

# The MTT/TON 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 layer shown in Figure 1. This layer is built from infinite building units, shown in Figure 2.

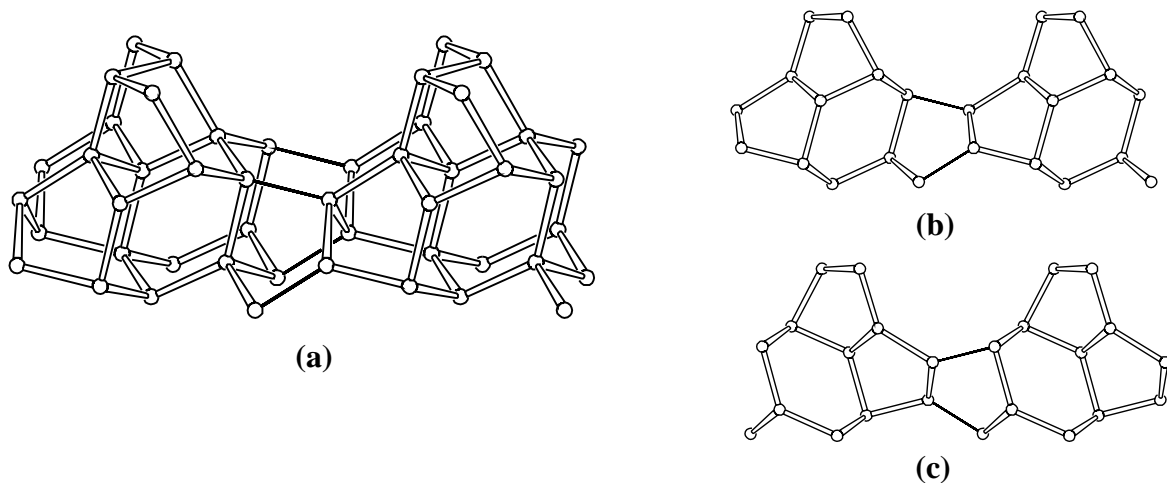


Figure 1: PerBU in the MTT/TON family of zeolite frameworks. (a): perspective view; (b) and (c): parallel projection along the zigzag chain axis

The PerBU in the MTT/TON family (Fig.1) is composed of infinite building units (Fig.2), related by pure translations. The PerBU's depicted in Figure 1b and 1c are identical and related by a rotation of 180° about the plane normal.

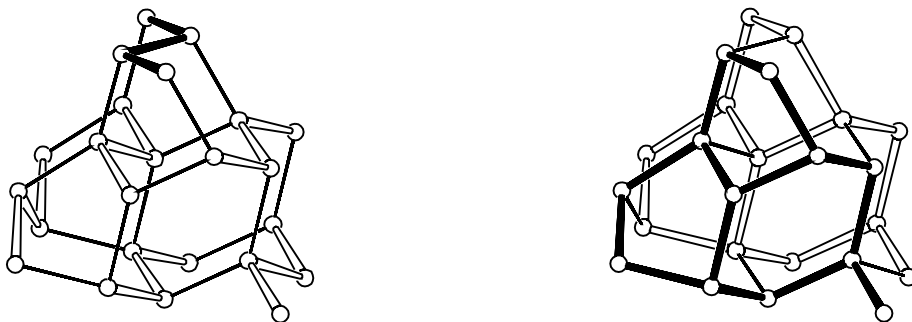


Figure 2: Infinite building unit constructed from six infinite zigzag (zz) chains running parallel to *a* (left) or from T12 units (right). For clarity only two repeat units along the zz chain axis are drawn. [Compare this building unit with the building unit in SFE constructed from seven zz chains] ▲

**2. Type of Faulting:** 1-dimensional stacking disorder of the PerBU's along the PerBU-plane normal.

**3. The Layer Symmetry:** the plane space group of the PerBU is  $Pm\bar{1}(1)$ . ▲

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

Neighbouring PerBU's can be connected in two different ways:

**(a):** neighbouring PerBU's are related by a pure translation. The resulting connectivity exhibits inversion symmetry (**i**; **o**) between successive layers.

