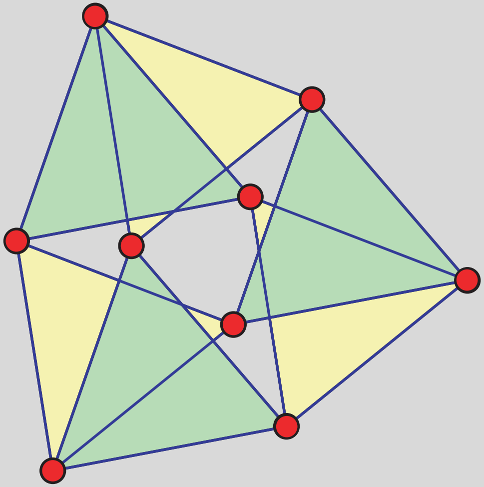
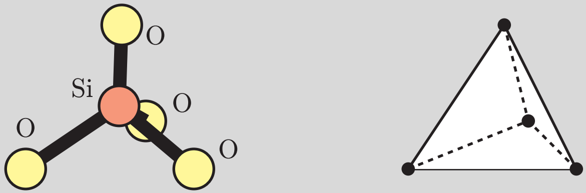
Kinematics of Zeolites

Brigitte Servatius — WPI

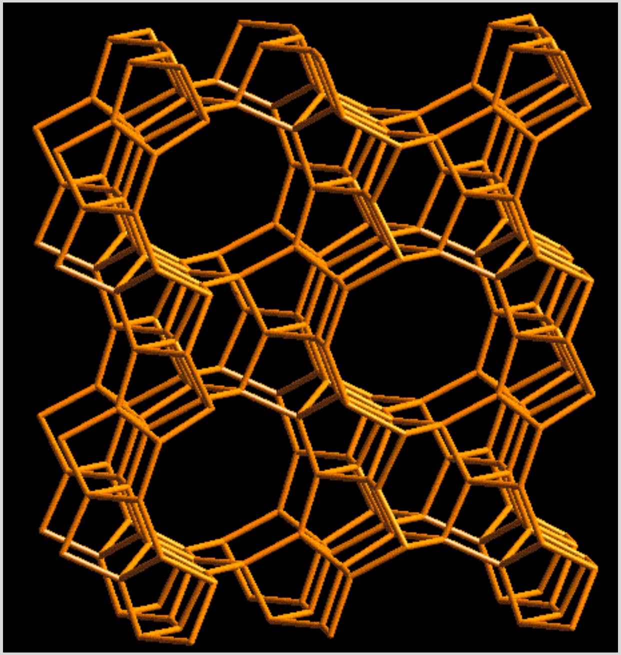


1. Chemical Zeolites

- 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) [5] 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

A 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

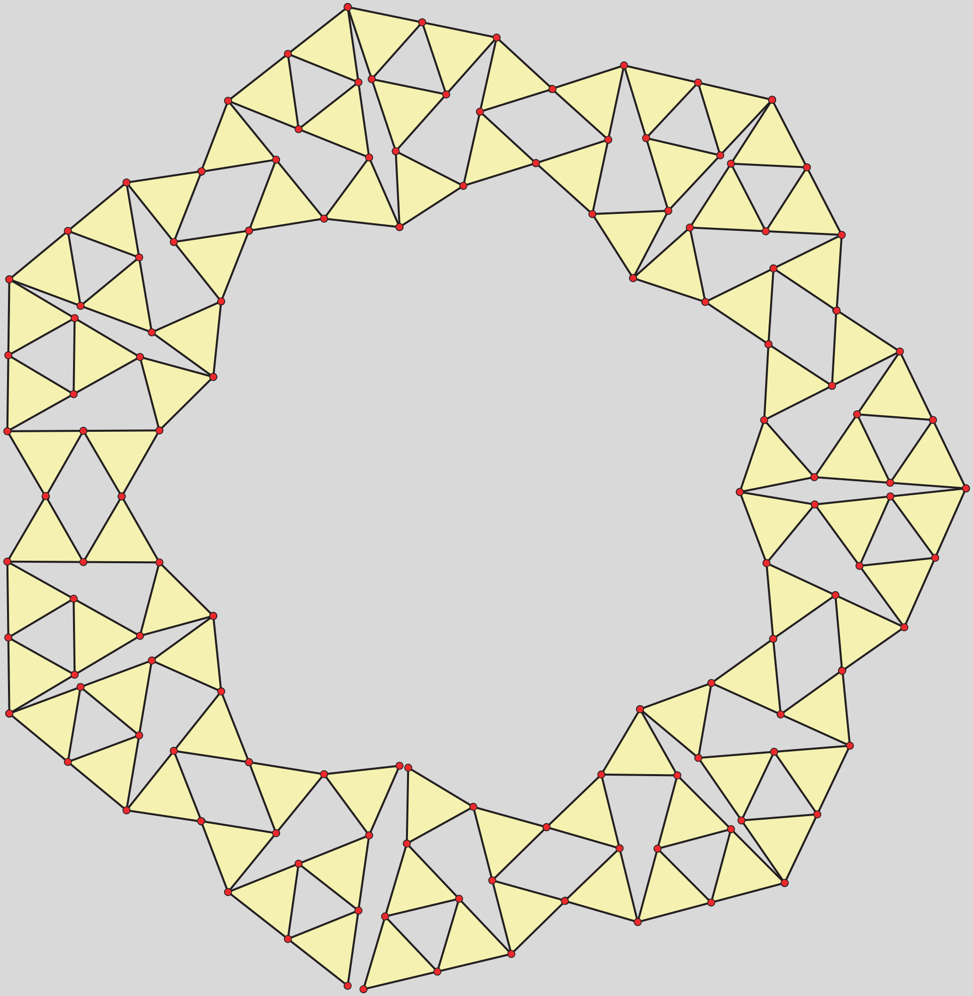
A realization where all edges join vertices distance 1 apart in $\mathbb{R}^d$.

non-interpenetrating realization

A realization where simplices are disjoint except at joined vertices.

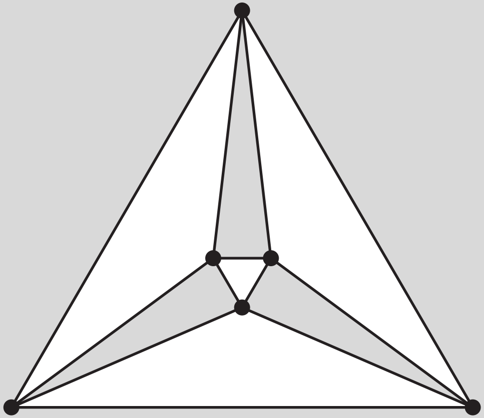
Home Page
Title Page
Page 7 of 43
Go Back
Full Screen
Close
Quit

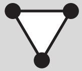
The typical(?) situation: Not unit distance realizable.



