# The Pentasil Family



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

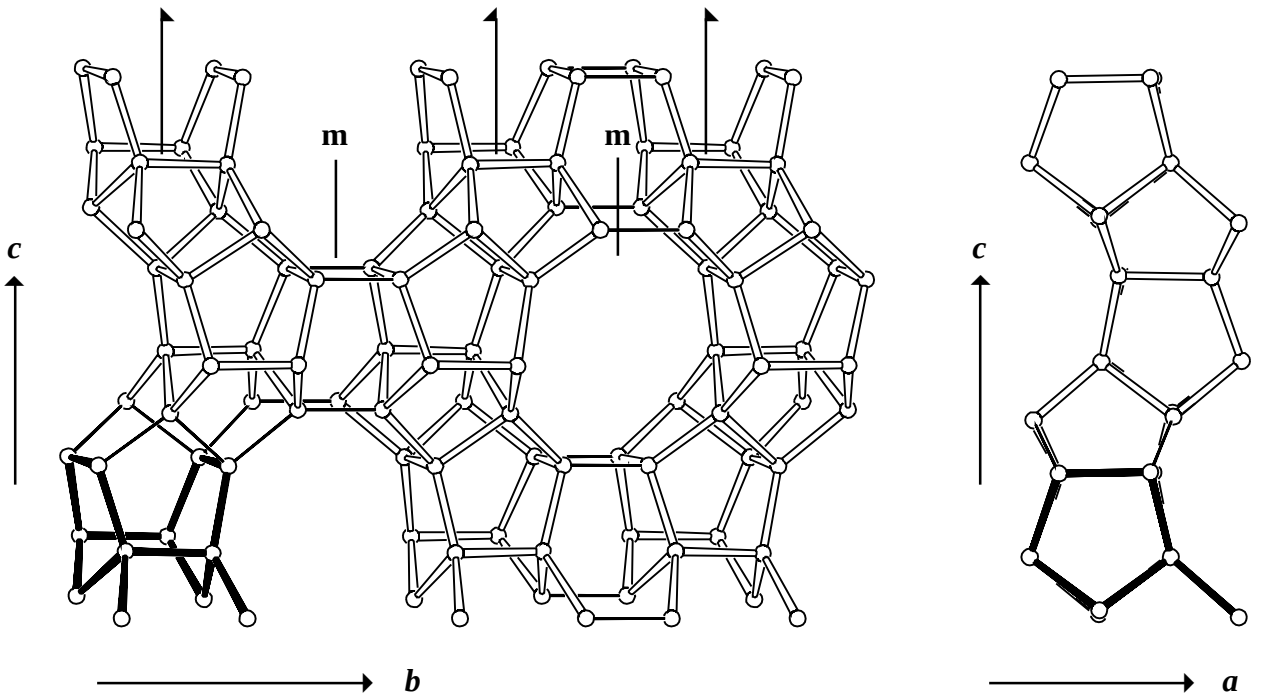


Figure 1: The Periodic Building Unit of the pentasil family of framework types

The PerBU in the pentasil family, the pentasil layer (Fig. 1(left)), is composed of T12-units (bold in Fig.1). T12-units, related by a rotation of 180º about ***c*** accompanied by a translation of ½***c***, form left- and right-handed chains along ***c***. The chains, related by a mirror plane **m** perpendicular to ***b***, are connected along ***b*** to give the characteristic ***bc*** pentasil layer. A parallel projection of the pentasil layer along ***b*** is shown at the right of Fig.1.

**2. Type of faulting:** 1-dimensional stacking disorder of the PerBU's along ***a***.

**3. The plane space group** of the PerBU is P 1 m (1).

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

Neighbouring PerBU's can be connected along ***a*** through O-bridges in two different ways:
**(a):** successive pentasil layers are connected after a rotation of 180º about ***a*** (or ***b***) with respect to each other. The resulting connectivity exhibits inversion symmetry (**i:** o) between successive layers.
**(b):** successive pentasil layers are connected after a rotation of 180º about ***c***. The connectivity now shows mirror symmetry (**m:** |) between successive layers.

