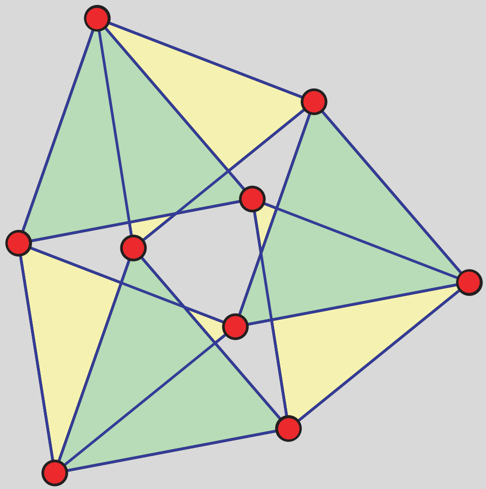
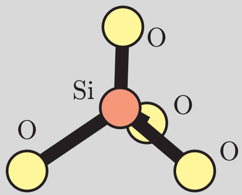
Combinatorial Zeolites

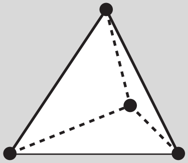
Herman Servatius — Clark University
(Brigitte Servatius — WPI)



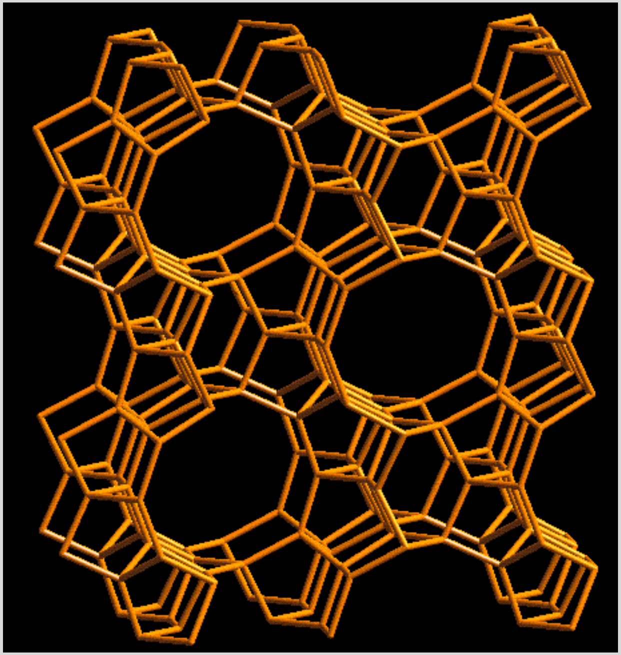
1. Chemical Zeolites

- 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

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

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.

