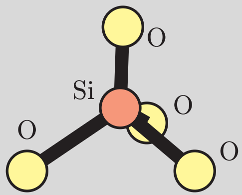
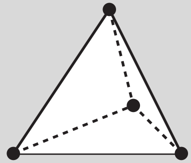
From combinatorial zeolites to geometric realizations

Brigitte Servatius — WPI

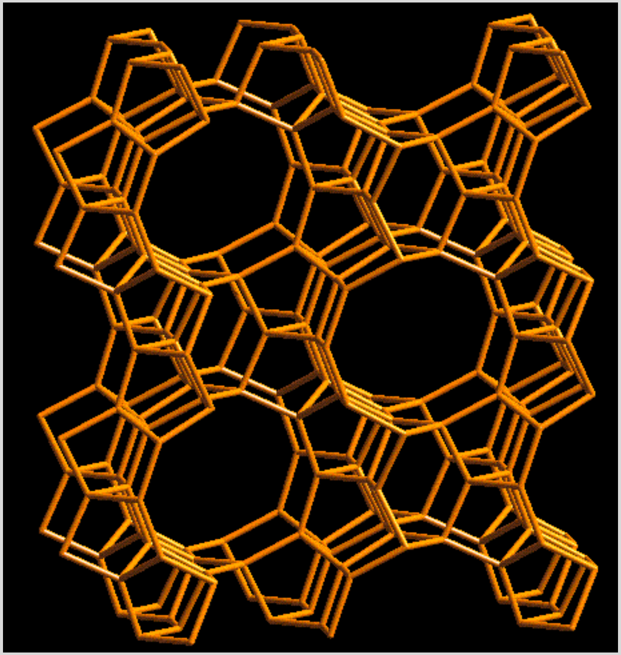
1. Chemical Zeolites

- 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

[9](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

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.

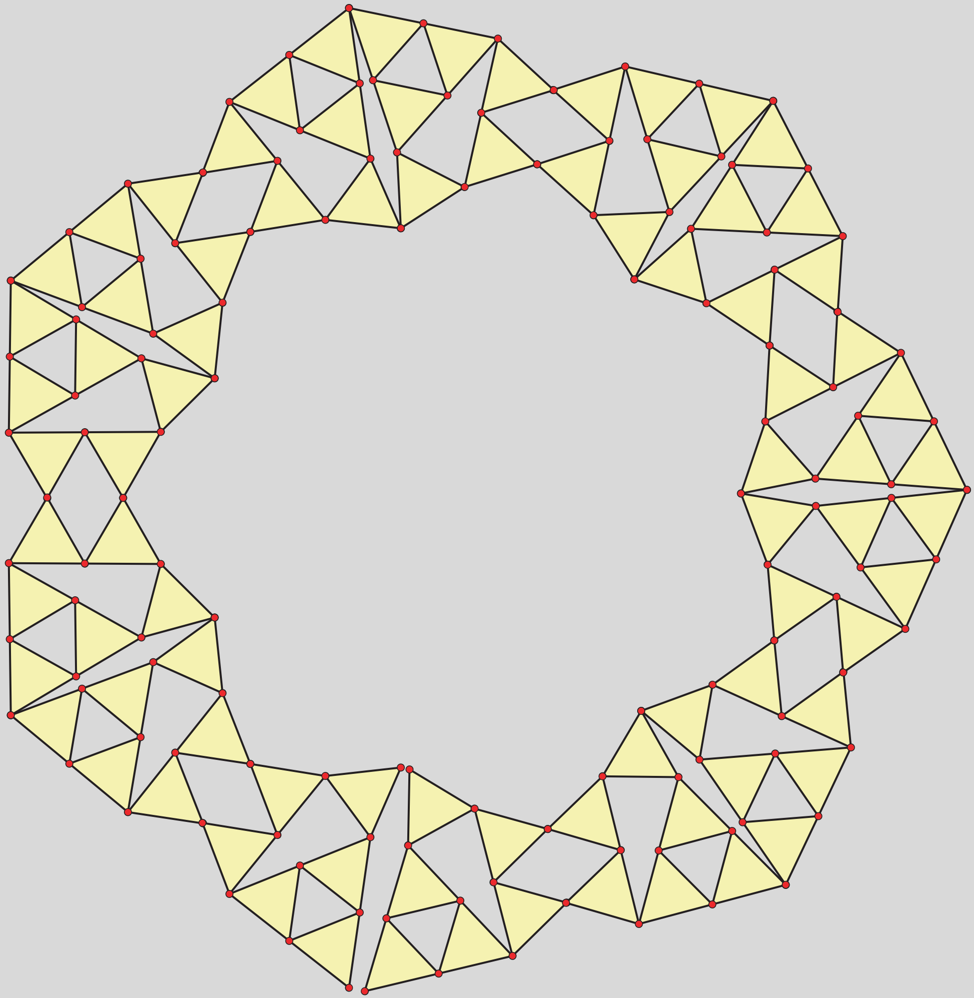
unit-distance realization

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

non-interpenetrating realization

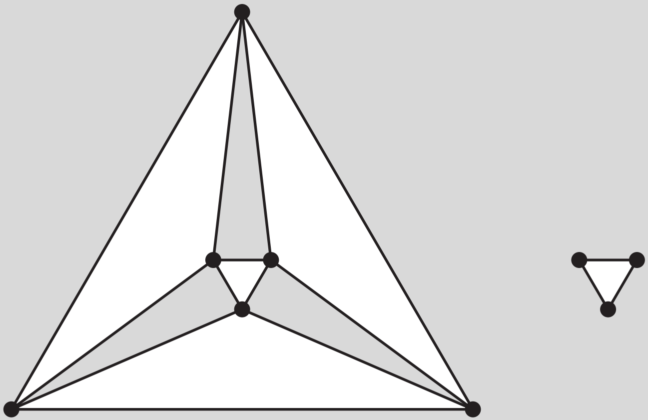
A realization where simplices are disjoint except at joined vertices.

The typical situation: Not unit distance realizable.

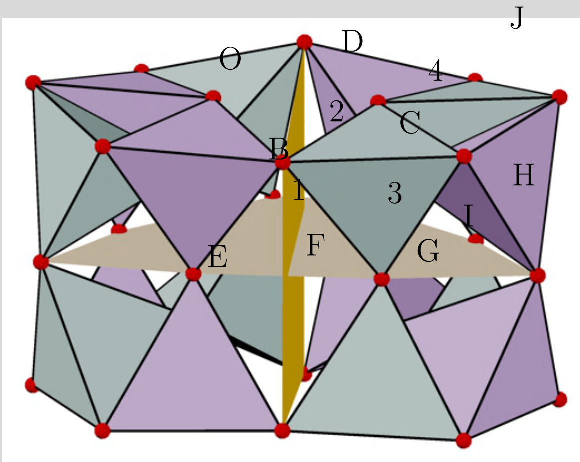


4. 2d Zeolites

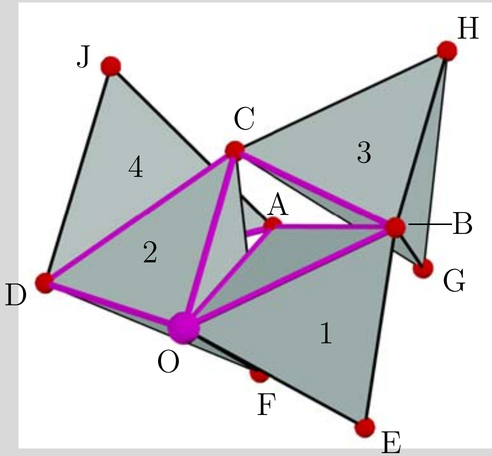
Smallest 2d zeolite is the line graph of K_4: The graph of the octahedron with four (edge disjoint) faces.
For body-pin graphs on more than 4 vertices, the zeolite can be recovered uniquely from the line-graph.



A finite 3-D symmetric example:

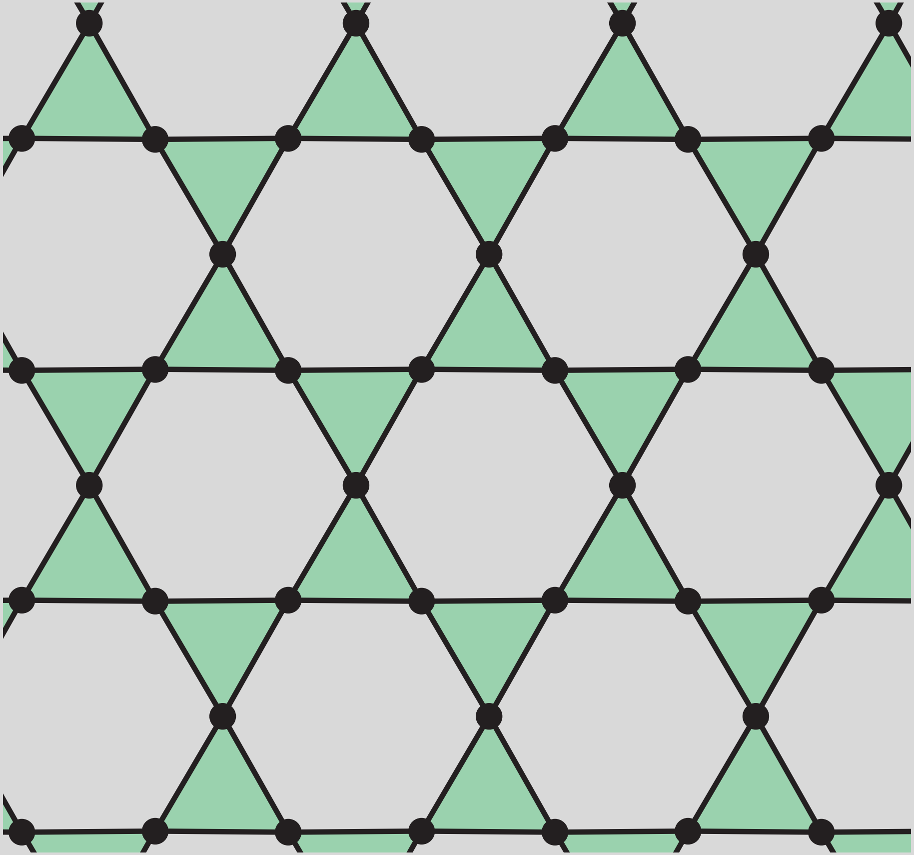


Model with its two planes of symmetry

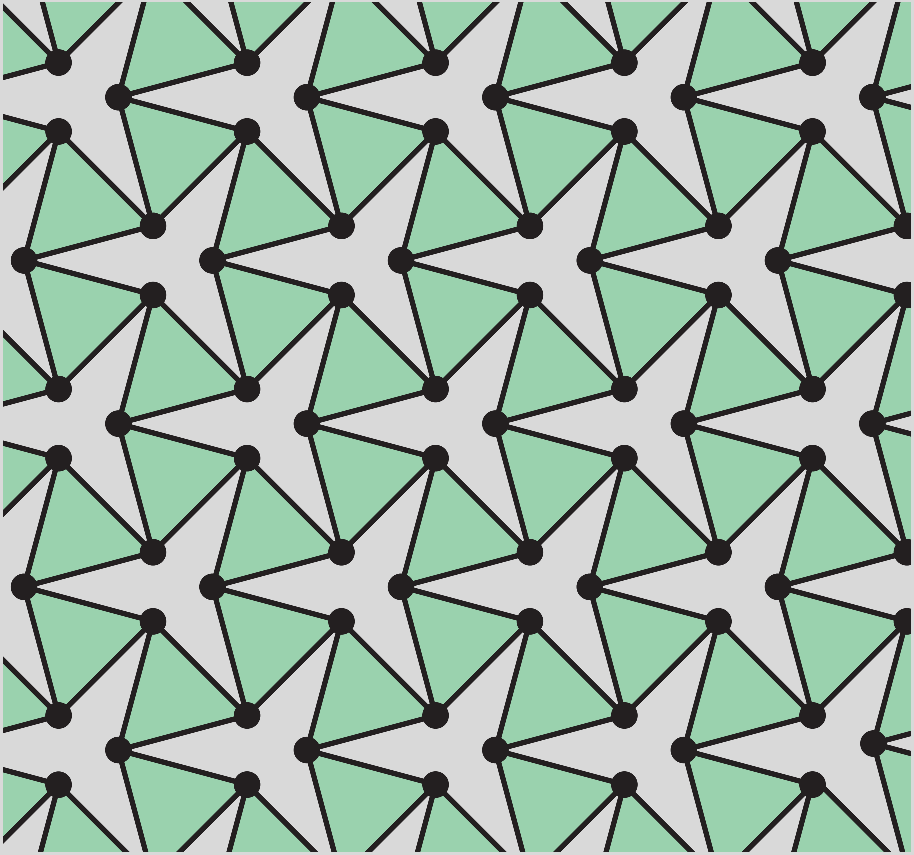


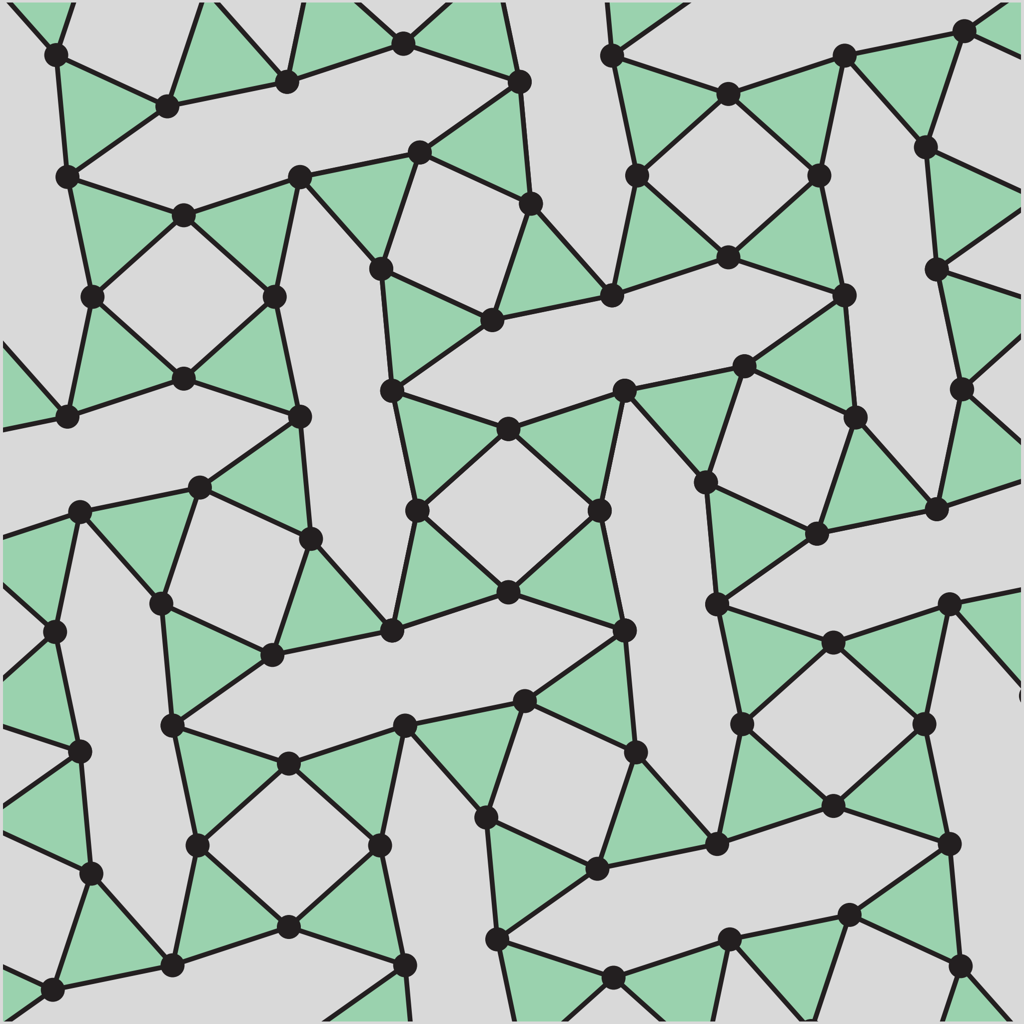
[2]