**(b):** neighbouring PerBU's are related by a rotation of  $180^\circ$  about the plane normal. The connectivity now shows mirror symmetry (**m**; **l**) between successive layers.

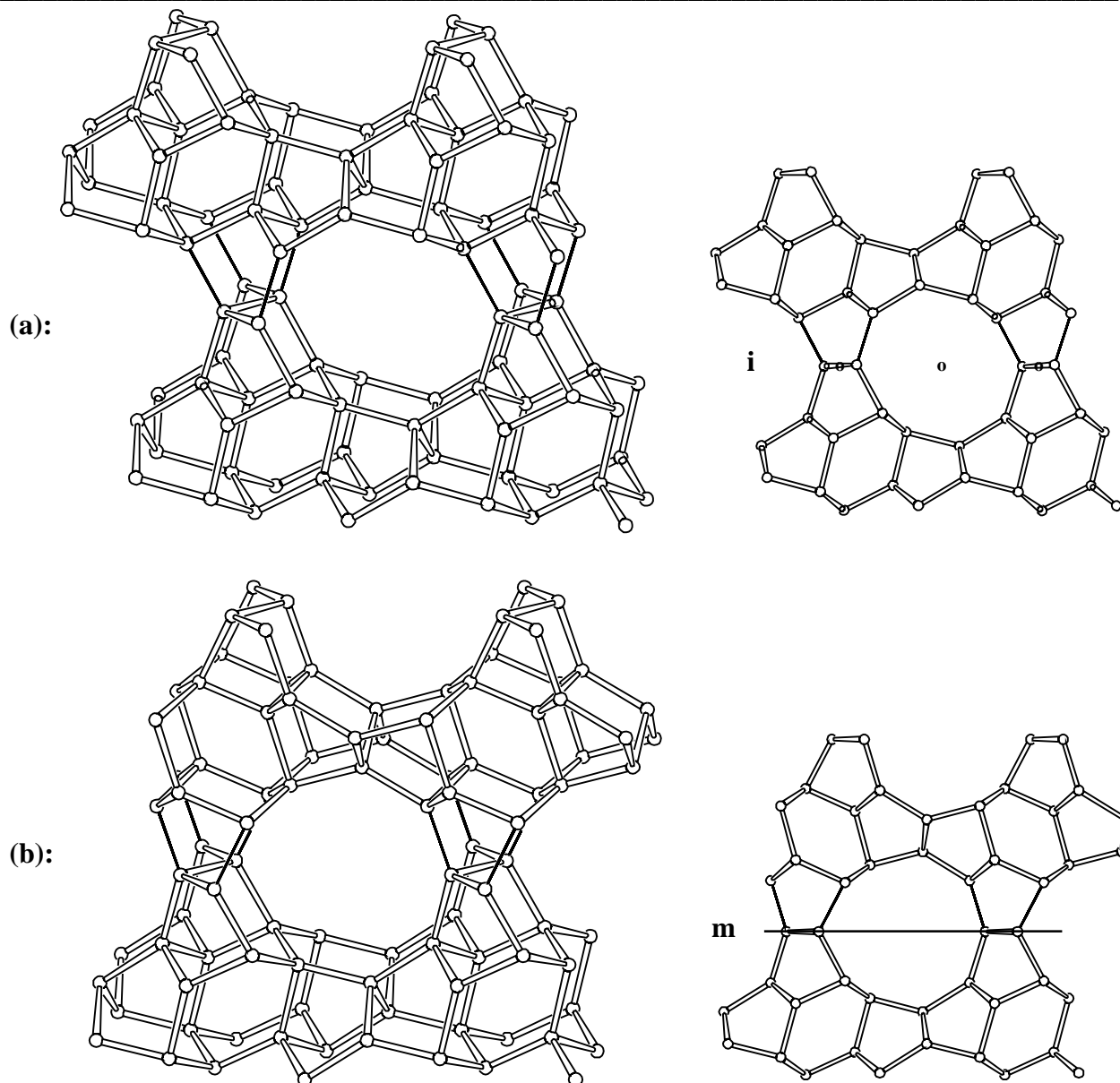


Figure 3: Perspective view (left) and parallel projection of the connection modes **(a)** and **(b)** in the MTT/TON family of zeolite frameworks seen perpendicular to the plane normal of the PerBU

