

The AEN/UEI family

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1. The Periodic Building Unit (PerBU) equals the xy layer shown in Figure 1. This layer is built from single T6-ring chains shown in Figure 2.

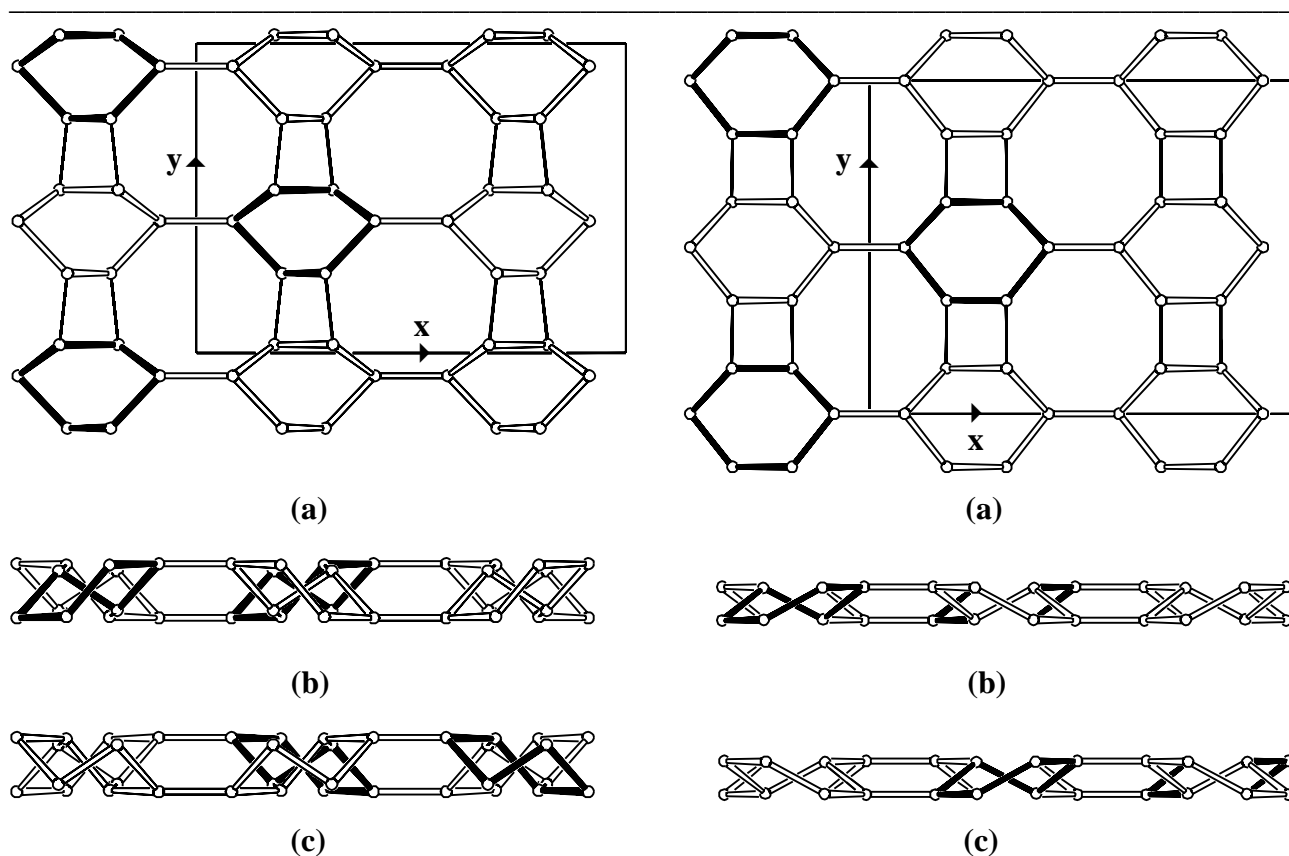


Figure 1: The PerBU of the AEN/UEI family of zeolite frameworks shown parallel to the plane normal z (a) and along y (b and c). At left and right different distortions of the PerBU are illustrated. The PerBU's, depicted in (b) and (c) at the left, are related by a rotation of 180° about z and the PerBU's in (b) and (c) at the right are related by a shift of $\frac{1}{2}x$.

