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#### Combinatorial Zeolites

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# 1. Chemical Zeolites

- crystalline solid
- $\bullet$  units: Si + 4O





two covalent bonds per oxygen



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- naturally occurring
- synthesized
- $\bullet$  theoretical

Used as microfilters.

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# 2. Combinatorial Zeolites

# Combinatorial d-Dimensional Zeolite

- $\bullet$  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.





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

## 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.

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## unit-distance realization

graph of the body-pin graph.

3. Realization

complex in  $\mathbb{R}^d$ .

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

An placement (embedding) of vertices of the the d-dimensional

Equivalently a placement (embedding) of the vertices of the line

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### non-interpenetrating realization

A realization of a  $d$ -dimensional zeolite

A realization where simplices are disjoint except at joined vertices.









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The typical situation: Not unit distance realizable.



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# 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.





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## It is just as easy to construct infinite symmetric examples:





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## Showing a different symmetry





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# 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.





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### Harborth's Example





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# 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 upper half space,

Call the Complex  $Z_a$  and its mirror image  $Z_b$ .



# Alternately staking  $Z_a$  and  $Z_b$  gives a *layered Zeolite* in  $\mathbb{R}^{d+1}$ .



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## Labels all  $+1$ A two layered zeolite.







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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  $d > 1$ .)





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#### Proof:



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# 7. Holes in Zeolites



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## 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.



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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]















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# 9. 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 a 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. Are there finite generically flexible 2D Zeolites?
- 5. Are there finite generically non-globally rigid 2D Zeolites?
- 6. Do there exist finite non-interpenetrating zeolites with unit distance plane realization which is non-rigid.







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### Harborth's Construction