It is just as easy to construct infinite symmetric examples:



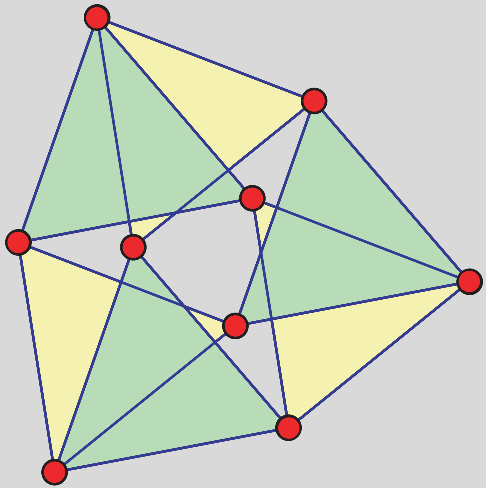
Showing a different symmetry



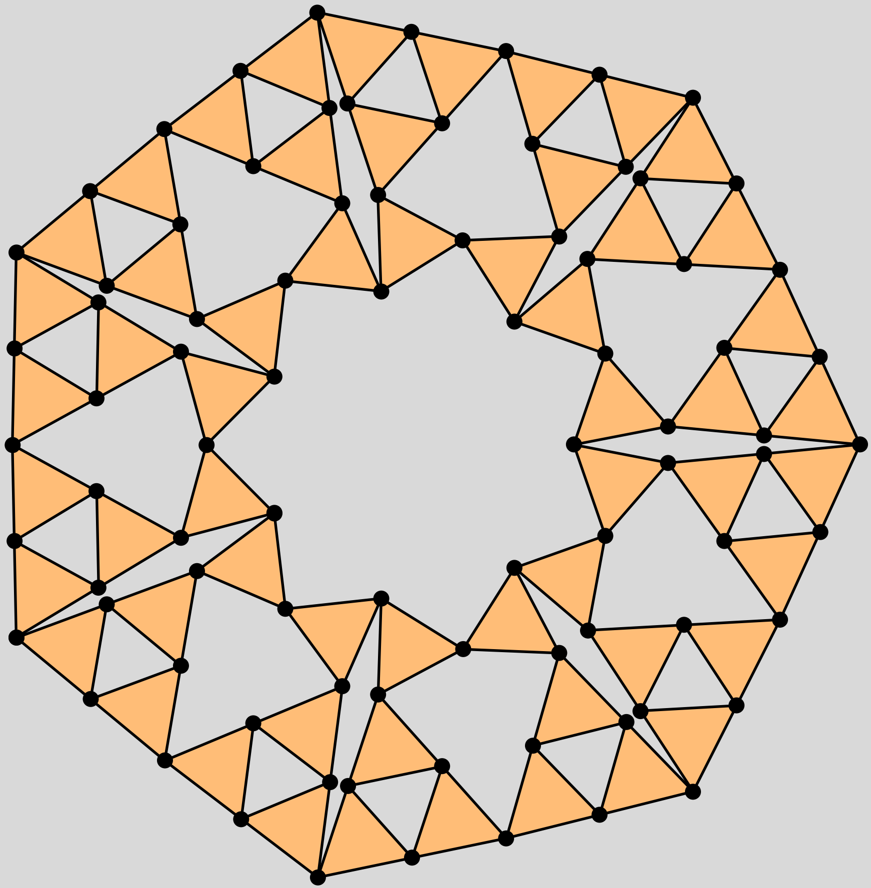


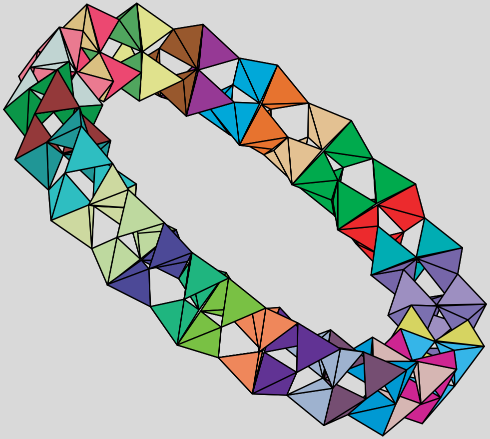
5. Finite Zeolites

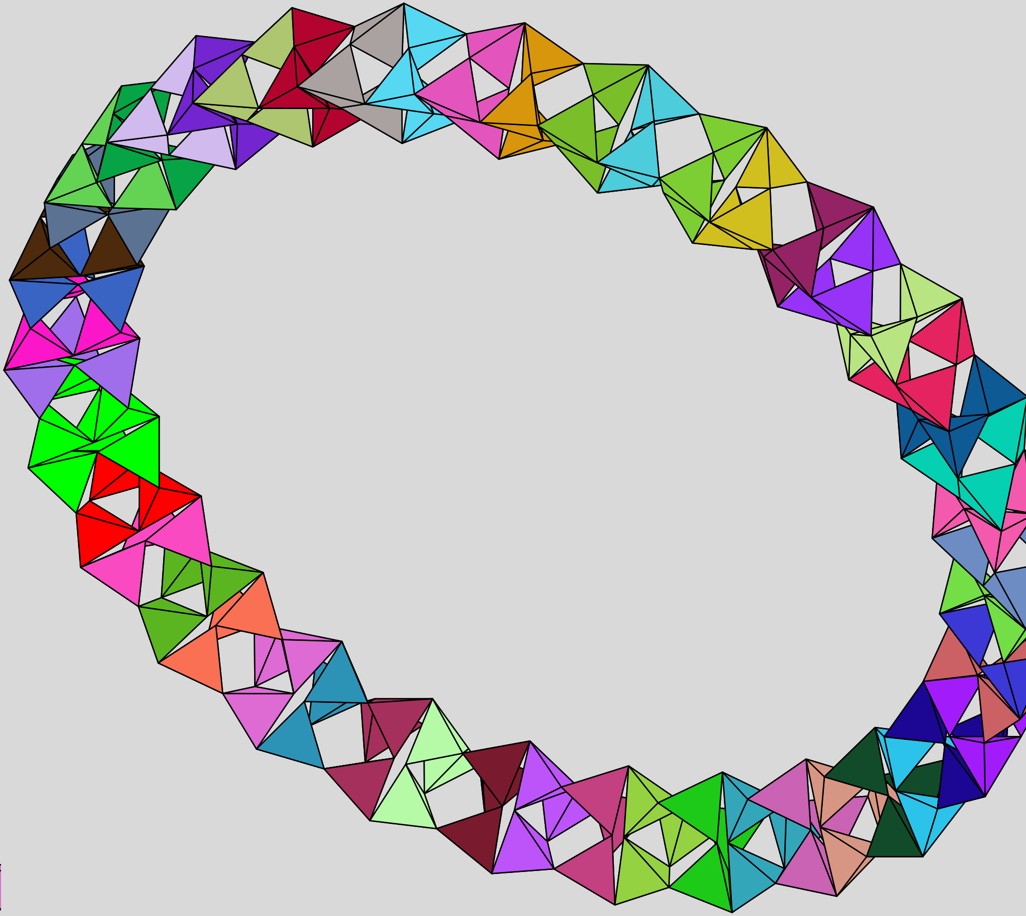
Body pin graph: $K_{3,3}$. Since the body pin graph is not planar, the resulting zeolite cannot be planar. Its underlying graph is generically globally rigid. However, it has a unit distance realization in the plane which is a mechanism.

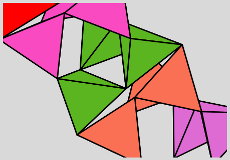


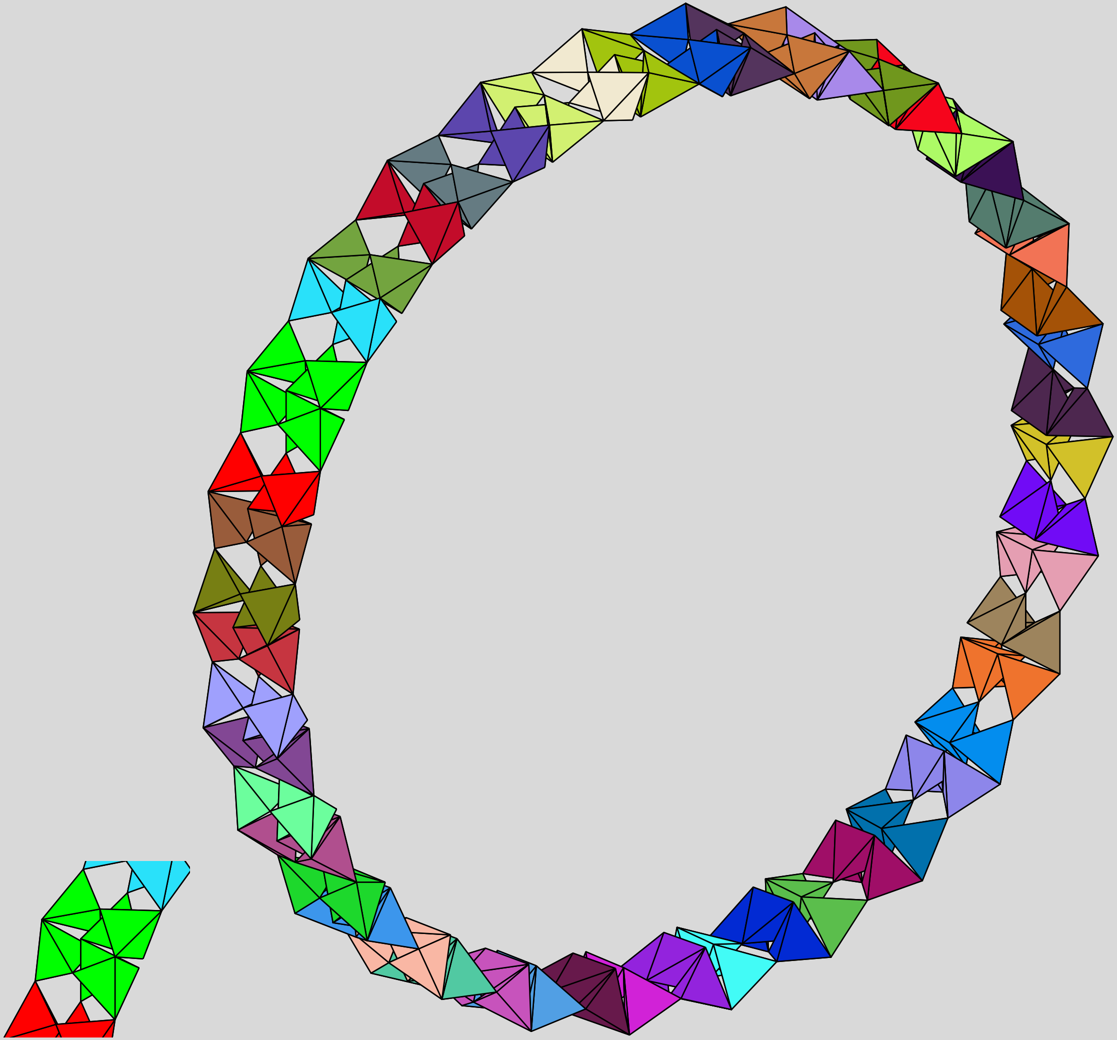
Harborth's Example [4, 3]





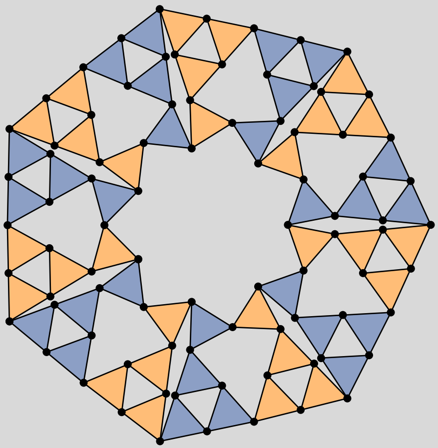






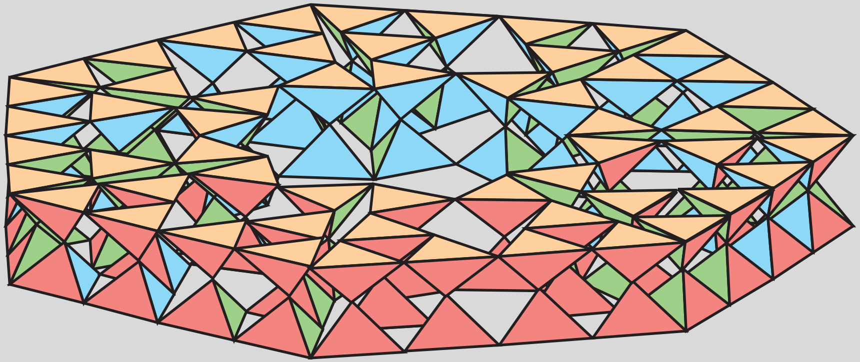
6. The Layer Construction

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

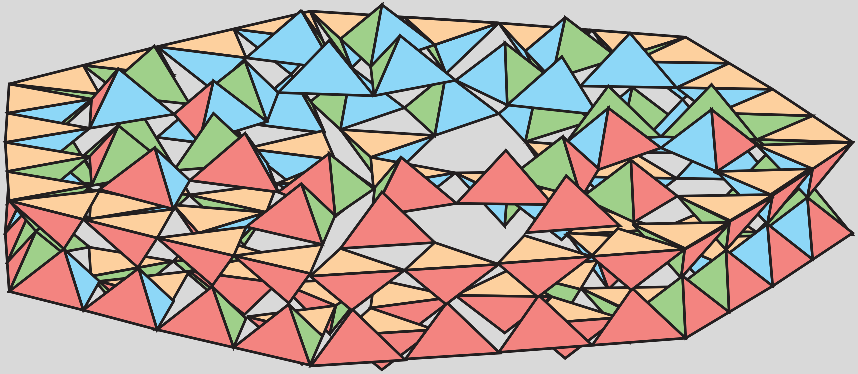


Alternately staking Z_a and Z_b gives a *layered Zeolite* in $\mathbb{R}^{d+1}$.

