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Vertex transitive . . .
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From combinatorial zeolites to geometric realizations

Brigitte Servatius — WPI

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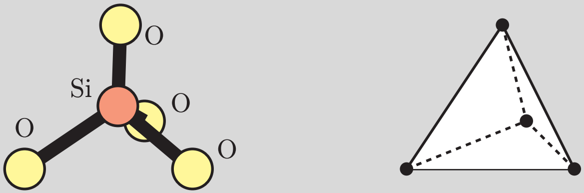
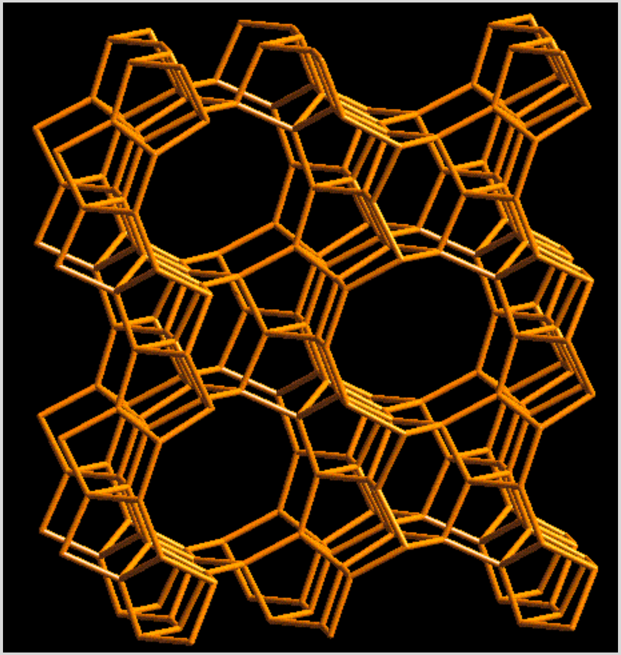
1. Chemical Zeolites

- crystalline solid
- units: Si + 4O



- two covalent bonds per oxygen



- naturally occurring
- synthesized
- theoretical

Used as microfilters.

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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.

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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, $Aut(X) \cong Aut(L(X))$.

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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.

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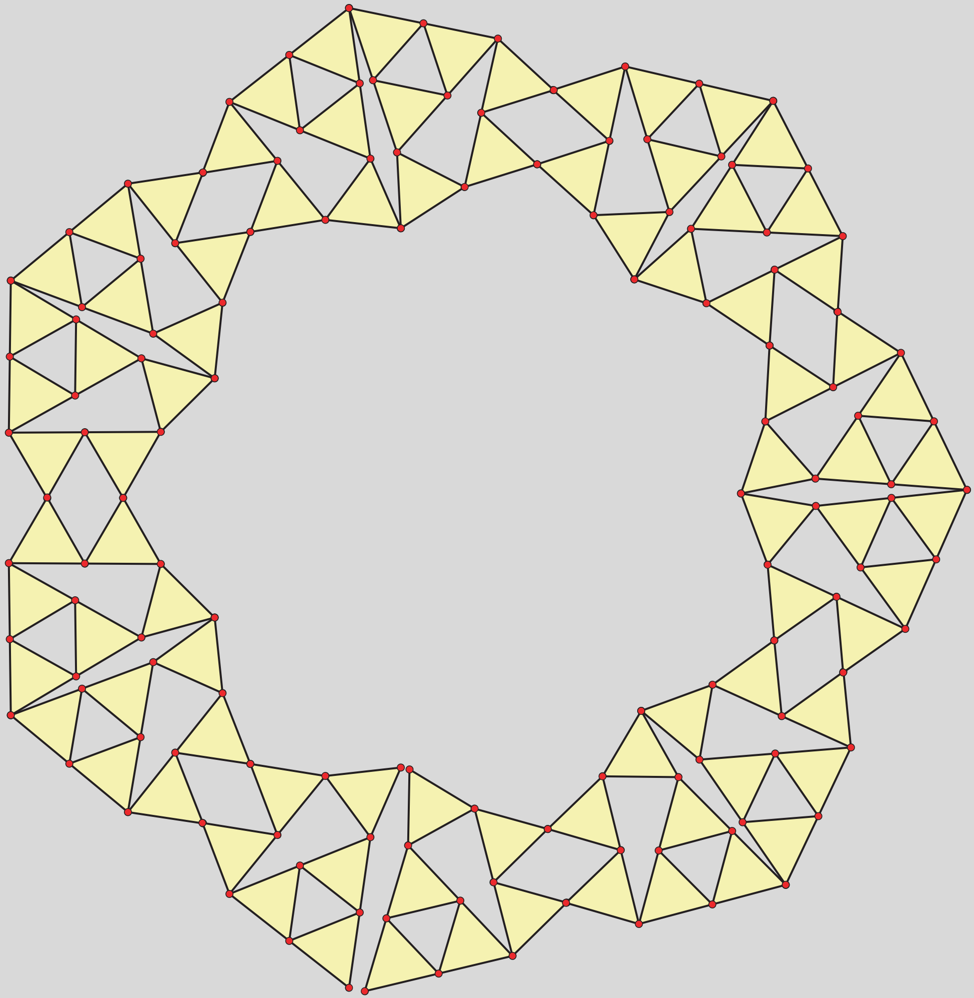
The typical situation: Not unit distance realizable.



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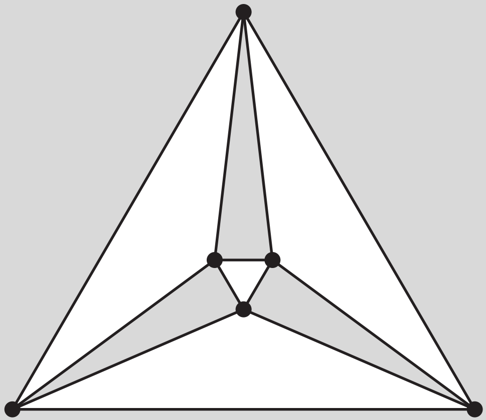
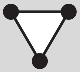
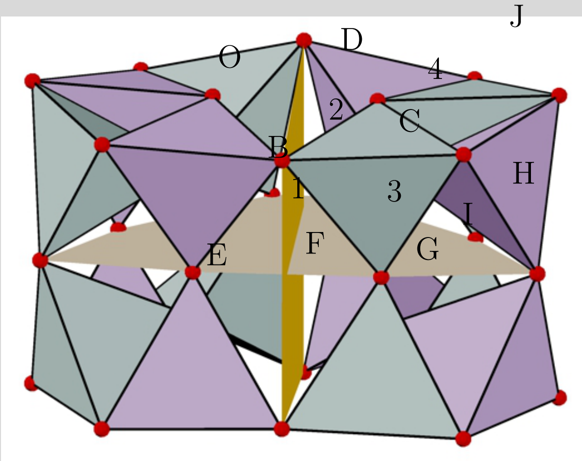
4. 2d Zeolites

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.

