The Faujasite Family

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

1. The Periodic Building Unit (PerBU) is the hexagonal layer shown in Figure 1. This layer is built from T24 units, the sodalite cages (sod-cages), shown in Figure 2.

Figure 1: The PerBU in the Faujasite family of zeolite frameworks is composed of sod-cages which are linked through double T6-rings into a hexagonal layer. The PerBU corresponds to the (001) layer in hexagonal EMT and to the (111) layer in cubic FAU. Hexagonal axes are given. Views along [001] (a), [010] (b) and [110] (c) are shown. The layers, depicted in Figure 1b and 1c are identical and related by a 60° rotation about the (hexagonal) \( \mathbf{c} \)-axis or by a mirror operation perpendicular to \( \mathbf{c} \).

Figure 2: The sod-cage. From left to right: perspective view perpendicular to \( \mathbf{c} \); parallel views perpendicular to \( \mathbf{c} \), after rotation of +30° and -30° about \( \mathbf{c} \) with respect to the most left drawing; and parallel view down \( \mathbf{c} \). [Compare the packing of sod-cages in LTA and SOD]
2. **Type of Faulting:** 1-dimensional stacking disorder of the PerBU’s along [001].

3. **The Layer Symmetry:** the plane space group of the PerBU is $P(\overline{3})m\ 1$.

4. **Connectivity Pattern of the PerBU:**

   Neighbouring PerBU’s can be connected along [001] through double T6-rings in two different ways:
   
   (a): the top layer is shifted over $\frac{1}{2}(-a + b)$ before connecting it to the bottom layer. The resulting connectivity exhibits inversion symmetry ($i\ o$) between successive layers.
   
   (b): the top layer is rotated over 60° about [001] (followed by the shift vector $\frac{1}{2}(-a + b)$) before connecting it to the bottom layer. The connectivity now shows mirror symmetry ($m\ |$) between successive layers (see also Fig. 1b and 1c).

---

Figure 3: Parallel projection along [010] of the connection modes (a) and (b) in the Faujasite family of zeolite frameworks

---

Once the distribution of the symmetry elements $i$ and $m$ between the layers stacked along [001] is known, the 3-dimensional structure is defined.
5. The Simplest Ordered End-Members in the Faujasite family are presented in Figure 5:

Pure EMT(1,2) and FAU(3,4) are obtained when neighbouring PerBU’s along the (hexagonal) [001] axis are exclusively related by \(m\) and \(i\), respectively.
6. Disordered Materials Synthesized and Characterized to Date:

CSZ-1 (5,6); CSZ-3 (5,7); ZSM-3 (5,8); ZSM-20 (5,9); ECR-30 (5,10).

7. Supplementary Information

7.1 Comparison with LTA:

In LTA, each sodalite(sod)-cage is connected to six nearest neighbouring sod-cages through double T4-rings (Fig.6). [In FAU/EMT each sod-cage is connected to four nearest neighbouring sod-cages through double T6-rings]. Eight sod-cages in a cubic packing enclose a RHO-cage (Fig.7). [For more details: see the building scheme of LTA in 'Schemes for Building Zeolite Framework Models' on http://www.iza-structure.org/databases/ ].

Figure 6: Sod-cage (left) connected through a double T4-ring to one of its nearest neighbours in perspective view (middle) and in parallel projection (right)

Figure 7: Cell content seen along a cube axis in perspective view (left) and in parallel projection (top right). For clarity, only one additional sod-cage along the viewing direction has been drawn (in bold)
7.2 Comparison with SOD:

In SOD, each sod-cage is connected to six nearest neighbouring sod-cages through common T4-rings (Fig. 8). Eight (fused) sod-cages in a cubic packing enclose 'new' sod-cages. [For more details: see the building scheme of SOD in 'Schemes for Building Zeolite Framework Models' on: http://www.iza-structure.org/databases/ ].

Figure 8: Sod-cage (left) connected through a common T4-ring (in bold) to one of its nearest neighbours in perspective view (middle) and in parallel projection (right)

Figure 9: Cell content seen along a cube axis in perspective view (left) and in parallel projection (right). For clarity, only one additional sod-cage along the viewing direction has been drawn (in bold)

8. References