Labels all +1
A two layered zeolite.

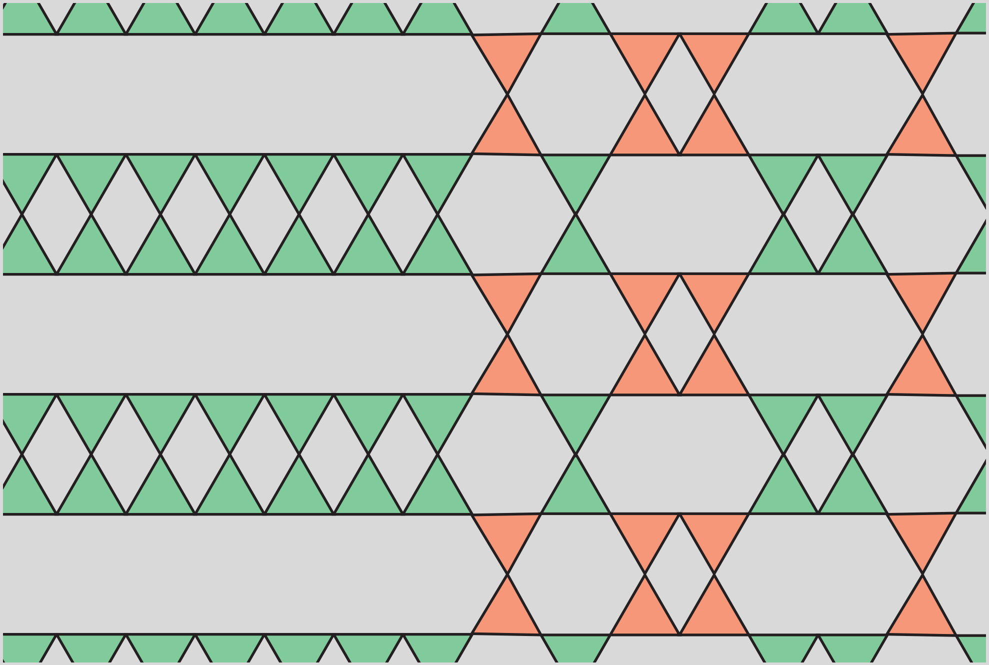


The general case starting from a finite zeolite.

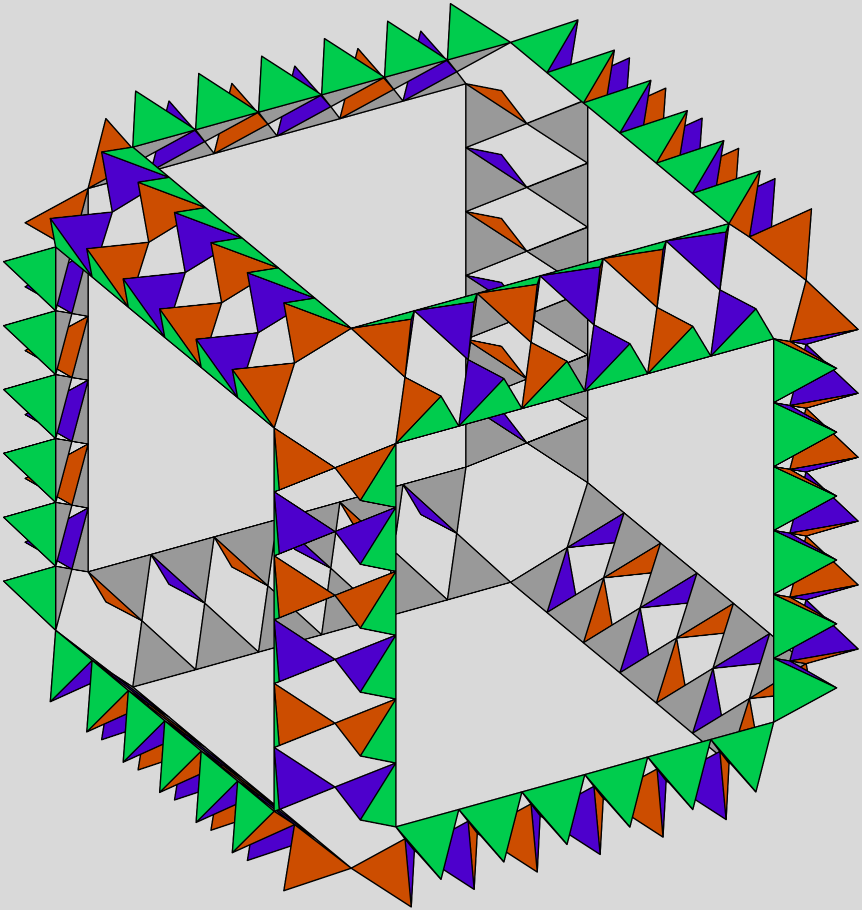


Theorem: There are uncountably many isomorphism classes of unit distance realizable zeolites in $\mathbb{R}^3$.
(actually in any dimension $d > 1$. [7])

Proof:



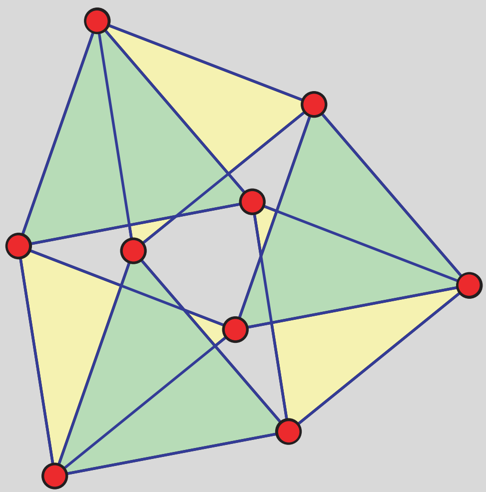
7. Holes in Zeolites



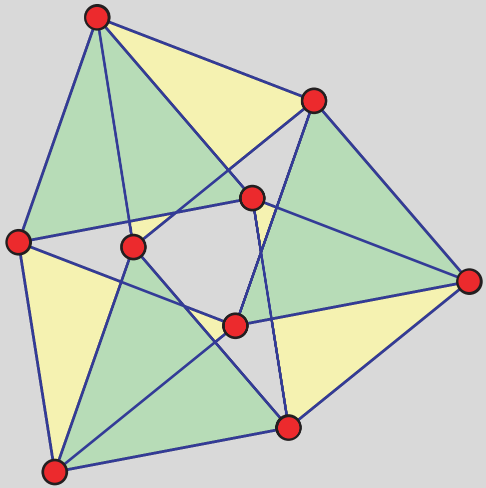
8. Motions

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

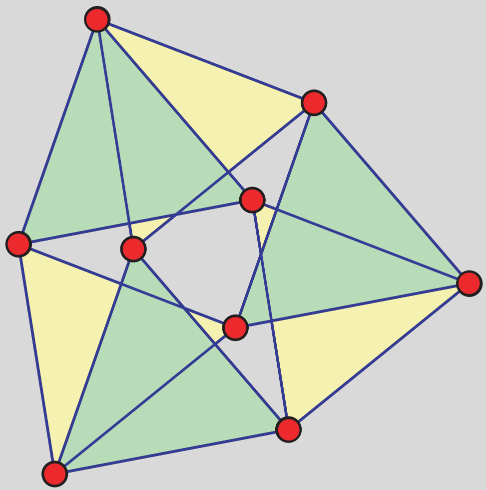


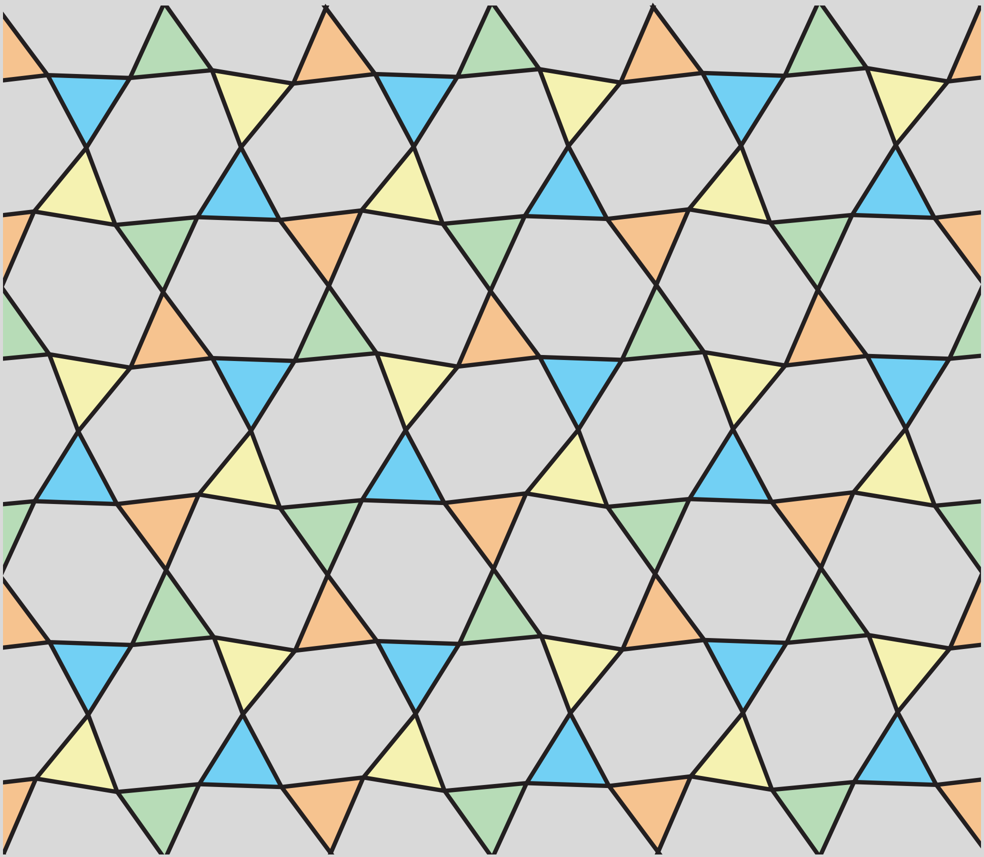
Generically globally rigid in the plane.

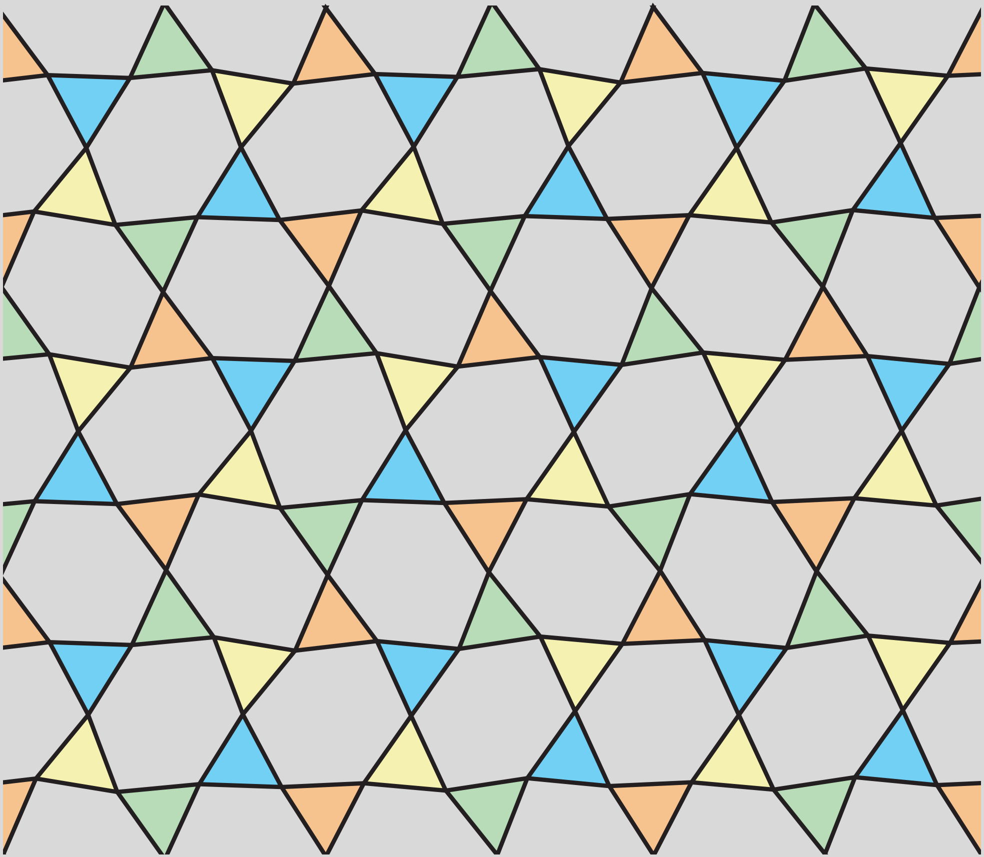


Generically globally rigid in the plane.