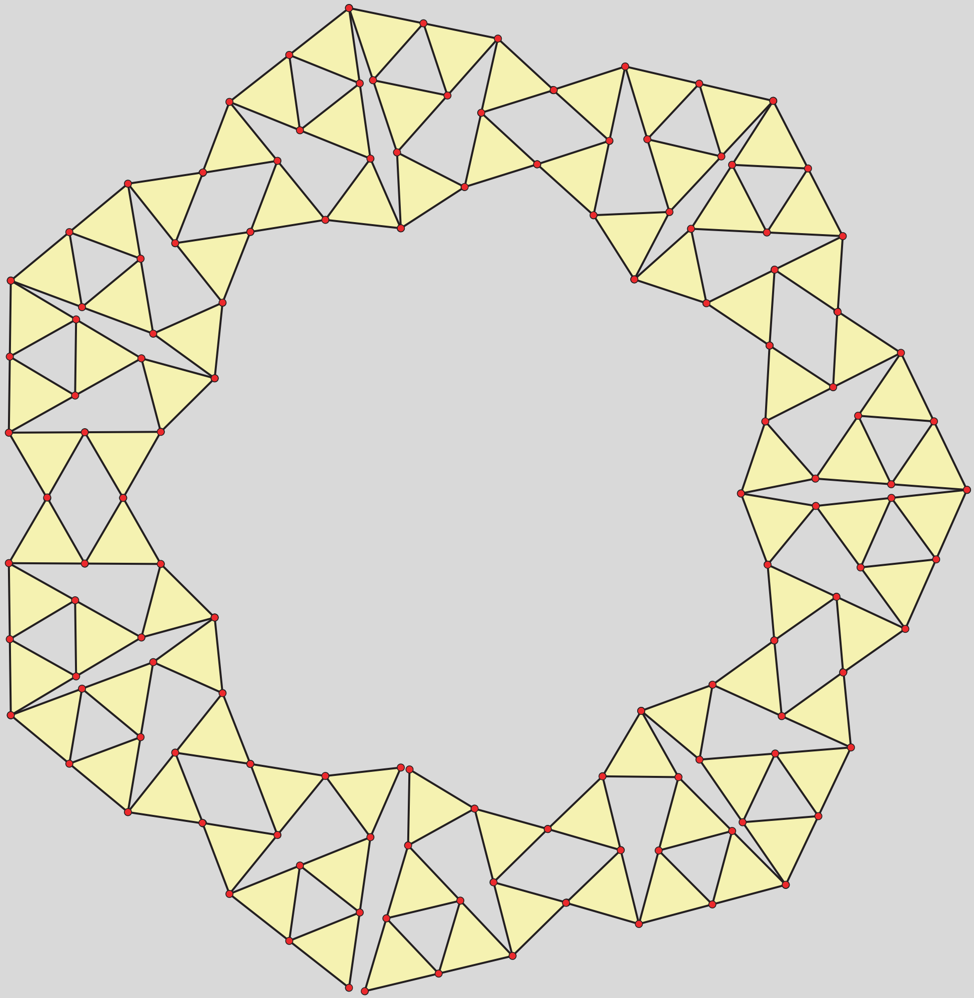
unit-distance realization

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

non-interpenetrating realization

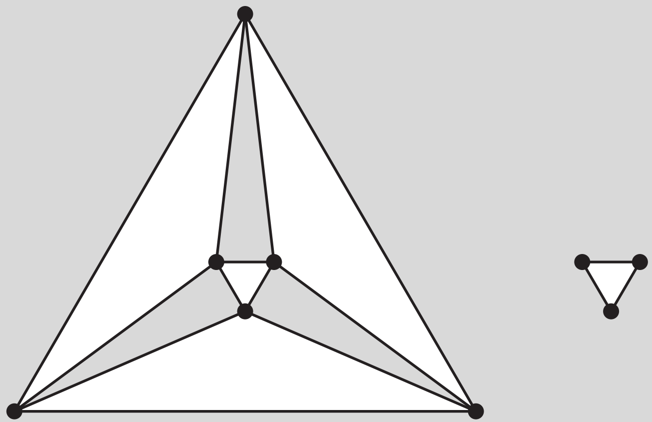
A realization where simplices are disjoint except at joined vertices.

The typical situation: Not unit distance realizable.