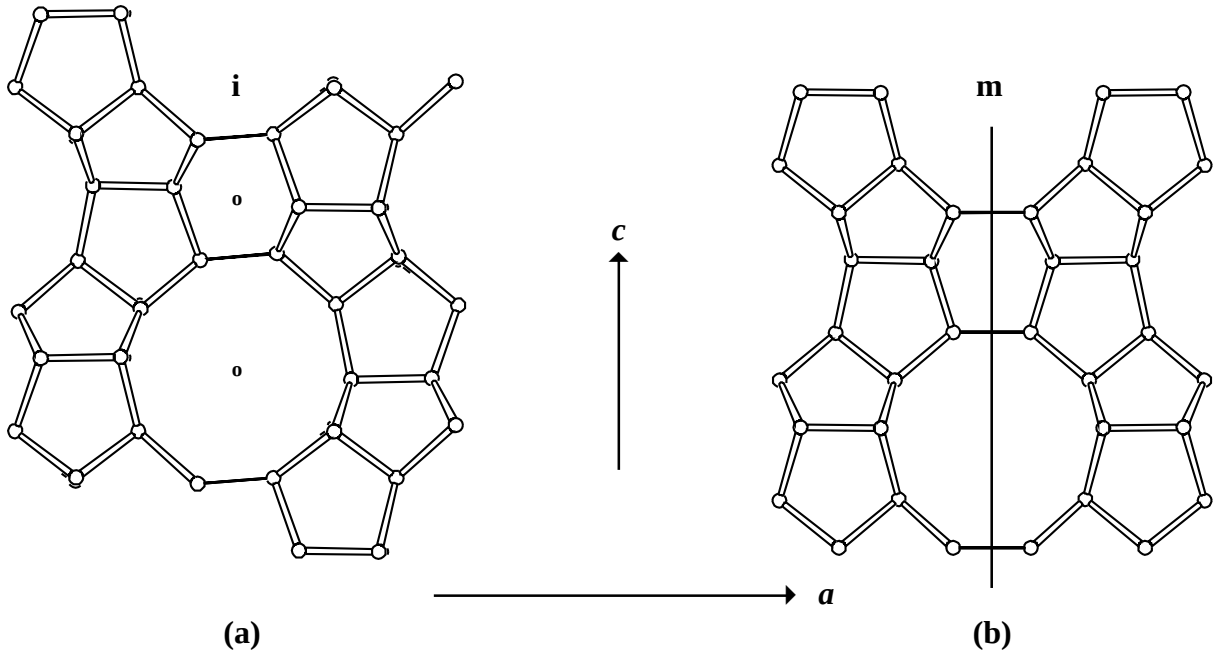


Figure 2: Parallel projection along ***b*** of the connection modes **(a)** and **(b)** in the pentasil family of framework types

Once the distribution of the symmetry elements **i** and **m** between the layers stacked along [100] is known, the 3-dimensional structure is defined.

An example of an intermediate structure in the pentasil family of zeolites is shown in Figure 3:

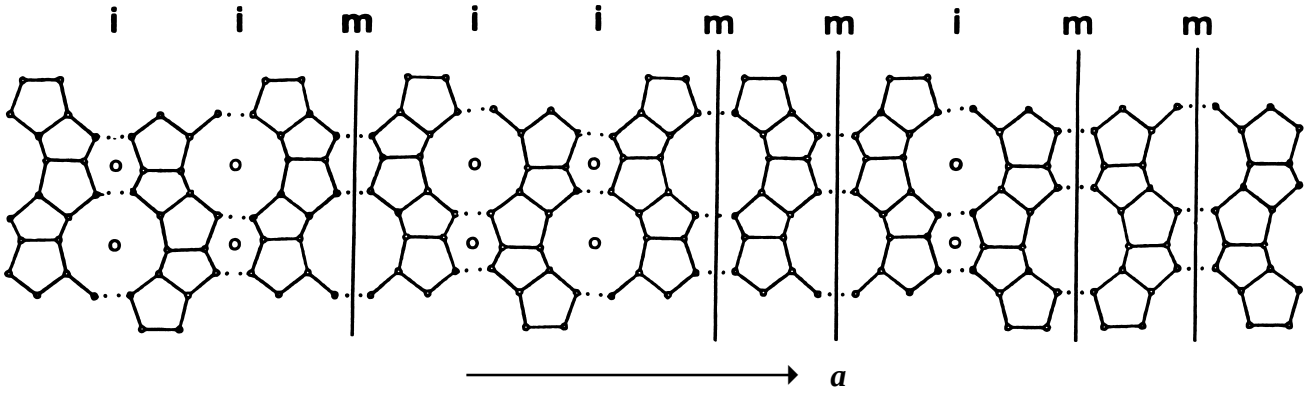


Figure 3: Connectivity sequence of PerBU's with **m** and **i** as symmetry elements