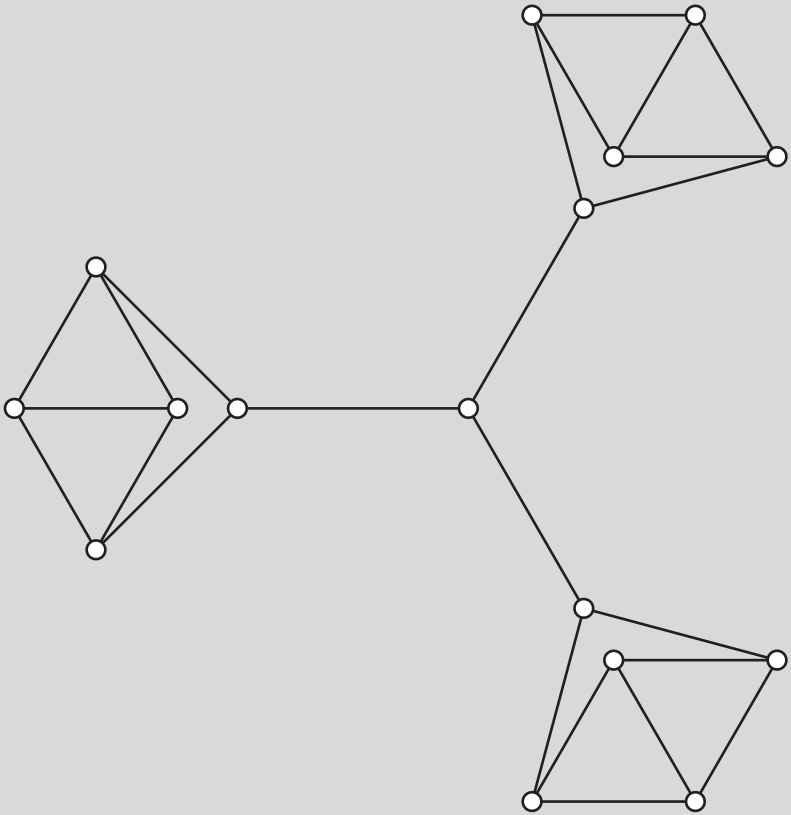
A 4-regular vertex transitive graph is globally rigid unless it has a 3-factor consisting of s disjoint copies of K_4 with $s \geq 3$. [Jackson, S, S – 2004]







Are there finite generically flexible 2D Zeolites?
Yes, line graphs of 3-regular graphs with edge connectivity less than 3.



Chemical Zeolites
Combinatorial . . .
Realization
2d Zeolites
Finite Zeolites
The Layer . . .
Holes in Zeolites
Motions
A geometric . . .
Vertex transitive . . .
Open Problems

Home Page

Title Page

Go Back

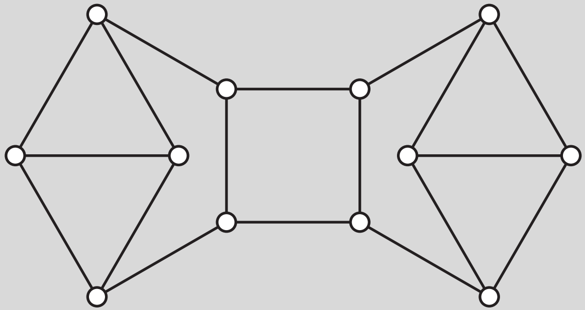
Full Screen

Close

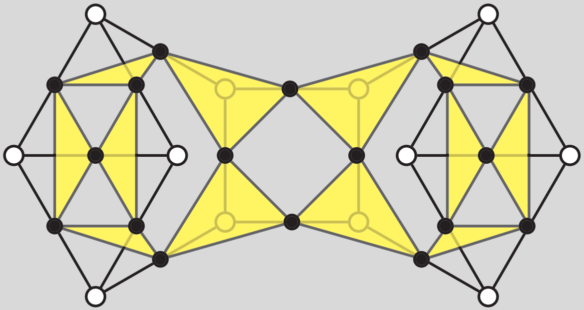
Quit

Are there finite generically rigid but not globally rigid 2D Zeolites?

Yes, line graphs of 3-regular graphs with edge connectivity less than 3.

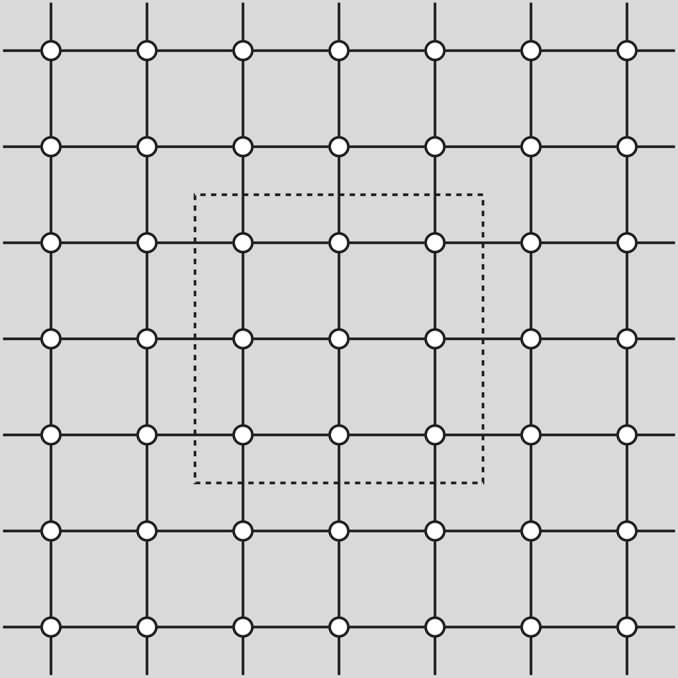


Are there finite generically rigid but not globally rigid 2D Zeolites?
Yes, line graphs of 3-regular graphs with edge connectivity less than 3.

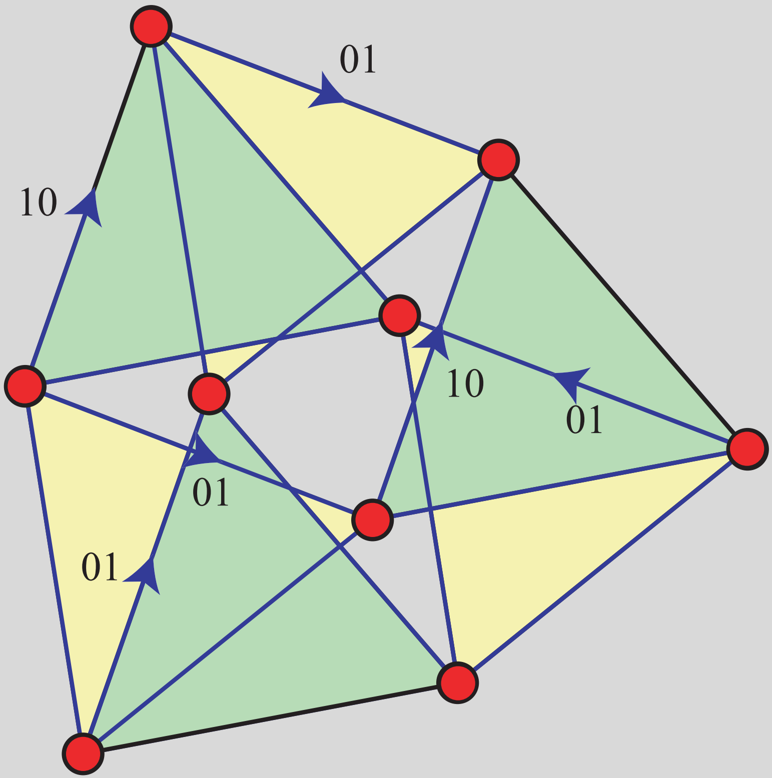


See [5]