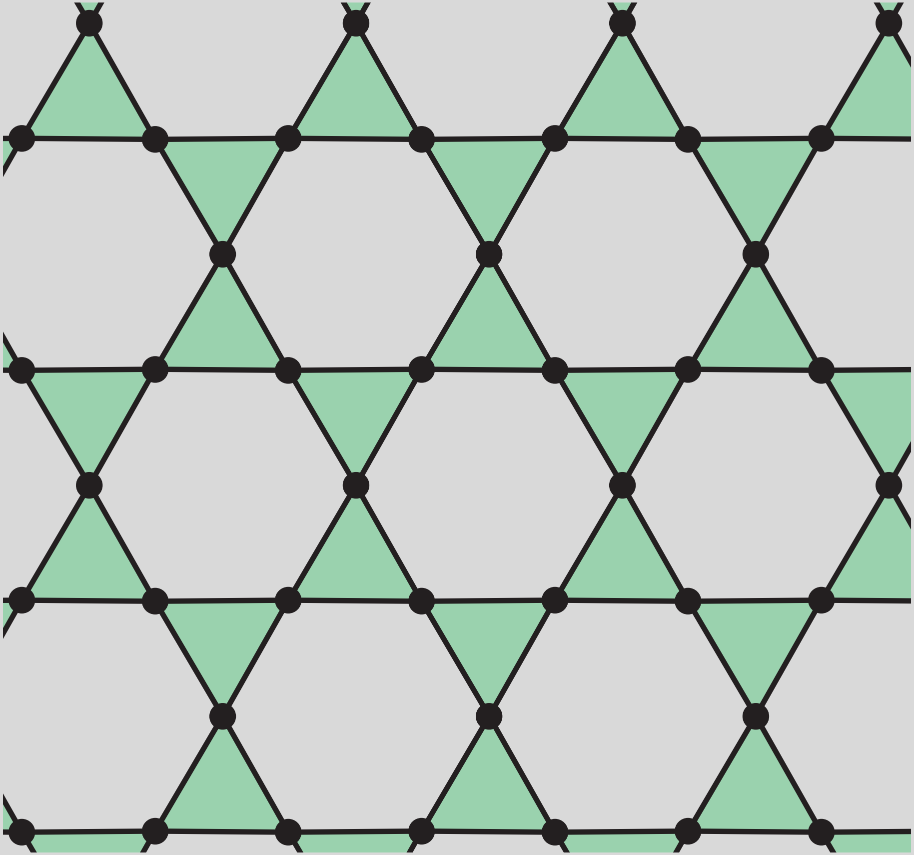


4. 2d Zeolites

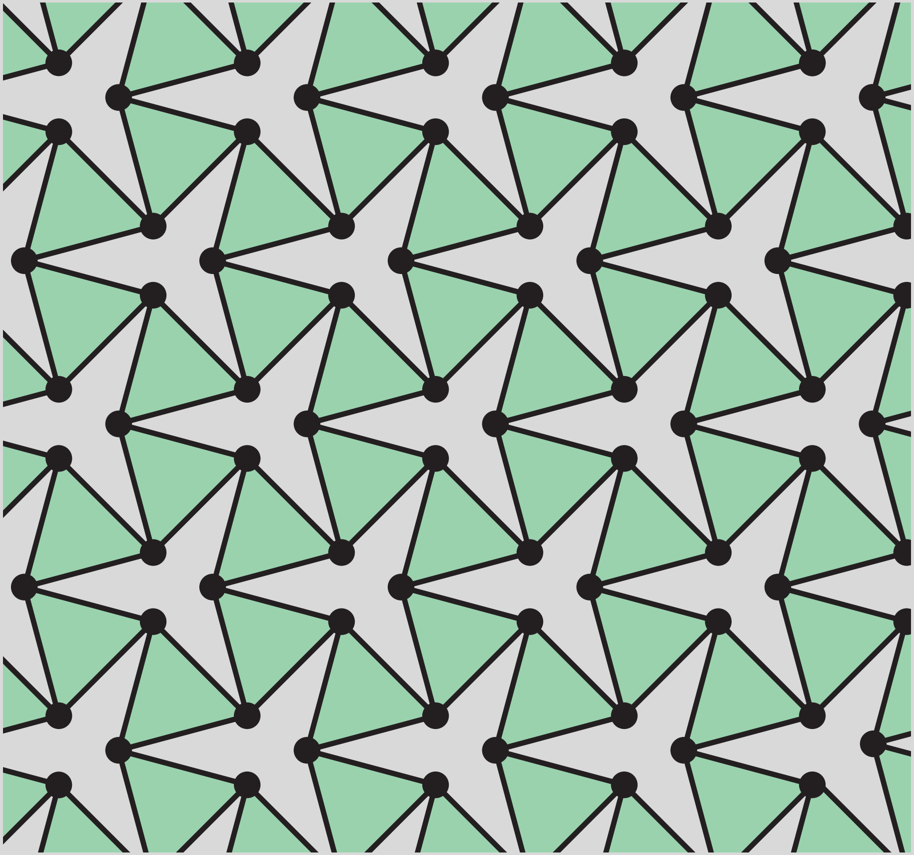
Smallest 2d zeolite is the line graph of K_4: The graph of the octahedron with four (edge disjoint) faces.
For body-pin graphs on more than 4 vertices, the zeolite can be recovered uniquely from the line-graph.

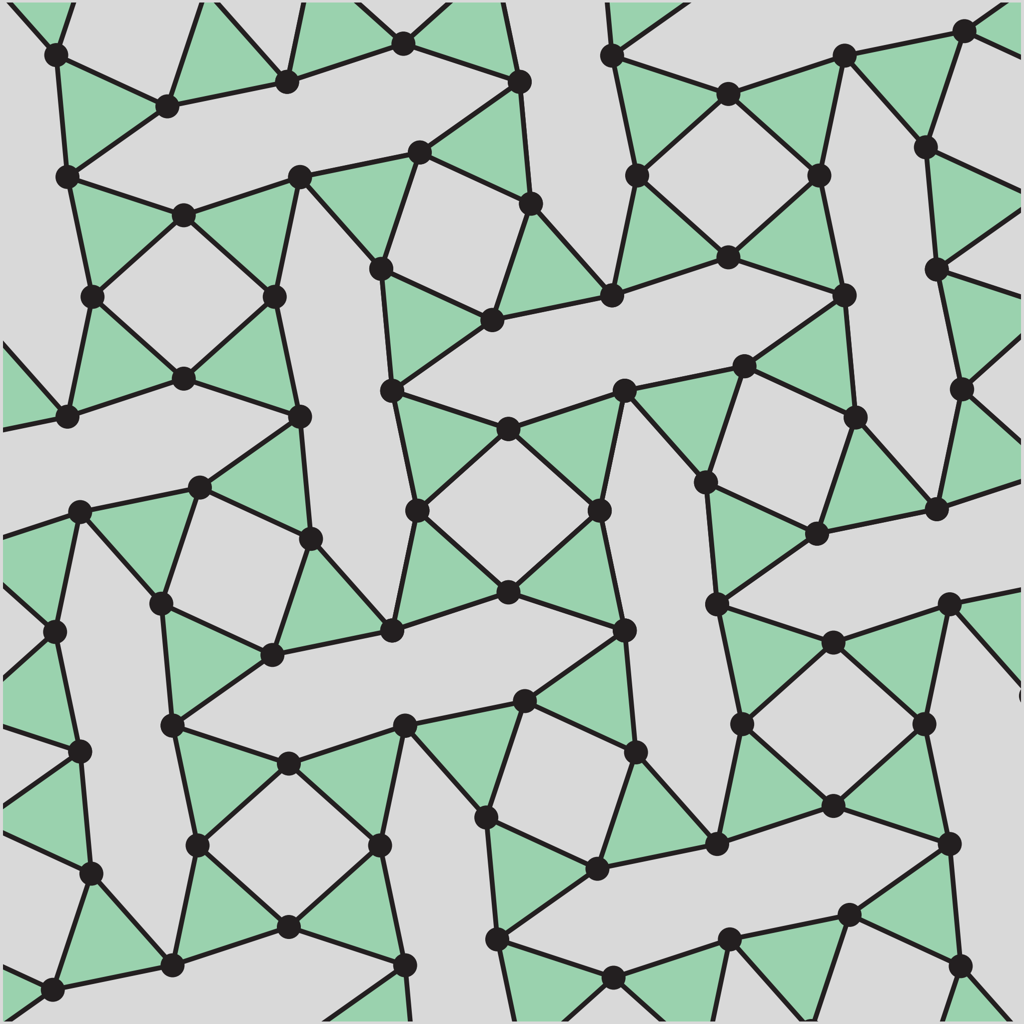


It is just as easy to construct infinite symmetric examples:



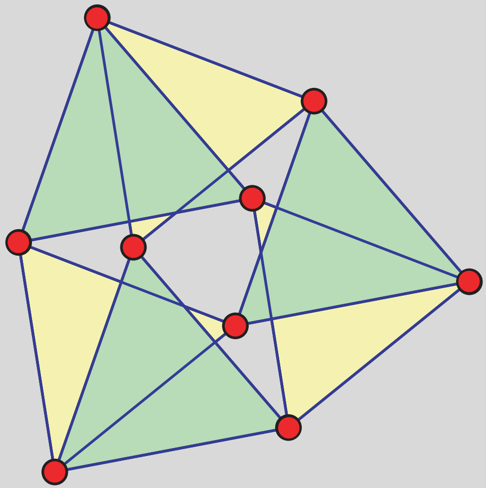
Showing a different symmetry



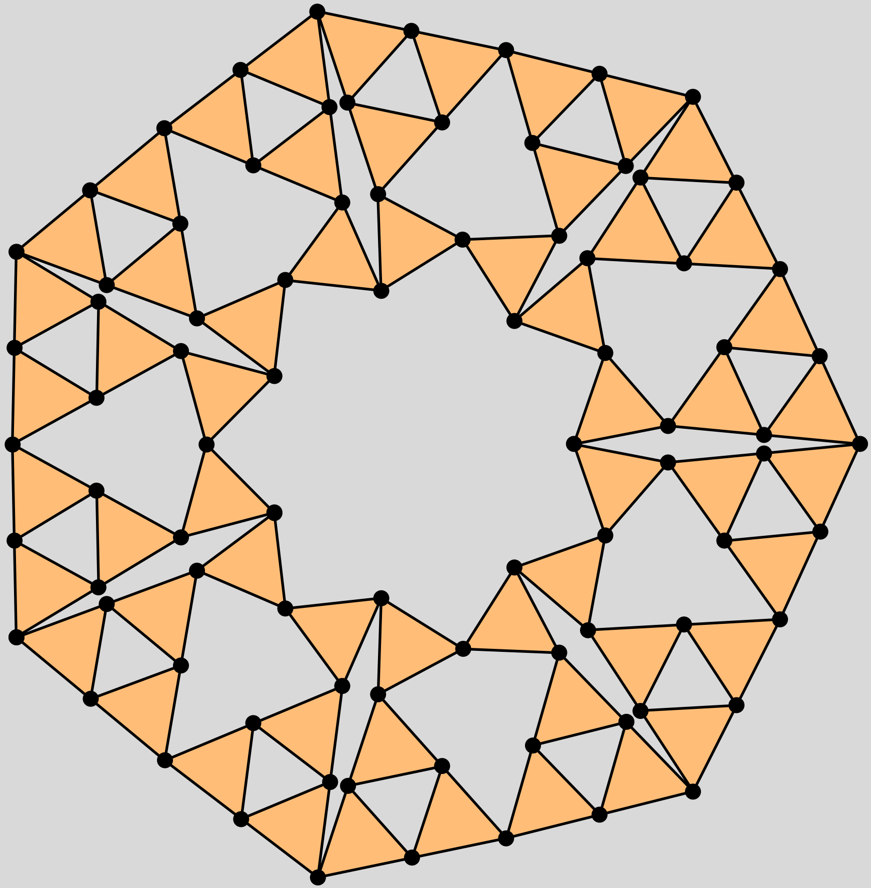


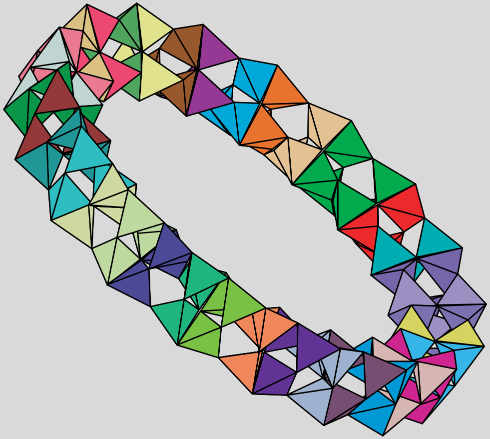
5. Finite Zeolites

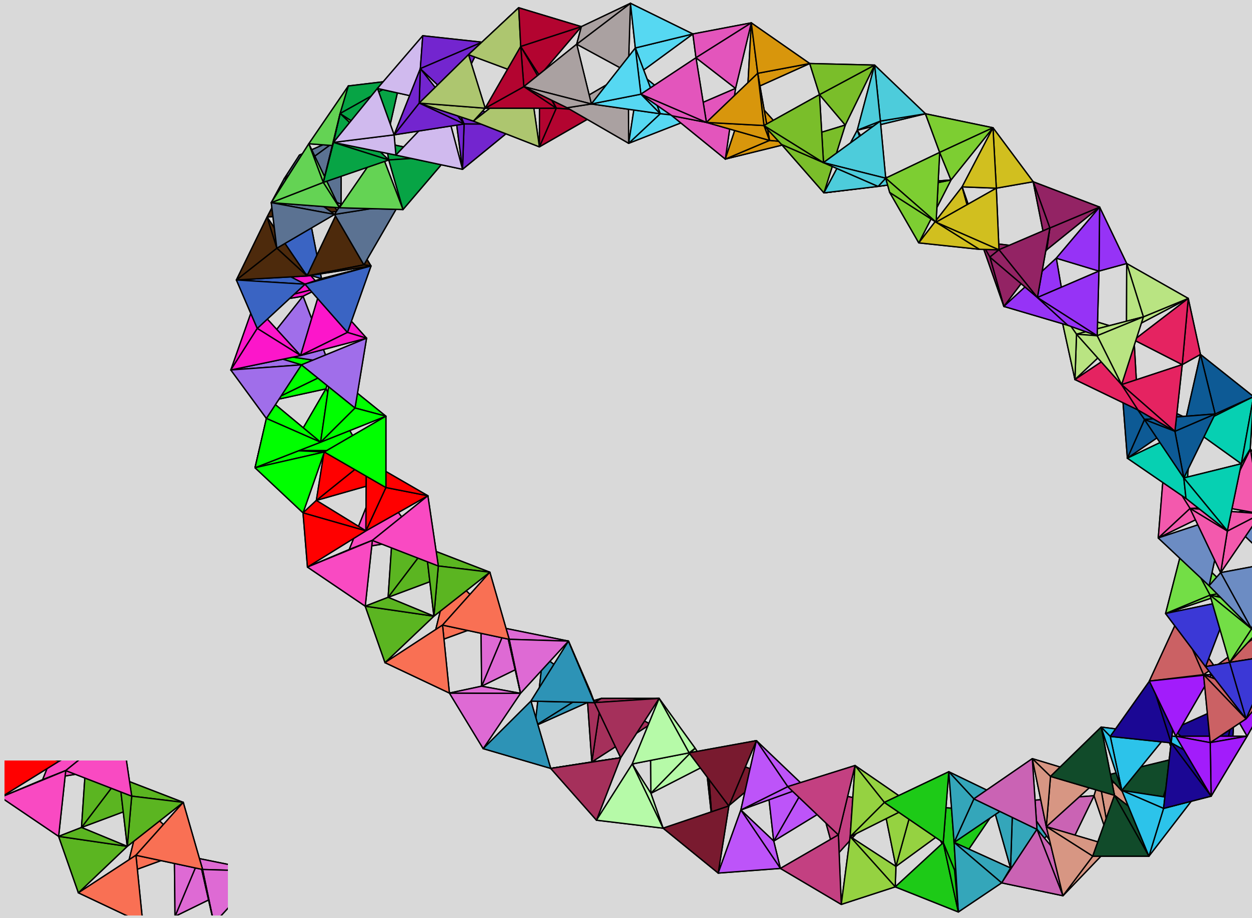
Body pin graph: $K_{3,3}$. Since the body pin graph is not planar, the resulting zeolite cannot be planar. Its underlying graph is generically globally rigid. However, it has a unit distance realization in the plane which is a mechanism.

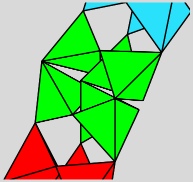


Harborth's Example