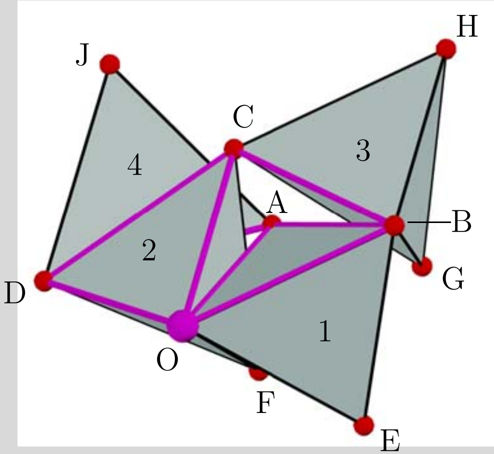




A finite 3-D symmetric example:



Model with its two planes of symmetry



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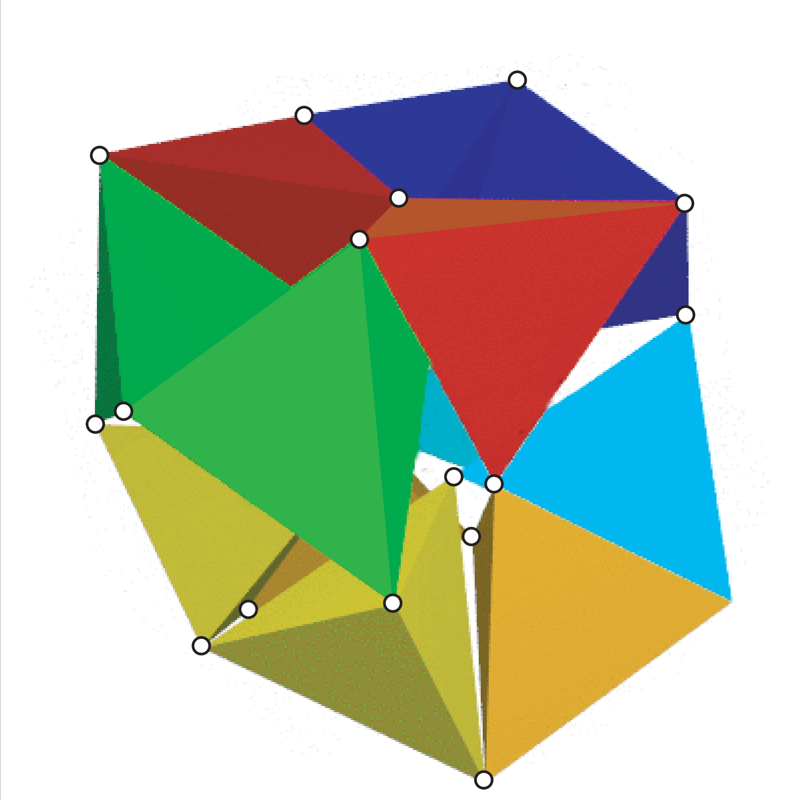

A saturated packing of 12 Tetrahedra found by Peter Dinkelacker

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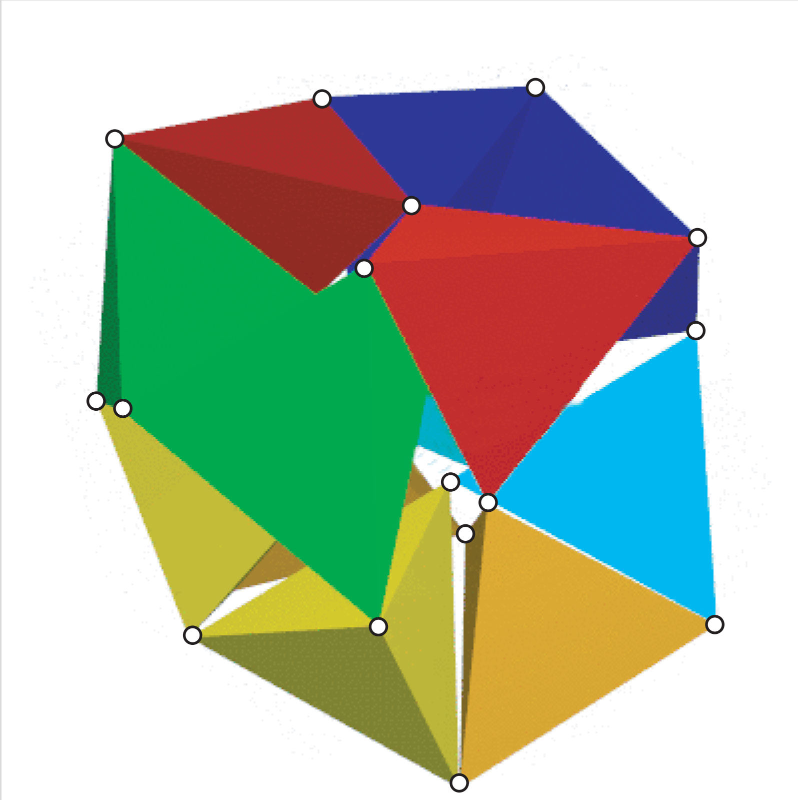

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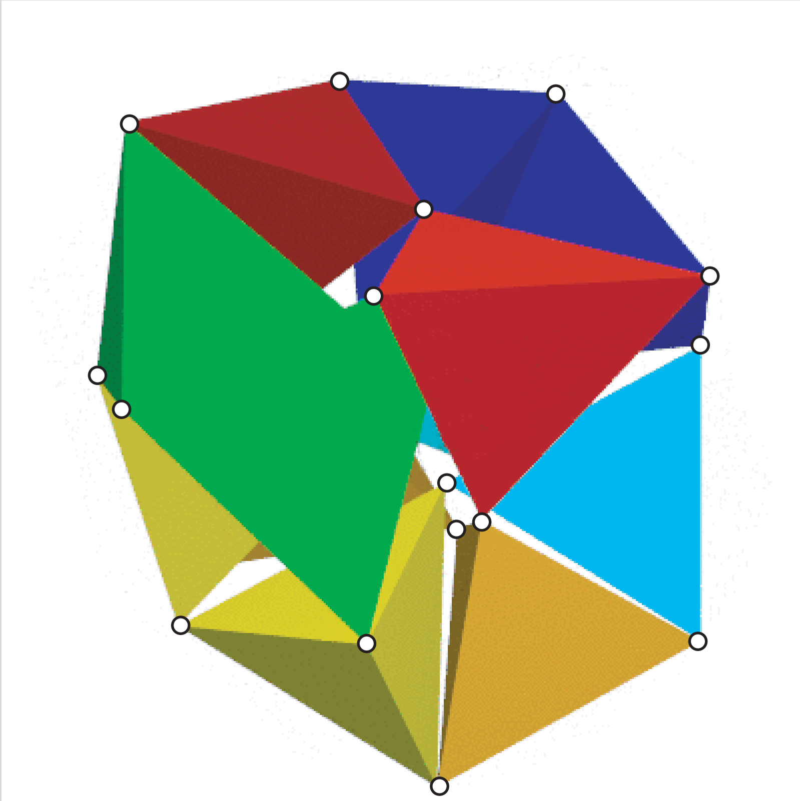

