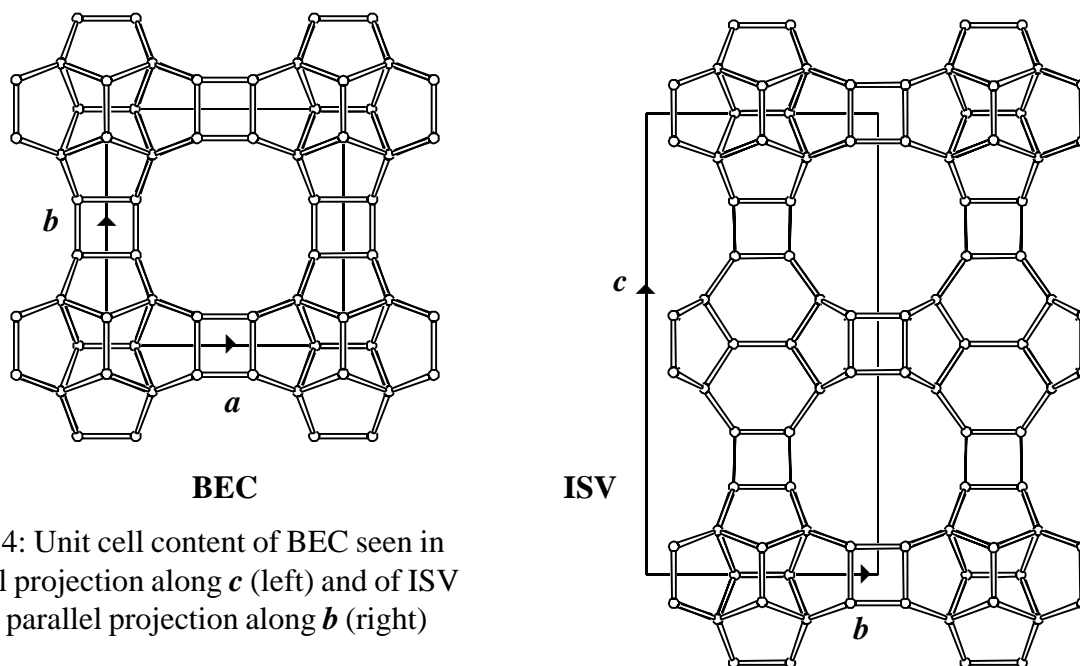


Figure 4: Unit cell content of BEC seen in parallel projection along c (left) and of ISV seen in parallel projection along b (right)

Pure BEC(1) and ISV(2) are obtained when neighbouring PerBU's, stacked along the plane normal of the PerBU, are exclusively related by \mathbf{m} and 4_2 , respectively.

6. Disordered Materials Synthesized and Characterized to Date: ▲

No disordered materials known to date.

7. Supplementary Information

7.1 Comparison with the BETA family:

The PerBU in the Beta family is the tetragonal ab layer depicted in Figure 5. The layer is composed of T16 units (in bold) related by pure translations along a and b .