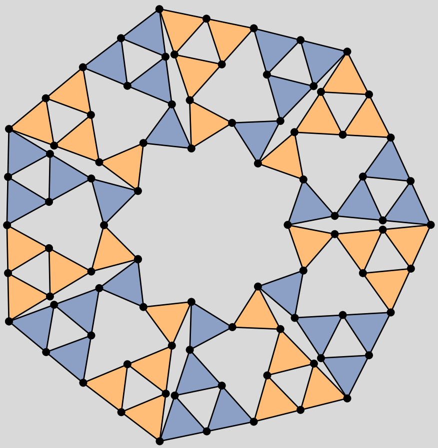




CLARK
Chemical Zeolites
Combinatorial . . .
Realization
2d Zeolites
Finite Zeolites
The Layer . . .
Holes in Zeolites
Motions
Open Problems
Home Page
Title Page
Page 17 of 100
Go Back
Full Screen
Close
Quit

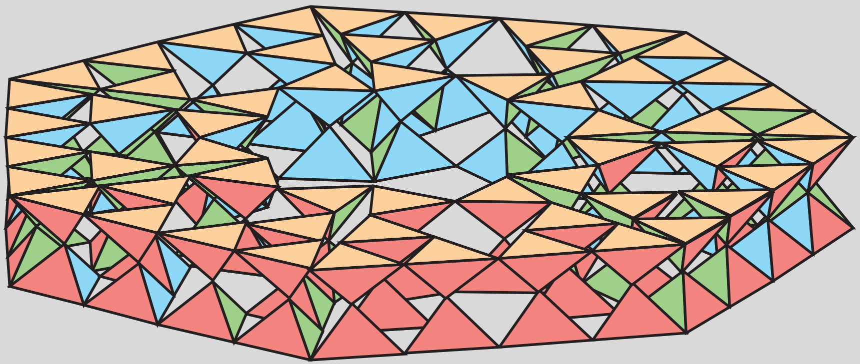
6. The Layer Construction

$Z = (T, C)$ is a combinatorial zeolite realizable in dimension d.
$\mathbb{R}^d \subseteq \mathbb{R}^{d+1}$
Label each $t \in T$ arbitrarily with ± 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.