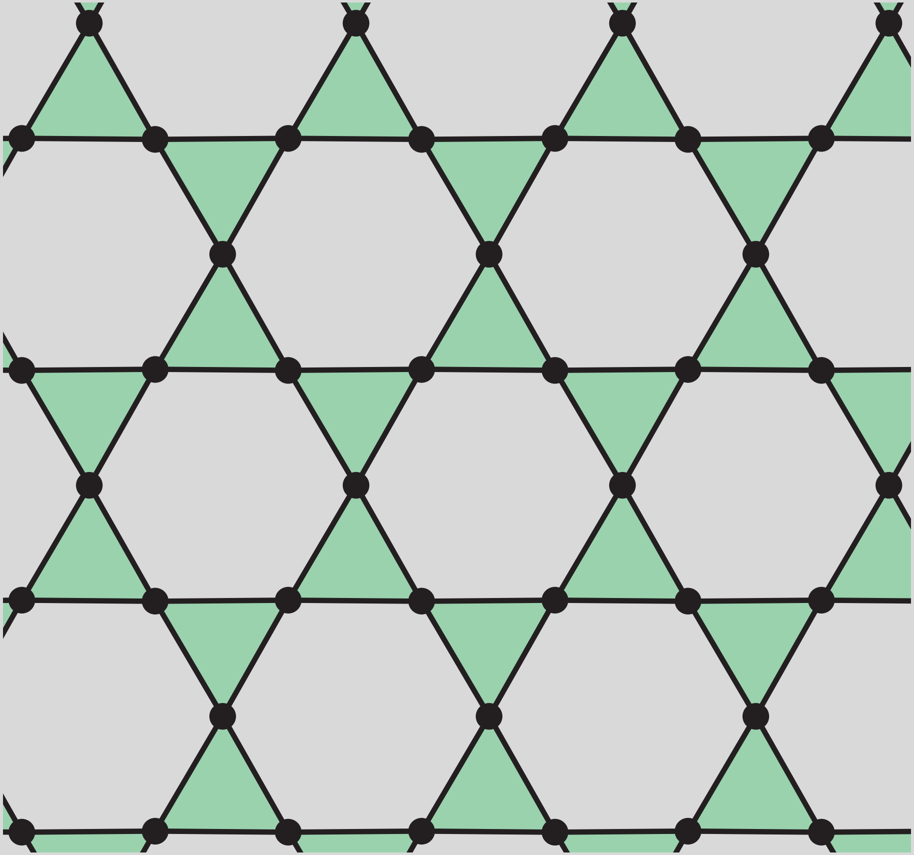
4. 2d Zeolites

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.

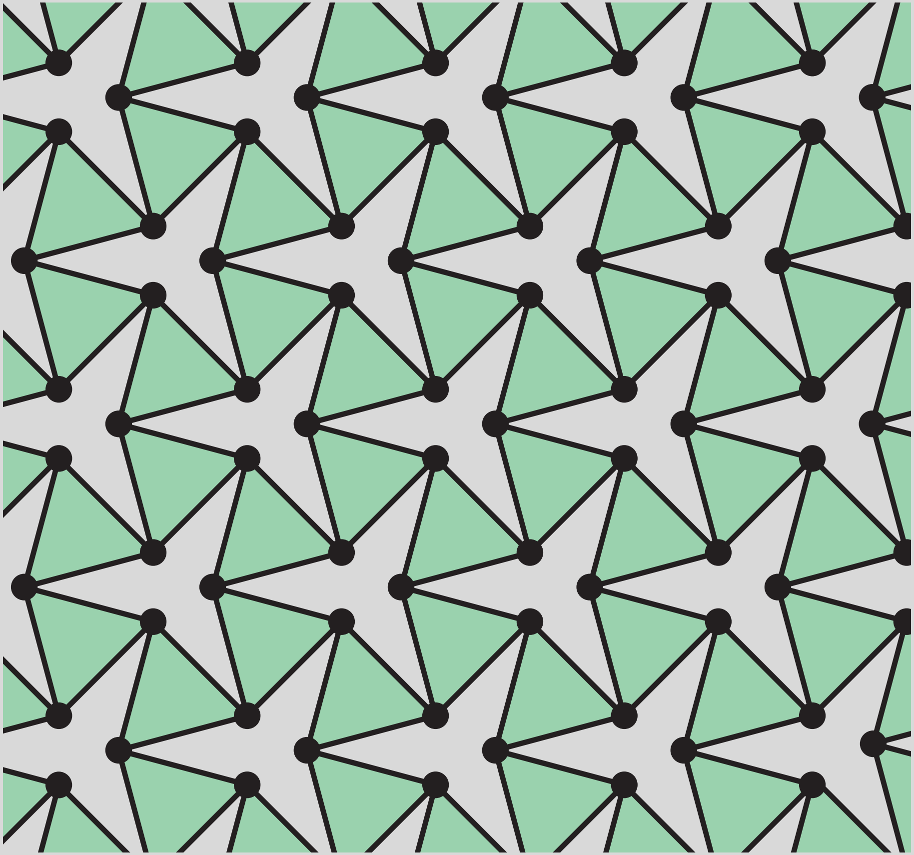


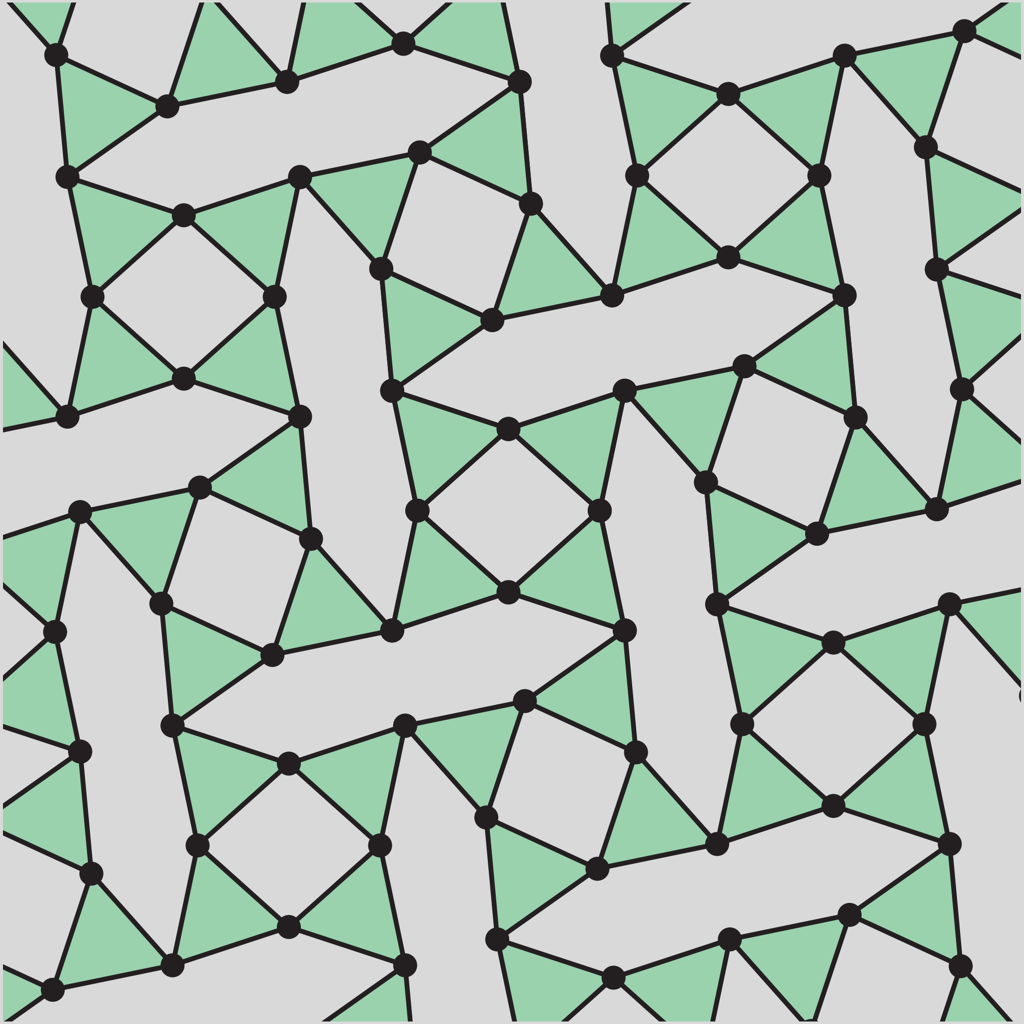


It is just as easy to construct infinite symmetric examples:



