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 90º 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 180º 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 180º 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).

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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)](image)

Pure BEC(1) and ISV(2) are obtained when neighbouring PerBU’s, stacked along the plane normal of the PerBU, are exclusively related by \( m \) 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)](image)
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