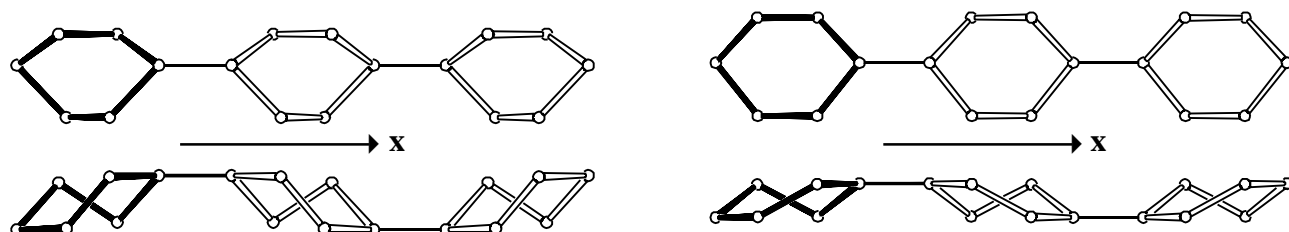


Figure 2: Chain of single T6-rings seen along z (top) and along y (bottom). Left and right: different distortions of the twisted-chair conformation of the T6-rings in the chain are shown ▲

The PerBU of the AEN/UEI family is composed of T6-rings (bold in Figs.1 and 2) with a twisted-chair conformation. T6-rings, related by a mirror plane perpendicular to x , are connected into chains along x (Fig.2). Chains, related by a shift of $\frac{1}{2}x$, are connected along y into the xy layer (Fig.1). [Compare with the xy layers in AWO, ATT and ATV depicted in the Supplementary Information].

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 $Cm1(1)$. ▲

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 rotation of 180° about z . The connectivity shows inversion symmetry ($i: \circ$) between successive layers (zigzag chains and (distorted) T6-rings are formed).

(b): neighbouring PerBU's are related by a translation of $\frac{1}{2}x$. The connectivity now exhibits mirror symmetry ($m: |$) between successive layers (double crankshaft chains parallel to z are formed).