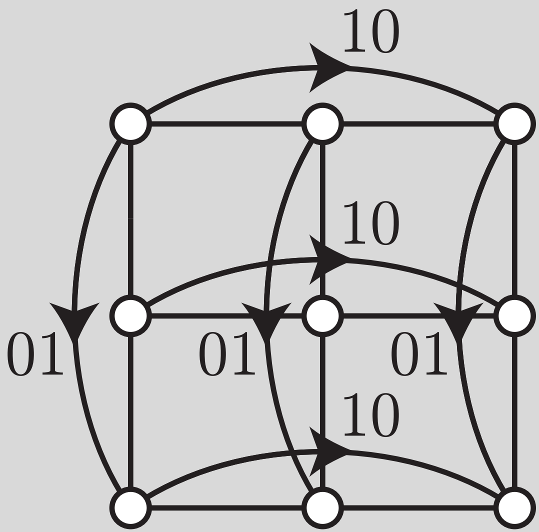
9. A geometric approach



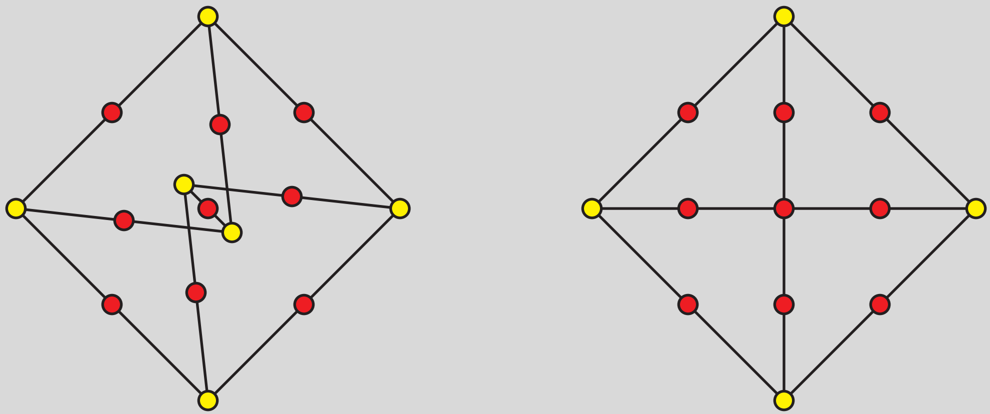
Combinatorial version of the gain graph



Geometric version of the gain graph

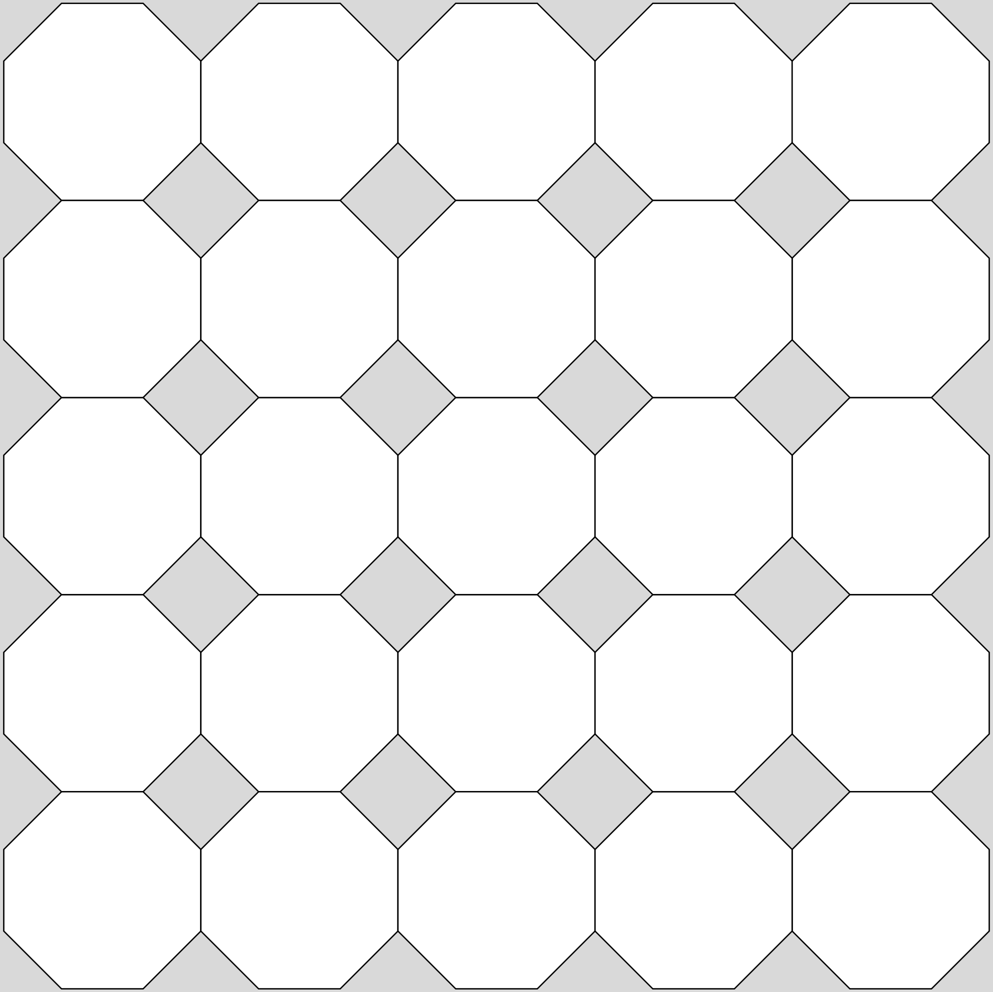


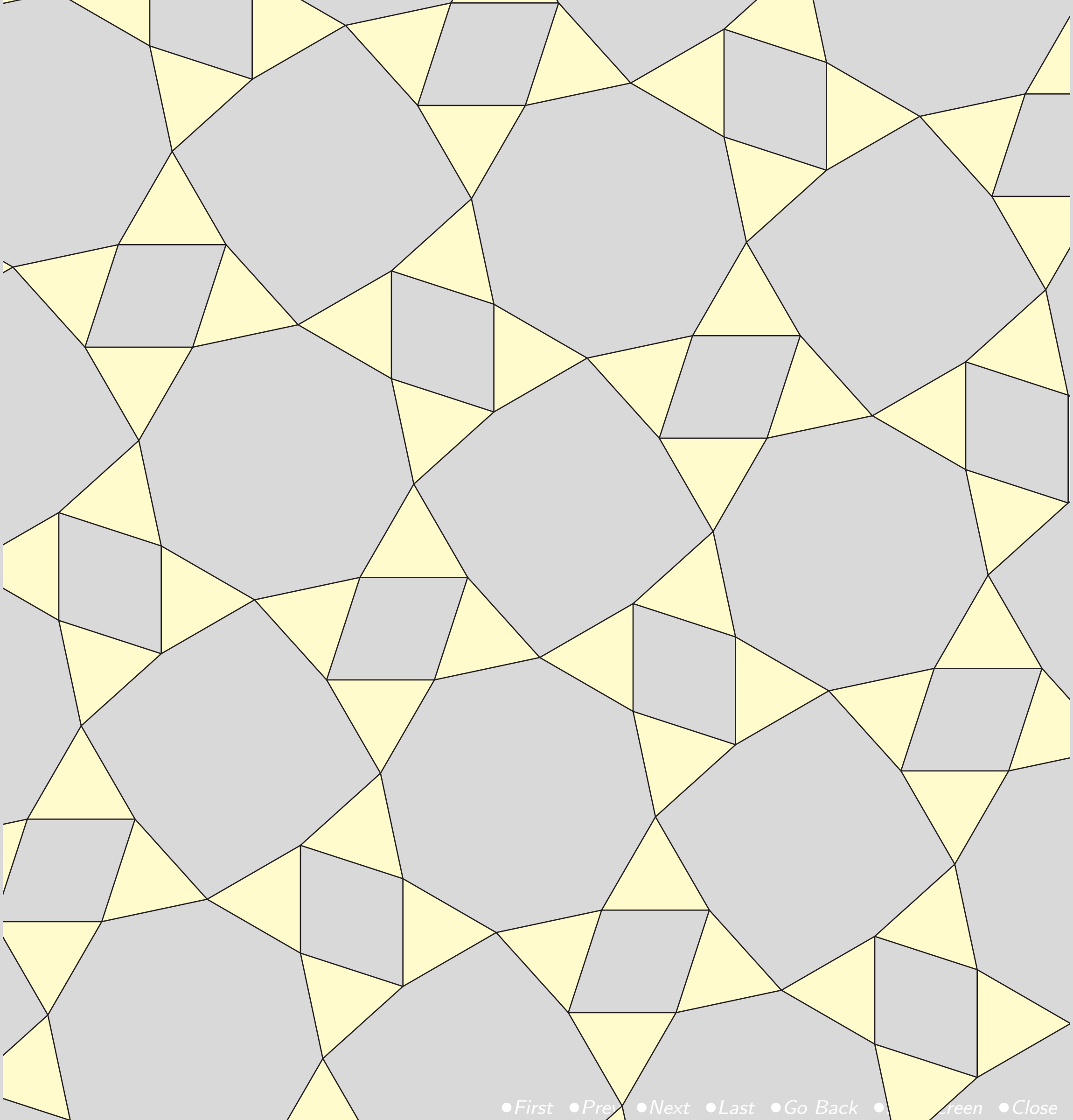
It's a geometric line graph!

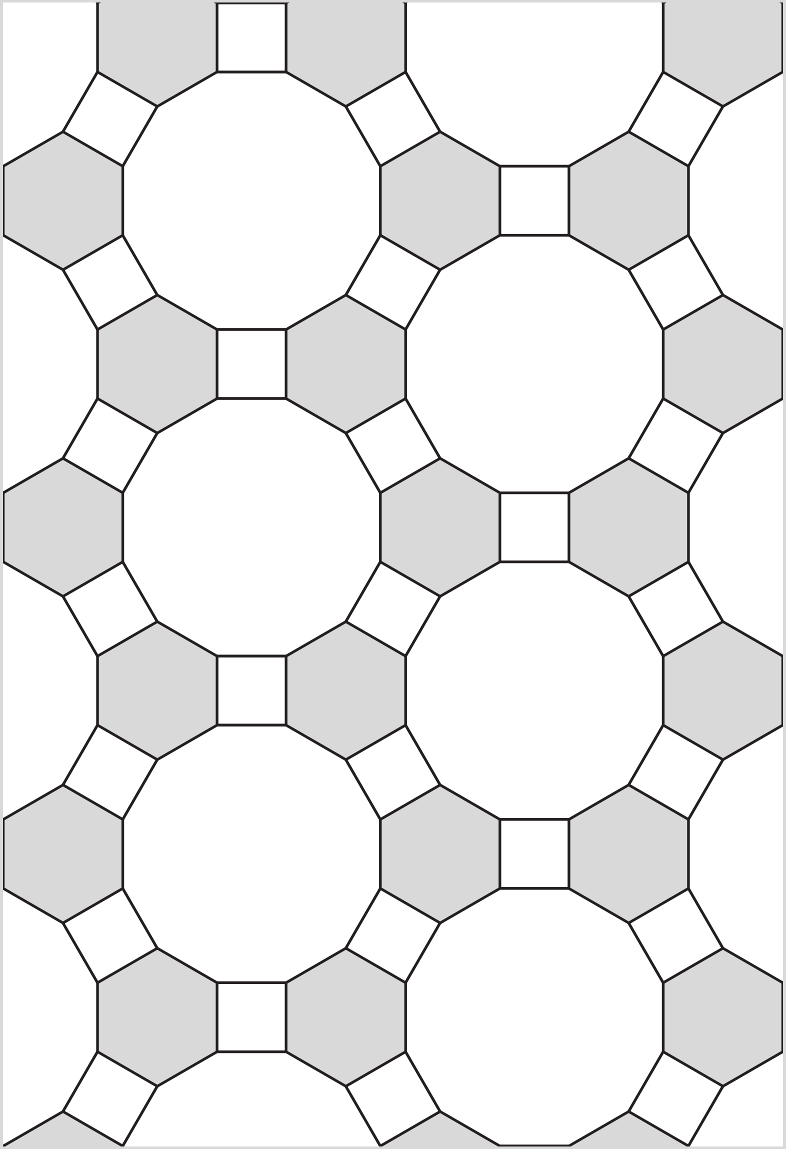


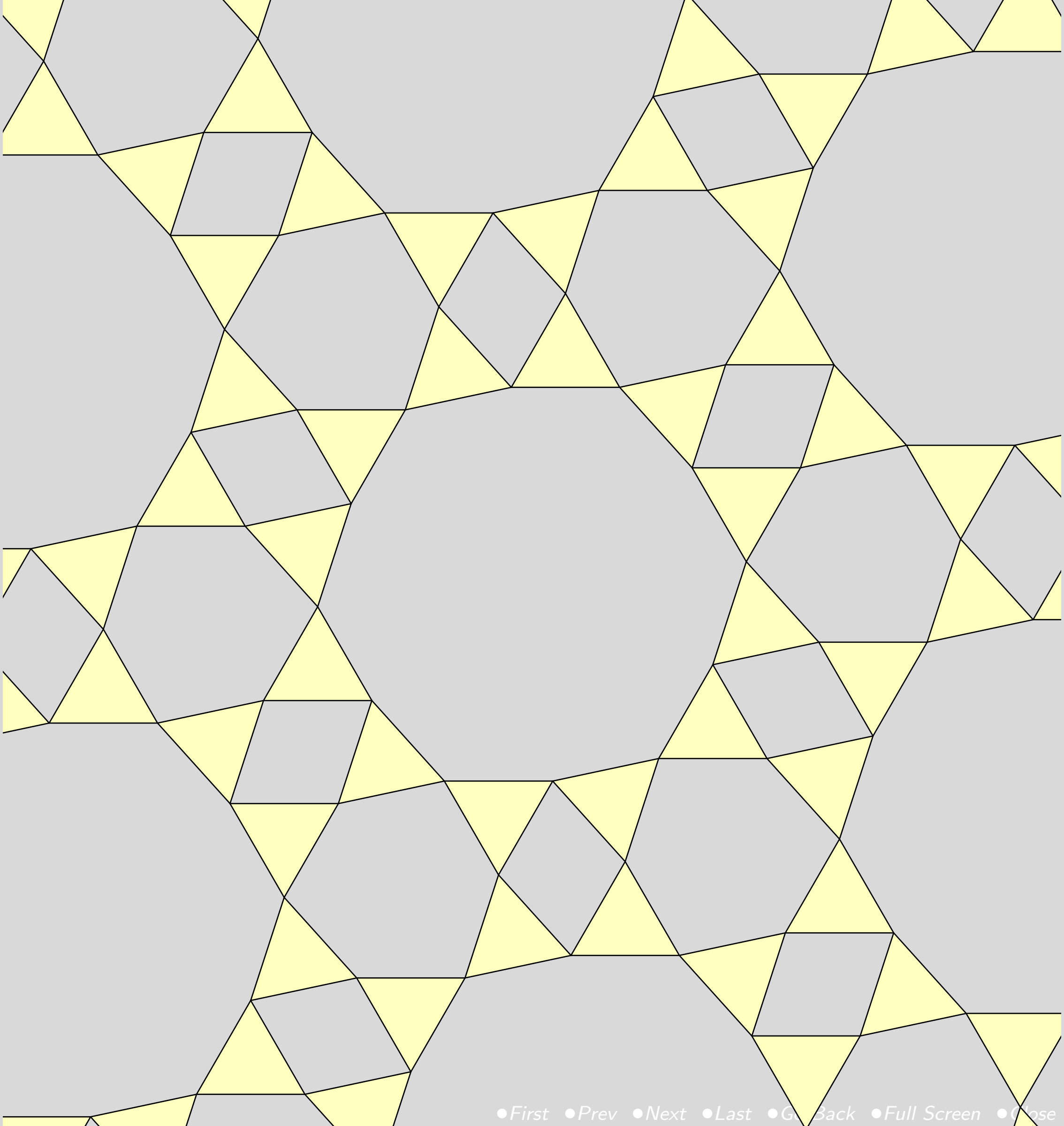
THEOREM [1] Let G be a locally finite 3-connected almost vertex-transitive planar graph with at most one end. Then G has an embedding on a natural geometry such that all automorphisms of G are induced by isometrics of the geometry. Straightening Lemma for maps on the sphere [6].

