

# The Pentasil Family



1. The Periodic Building Unit (PerBU) - 2. Type of Faulting - 3. The Layer Symmetry
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7. Supplementary Information - 8. References

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

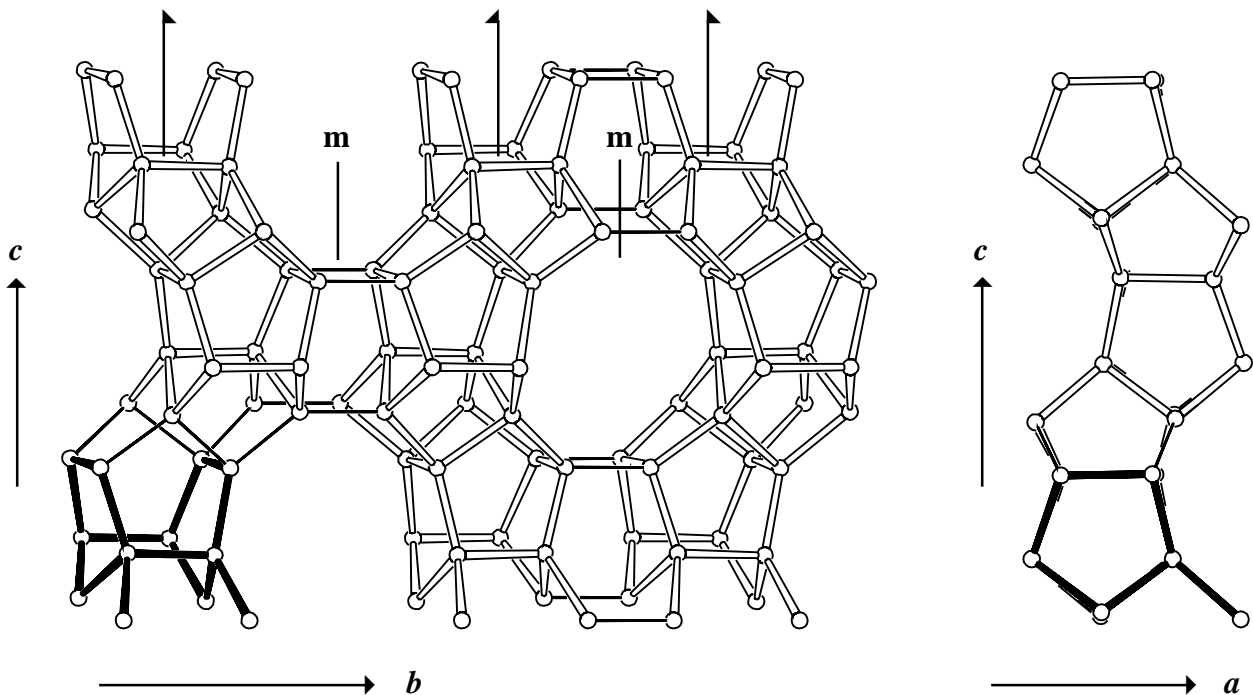


Figure 1: The Periodic Building Unit of the pentasil family of framework types

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  $180^\circ$  about  $c$  accompanied by a translation of  $\frac{1}{2}c$ , 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  $180^\circ$  about  $a$  (or  $b$ ) with respect to each other. The resulting connectivity exhibits inversion symmetry (**i**:  $\circ$ ) between successive layers.

(b): successive pentasil layers are connected after a rotation of  $180^\circ$  about  $c$ . The connectivity now shows mirror symmetry (**m**: |) between successive layers.