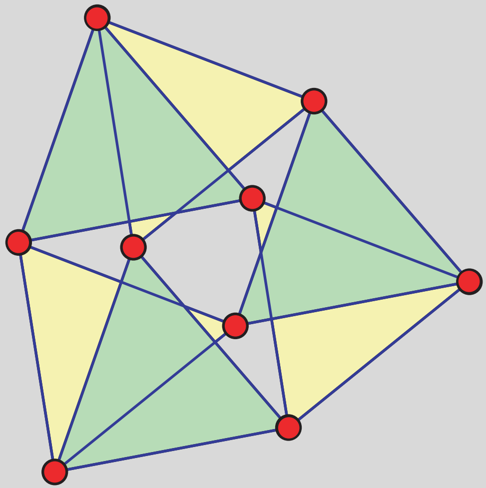
Showing a different symmetry



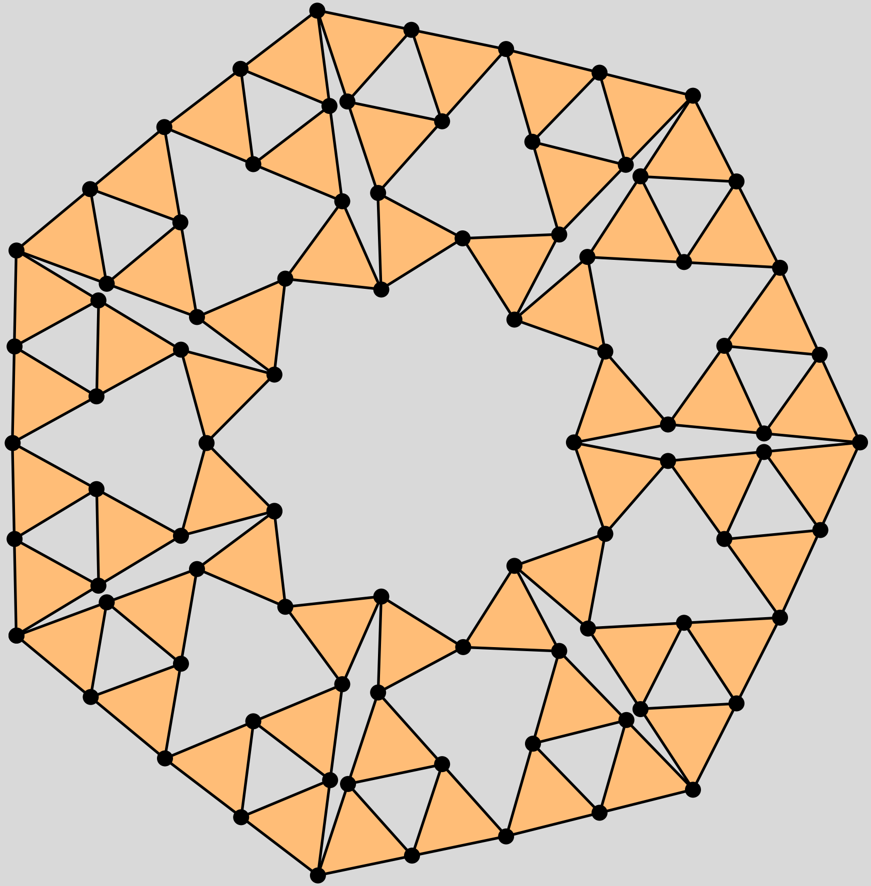


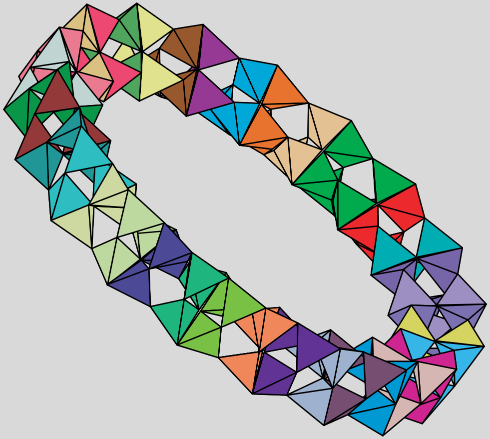
5. Finite Zeolites

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.