---

Once the distribution of the symmetry elements **i** and **m** between the PerBU's is known, the 3-dimensional structure is defined. ▲

5. The Simplest Ordered End-Members in the MTT/TON family are presented in Figure 4:

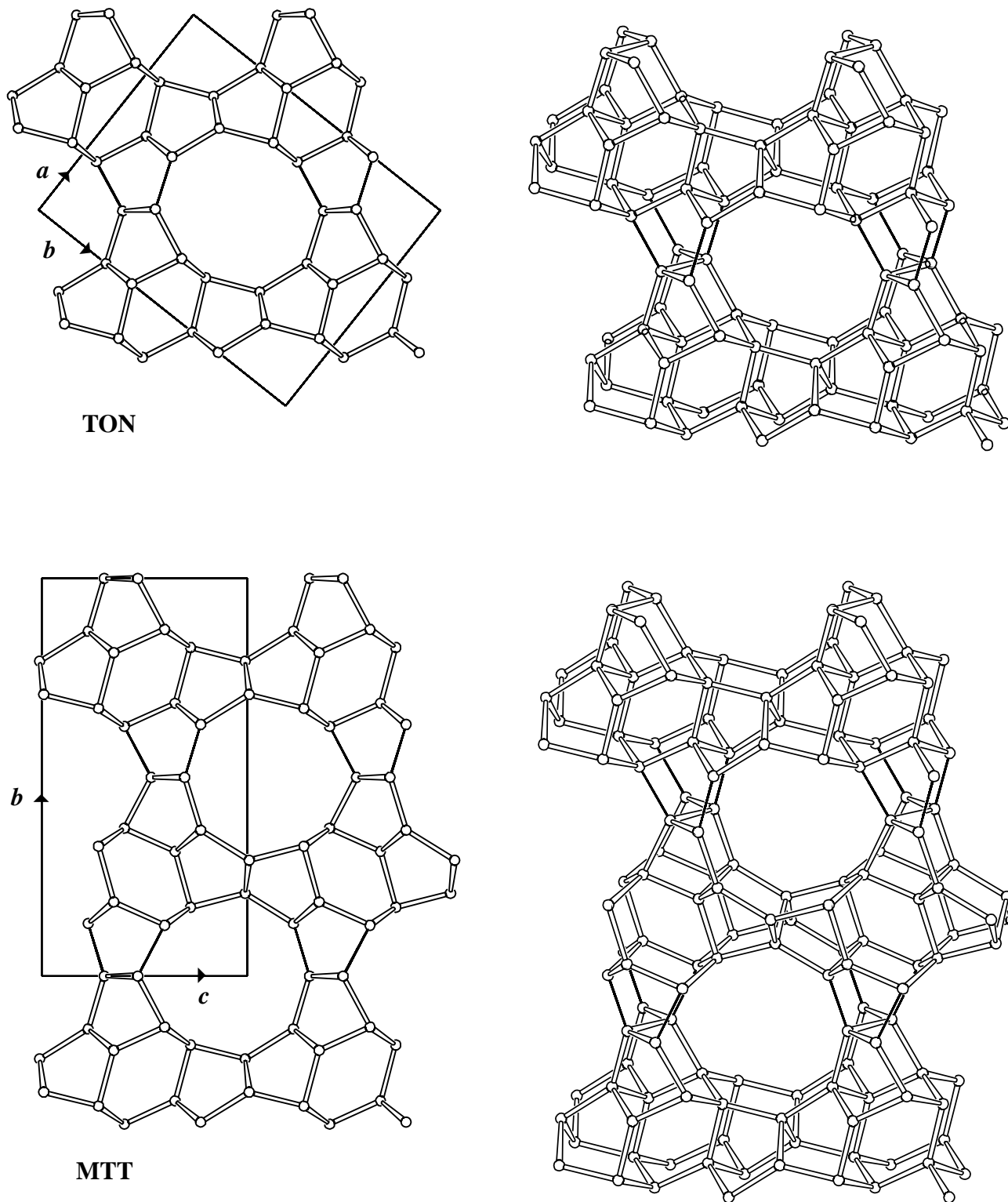


Figure 4: Perspective view and parallel projection along the zigzag chain axis of the unit cell content of the two simplest ordered end-members in the MTT/TON family: TON (top) and MTT (bottom)

Pure TON(1,2) and MTT(3,4) are obtained when neighbouring PerBU's, stacked along the plane normal, are exclusively related by  $\mathbf{i}$  and  $\mathbf{m}$ , respectively.



## 6. Disordered Materials Synthesized and Characterized to Date:

to be added



## 7. Supplementary Information

### 7.1 Comparison with SFE:

The PerBU in SFE is composed of infinite building units consisting of seven zz chains. PerBU's are connected after