Unit-distance Realizations of Combinatorial Zeolites

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1. Chemical Zeolites

- crystalline solid
- units: Si + 4O
- two covalent bonds per oxygen
- naturally occurring
- synthesized
- theoretical

Used as microfilters.
2. Combinatorial Zeolites

Combinatorial $d$-Dimensional Zeolite

- A connected complex of corner sharing $d$-dimensional simplices
- At each corner there are exactly two distinct simplices
- Two corner sharing simplices intersect in exactly one vertex.

$\textbf{body-pin graph}$

Vertices: simplices (silicon)
Edges: bonds (oxygen)

There is a one-to-one correspondence between combinatorial $d$-dimensional zeolites and $d$-regular body-pin graphs.
Graph of a Combinatorial Zeolite

is obtained by replacing each $d$-dimensional simplex with $K_{d+1}$.

The graph of the zeolite is the line graph of the Body-Pin graph.

**Whitney**

(1932) proved that connected graphs $X$ on at least 5 vertices are strongly reconstructible from their line graphs $L(X)$. Moreover, $\text{Aut}(X) \cong \text{Aut}(L(X))$. 
3. Realization

A realization of a $d$-dimensional zeolite

An placement (embedding) of vertices of the the $d$-dimensional complex in $\mathbb{R}^d$.
Equivalently a placement (embedding) of the vertices of the line graph of the body-pin graph.

unit-distance realization

A realization where all edges join vertices distance 1 apart in $\mathbb{R}^d$.

non-interpenetrating realization

A realization where simplices are disjoint except at joined vertices.
The typical situation: Not unit distance realizable.
4. 2d Zeolites

Smallest 2d zeolite is the line graph of $K_4$: The graph of the octahedron with four (edge disjoint) faces. For body-pin graphs on more than 4 vertices, the zeolite can be recovered uniquely from the line-graph.
It is just as easy to construct infinite symmetric examples:
Showing a different symmetry
5. Finite Zeolites

Body pin graph: $K_{3,3}$. Since the body pin graph is not planar, the resulting zeolite cannot be planar. Its underlying graph is generically globally rigid. However, it has a unit distance realization in the plane which is a mechanism.
Harborth’s Example
6. The Layer Construction

\( Z = (T, C') \) is a combinatorial zeolite realizable in dimension \( d \).
\( \mathbb{R}^d \subseteq \mathbb{R}^{d+1} \)

Label each \( t \in T \) arbitrarily with \( \pm 1 \).
For \( +1 \), erect a \( d+1 \) dimensional simplex in the upper half space,
For \( -1 \), erect a \( d+1 \) dimensional simplex in the lower half space,
Call the Complex \( Z_a \) and its mirror image \( Z_b \).

Alternately staking \( Z_a \) and \( Z_b \) gives a \textit{layered Zeolite} in \( \mathbb{R}^{d+1} \).
Labels all +1
A two layered zeolite.
The general case starting from a finite zeolite.

**Theorem:** There are uncountably many isomorphism classes of unit distance realizable zeolites in $\mathbb{R}^3$. (actually in any dimension $d > 1$.)
Chemical Zeolites
Combinatorial
Realization
2d Zeolites
Finite Zeolites
The Layer...
Holes in Zeolites
Motions
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Proof:
7. Holes in Zeolites
8. Motions

Degree of Freedom

Each simplex $d$-dimensional simplex has $d(d + 1)/2$ degrees of freedom.
Each contact of the $d + 1$ contacts removes $d$ degrees.
By a naïve count, a zeolite is rigid - (overbraced by $d(d + 1)/2$.)
Generically globally rigid in the plane.
Generically globally rigid in the plane.

A 4-regular vertex transitive graph is globally rigid unless it has a 3-factor consisting of $s$ disjoint copies of $K_4$ with $s \geq 3$. [Jackson, S, S – 2004]
Are there finite generically flexible 2D Zeolites? Yes, line graphs of 3-regular graphs with edge connectivity less than 3.
Are there finite generically rigid but not globally rigid 2D Zeolites?
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9. A geometric approach
Combinatorial version of the gain graph
Geometric version of the gain graph
It’s a geometric line graph!
10. Open Problems

1. Does there exist a finite 2D zeolite with a planar unit distance realization and having no non-simplex triangle?

2. Find \( f(n) \) so that, given a Unit Distance realization of an \( n \)-dimensional zeolite, its line graph has a unit distance realization in dimension \( f(n) \)

[If \( f(n) = 2n - 1 \), then the line graph corresponds to an \( 2n - 1 \) dimensional zeolite.]

3. In particular, find \( f(2) \).

4. Do there exist finite non-interpenetrating zeolites with unit distance plane realization which is non-rigid?
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