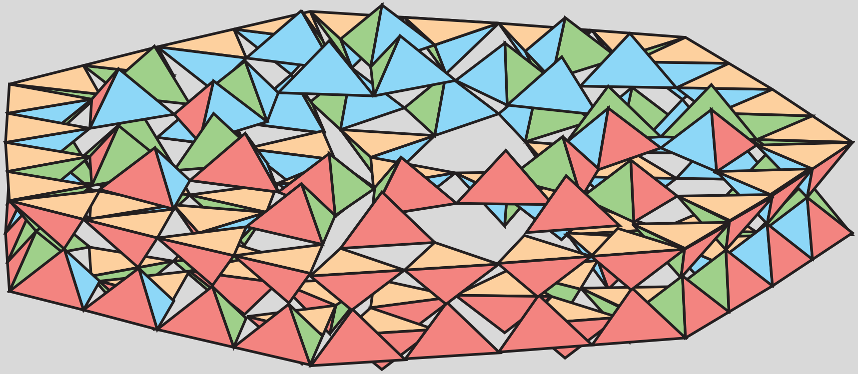


Alternately staking Z_a and Z_b gives a *layered Zeolite* in $\mathbb{R}^{d+1}$.

Labels all +1
A two layered zeolite.

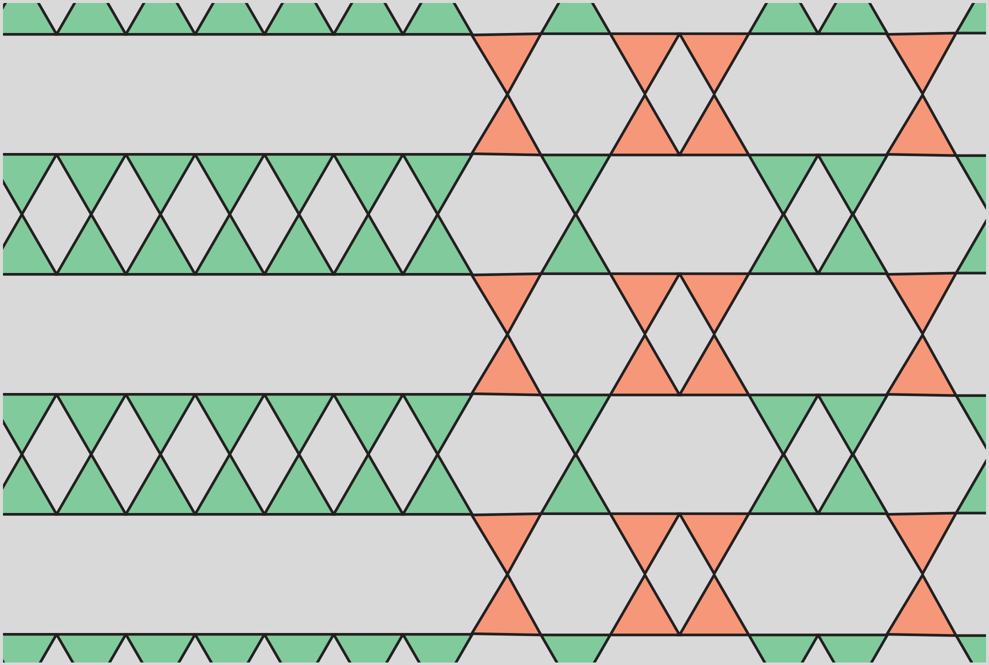


The general case starting from a finite zeolite.

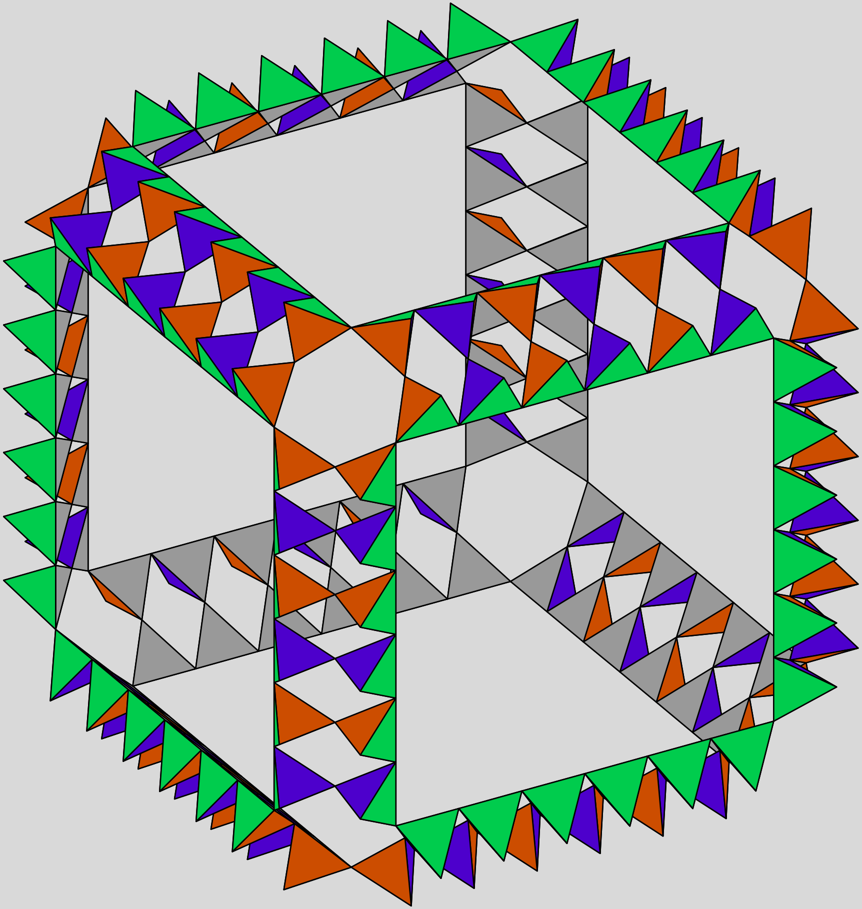


Theorem: There are uncountably many isomorphism classes of unit distance realizable zeolites in $\mathbb{R}^3$.
(actually in any dimension $d > 1$.)