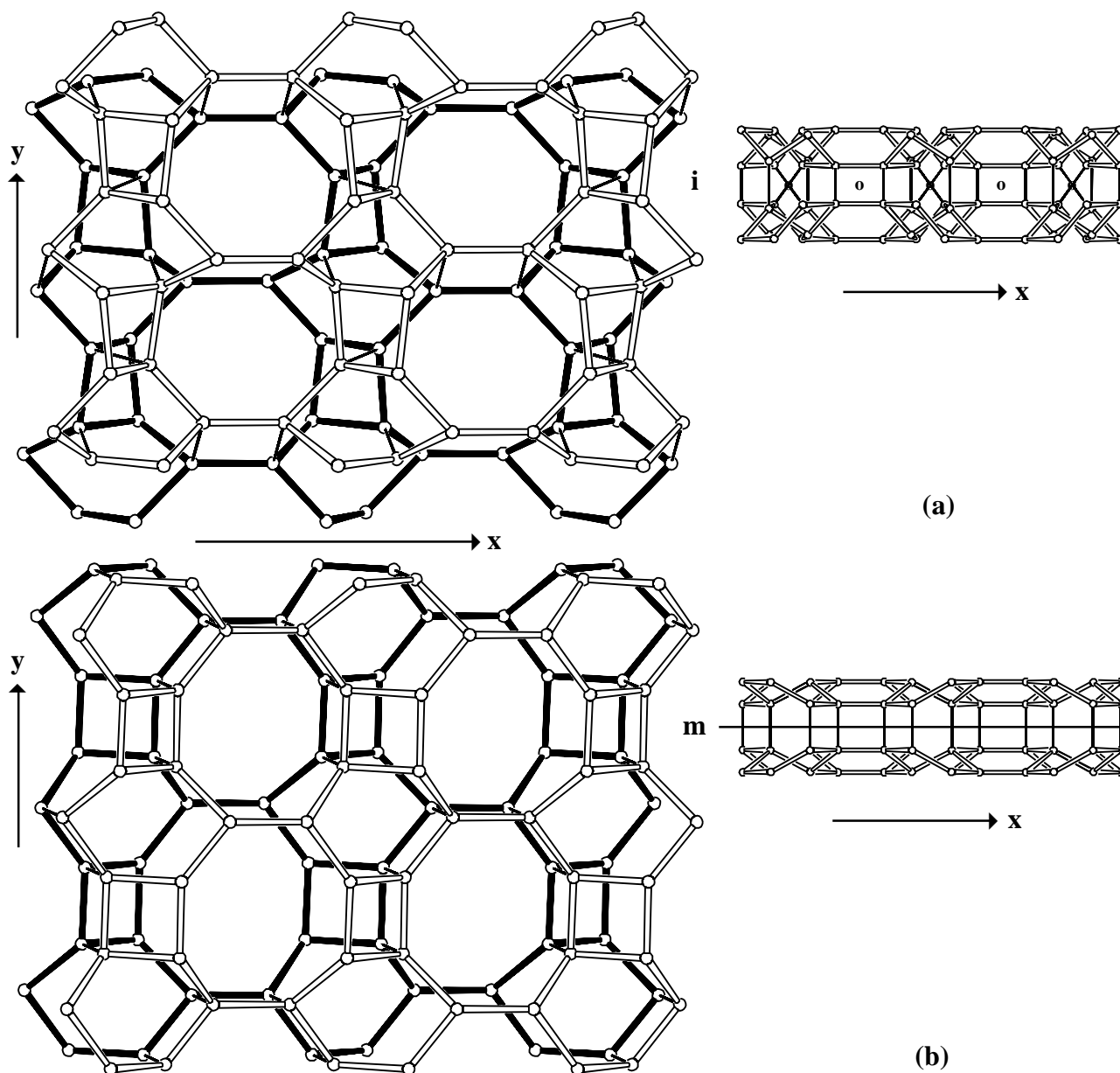


Figure 3: Perspective view along z (left) and parallel projection along y (right) of the connection modes (a) and (b) in the AEN/UEI family. (One PerBU is drawn in bold for clarity) ▲

Once the distribution of the symmetry elements \mathbf{i} and \mathbf{m} between the layers stacked along \mathbf{z} is known, the 3-dimensional structure is defined.

