

# The Decasil Family

1. The Periodic Building Unit (PerBU) -
2. Type of Faulting -
3. The Rod 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 chain shown in Figure 1:

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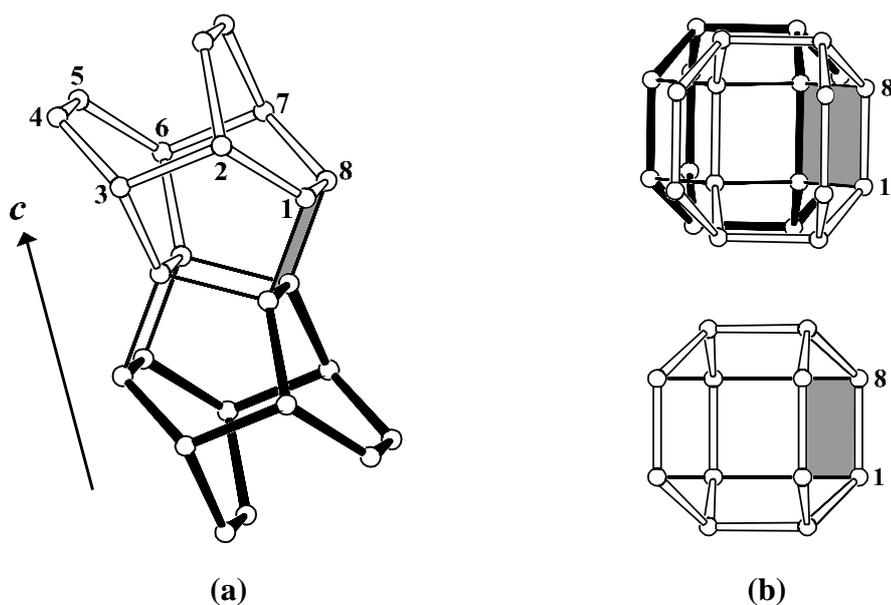


Figure 1: Perspective view of the PerBU in the Decasil family seen perpendicular to the chain axis  $c$  (a) and along  $c$  (b) in perspective view (top) and in parallel projection (bottom)

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The PerBU in the Decasil family of zeolite frameworks is formed by connecting T12 units (two-fold connected double T6-rings; depicted in Fig.1a in bold), related by pure translations along  $c$ , through T4-rings. As orientation sensitive indicator one of the T4-rings is shaded. The numbered T atoms are used in describing the connection modes.

**2. Type of Faulting:** 2-dimensional stacking disorder of the PerBU's along [100] and [010].

**3. The Rod Symmetry** of the PerBU is  $2/m$ .



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

Neighbouring PerBU's can be connected via O-bridges in several ways:

- the chains are connected after pure translations. The connection modes are shown in **a**, **d**, **e** and **g** in Figure 2a.
- the chains are connected after a translation accompanied by a  $180^\circ$  rotation about the chain axis as illustrated in connection modes **b** and **c** in Figure 2a.
- the chains are connected after translation followed by a  $+90^\circ$  or  $-90^\circ$  rotation about the chain axis. The resulting connection modes are given in **f** and **h** in Figure 2a.