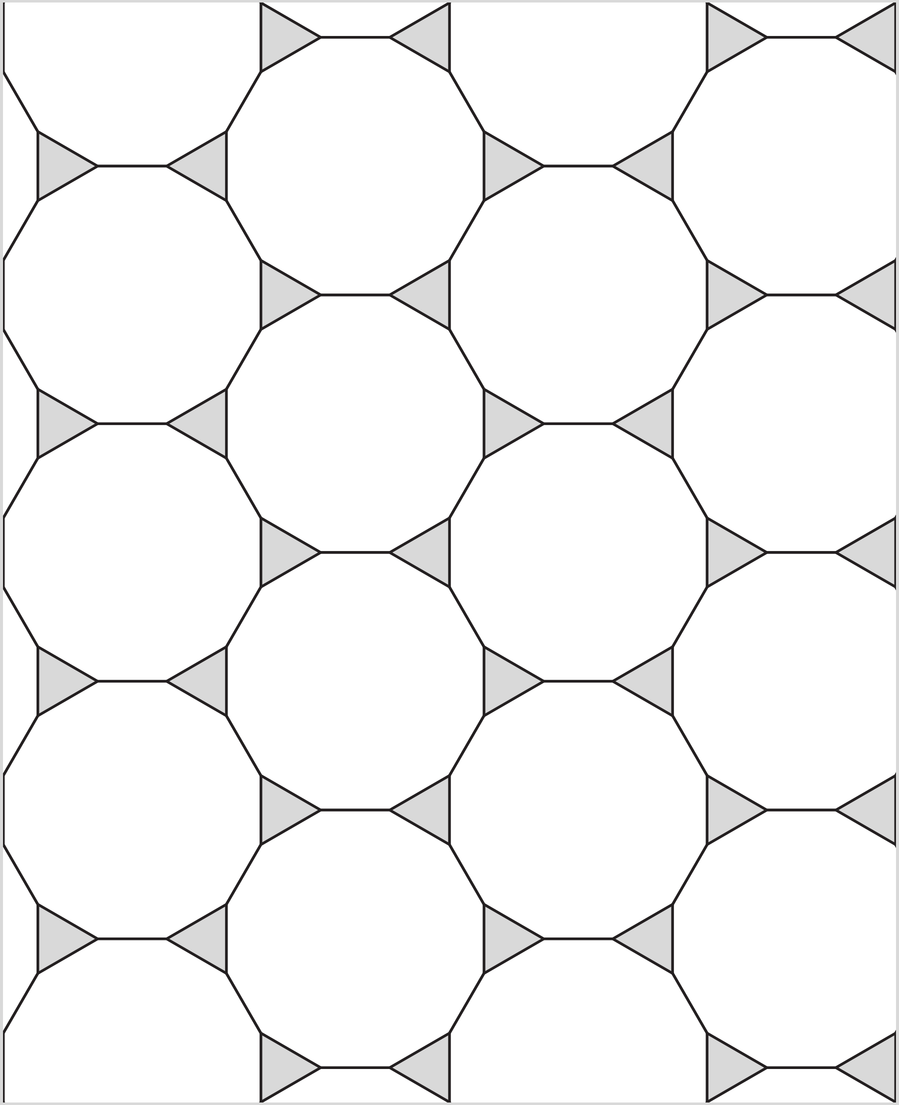
10. Vertex transitive 3-regular

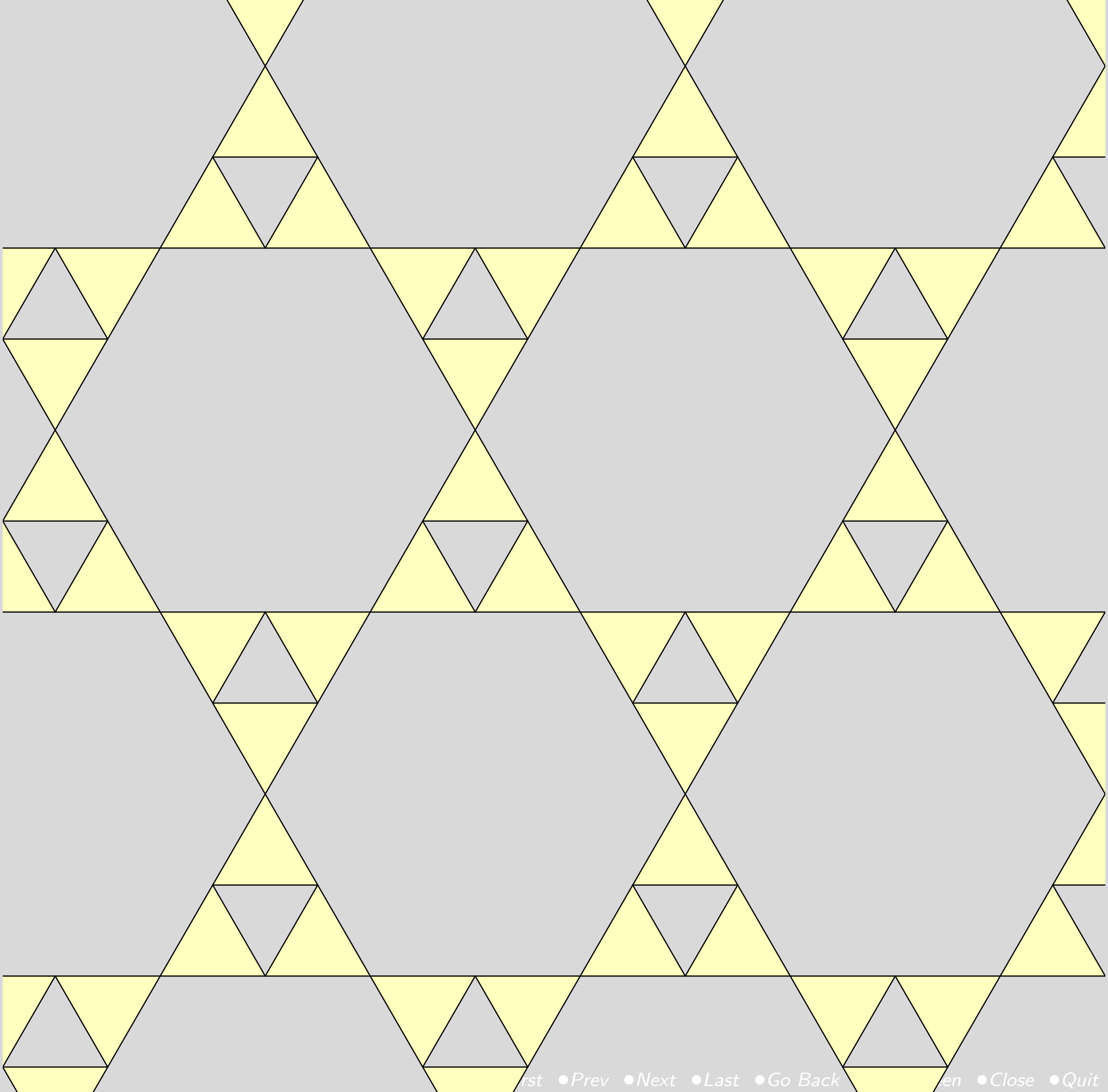


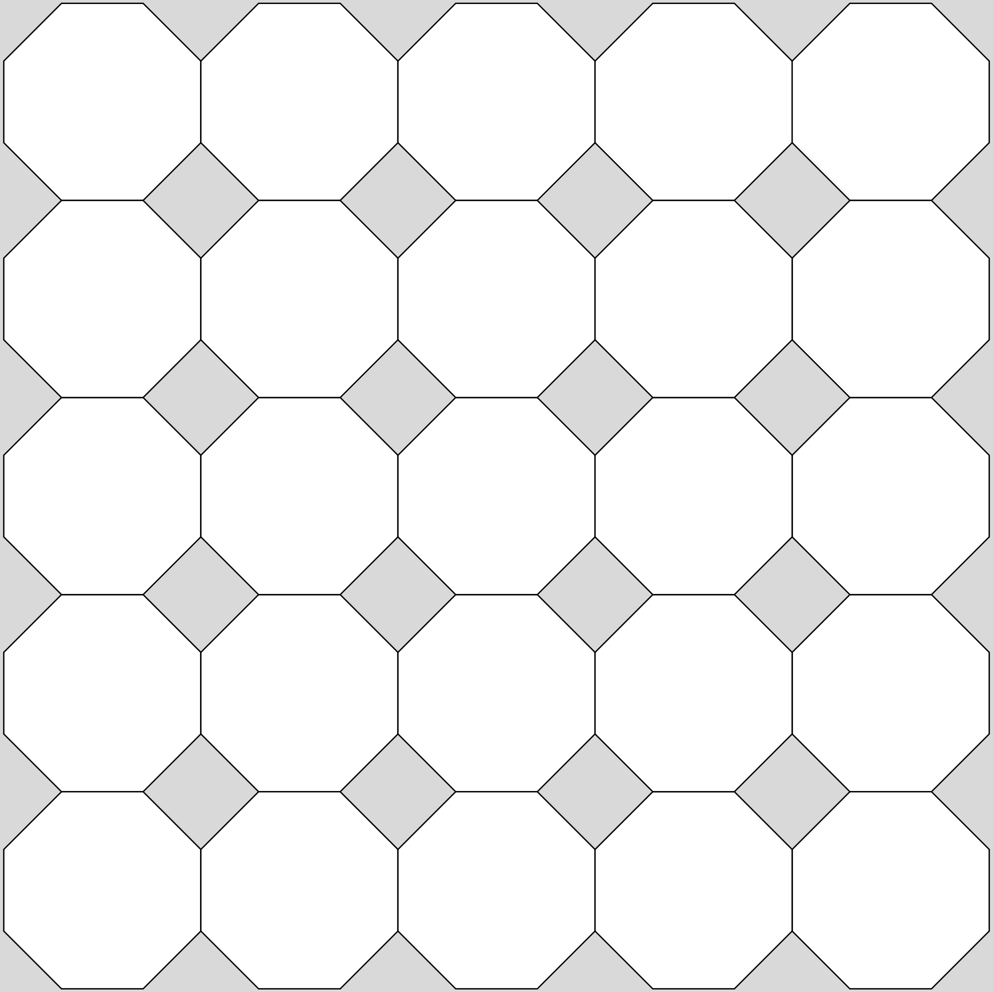


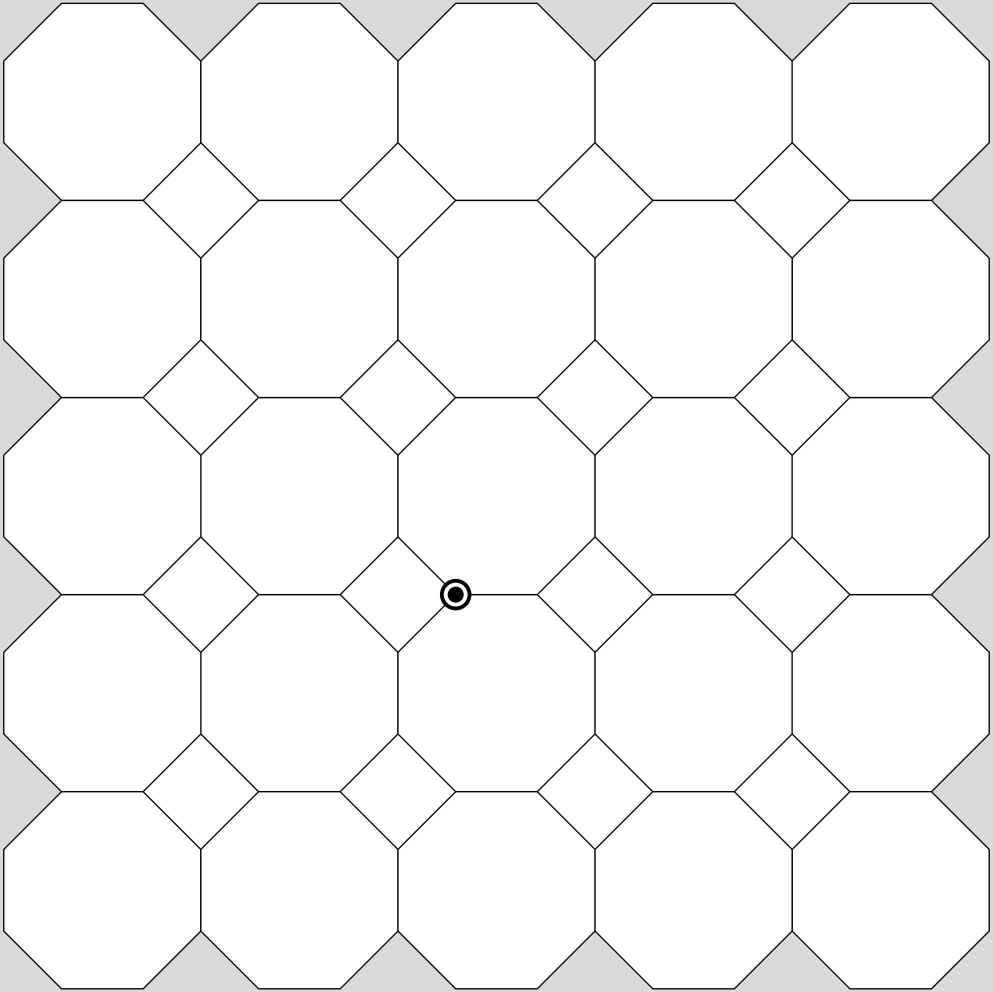


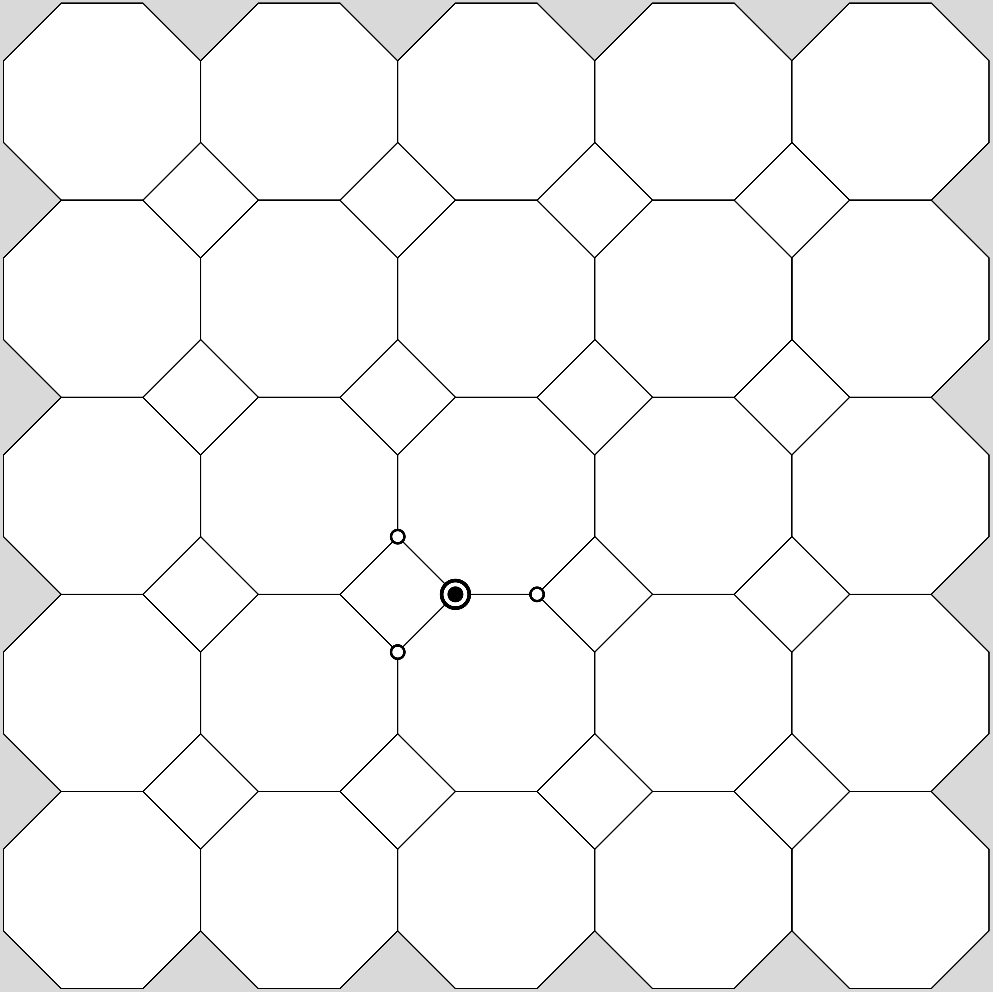


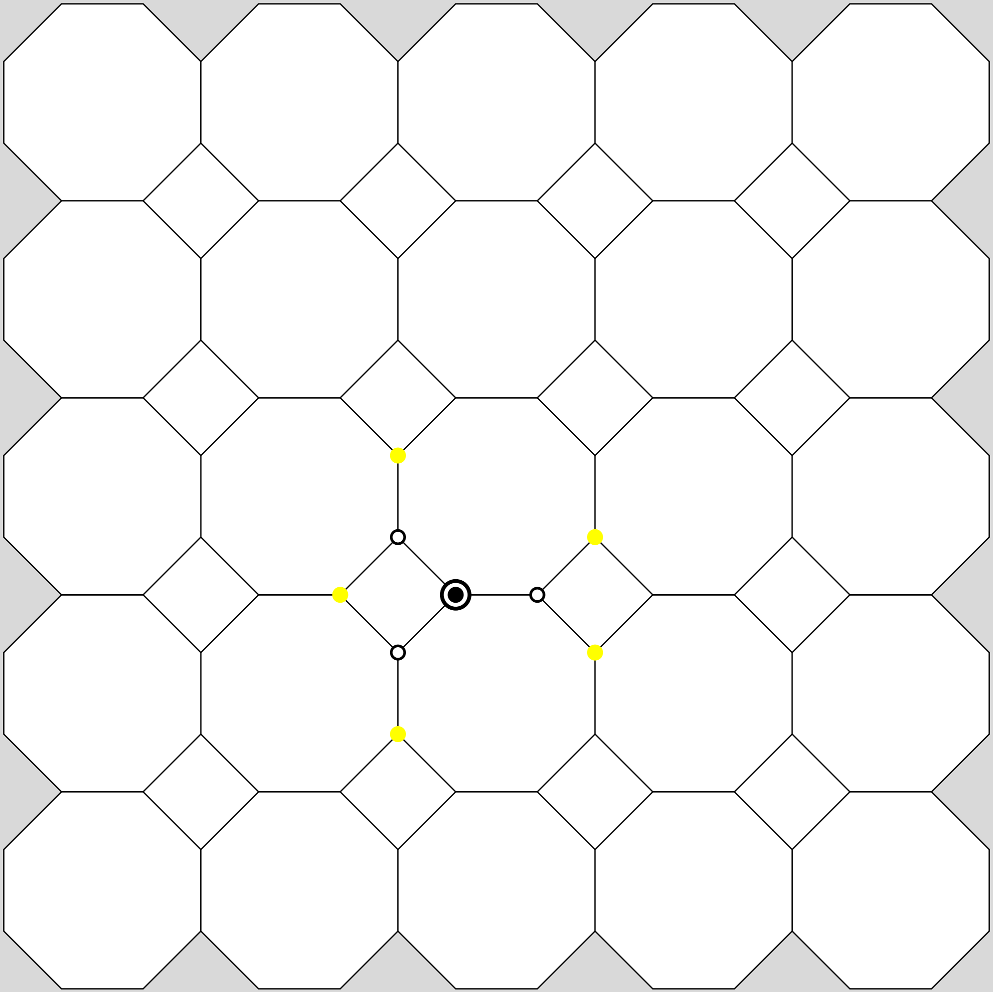


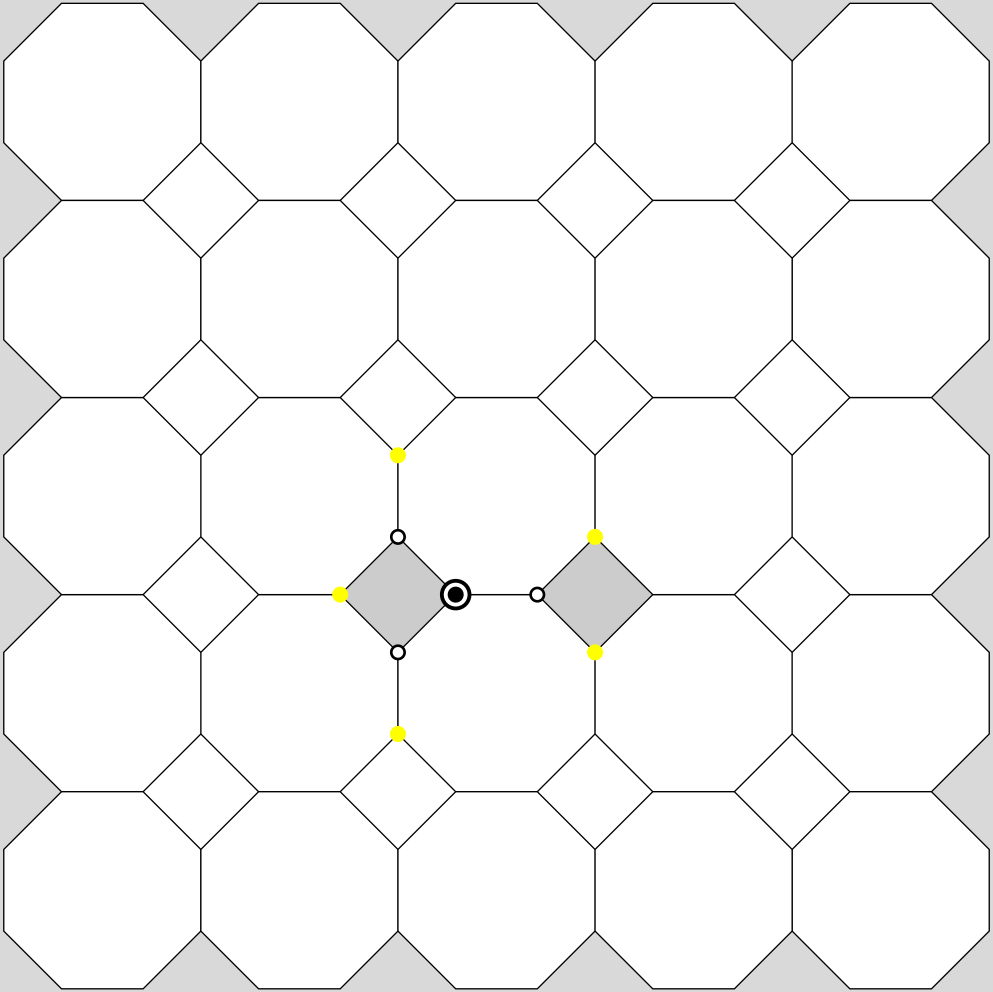


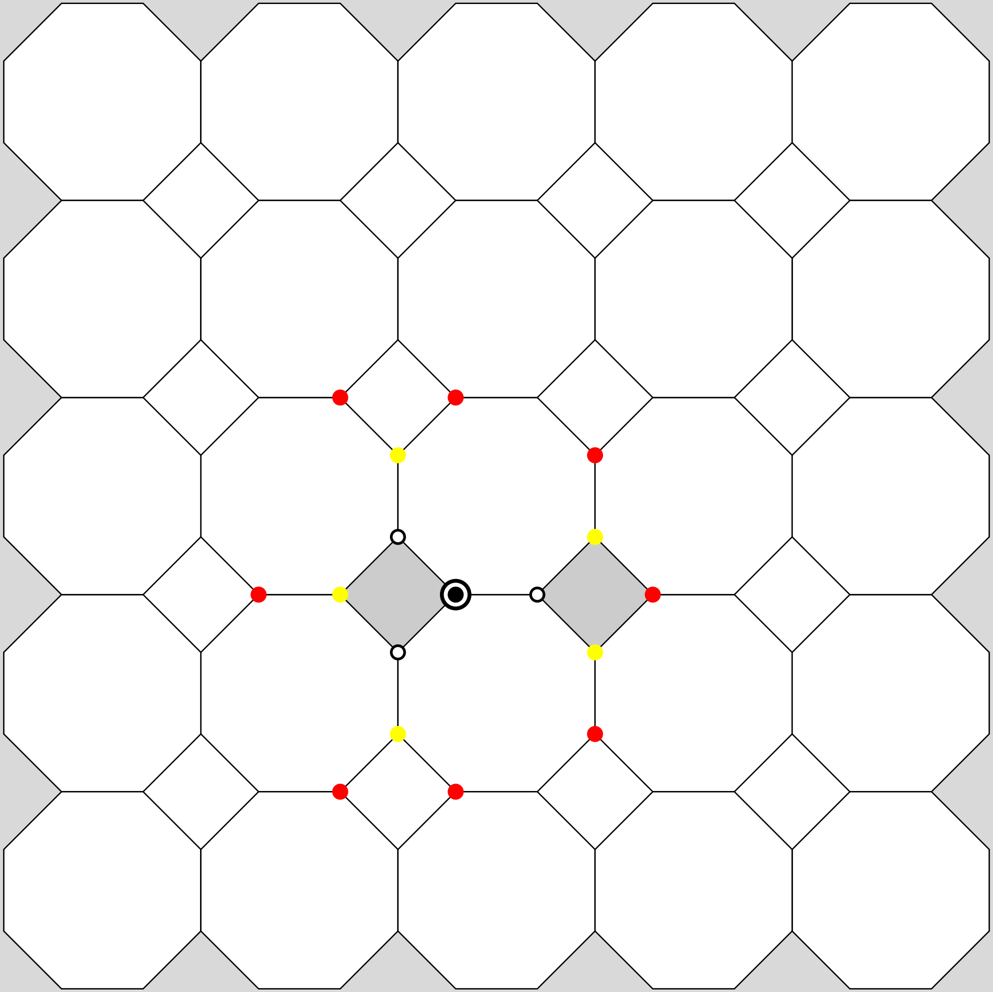


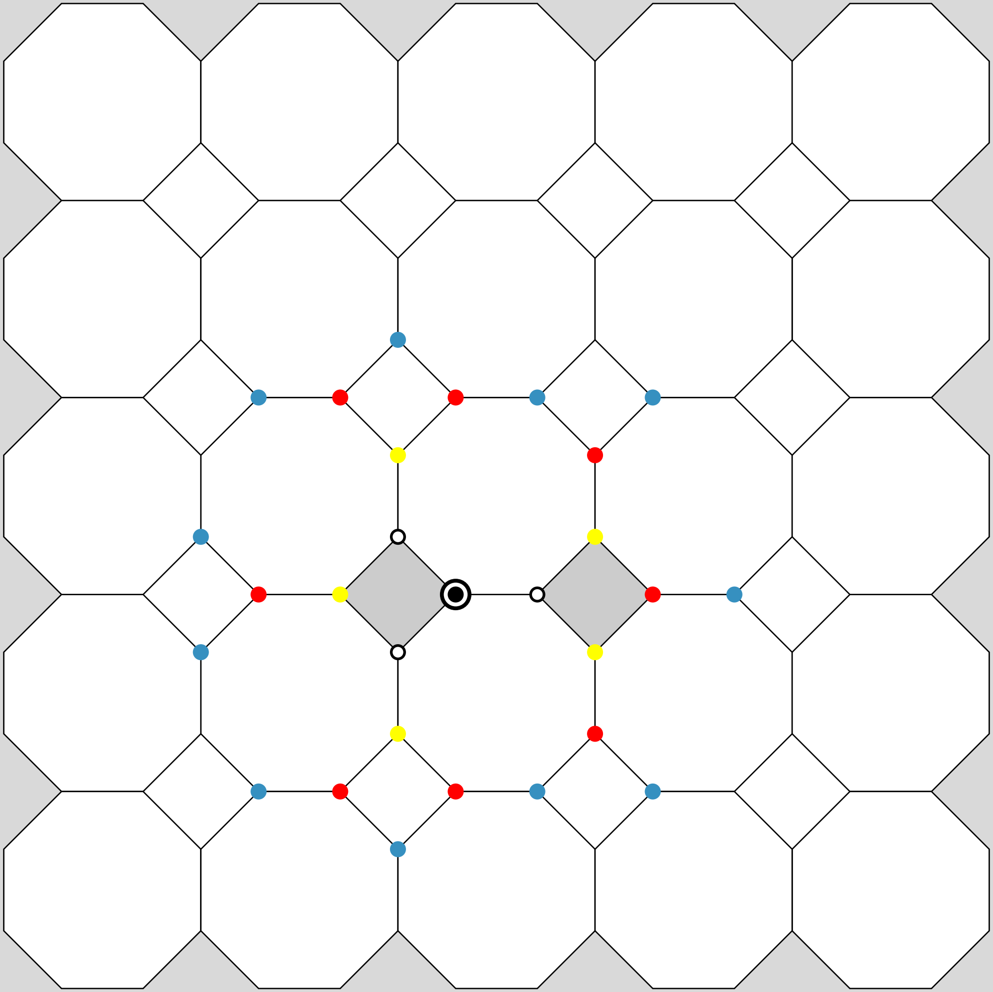




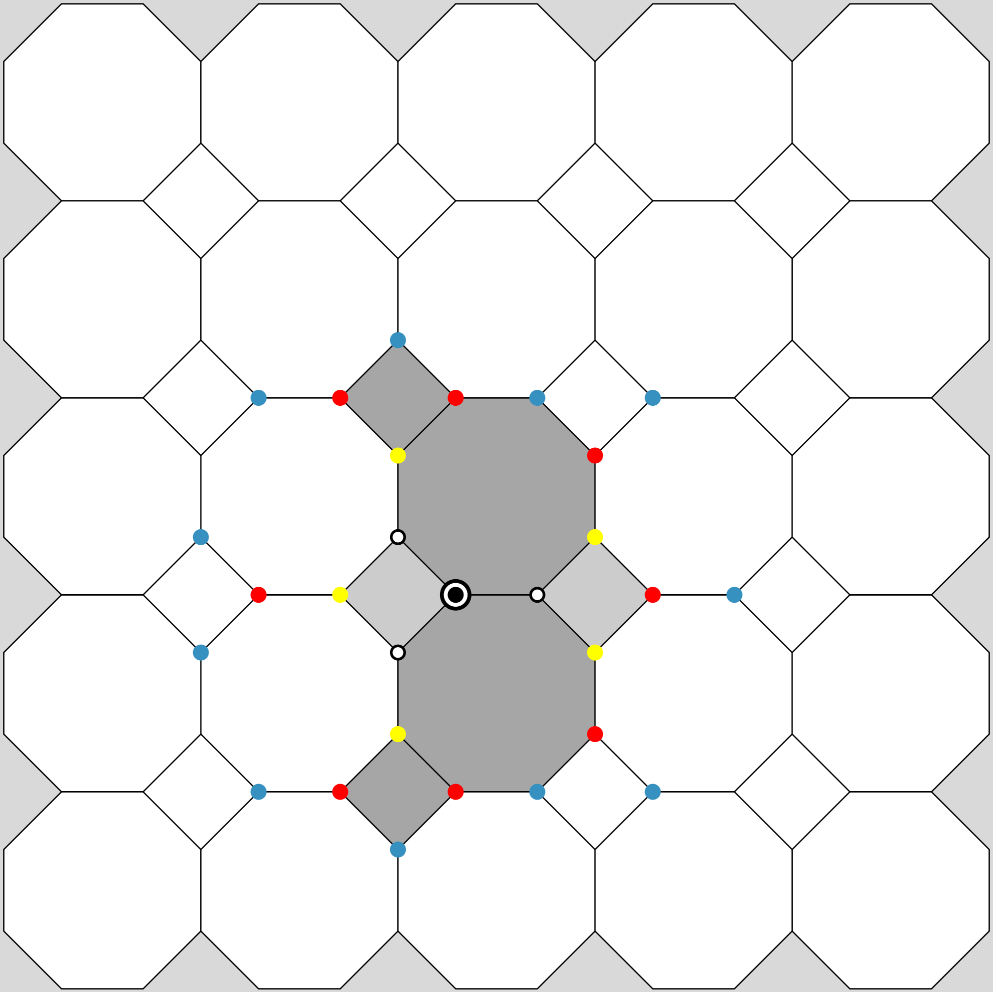


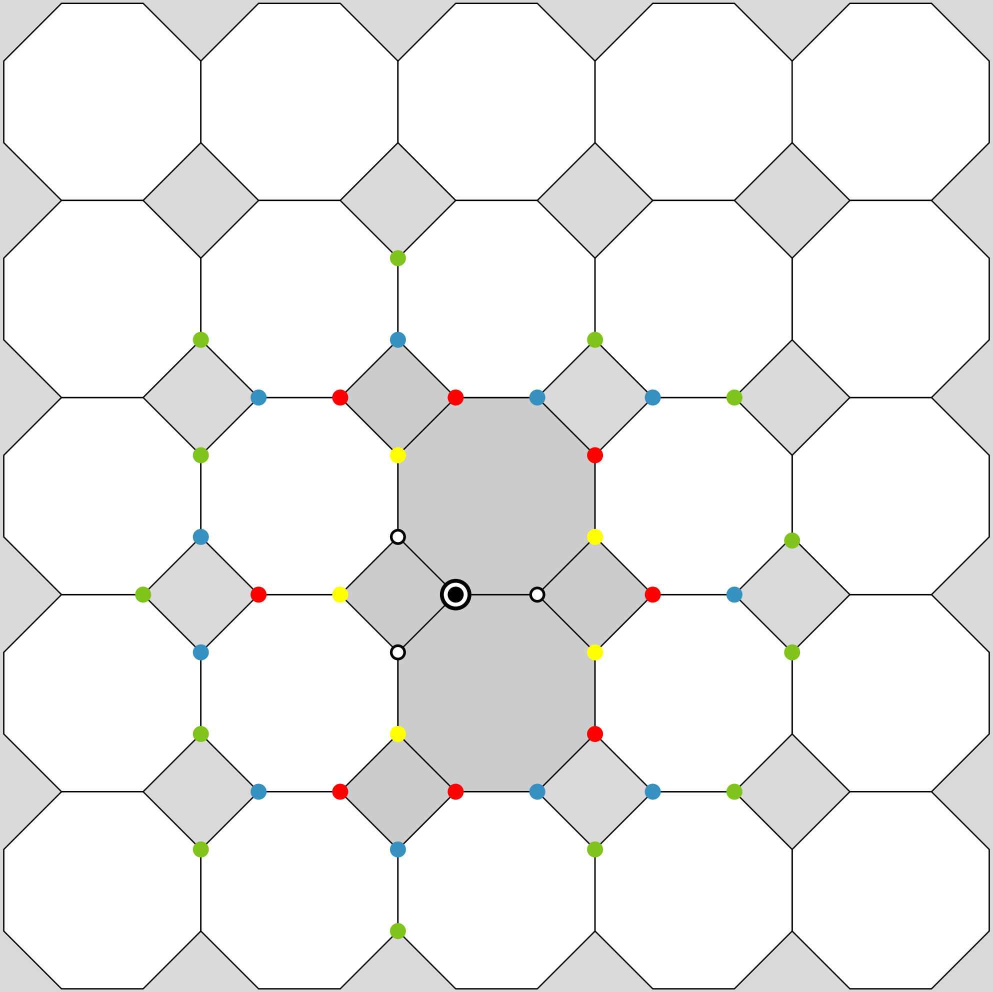


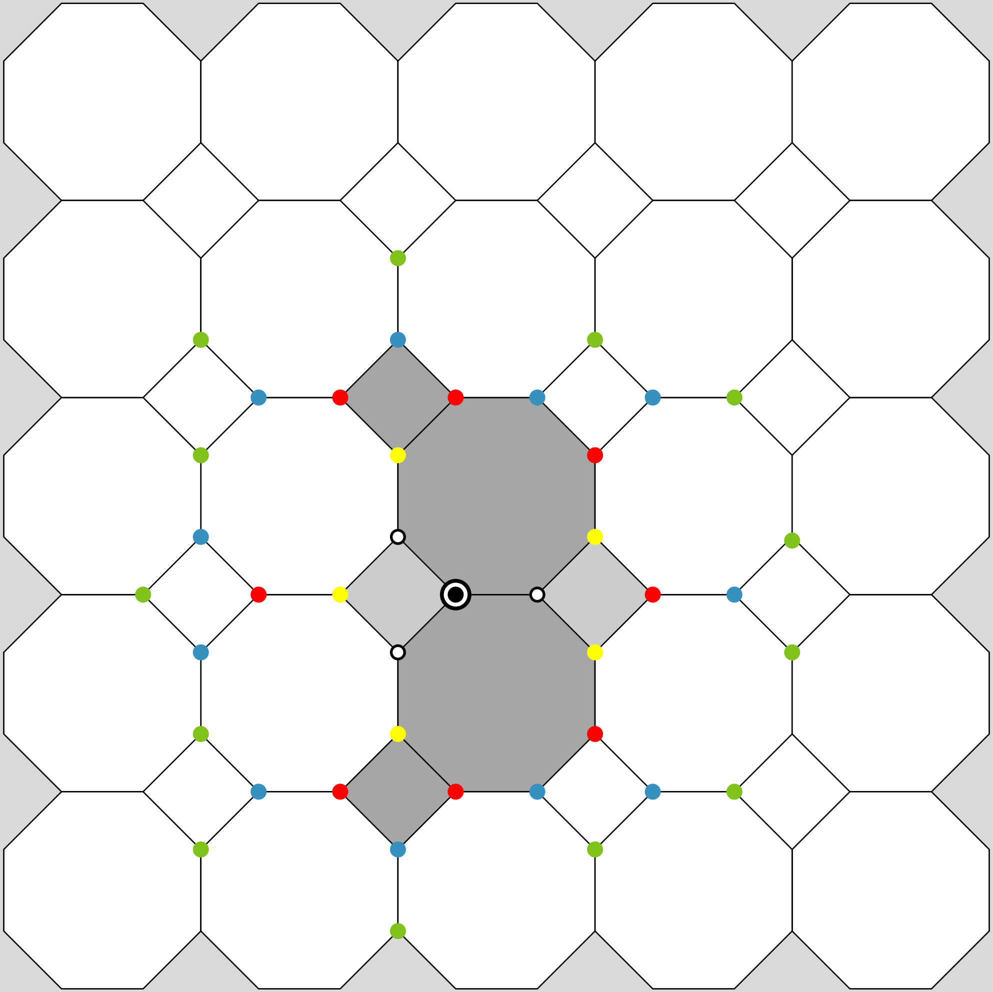


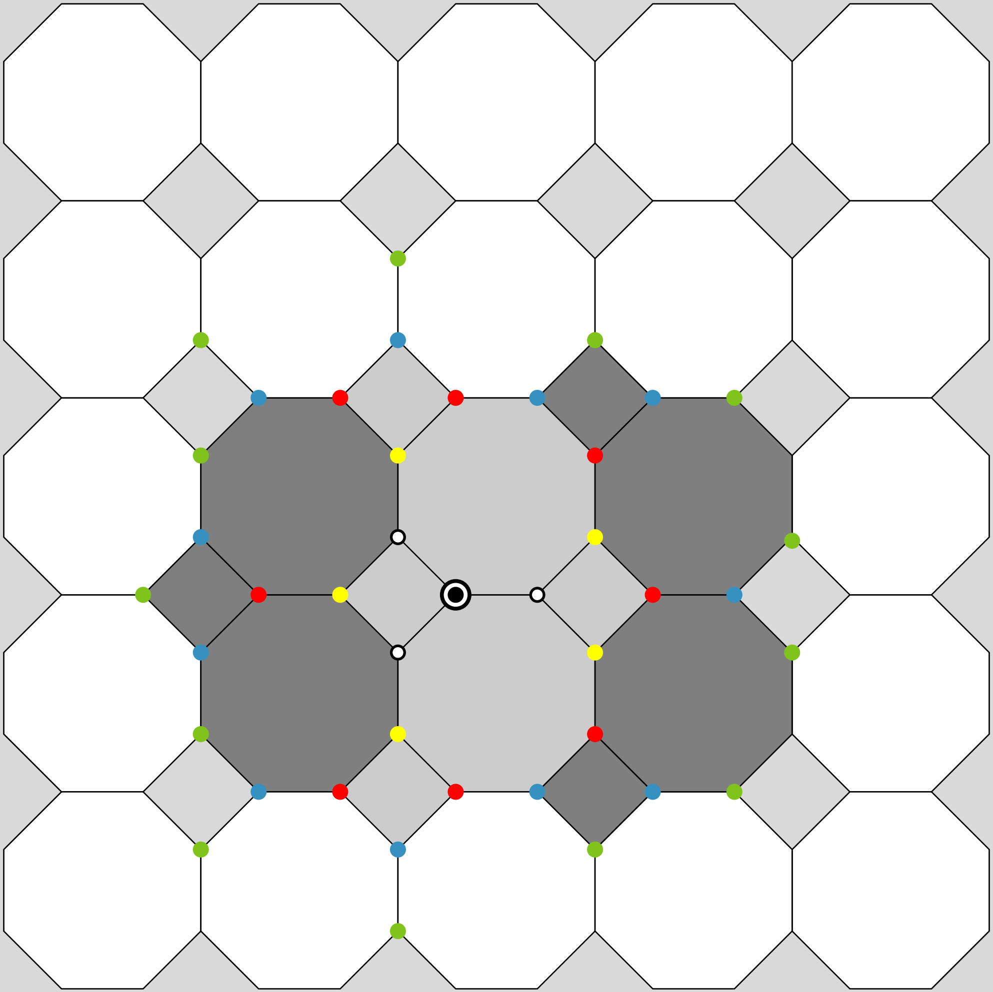


May be pinned isostatically [8].



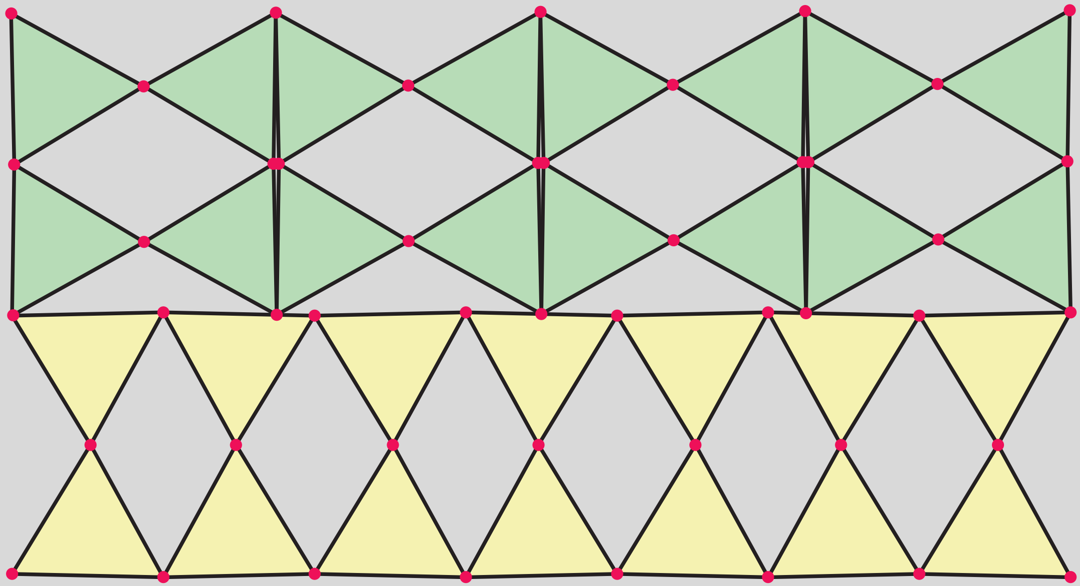






11. Open Problems

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