5. The Simplest Ordered End-Members in the AEN/UEI family are shown in Figure 4:

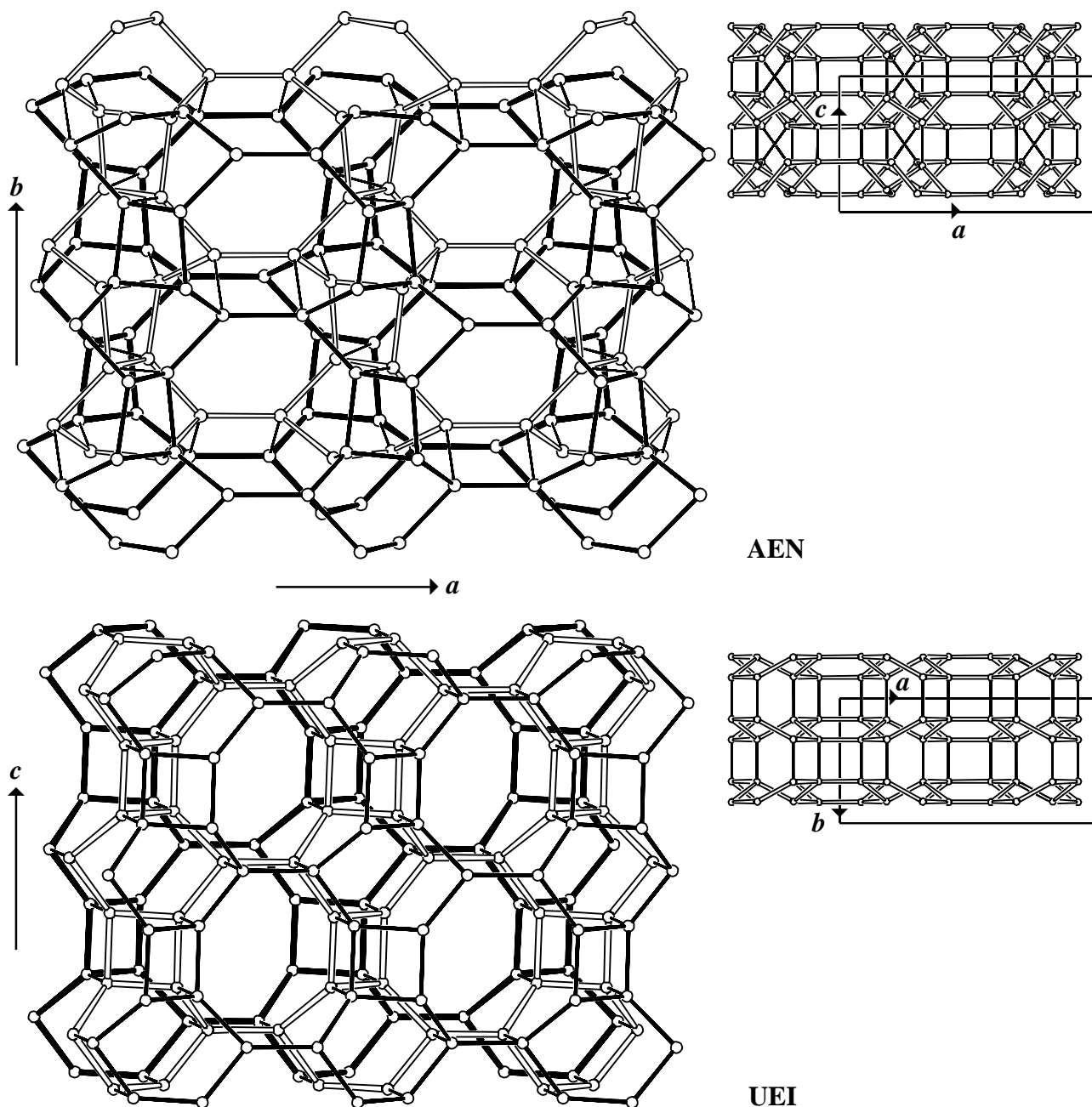


Figure 4: Unit cell content of AEN in perspective view along \mathbf{c} (top left) and in parallel projection along \mathbf{b} (top right) and of UEI seen along \mathbf{b} (bottom left) and along \mathbf{c} (bottom right). In the perspective drawings, two PerBU's are drawn in bold for clarity

Pure AEN(1) and UEI(2) are obtained when neighbouring PerBU's, stacked along the plane normal of the PerBU, are exclusively related by \mathbf{i} and \mathbf{m} , respectively.

6. Disordered Materials Synthesized and Characterized to Date:

No disordered materials known to date.



7. Supplementary Information

7.1 Comparison with AWO:

The PerBU in AWO is the xy layer composed of chains of T6-rings depicted in Figure 5. Neighbouring T6-rings within the chains are related by a rotation of 180° about the chain axis x (and not by a mirror plane perpendicular to x as in AEN and UEI). Neighbouring chains, related by a mirror operation perpendicular to y accompanied by a translation of $\frac{1}{2}x$, are connected along y through T4-rings into the xy layer. The T6-rings exhibit the same twist-chair conformation as the T6-rings in AEN and UEI. [For more details: see the building scheme of AWO in 'Schemes for Building Zeolite Framework Models' on <http://www.iza-structure.org/databases/>].