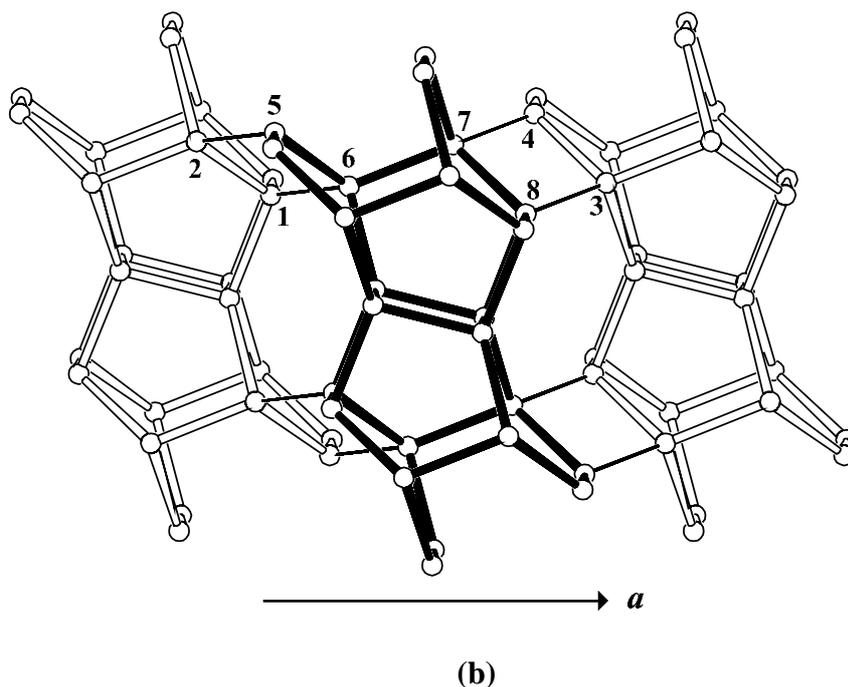
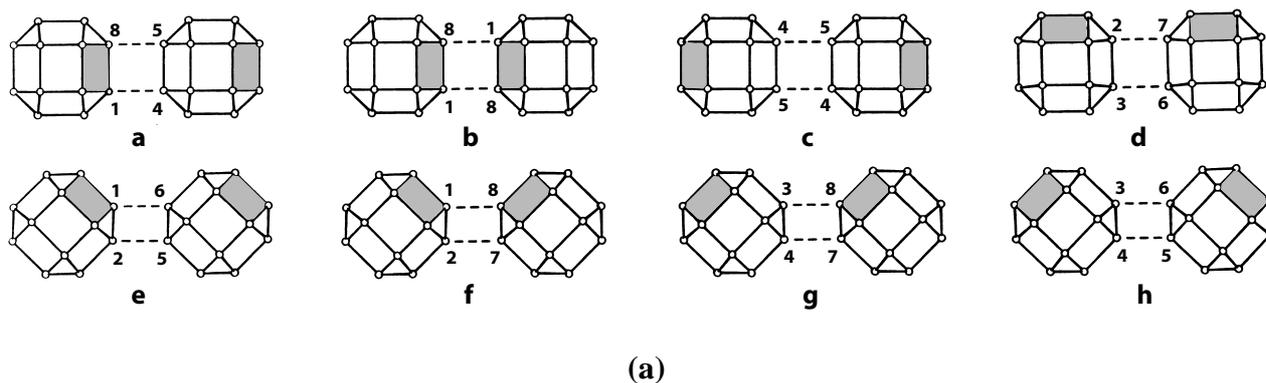


Figure 2(a): Connection modes, denoted **a** to **h**, of neighbouring PerBU's and (b): perspective view of the connection modes **e** and **g** where one of the PerBU's is drawn in bold

The connectiomodes **b** and **c**, **e** and **g**, and **f** and **h** are pairwise identical. The modes in each pair are related by a  $180^\circ$  rotation about an axis perpendicular to the plane of the connected chains. Once the distribution of the connection modes in two dimensions is known the 3-dimensional structure is defined.



**5. The Simplest Ordered End-Members** in the decasil family are shown in Figure 3. Only end-member **1** has been observed as pure single crystal material and represents the framework with framework type code RTE (1,2).