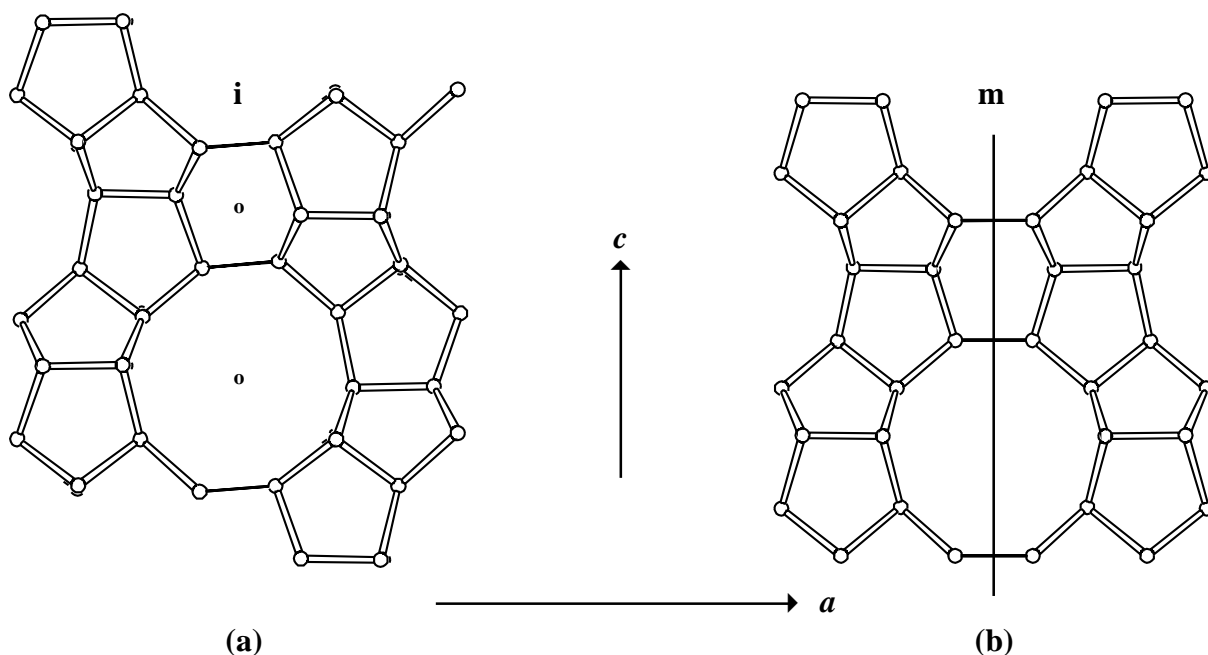


Figure 2: Parallel projection along  $b$  of the connection modes (a) and (b) in the pentasil family of framework types

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:

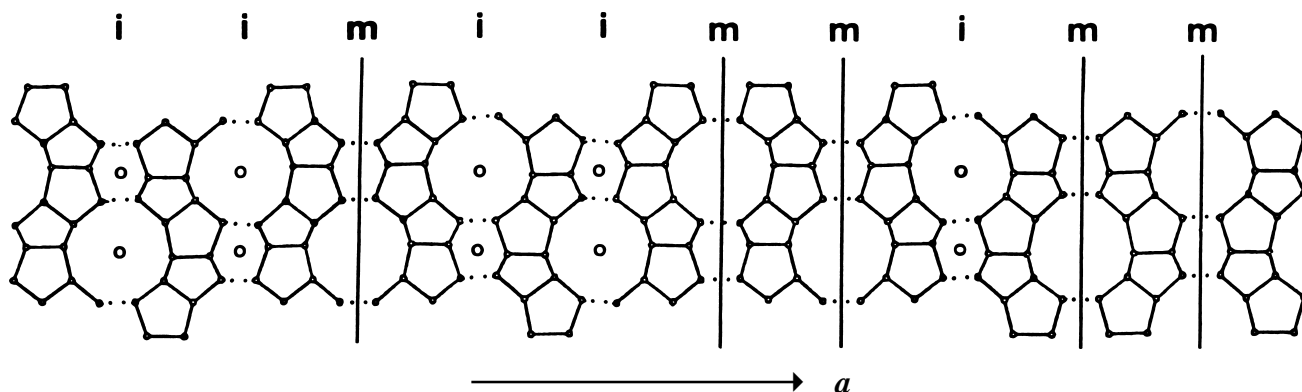


Figure 3: Connectivity sequence of PerBU's with **m** and **i** as symmetry elements ▲