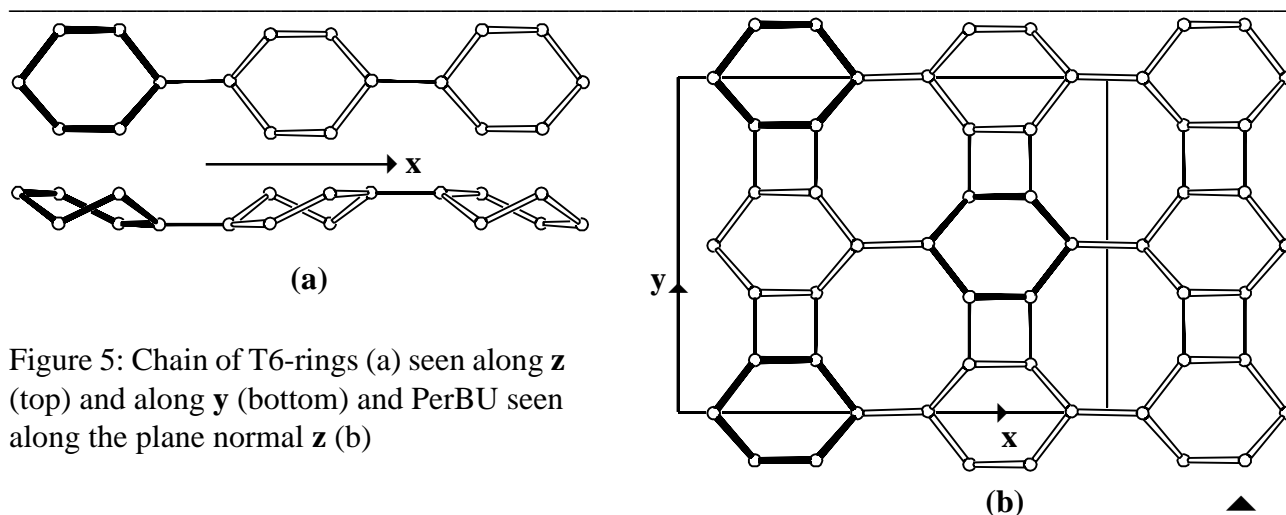


Figure 5: Chain of T6-rings (a) seen along z (top) and along y (bottom) and PerBU seen along the plane normal z (b)

7.2 Comparison with ATT:

The PerBU in ATT is the xy layer composed of chains of T6-rings depicted in Figure 6. Neighbouring T6-rings within the chains, related by pure translations along the chain axis x (and not by a mirror perpendicular to x as in AEN and UEI), are axially connected along x . Neighbouring chains, related by pure translations along y , are connected along y through T4-rings into the xy layer. The T6-rings exhibit a chair conformation (as in ATV). This conformation is different from the T6-ring conformation in AEN and UEI. [For more details: see the building scheme of ATT in 'Schemes for Building Zeolite Framework Models' on <http://www.iza-structure.org/databases/>].