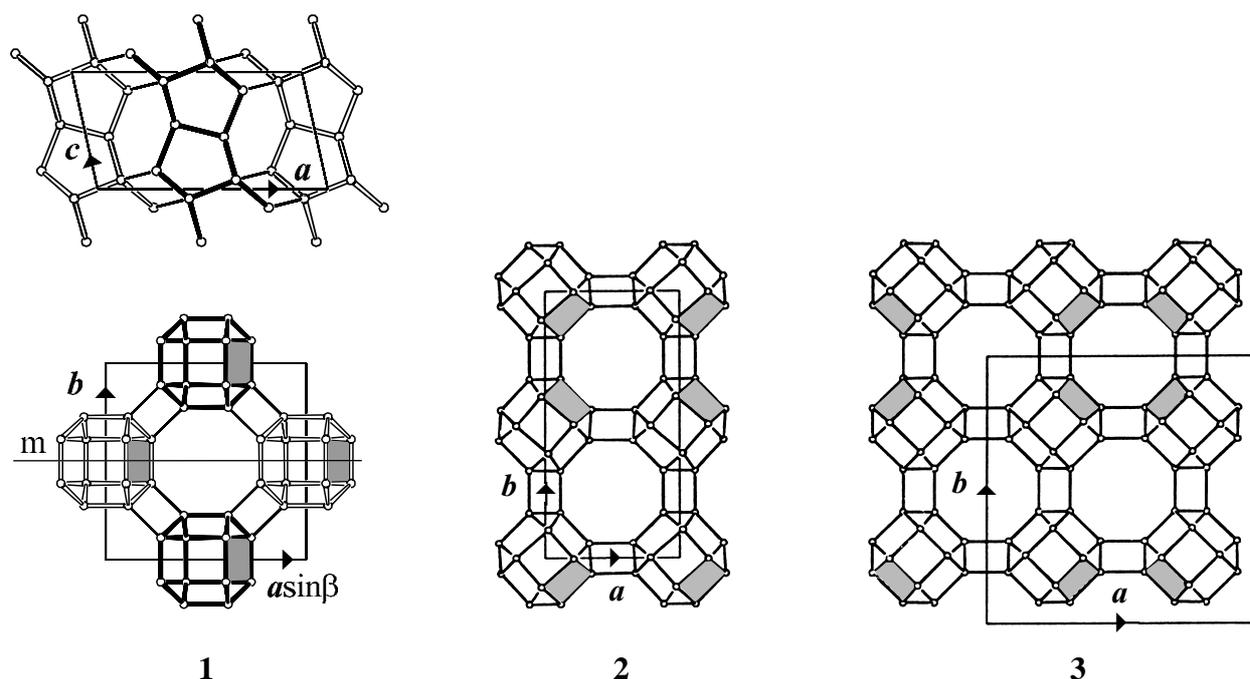


Figure 3: Projections of the unit cell content of the three simplest ordered end-members in the Decasil family (cf. Table 1). End-member **1**, seen along **b** (top) and along **c** (bottom), corresponds to the zeolite with framework type code RTE. The fourth PerBU, completing the cell content in RTE, is obtained by applying to the heavy bold PerBU in Figure 2b a mirror operation perpendicular to **b** (equal to the *m* operation indicated in Fig.3)

Table1: Connection mode of the rod-like PerBU along **a** and **b** for the simplest end-members in the decasil family. The end-member number refers to the framework plots given in Figure 3

<i>End-member</i>	<i>Sequence of the Connection Modes along a and b:</i> ( <i>along a,.....; b,.....</i> )	<i>Space Group</i>
<b>1</b>	( <b>e,e,.....; g,g,.....</b> )	C2/m <sup>1</sup>
<b>2</b>	( <b>g,g,.....; h,f,h,.....</b> )	P2/m
<b>3</b>	( <b>h,f,h,.....; h,f,h,.....</b> )	P4/mmm

<sup>1</sup> This is end-member with framework type code RTE (1,2); in this framework the sequence of the connection modes given is along  $(-a + b)$  and  $(a + b)$ , respectively.

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

RUB-4 (1,3)



## 7. Supplementary Information

to be added

## 8. References

- (1) B. Marler, A. Grünewald-Lüke and H. Gies *Zeolites* **15**, 388 (1995).
- (2) B. Marler, A. Grünewald-Lüke and H. Gies, *Microp. Mesopor. Mater.* **26**, 49 (1998).
- (3) A. Grünewald-Lüke and H. Gies, *Microp. Mater.* **3**, 159 (1994).
- (4) P. Daniels, *J. Appl. Cryst.* **31**, 559 (1998). 