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

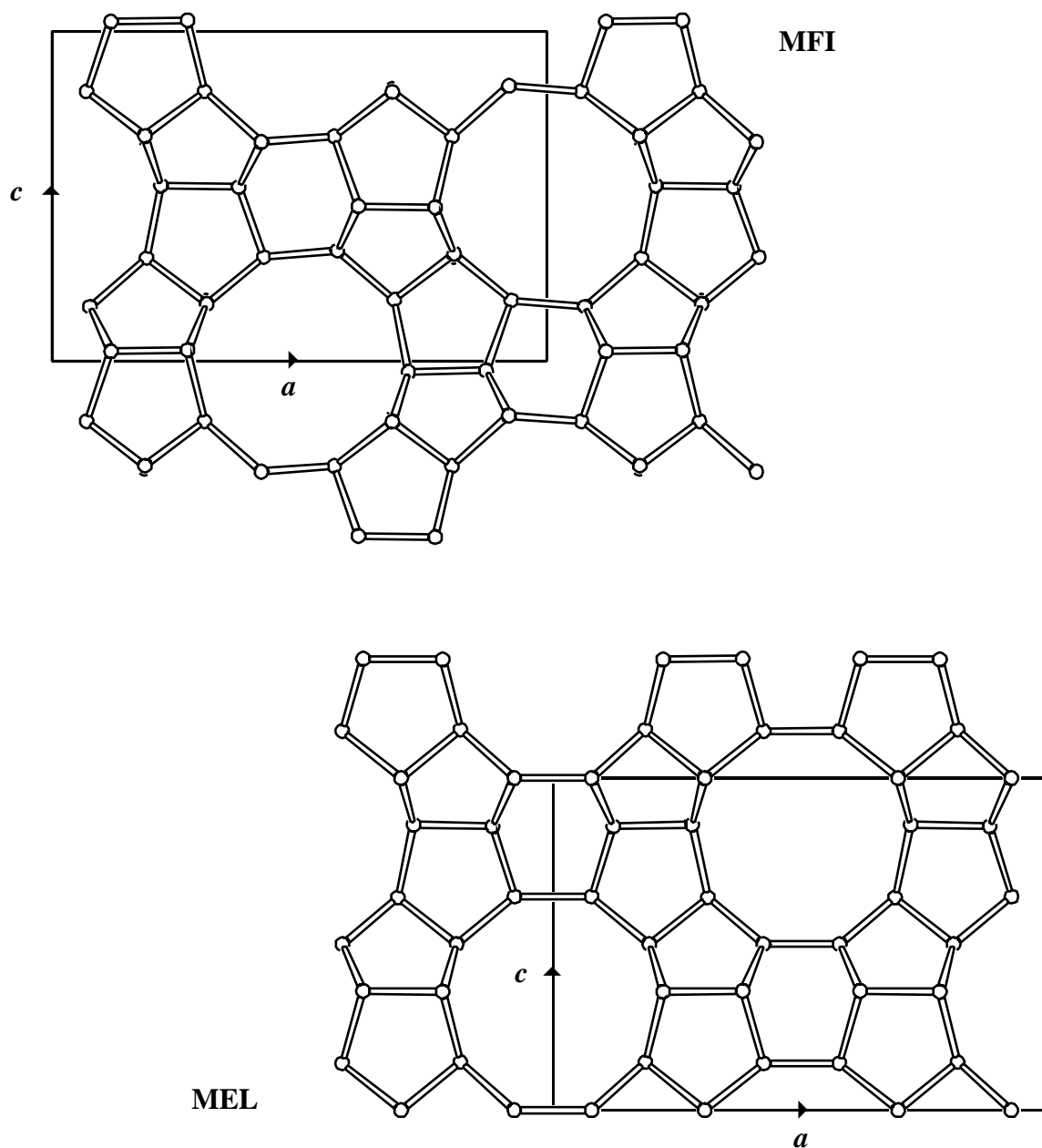


Figure 4: Parallel projection of the unit cell content along  $b$  of the two simplest ordered end-members of the Pentasil family: MFI (top) and MEL (bottom)

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 powdred pattern for the MFI-MEL intergrowth.