[1] L. Babai, *The growth rate of vertex-transitive planar graphs*, in Proceedings of the Eighth Annual ACM-SIAM Symposium on Discrete Algorithms (New Orleans, LA, 1997), New York, 1997, ACM, pp. 564–573.

[2] P. Fazekas, O. Röschel, and B. Servatius, *The kinematics of a framework presented by H. Harborth and M. Möller*, Beiträge zur Algebra und Geometrie / Contributions to Algebra and Geometry, pp. 1–9. 10.1007/s13366-011-0079-x.

[3] H. Harborth and M. Möller, *Complete vertex-to-vertex packings of congruent equilateral triangles*, Geombinatorics, 11 (2002), pp. 115–118.

[4] ——, *Vertex-to-vertex packings of congruent triangles*, Abh. Braunschw. Wiss. Ges., 51 (2002), pp. 49–54.

[5] T. Jordán, *Generically globally rigid zeolites in the plane*, Tech. Rep. TR-2009-08, Egerváry Research Group, Budapest, 2009. `www.cs.elte.hu/egres`.

[6] B. Servatius and H. Servatius, *The 24 symmetry pairings of self-dual maps on the sphere*, Discrete Mathematics, 140 (1995), pp. 167 – 183.

[7] B. Servatius, H. Servatius, and M. F. Thorpe, *Zeolites: Geometry and combinatorics*, International Journal of Chemical Modeling, 4 (2012), pp. 253–267.

[8] L. Theran, A. Nixon, E. Ross, M. Sadjadi, B. Servatius, and M. F. Thorpe, *Anchored boundary conditions for locally isostatic networks*, Phys. Rev. E, 92 (2015), p. 053306.

[9] H. Whitney, *Congruent Graphs and the Connectivity of Graphs*, Amer. J. Math., 54 (1932), pp. 150–168.