The BEC/ISV family

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

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 \mathbf{z} (a) and in projection parallel to \mathbf{y} (b) and parallel to \mathbf{x} (c). The PerBU's, depicted in (b) and (c), are identical and related by a rotation of 90° about \mathbf{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 <u>Beta</u> 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).



Once the distribution of the symmetry elements \mathbf{m} and $\mathbf{4}_2$ between the layers stacked along \mathbf{z} is known, the 3-dimensional stucture is defined.

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



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 $\mathbf{4}_2$, 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).