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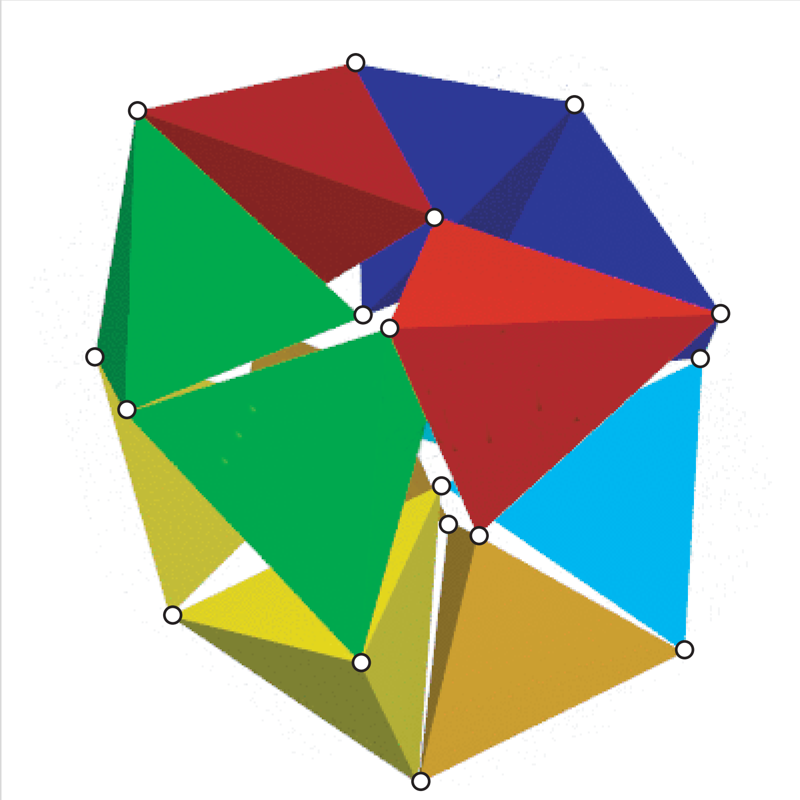

A saturated packing of 12 Tetrahedra found by Peter Dinkelacker

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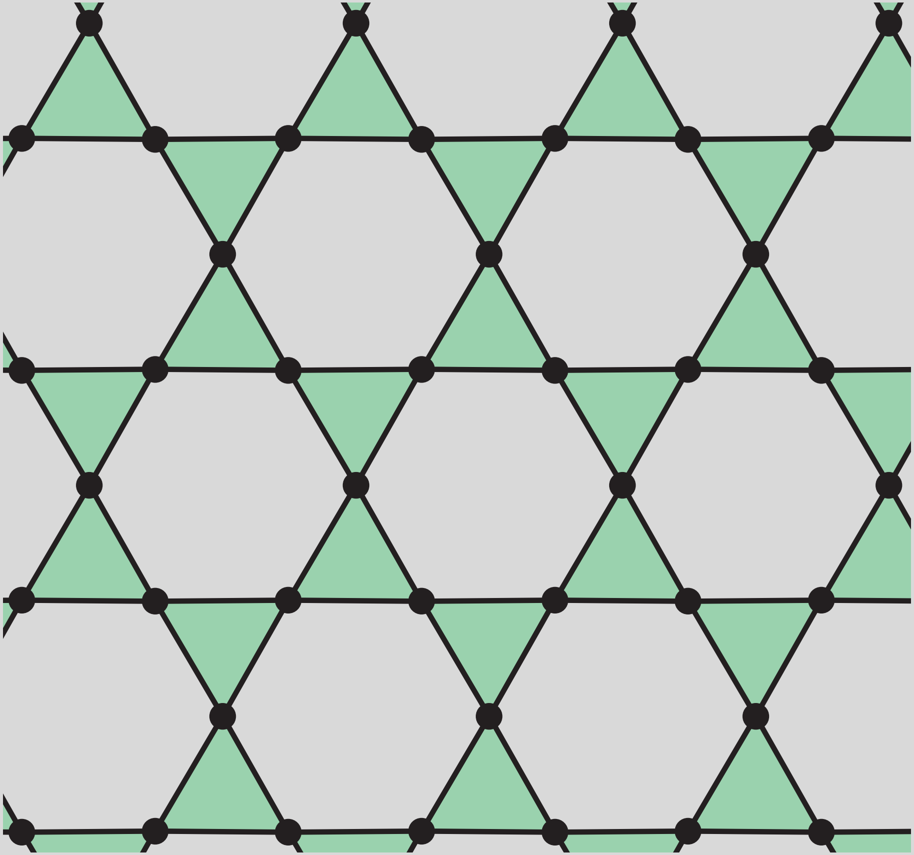
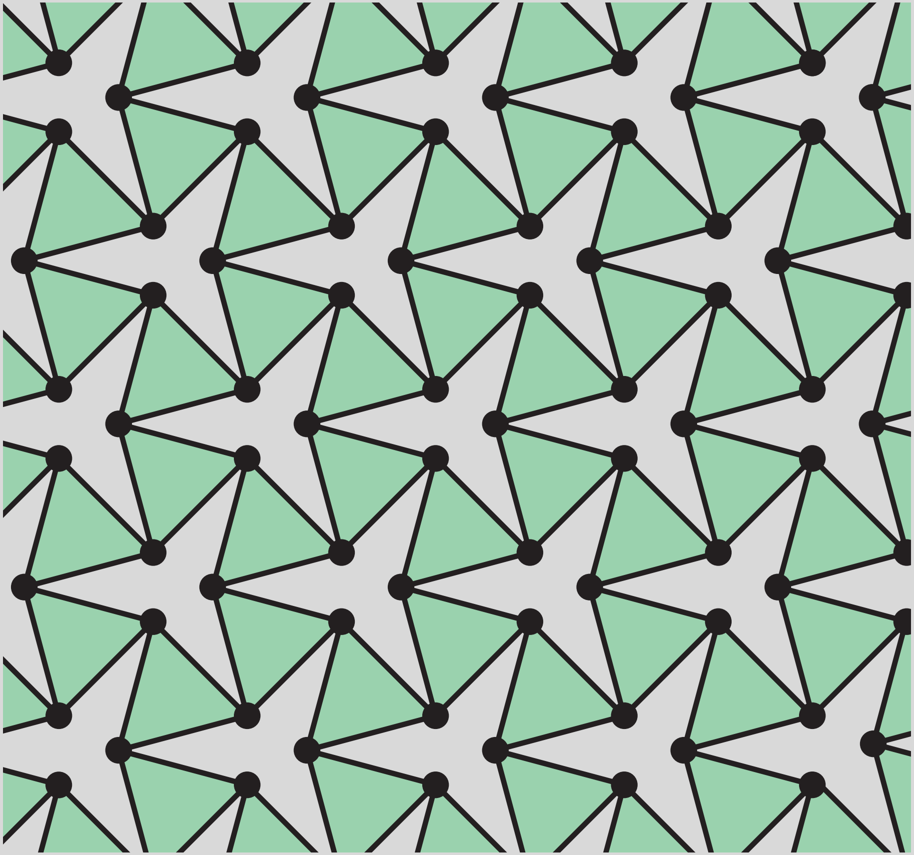
It is just as easy to construct infinite symmetric examples:



