From combinatorial zeolites to geometric realizations

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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.

**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

[9](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

A placement (embedding) of the vertices of 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.
A finite 3-D symmetric example:

Model with its two planes of symmetry
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 [4, 3]
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 \( \mathbb{R}^{d+1} \).

\[ \text{Diagram of layered zeolite} \]
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 $d > 1$. [7])
Proof:
7. Holes in Zeolites
8. Motions

Degree of Freedom

Each $d$-dimensional simplex has $d(d + 1)/2$ degrees of freedom. Each 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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See [5]
9. A geometric approach
Combinatorial version of the gain graph
Geometric version of the gain graph
It’s a geometric line graph!
THEOREM [1] Let $G$ be a locally finite 3-connected almost vertex-transitive planar graph with at most one end. Then $G$ has an embedding on a natural geometry such that all automorphisms of $G$ are induced by isometrics of the geometry. Straightening Lemma for maps on the sphere [6].
10. Vertex transitive 3-regular
May be pinned isostatically [8].
11. Open Problems

1. Use growth rate result to show unit distance embeddability of the line graph of $B_r$ in the almost vertex-transitive case.

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

3. Design nano lentils and prove their realization

4. Line graphs of line graphs?

5. Do there exist finite non-interpenetrating zeolites with unit distance plane non-rigid realizations?
Harborth’s Construction
References