Proof:



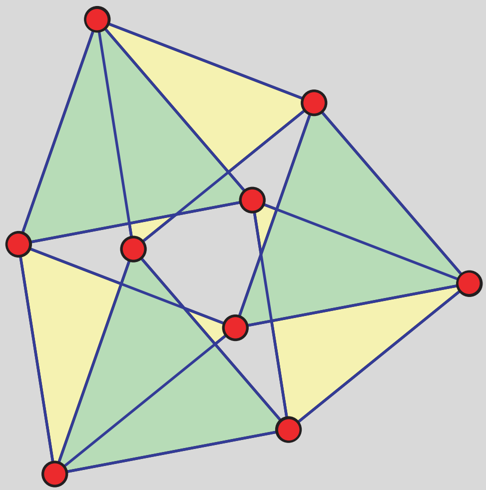
7. Holes in Zeolites



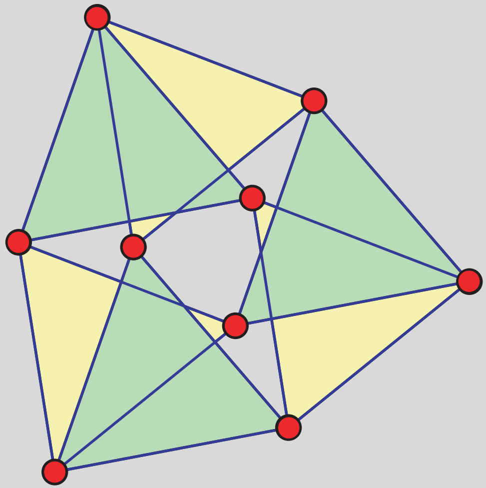
8. Motions

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 $d(d+1)/2$.)

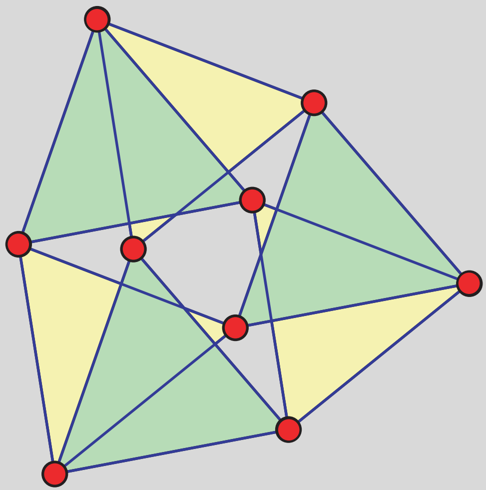


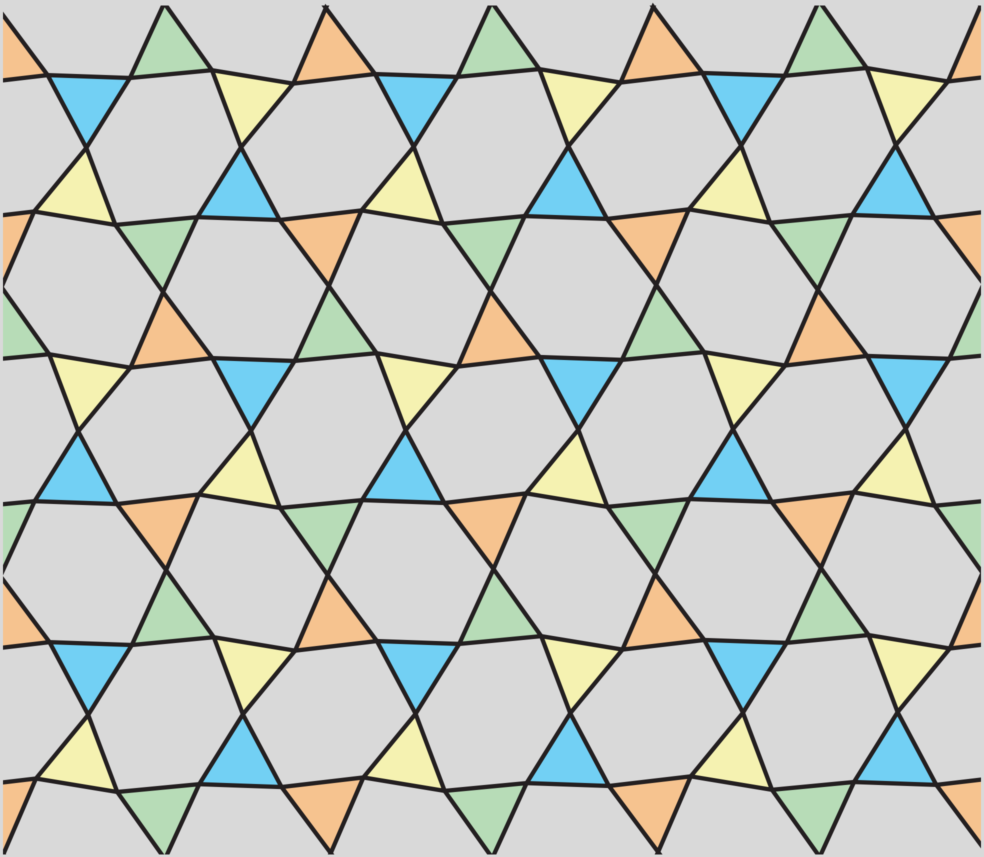
Generically globally rigid in the plane.