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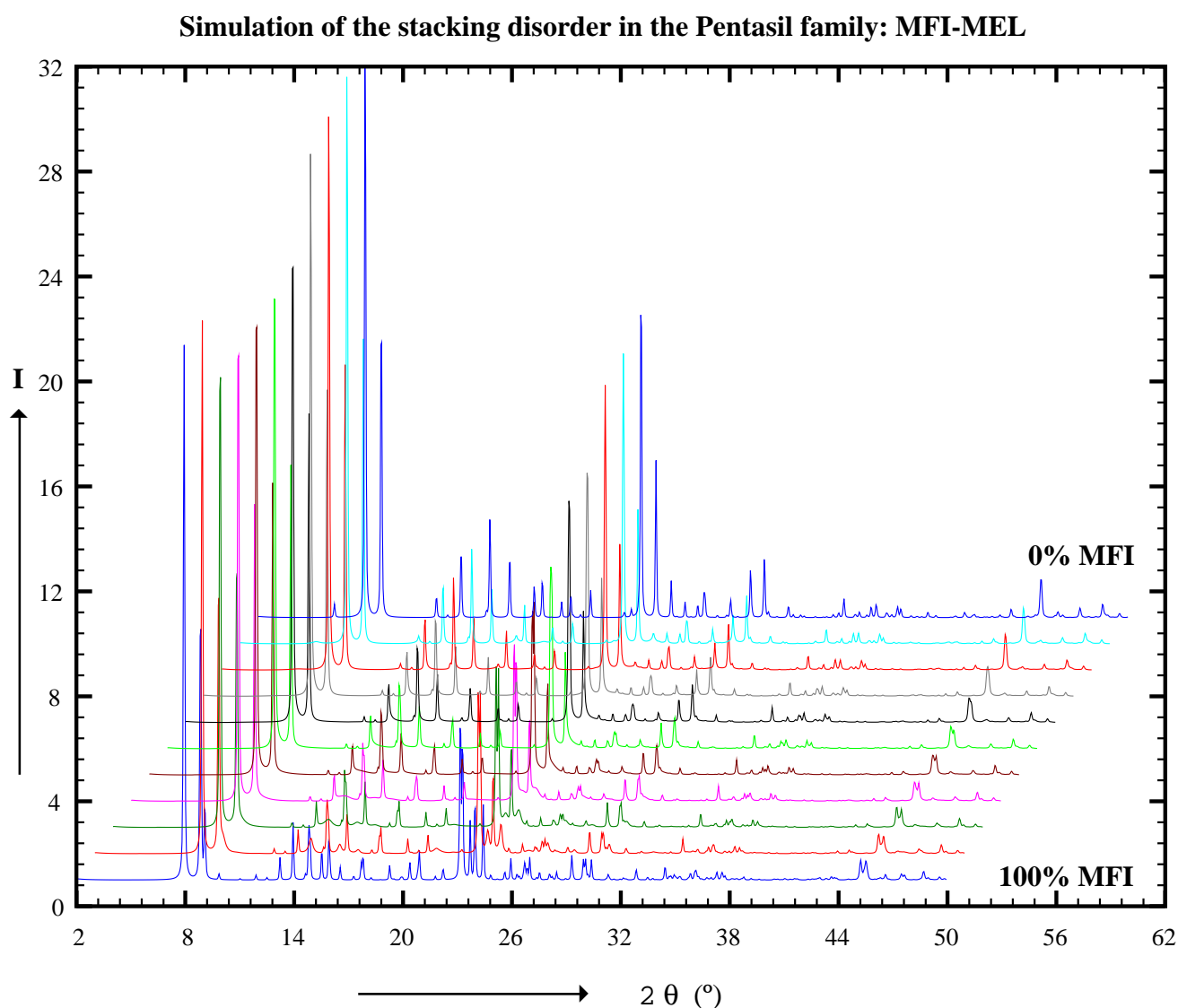


Figure 5: Intensity (I, a.u.) of simulated powder patterns versus diffraction angle ( $2\theta$ ) of disordered materials in the MFI-MEL series in steps of 10% intergrowth. The 0% MFI pattern corresponds to the 100% MEL pattern

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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). ▲