pure translations along the cell axes as shown in Figure 5. [For more details: see the building scheme of SFE in 'Schemes for Building Zeolite Framework Models' on <http://www.iza-structure.org/databases/>]

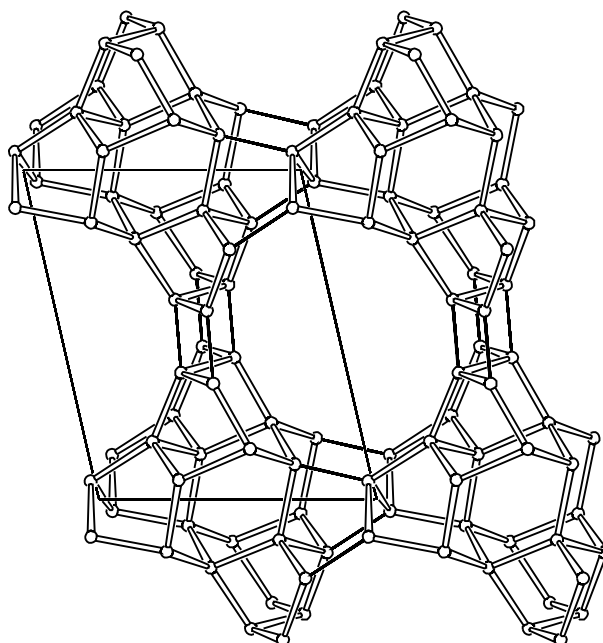
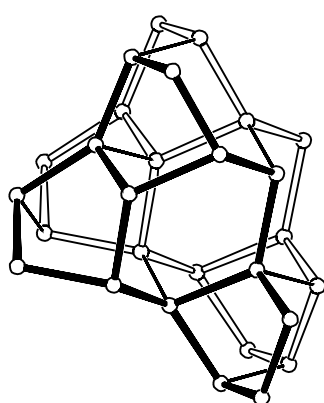


Figure 5: Infinite building unit, (top left) and perspective view (right) of the unit cell content of SFE



## 8. References

- (1) S.A.I. Barri, G.W. Smith, D. White and D. Young, *Nature* **312**, 533 (1984).
- (2) R.M. Highcock, G.W. Smith and D. Wood, *Acta Cryst.* **C41**, 1391 (1985).
- (3) A.C. Rohrman Jr., R.B. LaPierre, J.L. Schlenker, J.D. Wood, E.W. Valyocsik, M.K. Rubin, J.B. Higgins and W.J. Rohrbaugh, *Zeolites* **5**, 352 (1985).
- (4) B. Marler, C. Deroche, H. Gies, C.A. Fyfe, H. Grondey, G.T. Kokotailo, Y. Feng, S. Ernst, J. Weitkamp and D.E. Cox, *J. Appl. Cryst.* **26**, 636 (1993).

