

The Montesommaite 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) equals the T4-ring layer depicted in Figure 1:

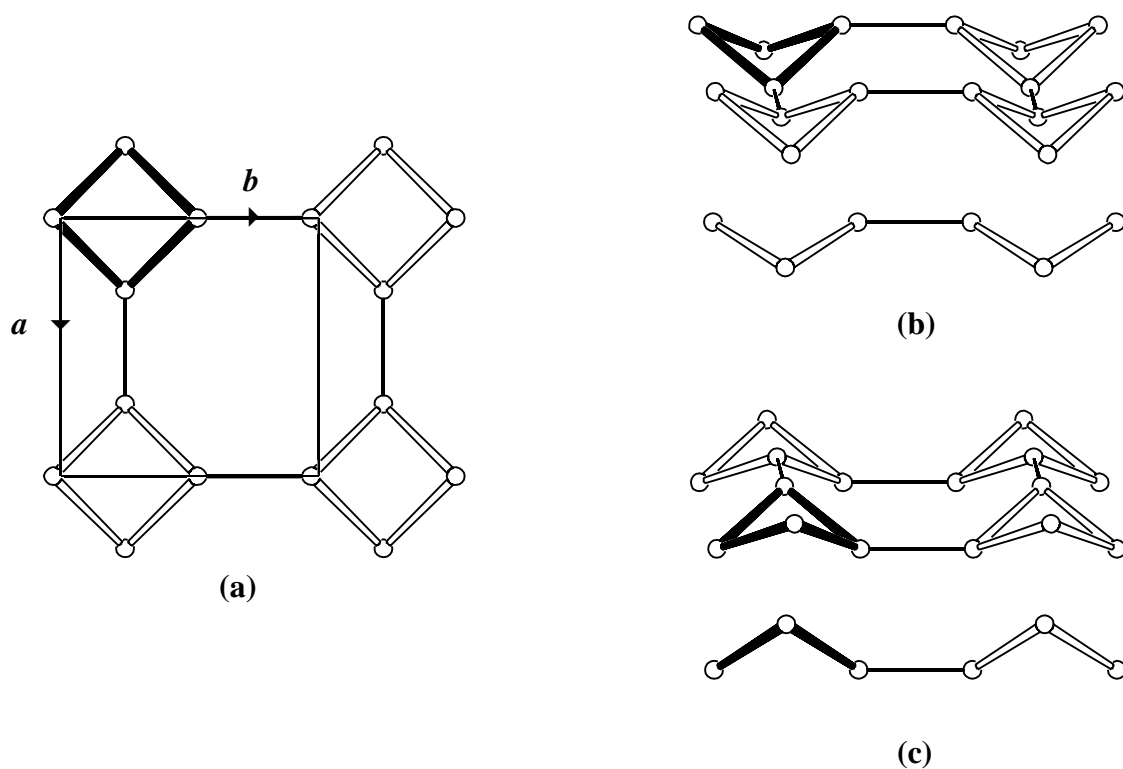


Figure 1: PerBU of the montesommaite family of zeolite frameworks seen along *c* (a) and perpendicular to *c* (b and c) in perspective view (top) and in parallel projection (bottom)

The PerBU of the montesommaite family is composed of T4 rings (in bold) related by pure translations along *a* and *b*. Views along [001] (Fig.1a), [100] (Fig.1b) and [010] (Fig.1c) are shown. The layers depicted in Figure 1b and 1c are identical and related by a 90° rotation about the plane normal or by a mirror operation perpendicular to the plane normal.

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 $P(\bar{4})m2$.

4. Connectivity Pattern of the PerBU:

Neighbouring PerBU's, related by a mirror operation, can be connected along c in two different ways:

(a) the lateral shift of the top layer along a or b is zero; denoted as (0,0). This connectivity, which shows mirror symmetry (\mathbf{m} ; |) between successive layers, has not been observed yet.

(b) the lateral shift of the top layer is (plus or minus) $\frac{1}{2}a$ or $\frac{1}{2}b$; denoted as $(\frac{1}{2},0)$ or $(0,\frac{1}{2})$, respectively. The connectivity exhibits inversion symmetry (\mathbf{i} ; \circ) between successive layers.