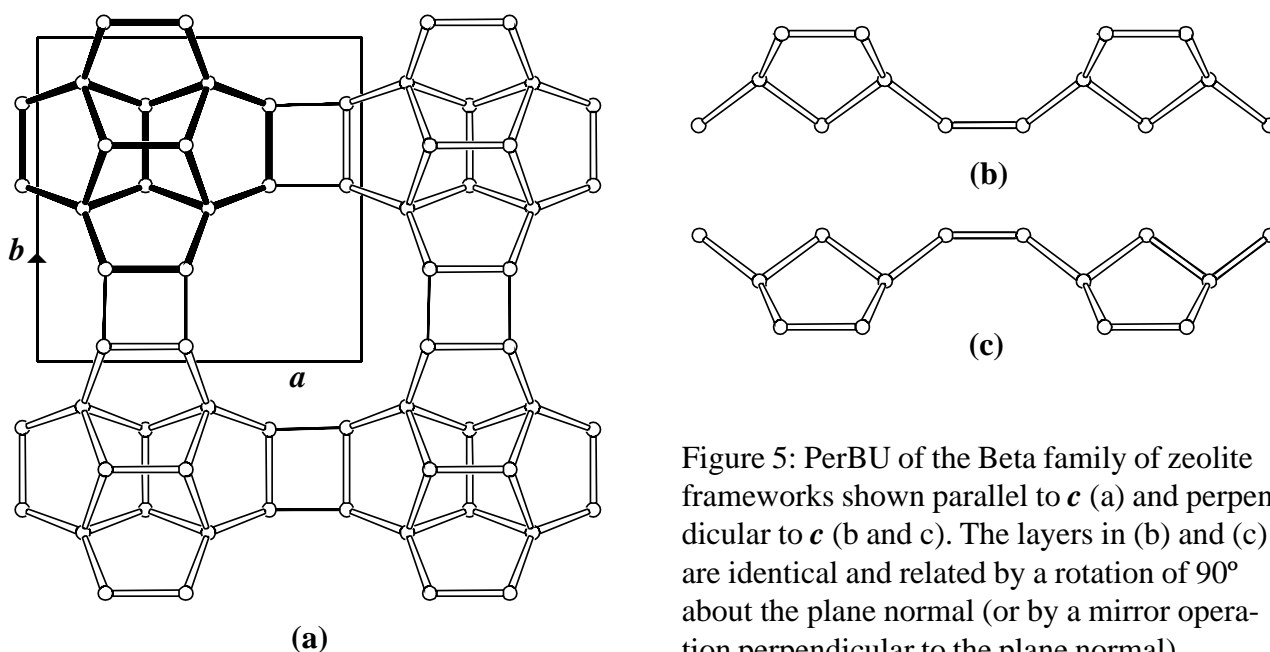


Figure 5: PerBU of the Beta family of zeolite frameworks shown parallel to c (a) and perpendicular to c (b and c). The layers in (b) and (c) are identical and related by a rotation of 90° about the plane normal (or by a mirror operation perpendicular to the plane normal)

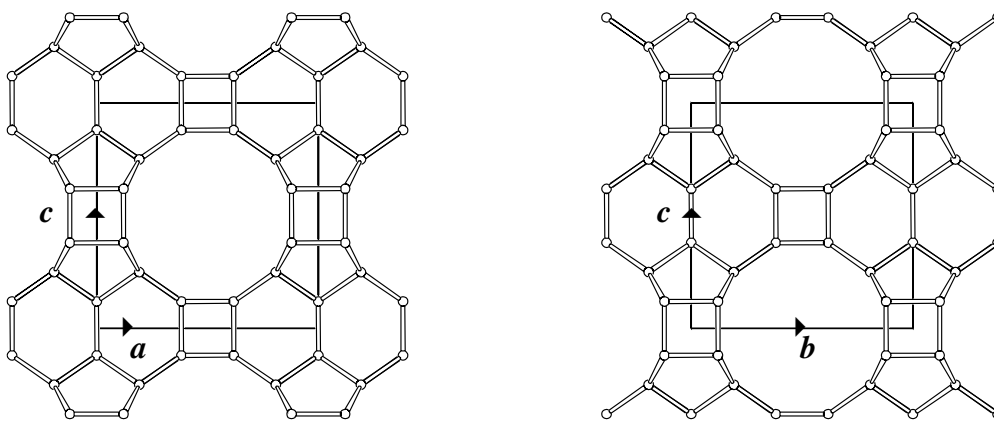


Figure 6: Unit cell content of the end-member BEC seen along b (left) and along a (right)

For more details: see the description of the Beta family in this 'Catalog'.

8. References

- (1) L.A. Villaescusa, P.A. Barrett and M.A. Camblor, *Angew. Chem., Int. Ed.* **38**, 1997 (1999).
- (2) T. Conradsson, M.S. Dadachov and X.D. Zou, *Microp. and Mesop. Mat.*, **41**, 183 (2000).