Showing a different symmetry



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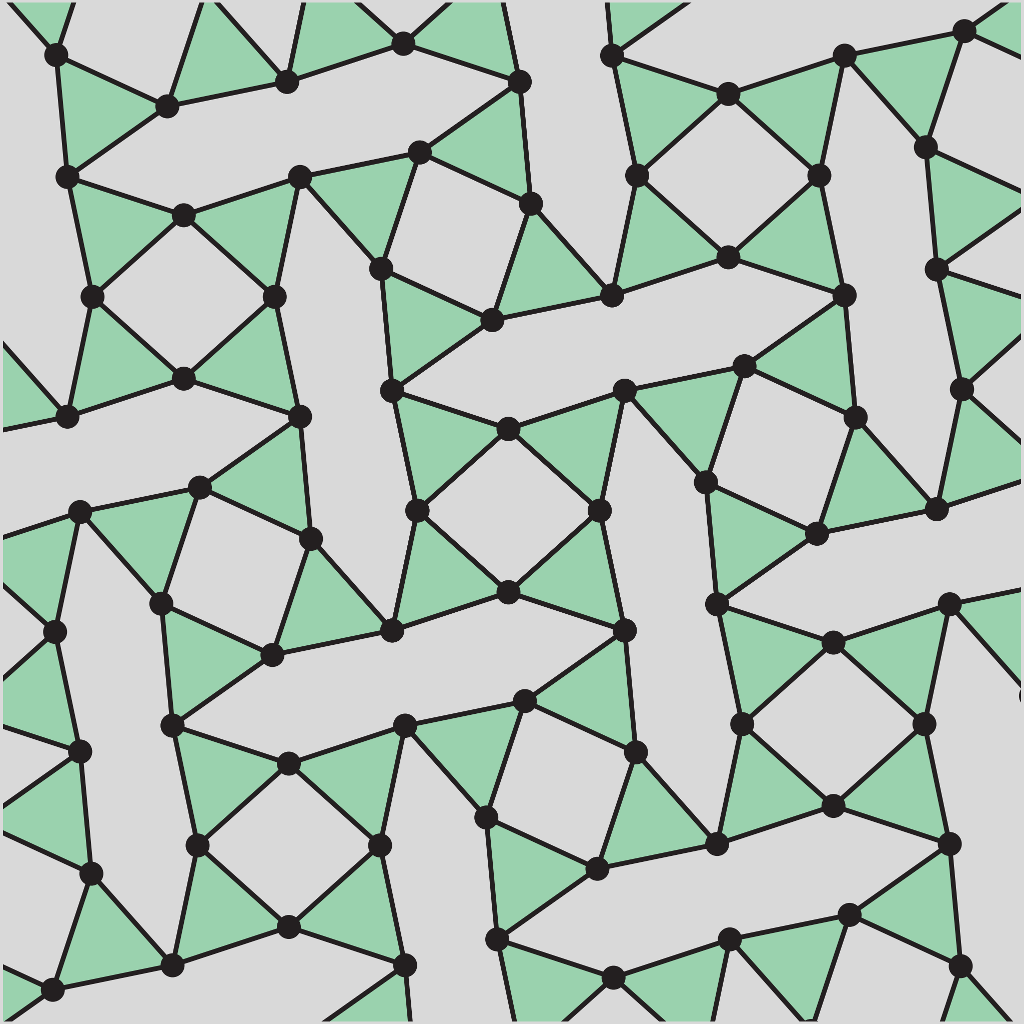

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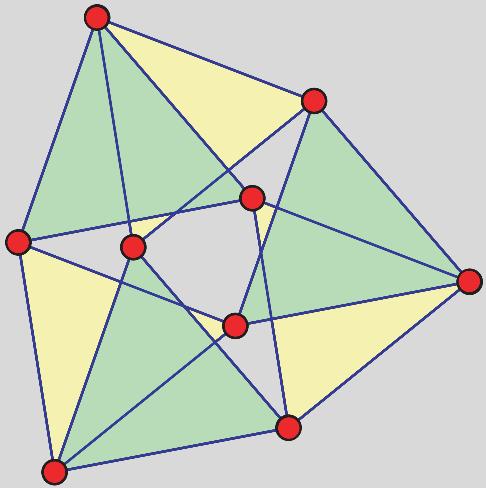
5. Finite Zeolites

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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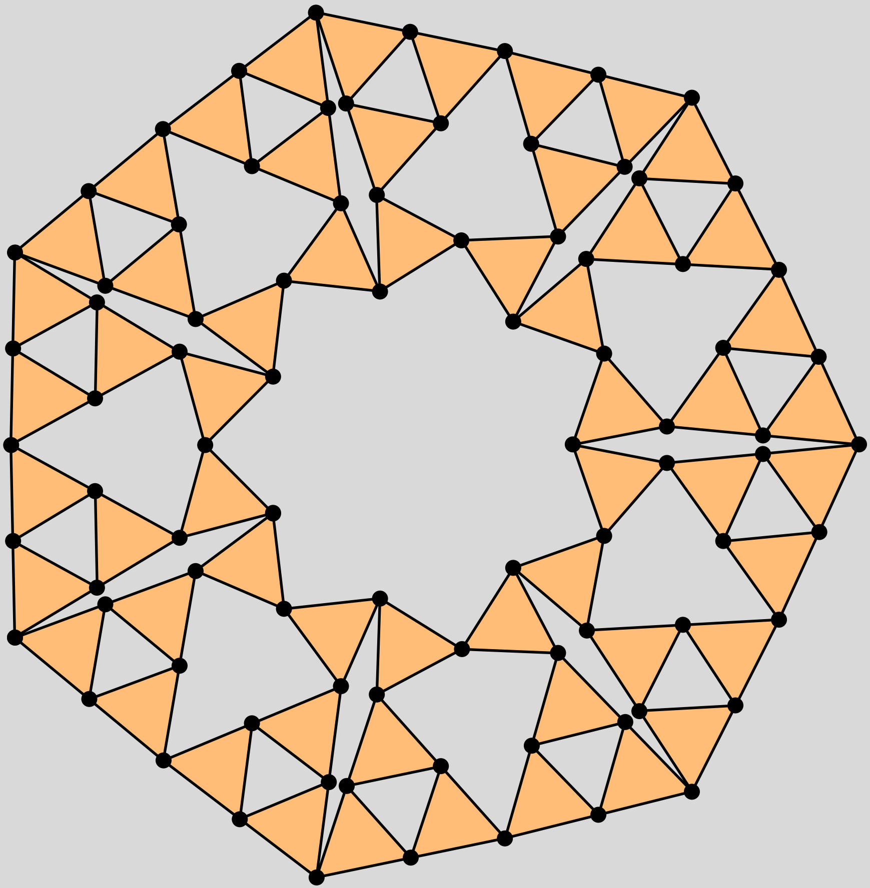
Harborth's Example [4, 3]



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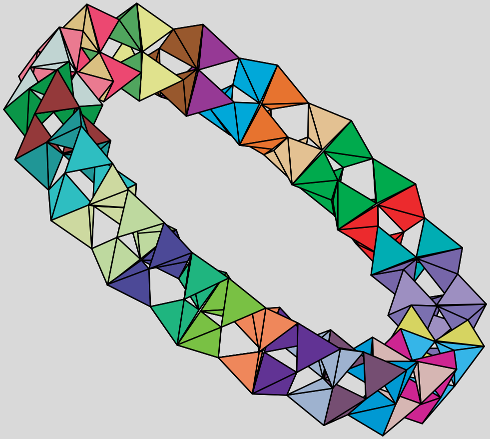