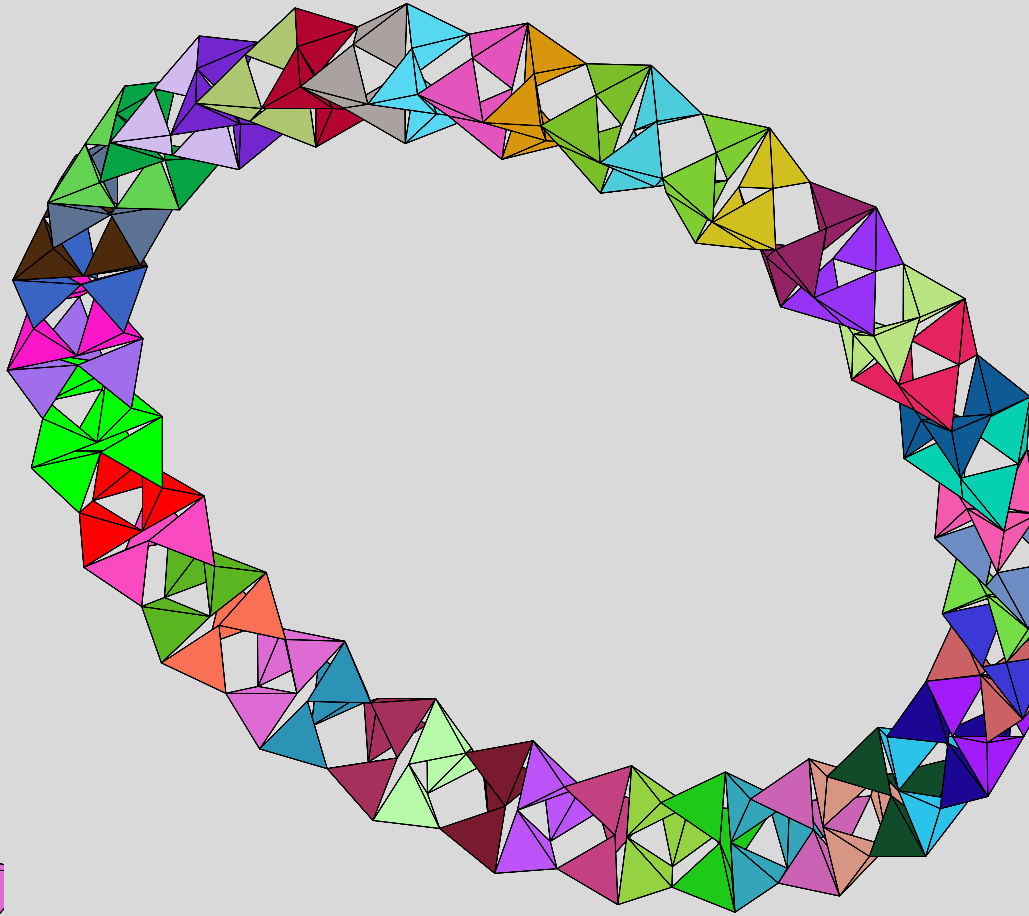
Harborth's Example

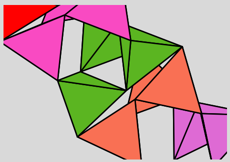


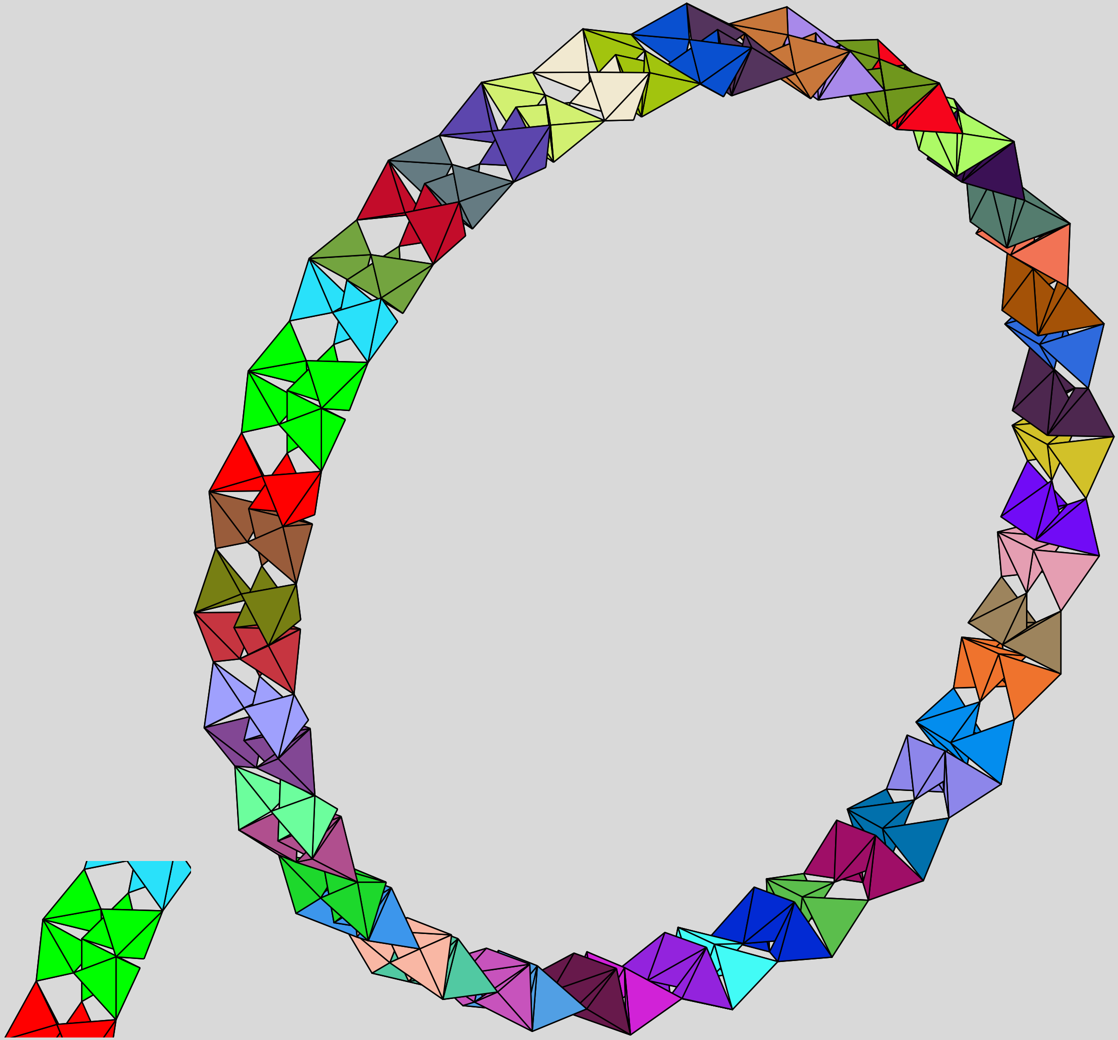


Chemical Zeolites
Combinatorial . . .
Realization
2d Zeolites
Finite Zeolites
The Layer . . .
Holes in Zeolites
Motions
Open Problems

Home Page
Title Page
Page 15 of 43
Go Back
Full Screen
Close
Quit

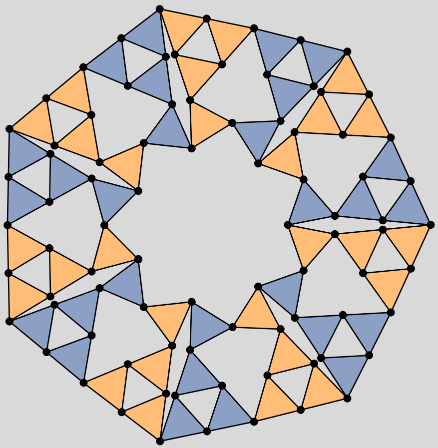






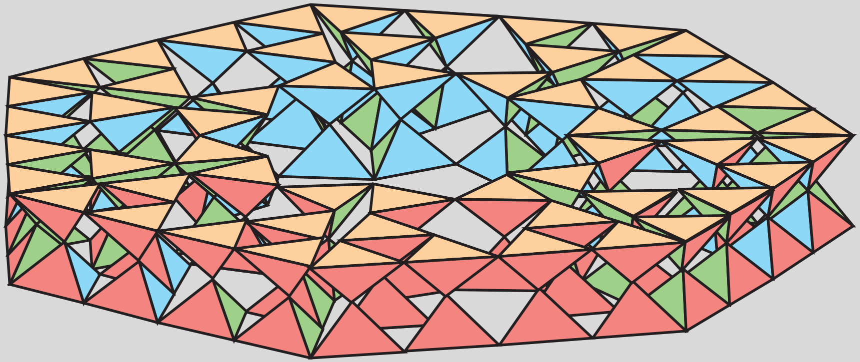
6. The Layer Construction

$Z = (T, C)$ 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.

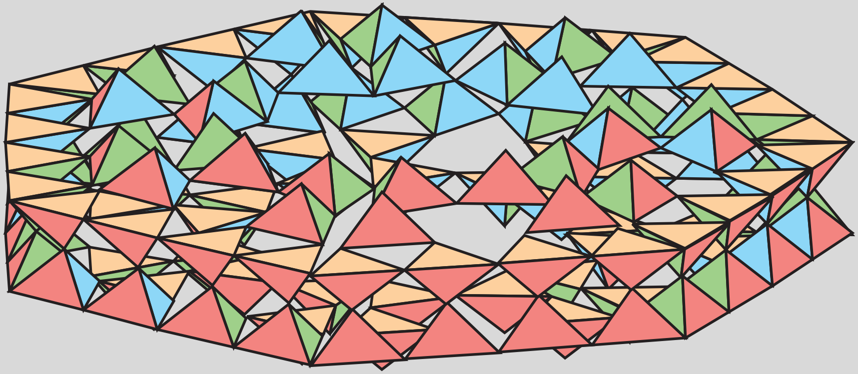


Alternately staking Z_a and Z_b gives a *layered Zeolite* in $\mathbb{R}^{d+1}$.

Labels all +1
A two layered zeolite.

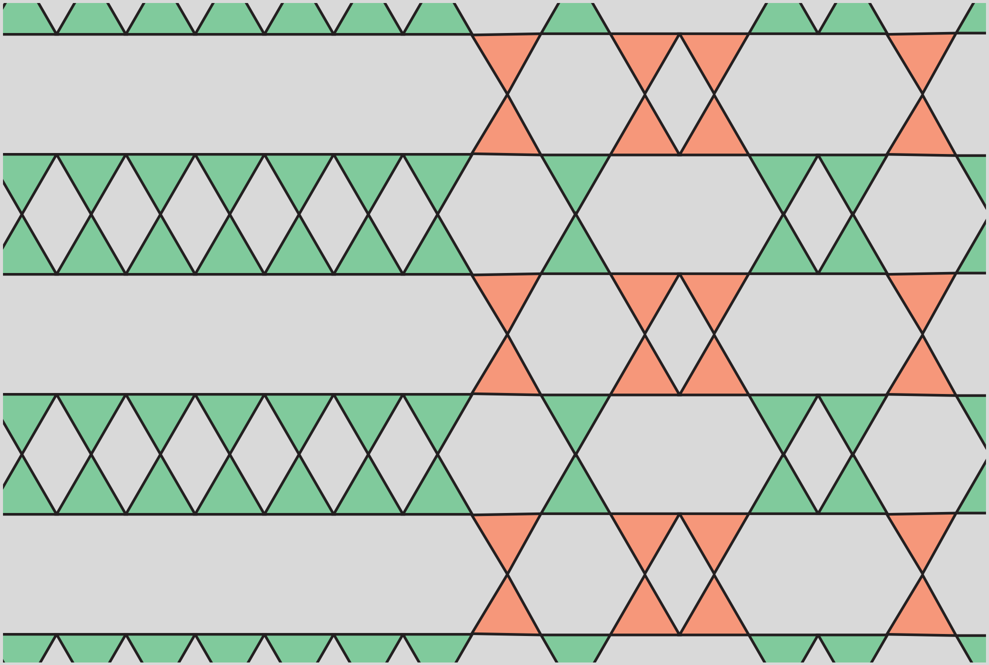


The general case starting from a finite zeolite.