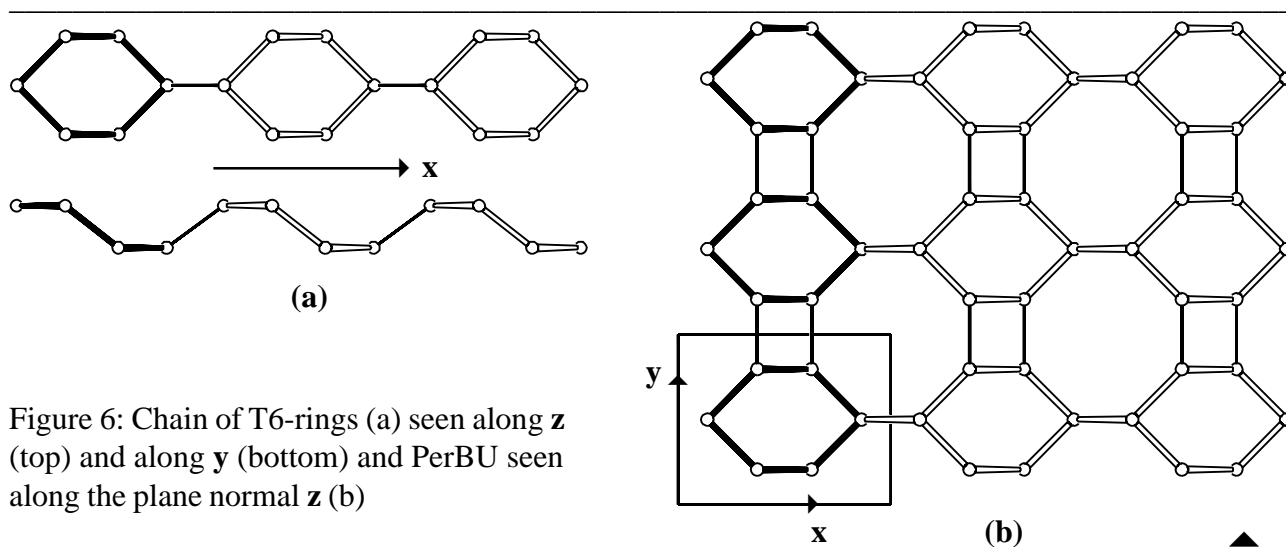


Figure 6: Chain of T6-rings (a) seen along z (top) and along y (bottom) and PerBU seen along the plane normal z (b)

7.3 Comparison with ATV:

The PerBU in ATV is the **xy** layer composed of chains of T6-rings depicted in Figure 7. Neighbouring T6-rings within the chains, related by pure translations along the chain axis **x** (and not by a mirror plane perpendicular to **x** as in AEN and UEI), are equatorially connected along **x**. Neighbouring chains, related by a rotation of 180° about the chain axis **x**, are connected through T4-rings into the **xy** layer. The T6-rings exhibit a chair conformation (as in ATT). This conformation is different from the T6-ring conformation in AEN and UEI. [For more details: see the building scheme of ATV in 'Schemes for Building Zeolite Framework Models' on <http://www.iza-structure.org/databases/>].

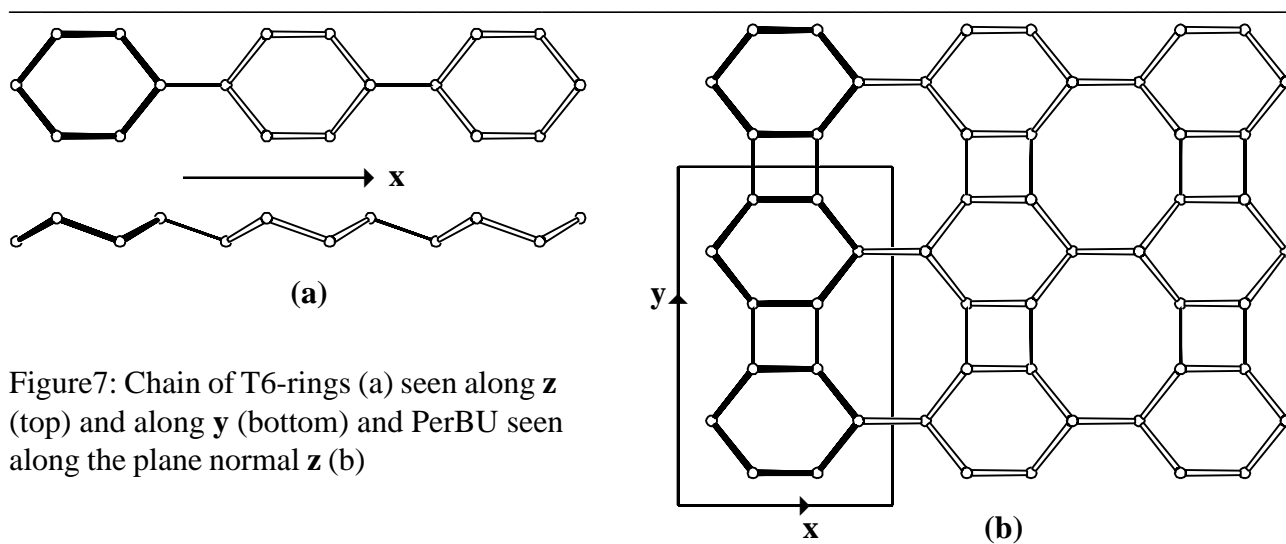


Figure7: Chain of T6-rings (a) seen along **z** (top) and along **y** (bottom) and PerBU seen along the plane normal **z** (b)

8. References

- (1) J.B. Parise, *Stud. Surf. Sci. Catal.* **24**, 271 (1985).
- (2) L. Josten, A. Simon, V. Gramlich and J. Patarin, *Chem. Mater.* **13**, 1305 (2001).