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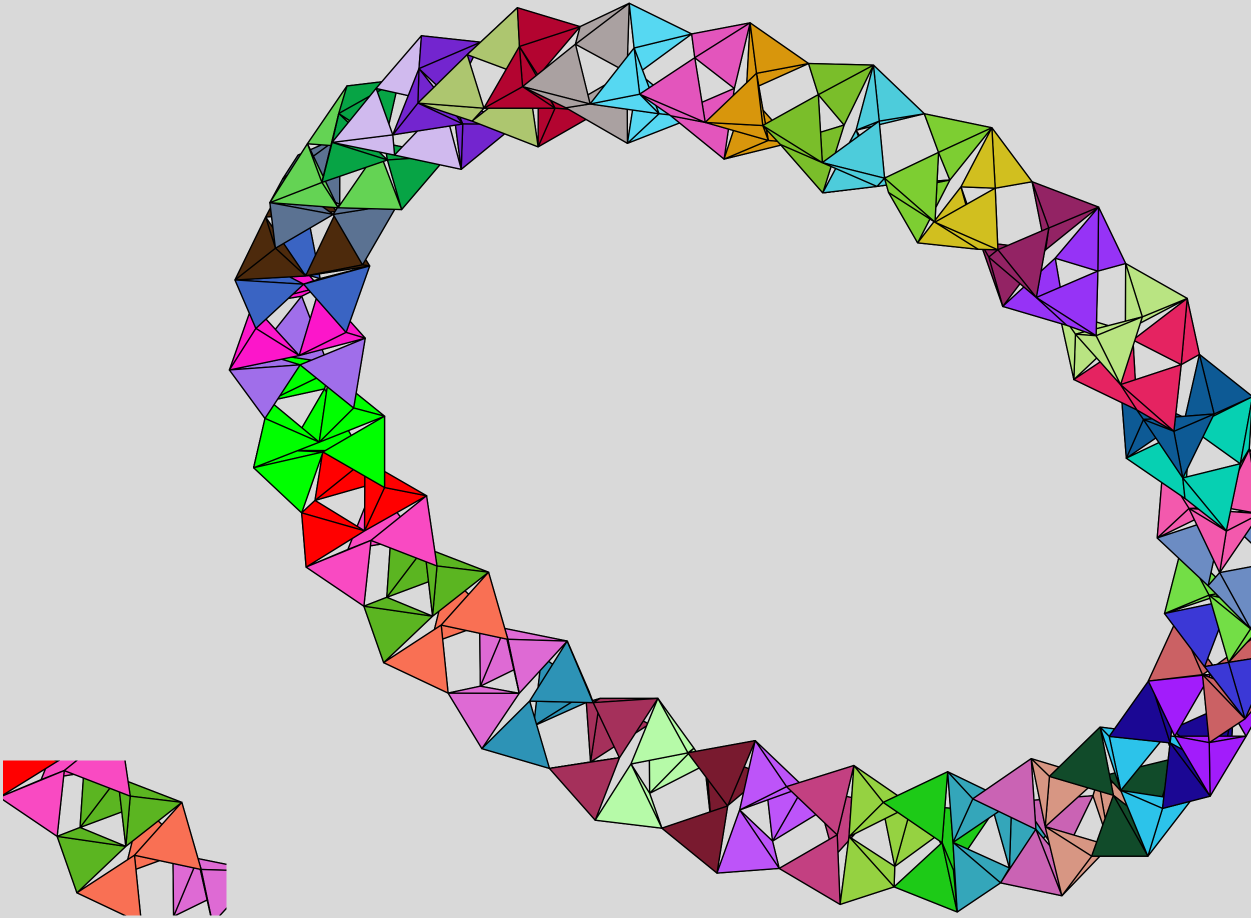

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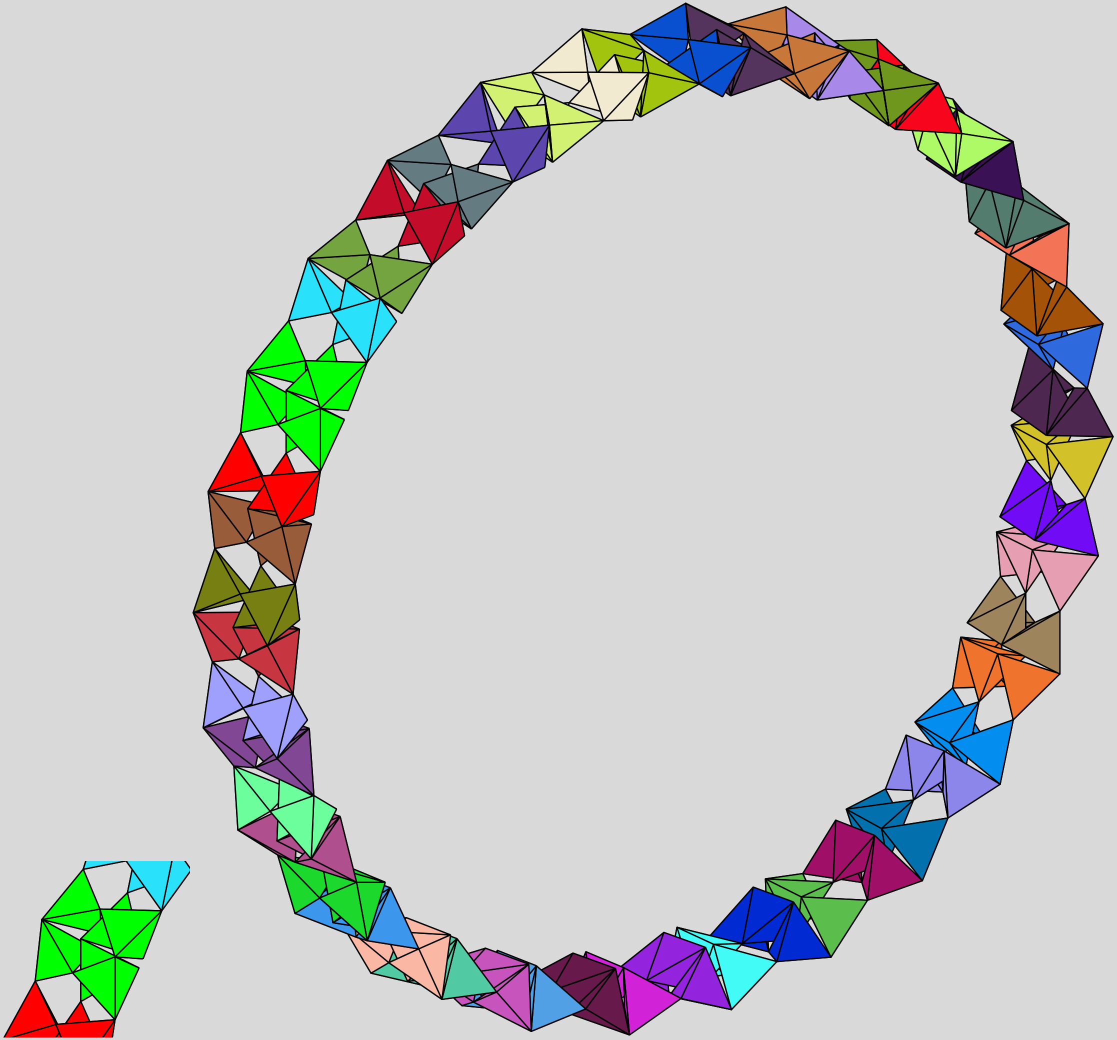

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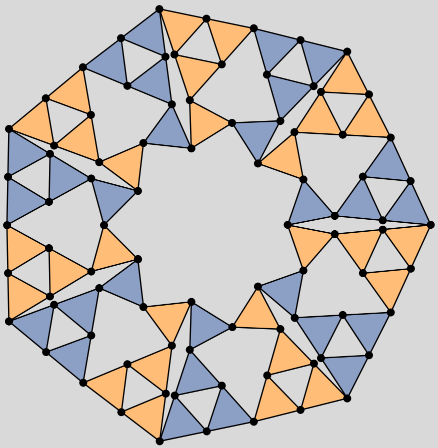
6. The Layer Construction

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

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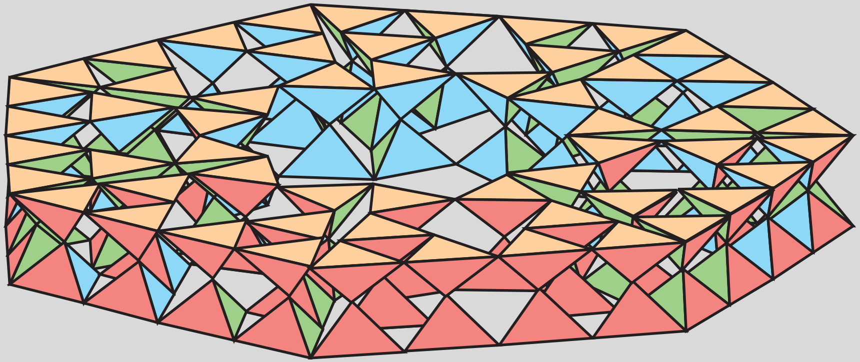
Labels all +1
A two layered zeolite.