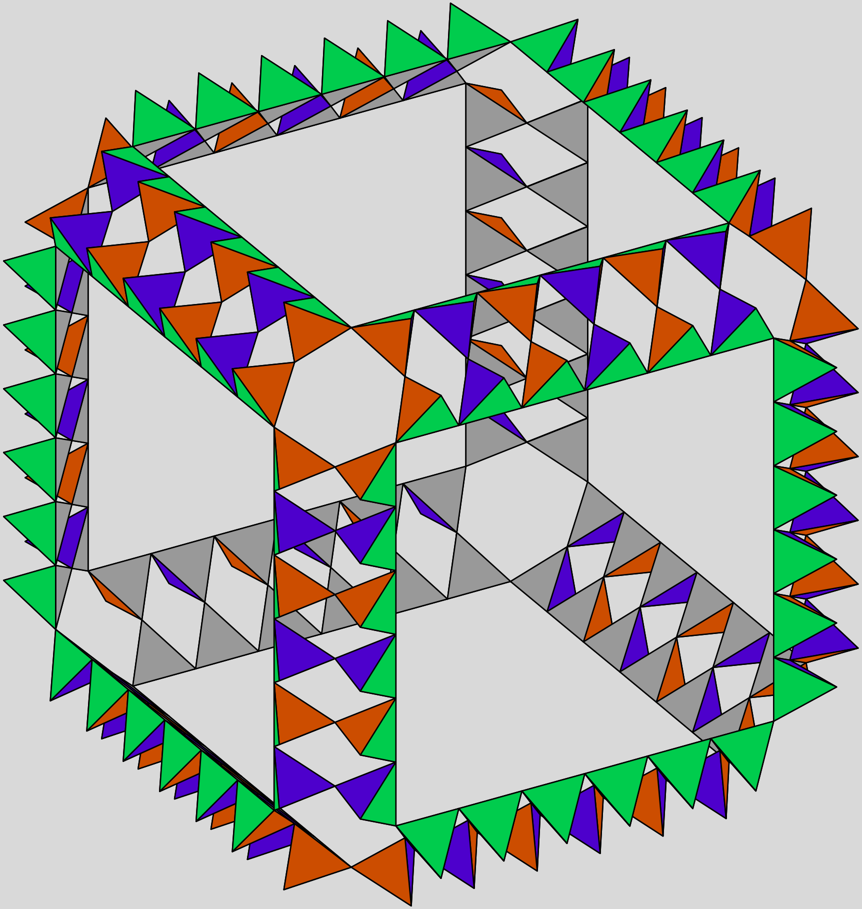


Theorem: There are uncountably many isomorphism classes of unit distance realizable zeolites in $\mathbb{R}^3$.
(actually in any dimension $d > 1$.)

Proof:



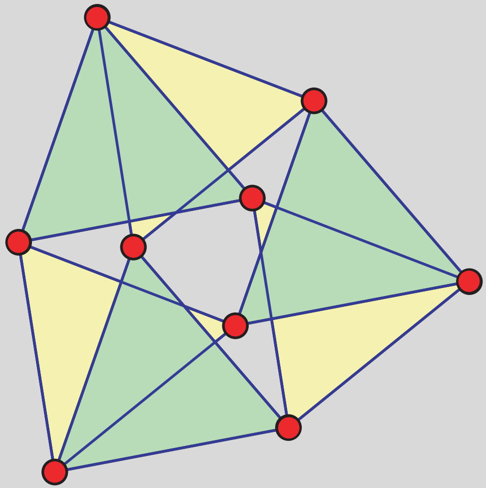
7. Holes in Zeolites



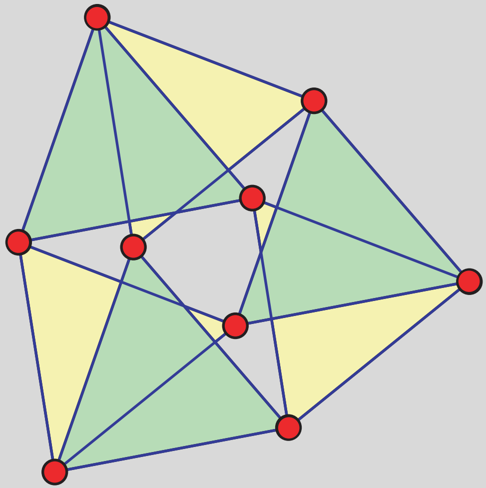
8. Motions

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.



Chemical Zeolites
Combinatorial . . .
Realization
2d Zeolites
Finite Zeolites
The Layer . . .
Holes in Zeolites
Motions
Open Problems