**5. The simplest ordered end-members** in the pentasil family are shown in Figure 4:

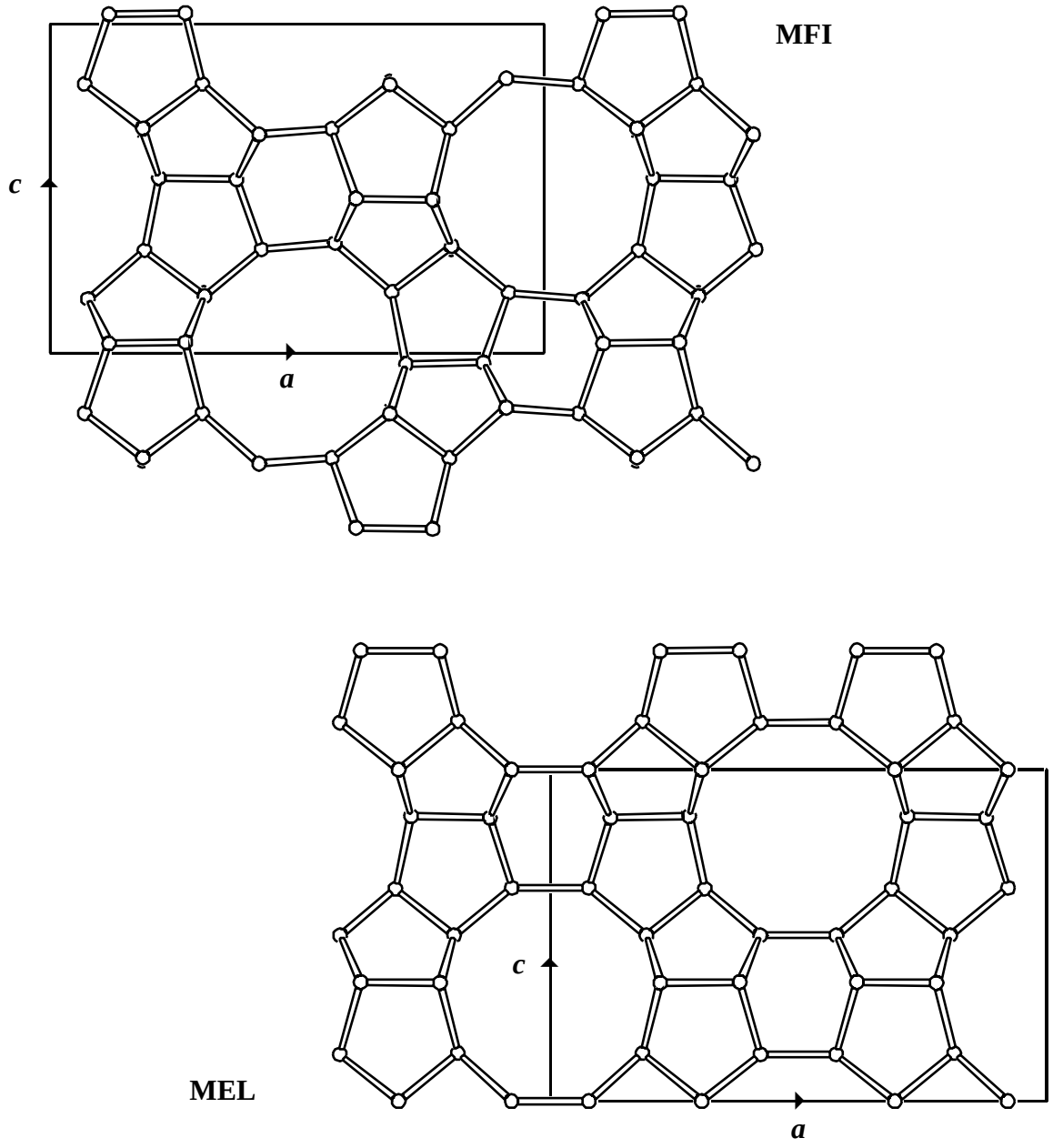


Figure 4: Parallel projection of the unit cell content along ***b*** of the two simplest ordered end-members of the Pentasil family: MFI (top) and MEL (bottom)

Pure MFI (1) and MEL (2) are obtained when neighbouring PerBU's along ***a*** are exclusively related by inversion and reflection, respectively.

**6. Disordered materials synthesized and characterized to date:**

Bor-D (3)

## 7. Supplementary material

Diffax-Simulation of X-ray powdre pattern for the MFI-MEL intergrowth.