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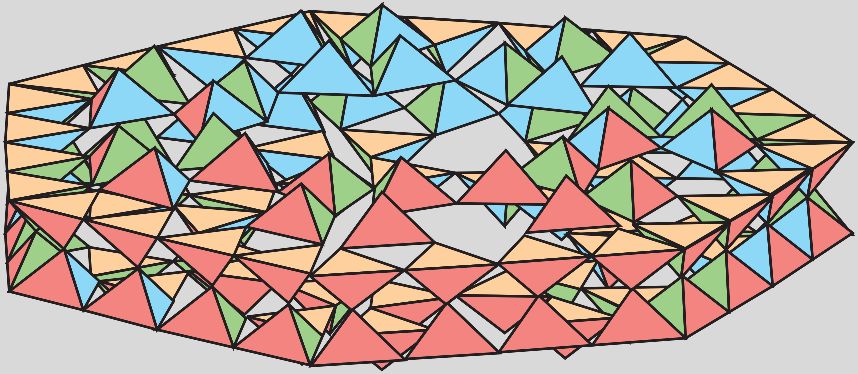
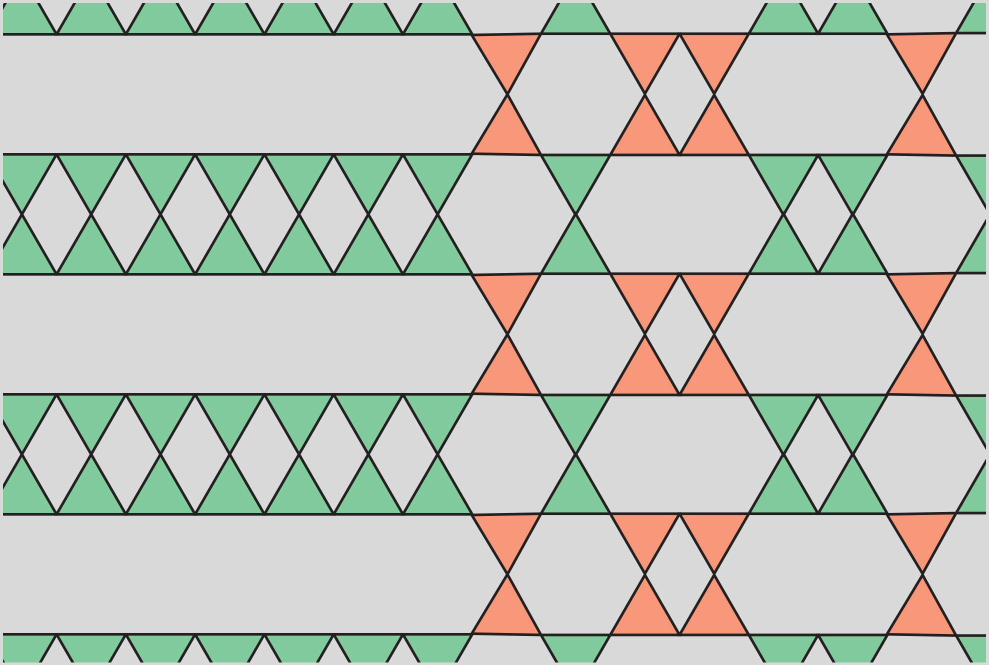
The general case starting from a finite zeolite.



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

Proof:



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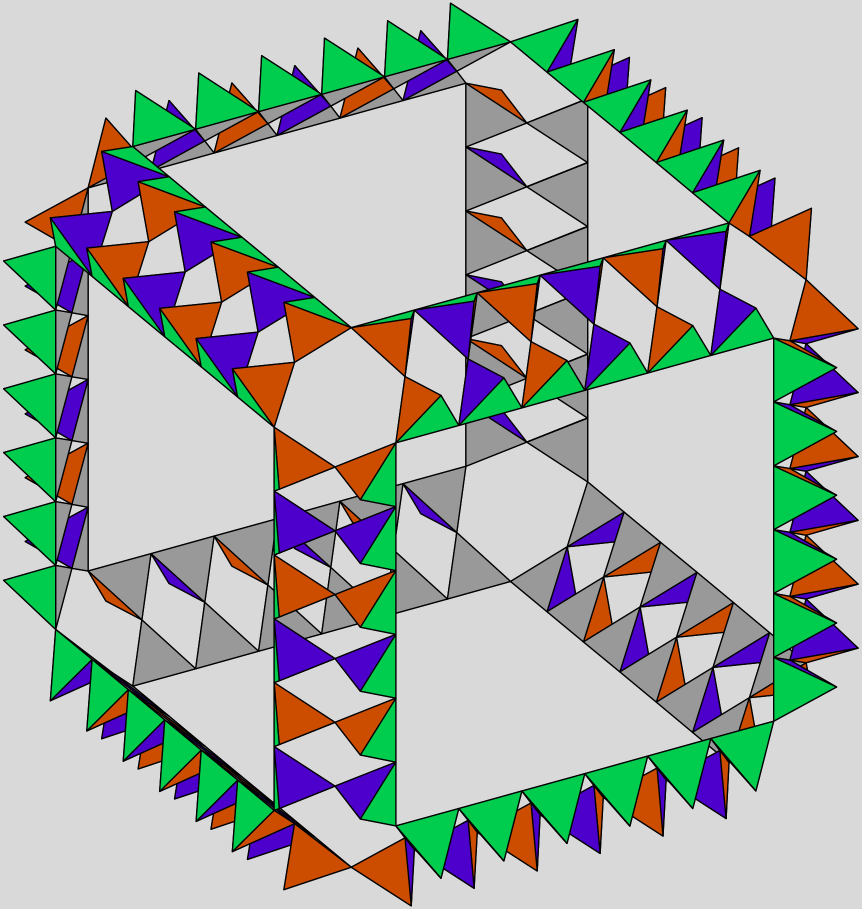
7. Holes in Zeolites



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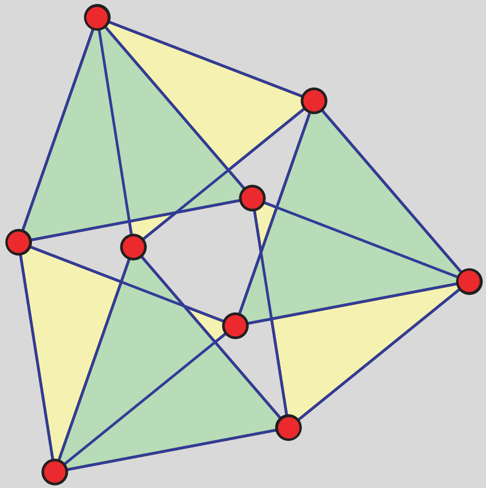
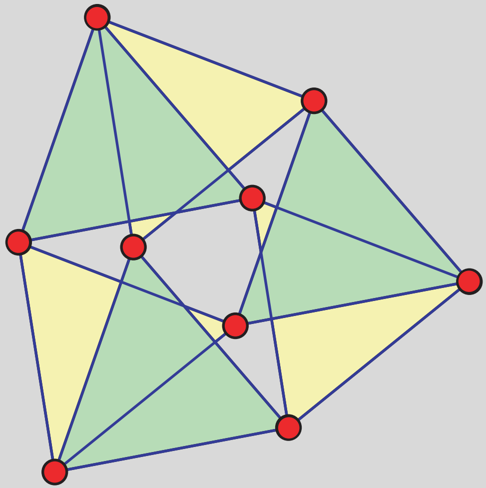
8. Motions

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.