Home Page

Title Page

Go Back

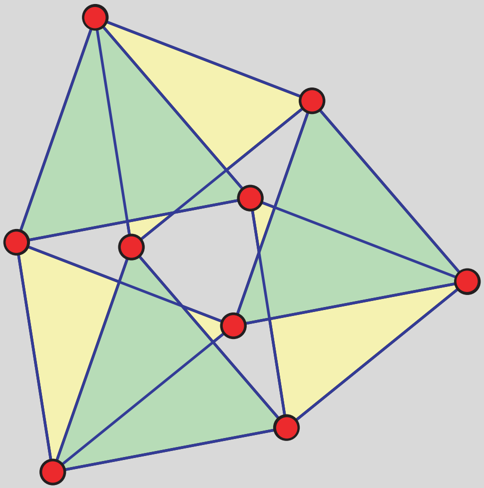
Full Screen

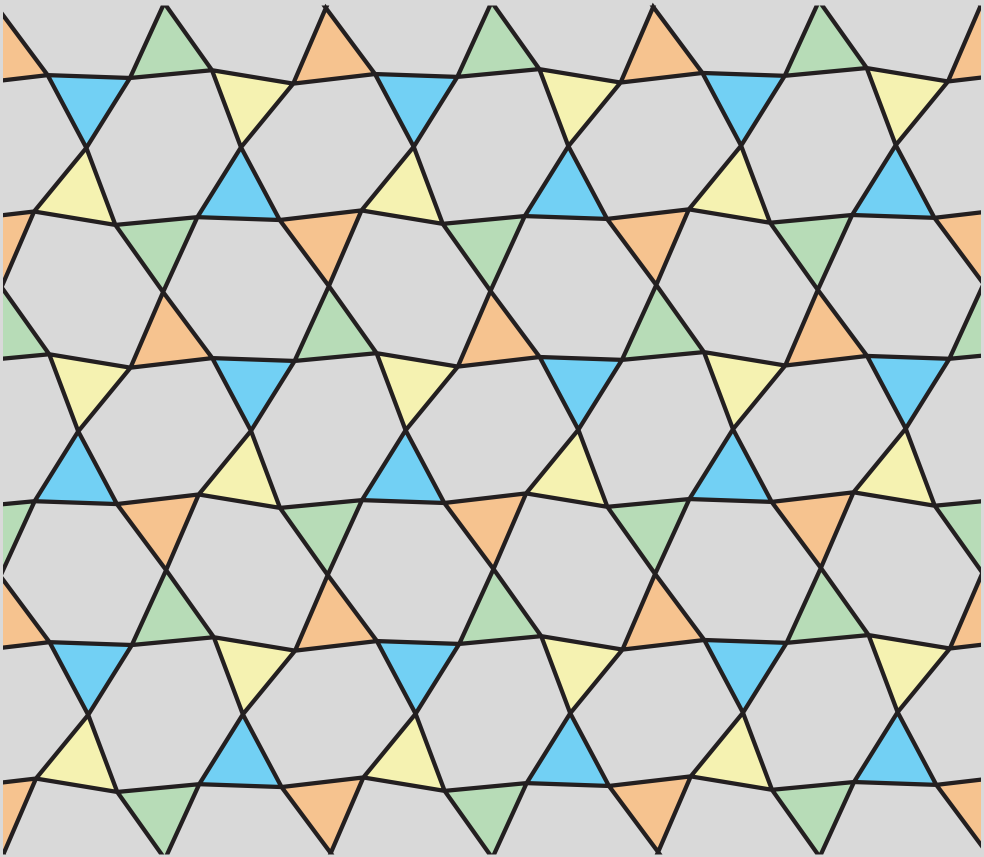
Close

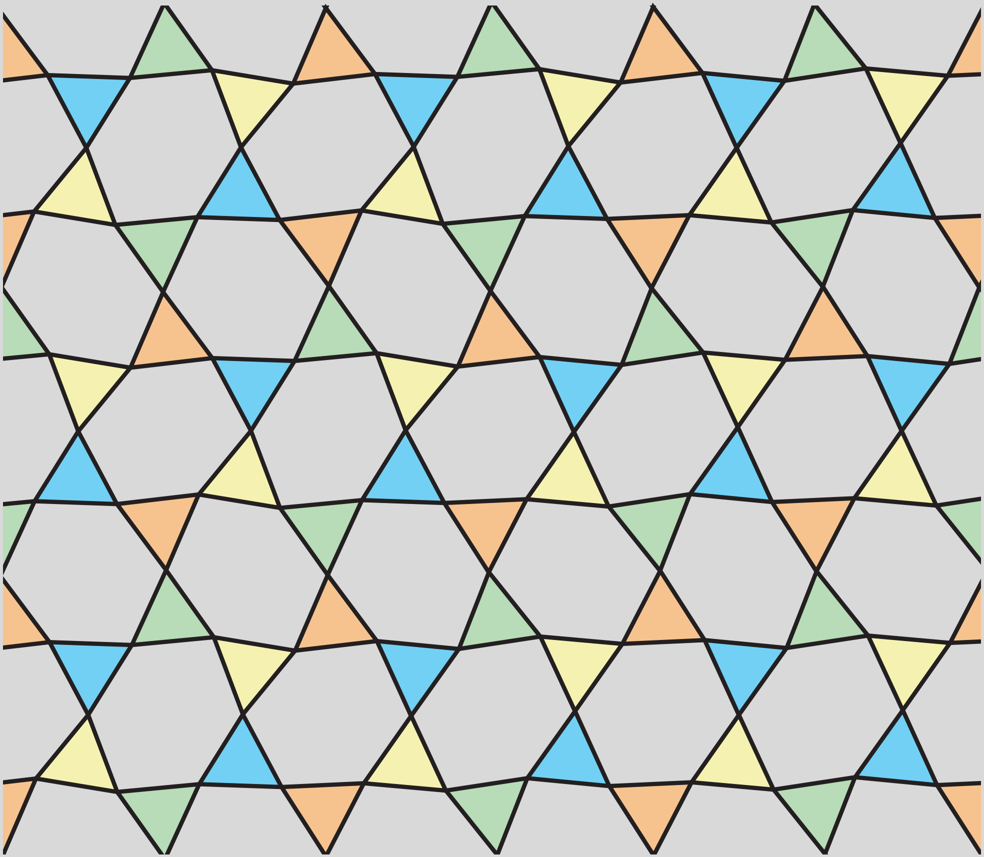
Quit

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 $s \geq 3$. [3]







The *chromatic index*, $\chi'(G)$: the minimum number of colors needed to color the edges of G such that incident edges have different colors
The *chromatic number*, $\chi(G)$ denotes the analogous number for vertex colorings.
If the chromatic index a body pin graph G is $d+1$, which is for example always the case if G is bipartite of maximal valence $d+1$, then its combinatorial zeolite $L(G)$ has chromatic number $d+1$ and we can use a $d+1$ coloring to obtain a mapping from $L(G)$ to the vertices of a regular simplex.

We call a d-dimensional zeolite with body-pin graph of chromatic index $d+1$ *collapsible*. Since the d-dimensional regular simplex is a unit distance graph in $\mathbb{R}^d$, we have the following.

Theorem 1 *A collapsible d-dimensional combinatorial zeolite is realizable as a fictitious zeolite.*
In particular, a combinatorial zeolite corresponding to a bipartite body-pin graph is realizable as a fictitious zeolite.

See [4].

With Peter Fazekas and Otto Röschel [1] we studied the Harborth-Möller example [2].

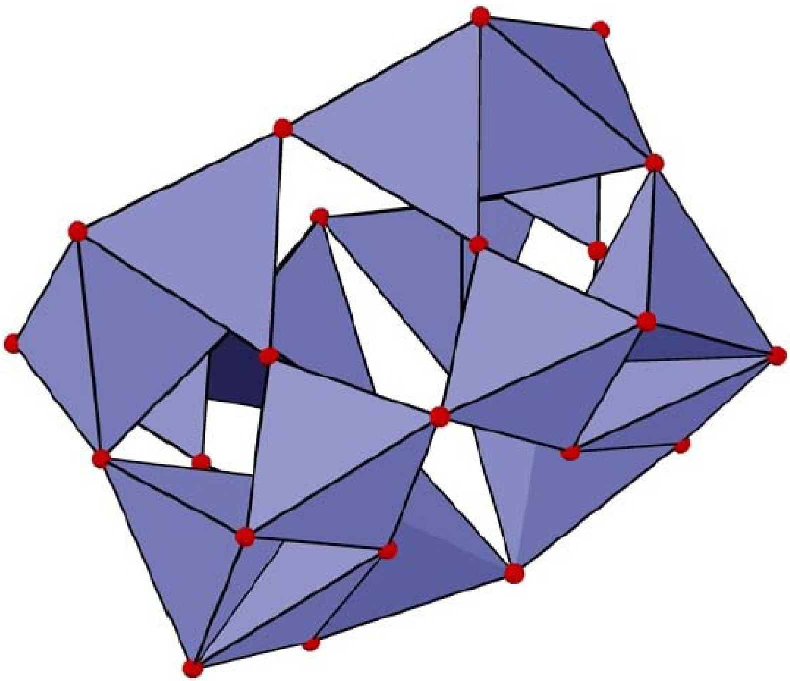
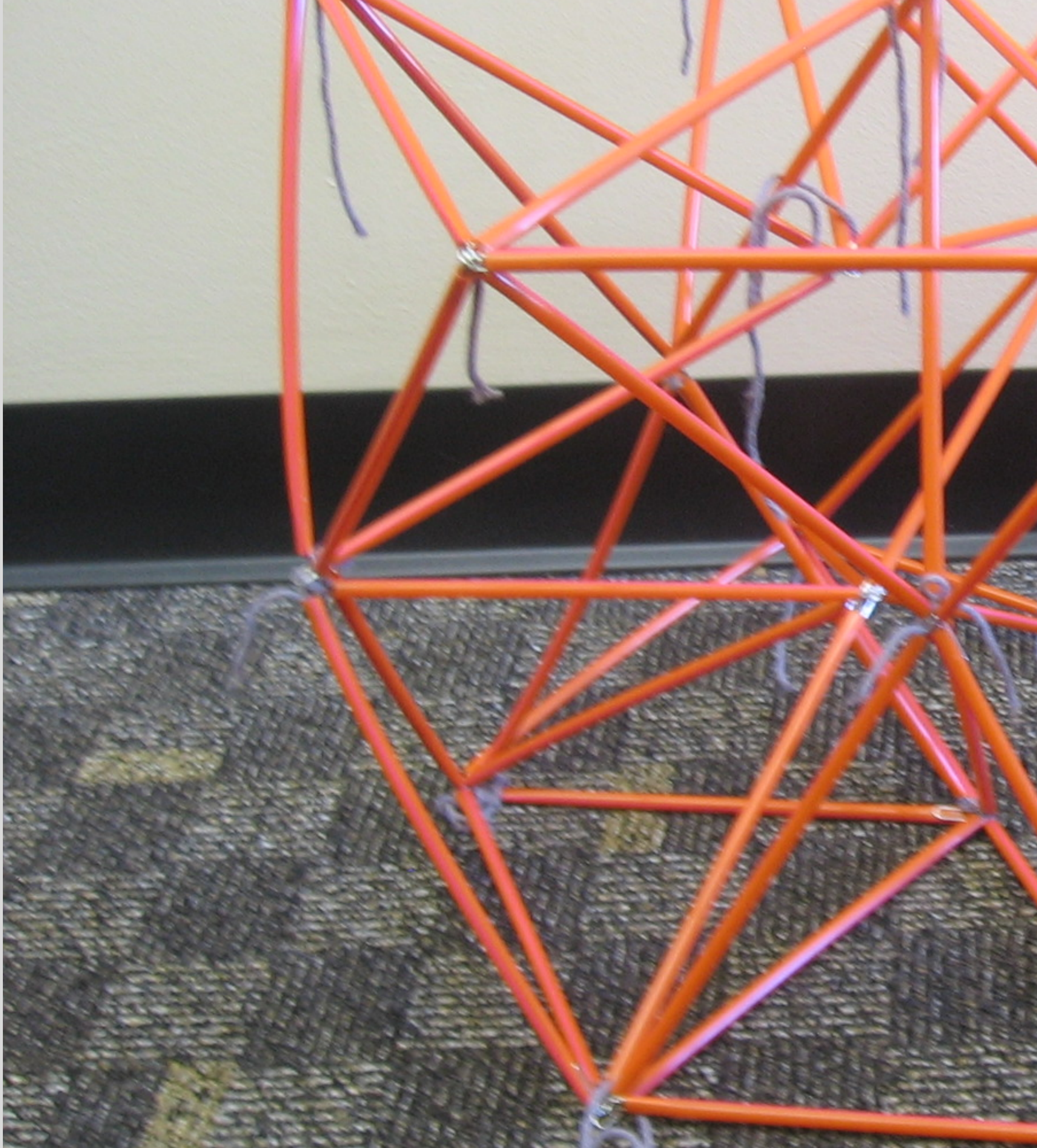