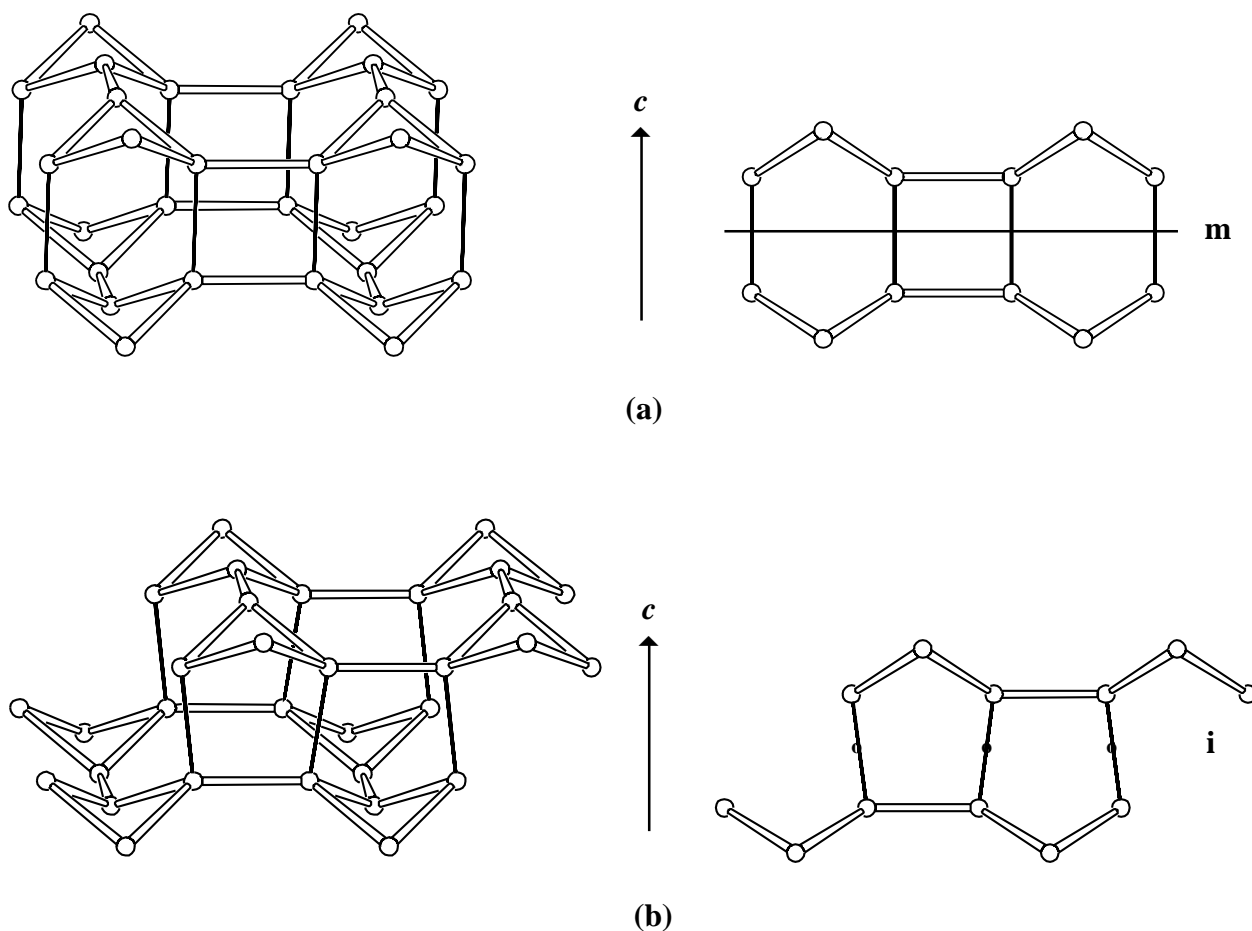


Figure 2: Perspective view (left) and parallel projection (right) of the connection modes (a) and (b) in the montsommaite family of zeolite frameworks seen perpendicular to c . In connection mode (a) the neighbouring PerBU's are connected through (fused) T6-T4-T6 ring sequences and in connection mode (b) through (fused) T5-T5-T5 ring sequences

Once the distribution of the lateral shifts between the layers stacked along c is known, the 3-dimensional structure is defined.

5. The Simplest Ordered End-Members in the montesommaite family are given below. Only end-member number **2** has been observed as pure single crystal material and represents the structure with framework type code MON(1).