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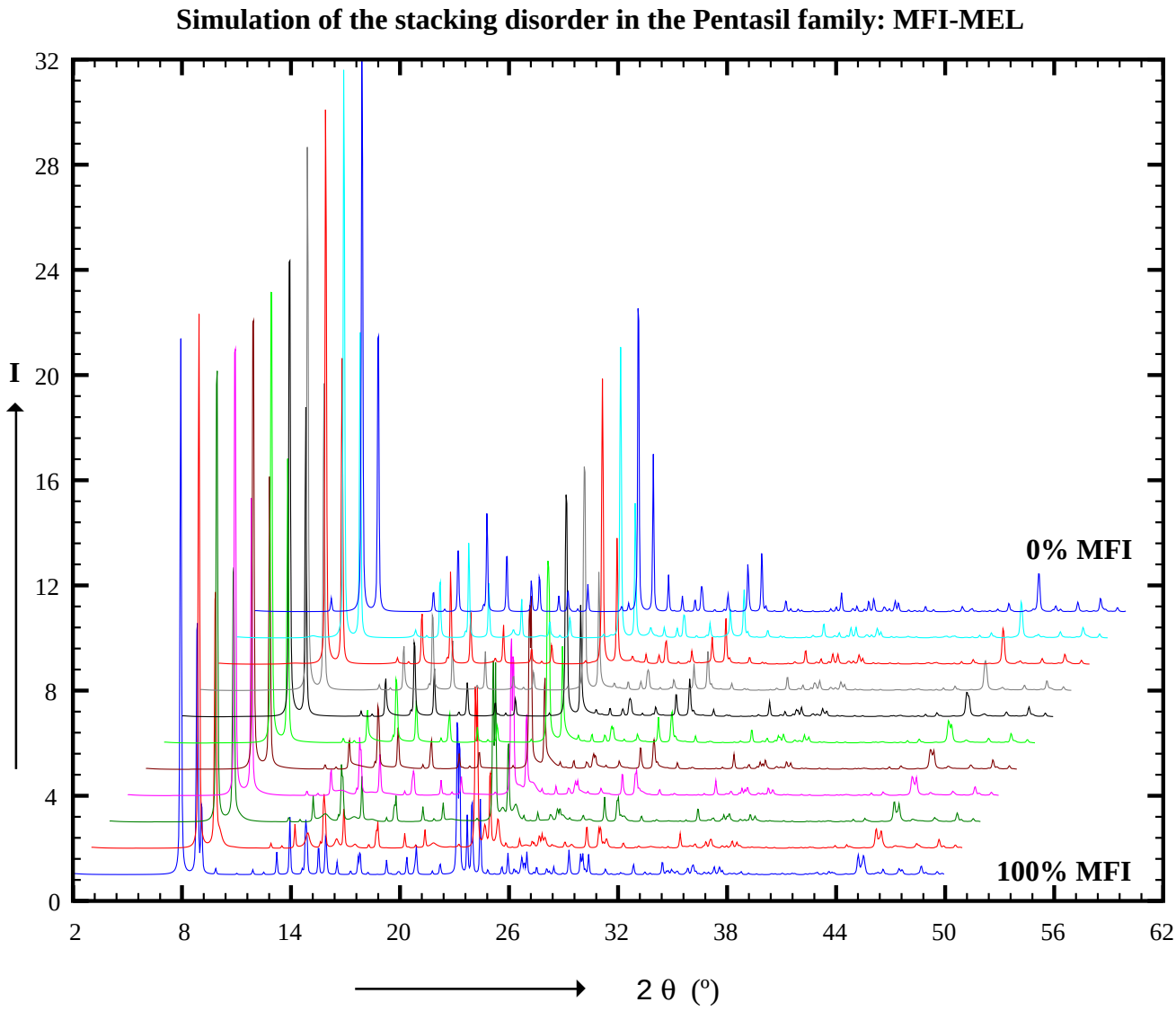


Figure 5: Intensity (**I**, a.u.) of simulated powder patterns versus diffraction angle (**2 θ**) of disordered materials in the MFI-MEL series in steps of 10% intergrowth. The 0% MFI pattern corresponds to the 100% MEL pattern

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## 8. References


(1) G.T. Kokotailo, S.L. Lawton, D.H. Olson and W.M. Meier, Nature **272**, 437 (1978).

(2) G.T. Kokotailo, P. Chu, S.L. Lawton and W.M. Meier, Nature **275**, 119 (1978).

(3) G. Perego, M. Cesari, J. Appl. Cryst. **17**, 403 (1984).