Figure 1: Saturated Packing of 16 tetrahedra



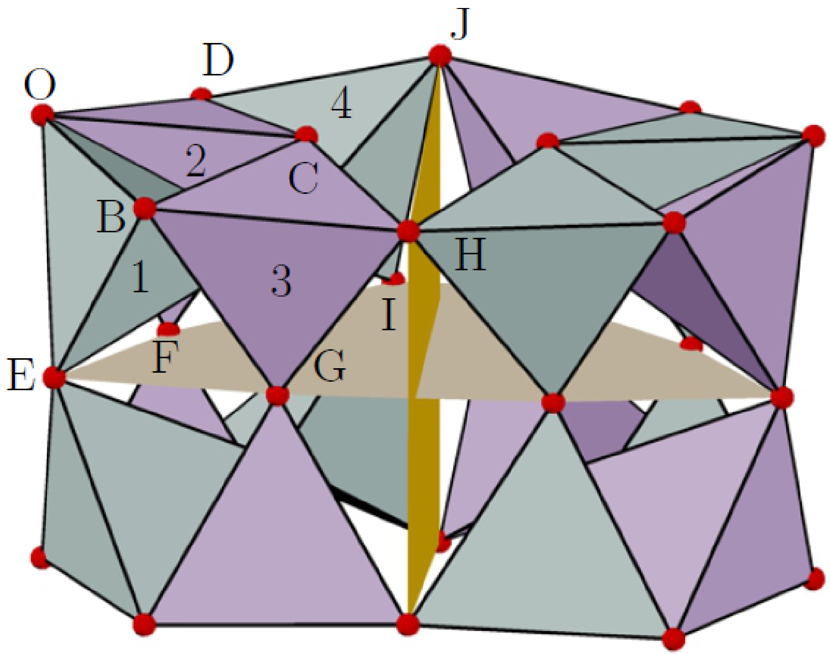


Figure 3: Model with its two planes of symmetry

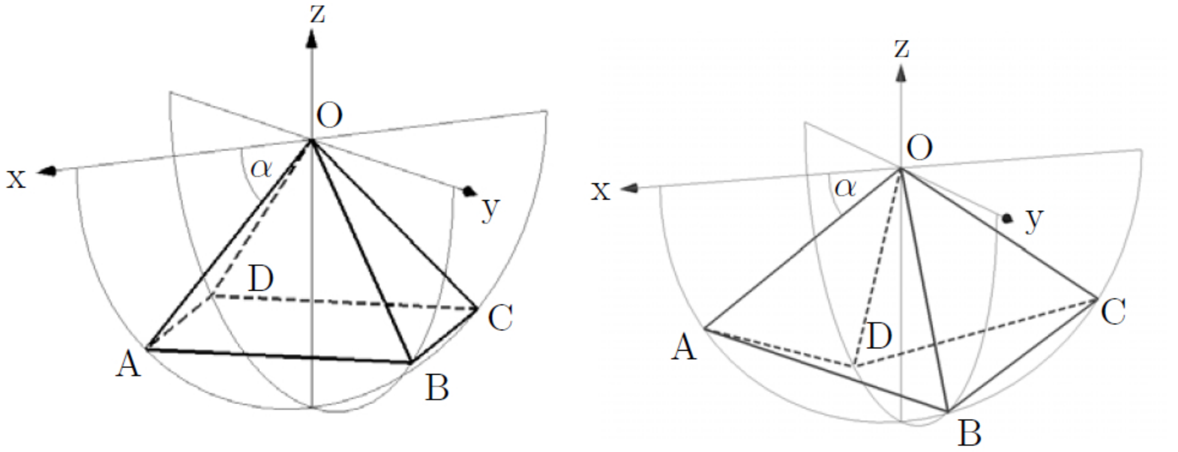


Figure 2: Half an octahedron

$$A(\alpha) = \begin{pmatrix} \cos\alpha \\ 0 \\ -\sin\alpha \end{pmatrix} \qquad B(\beta) = \begin{pmatrix} 0 \\ \cos\beta \\ -\sin\beta \end{pmatrix} \tag{1}$$

$$C(\alpha) = \begin{pmatrix} -\cos\alpha \\ 0 \\ -\sin\alpha \end{pmatrix} \qquad D(\beta) = \begin{pmatrix} 0 \\ -\cos\beta \\ -\sin\beta \end{pmatrix} \tag{2}$$

$$E = \frac{1}{3}\begin{pmatrix} \cos\alpha + 2\sqrt{2}\cos\beta \ \ \sin\alpha \\ \cos\beta + 2\sqrt{2}\cos\alpha \ \ \sin\beta \\ -\sin\alpha - \sin\beta + 2\sqrt{2}\cos\alpha \ \ \cos\beta \end{pmatrix} \tag{3}$$

$$F = \frac{1}{3}\begin{pmatrix} -\cos\alpha + 2\sqrt{2}\cos\beta \ \ \sin\alpha \\ -\cos\beta + 2\sqrt{2}\cos\alpha \ \ \sin\beta \\ -\sin\alpha - \sin\beta - 2\sqrt{2}\cos\alpha \ \ \cos\beta \end{pmatrix}. \tag{4}$$

$$k_1(s) = \frac{1-\cos s}{2}\begin{pmatrix} \cos\alpha \\ -\cos\beta \\ -\sin\alpha - \sin\beta \end{pmatrix} + \sin s \begin{pmatrix} \sin\alpha \ \cos\beta \\ -\cos\alpha \ \sin\beta \\ \cos\alpha \ \cos\beta \end{pmatrix} \tag{5}$$

$$k_2(t) = \frac{1-\cos t}{2}\begin{pmatrix} -\cos\alpha \\ \cos\beta \\ -\sin\alpha - \sin\beta \end{pmatrix} + \sin t \begin{pmatrix} -\sin\alpha \ \cos\beta \\ \cos\alpha \ \sin\beta \\ \cos\alpha \ \cos\beta \end{pmatrix} \tag{6}$$