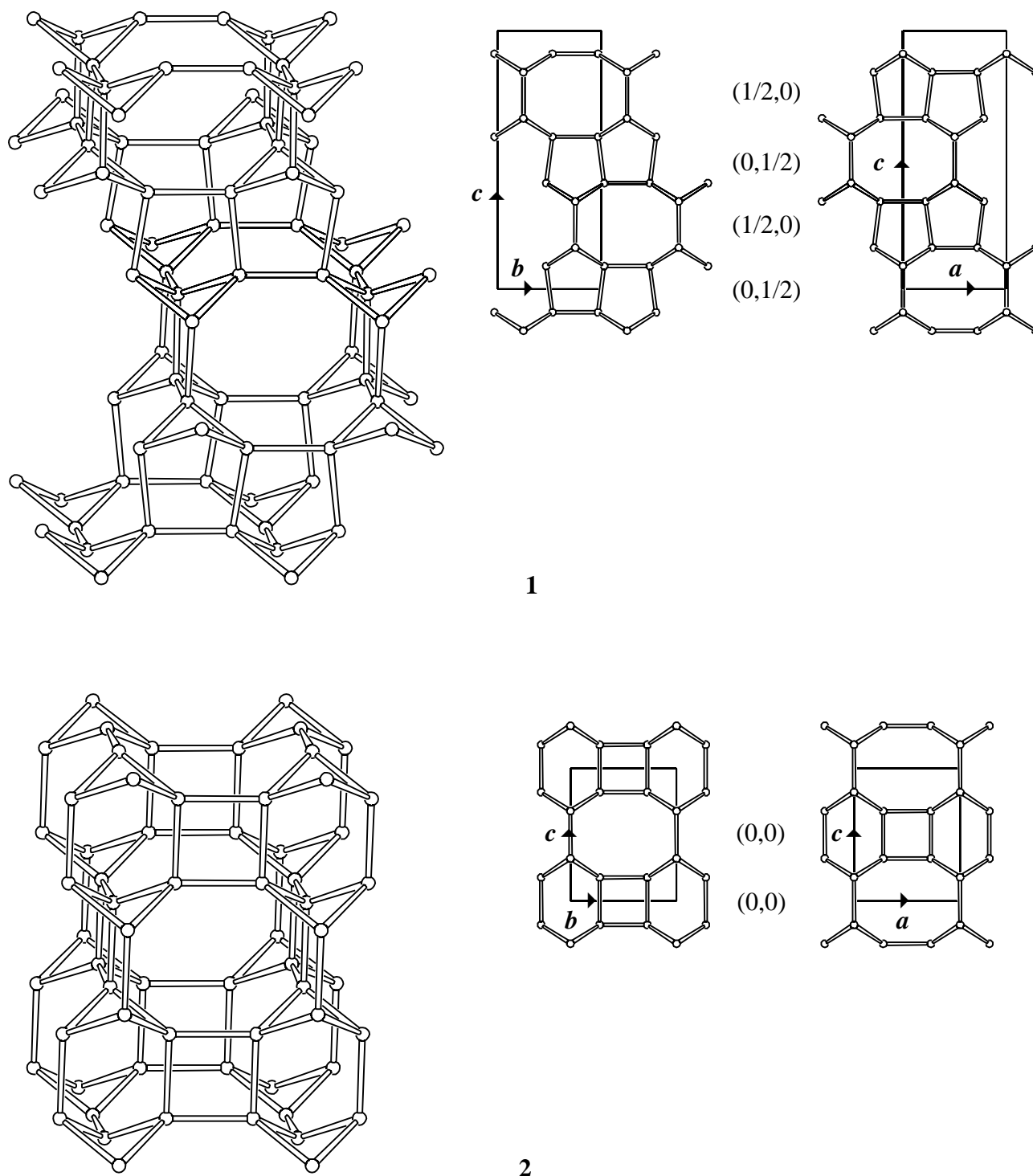


Figure 3: Perspective drawing (left) and parallel projection along a (middle) and b (right) of the two simplest ordered end-members in the montesommaite family. The connectivity codes are given (cf. Table 1 on next page)

Table 1: Stacking sequences of PerBU’s for the simplest ordered end-members in the montesommaite family. The end-member numbers refer to the framework plots **1** and **2** in Figure 3 on the previous page.

<i>End-Member</i>	<i>Lateral shifts between subsequent PerBU's stacked along c; shifts are in fractions of (a, and b)</i>					<i>space group</i>
1	(0,0);	(0,0);	(0,0);.....			P4 ₂ /mmc
2	(0,1/2);	(1/2,0);	(0,1/2);	(1/2,0);	(0,1/2);.....	I4 ₁ /amd *

* This is the end-member with framework type code MON.

6. Disordered Materials Synthesized and Characterized to Date:

none

7. Supplementary Information

to be added

8. References

(1) R.C. Rouse, P.J. Dunn, J.D. Grice, J.L. Schlenker, and J.B. Higgins, Am. Mineral. **75**, 1415 (1990).