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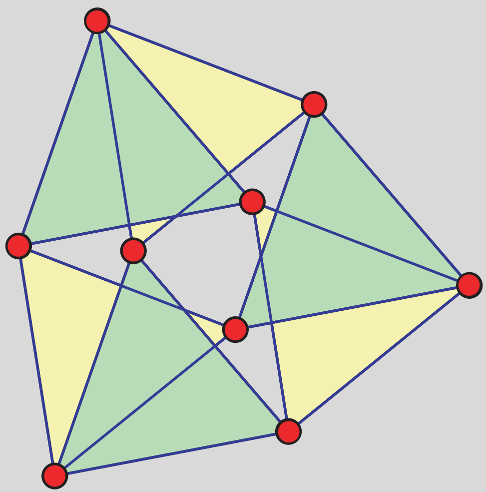
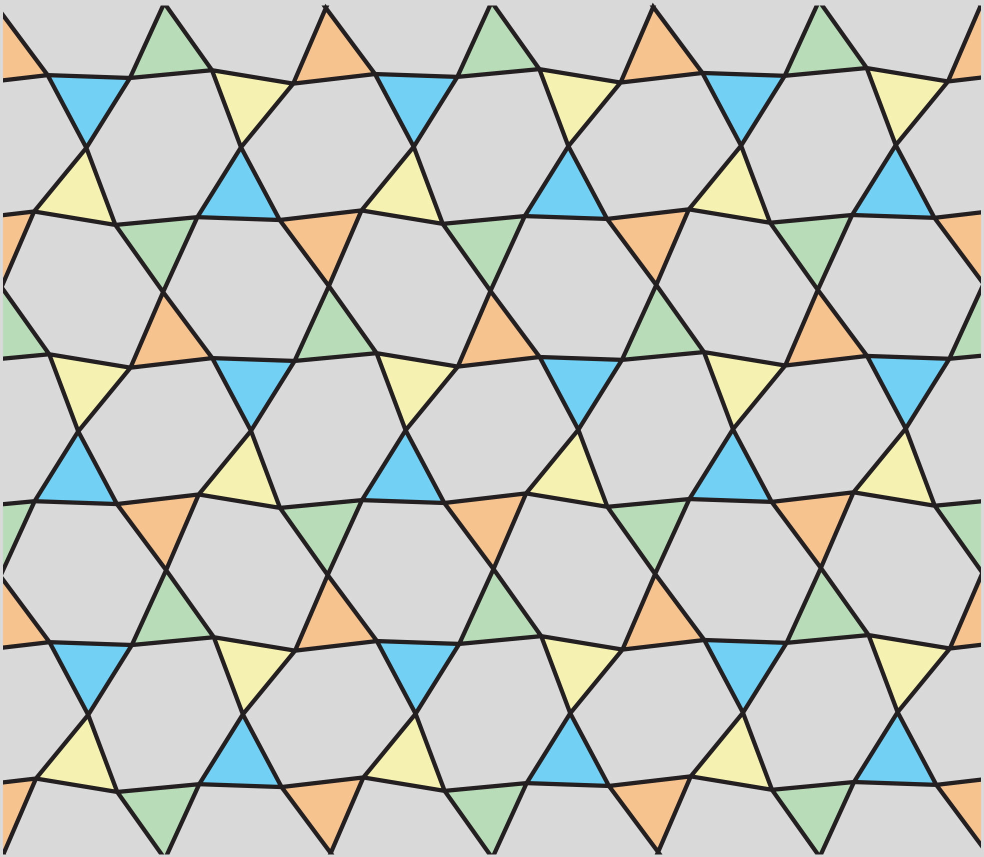
Generically globally rigid in the plane.

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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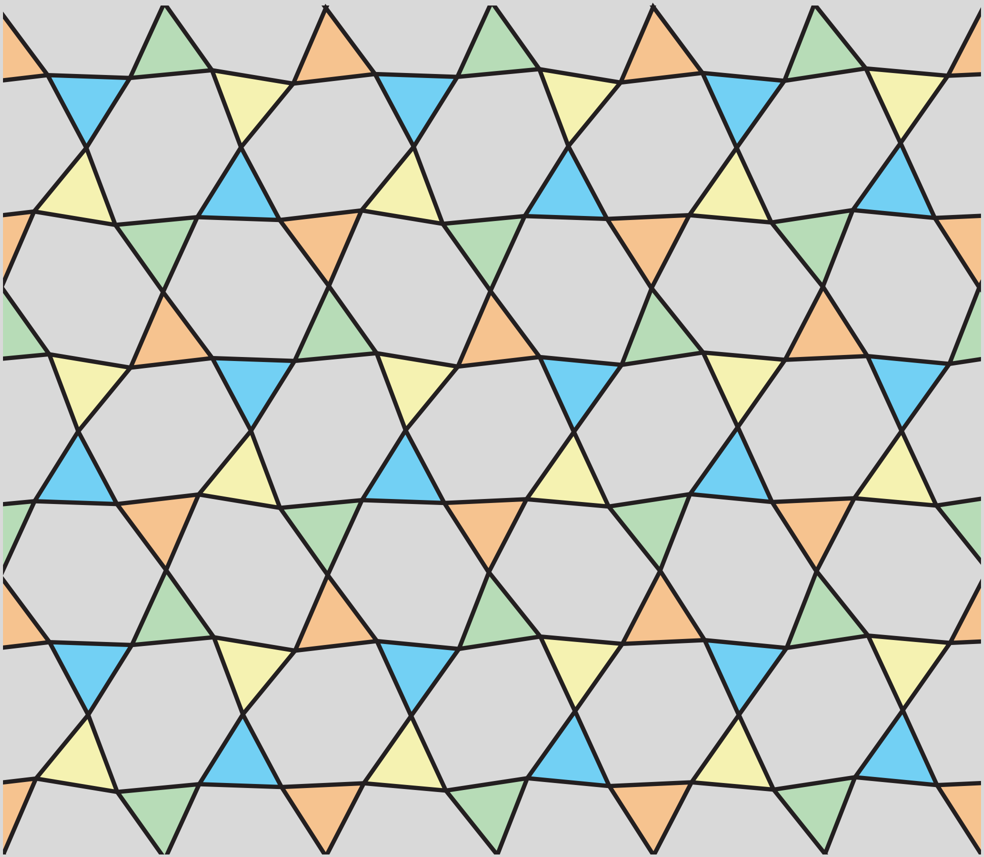