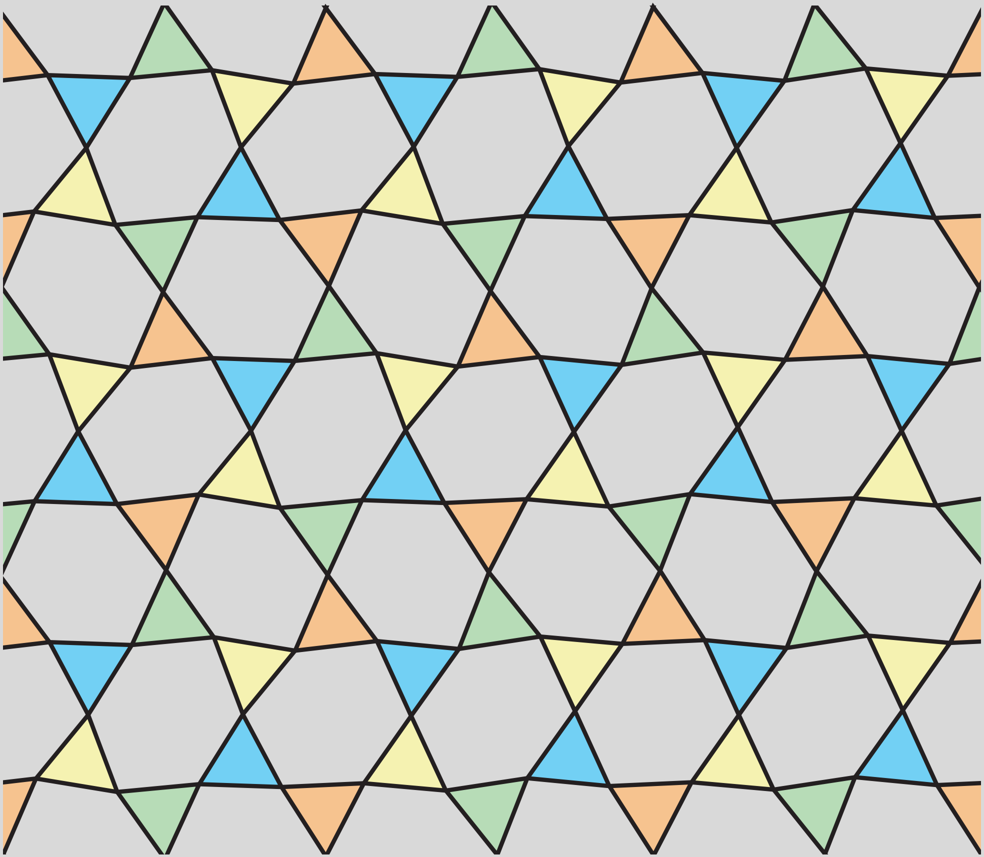


Generically globally rigid in the plane.

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]

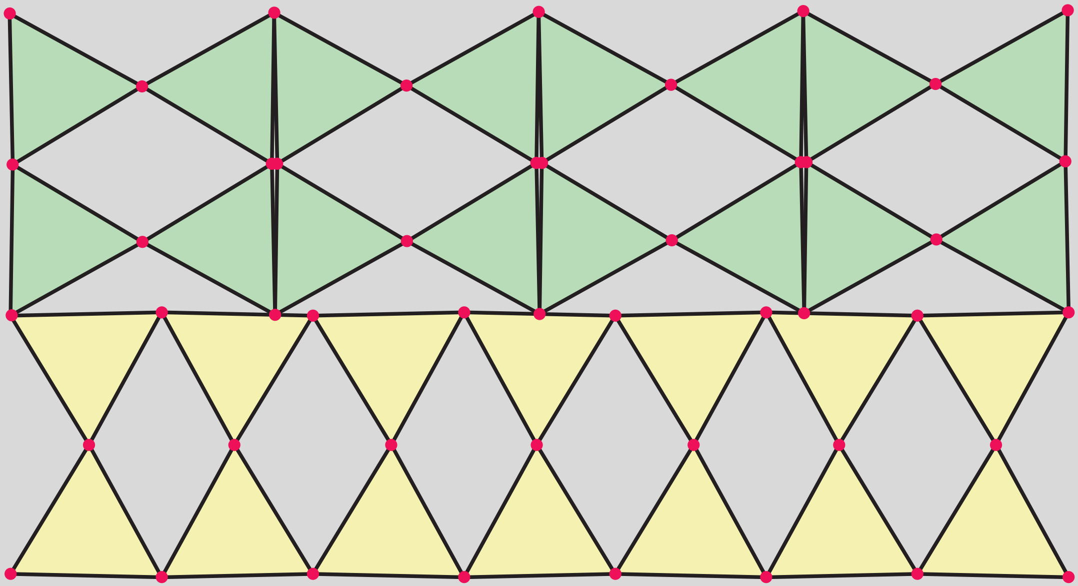






9. Open Problems

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.



Harborth's Construction