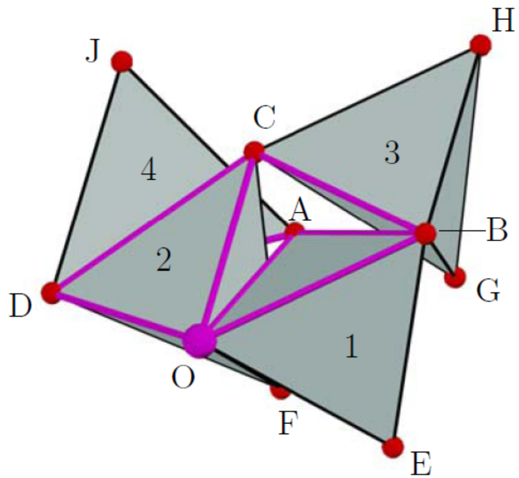


Figure 4: Half-octahedron in one fourth of the model: Vertex O and basic quadrangle $ABCD$

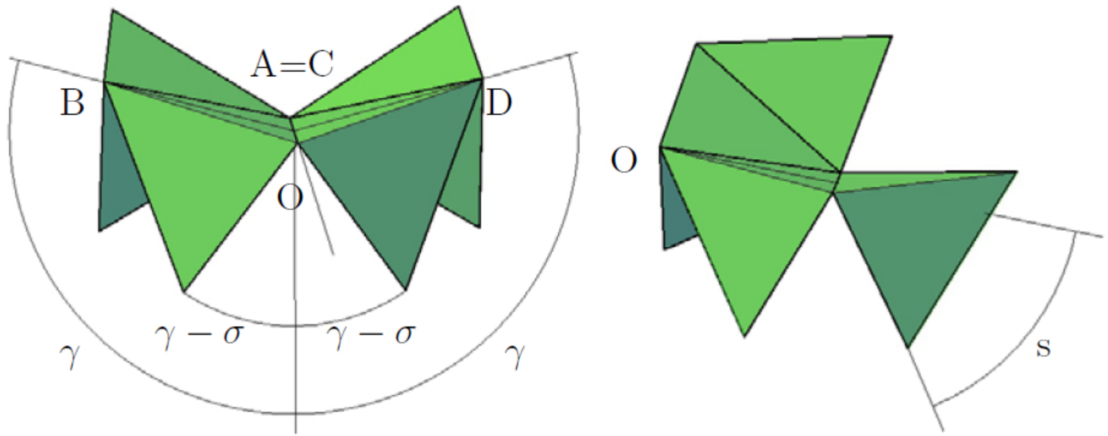


Figure 5: The two motion-parameters γ and s in the degenerate case

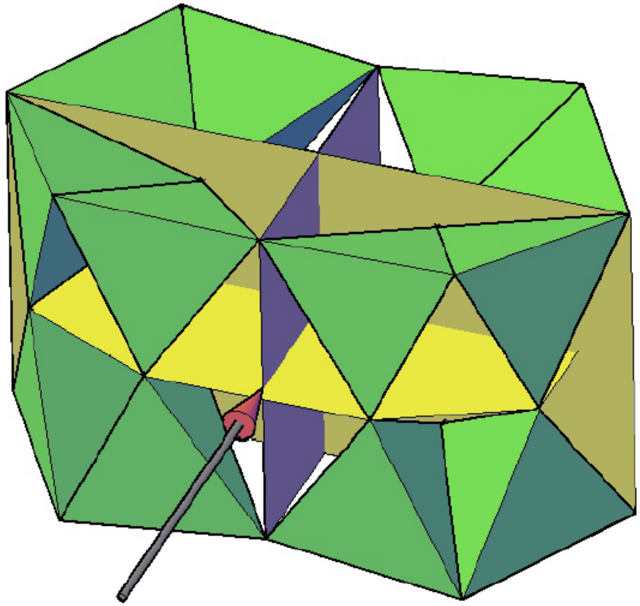


Figure 6: Degenerate case of the model with its three mirror planes

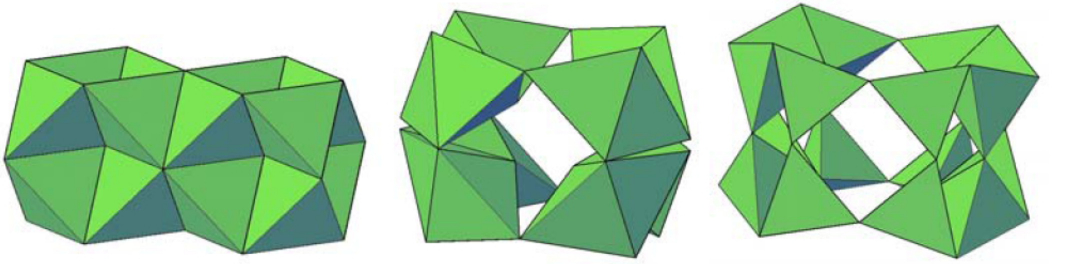
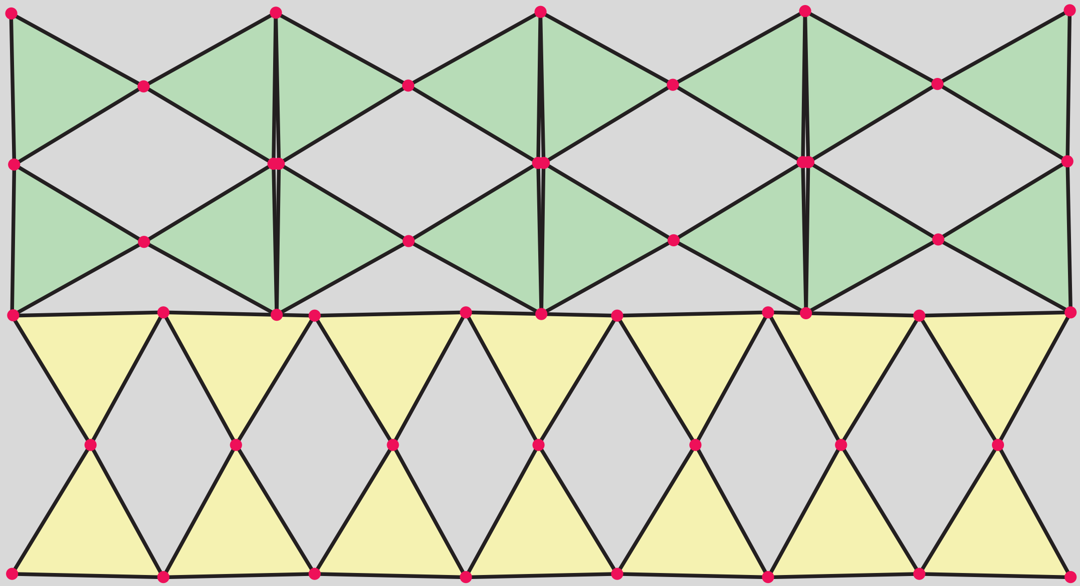


Figure 7: Positions of the model where the channel reaches the minimal and the maximal cross section

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

References

[1] P. Fazekas, O. Rschel, and B. Servatius. The kinematics of a framework presented by h. harborth and m. mller. *Beitrge zur Algebra und Geometrie / Contributions to Algebra and Geometry*, pages 1–9. 10.1007/s13366-011-0079-x.

[2] Heiko Harborth and Meinhard Möller. Complete vertex-to-vertex packings of congruent equilateral triangles. *Geombinatorics*, 11(4):115–118, 2002.

[3] Bill Jackson, Brigitte Servatius, and Herman Servatius. The 2-dimensional rigidity of certain families of graphs. *J. Graph Theory*, 54(2):154–166, 2007.

[4] Brigitte Servatius, Herman Servatius, and M. F. Thorpe. Zeolites: Geometry and combinatorics. *International Journal of Chemical Modeling*, to appear.

[5] Hassler Whitney. Congruent Graphs and the Connectivity of Graphs. *Amer. J. Math.*, 54(1):150–168, 1932.