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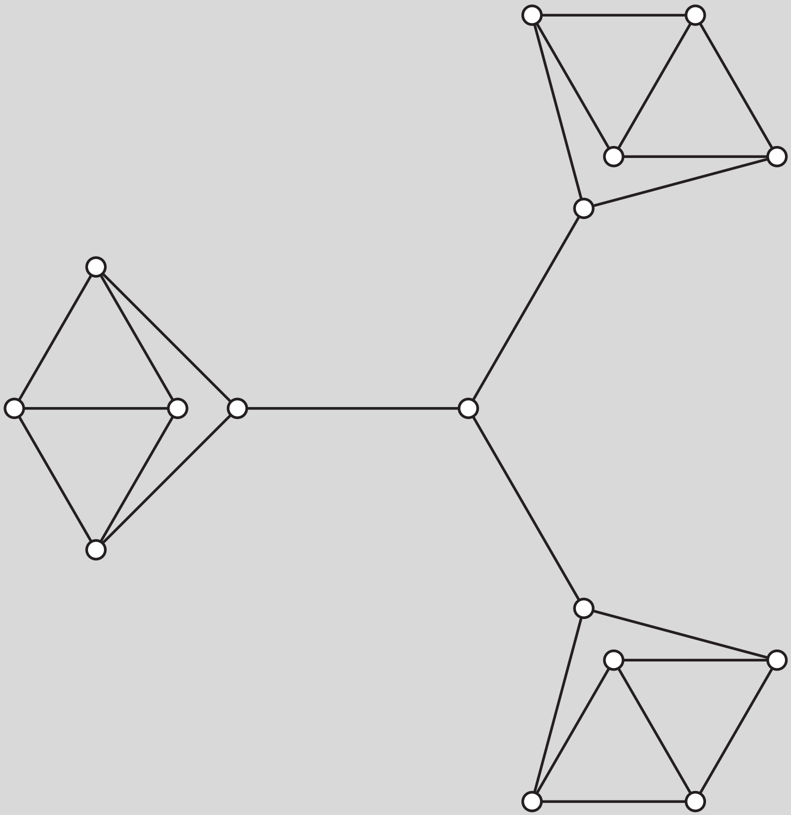
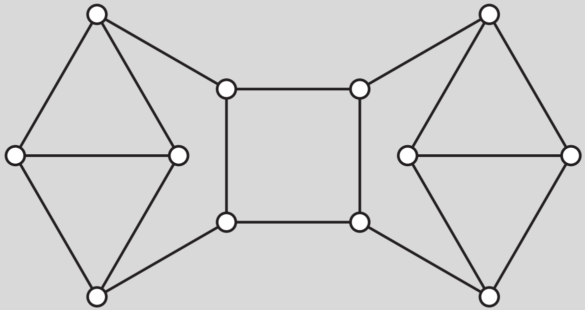
Are there finite generically flexible 2D Zeolites?
Yes, line graphs of 3-regular graphs with edge connectivity less than 3.



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

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



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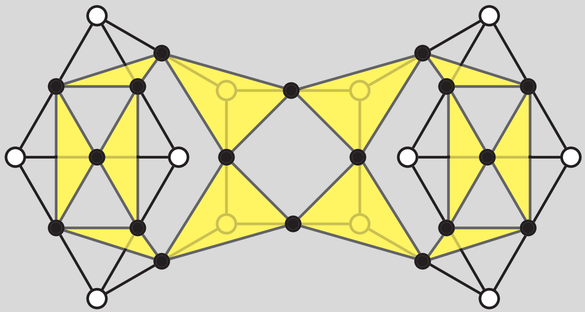
Yes, line graphs of 3-regular graphs with edge connectivity less than 3.



See [5]

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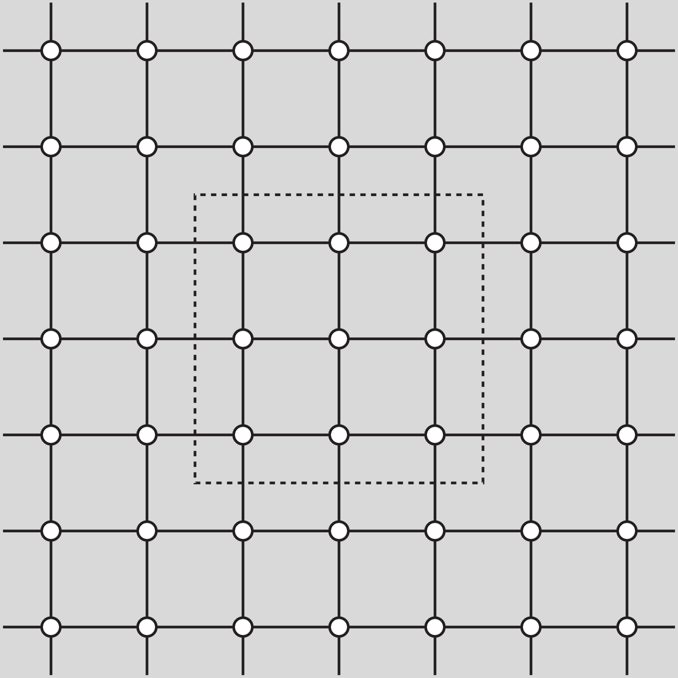
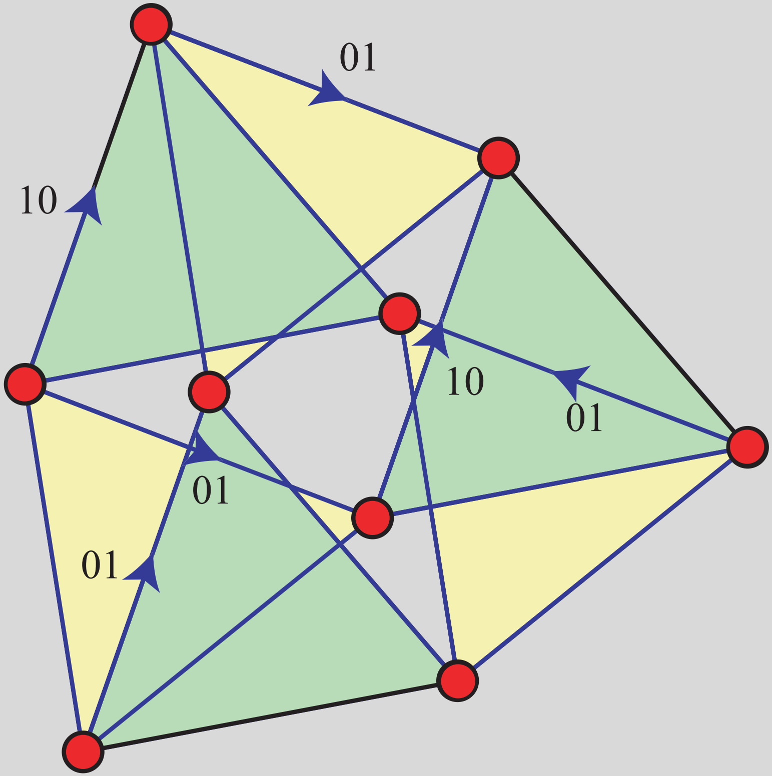
9. A geometric approach



Combinatorial version of the gain graph



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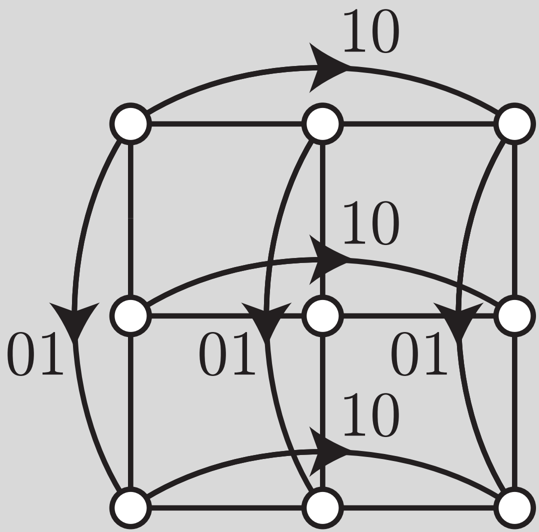
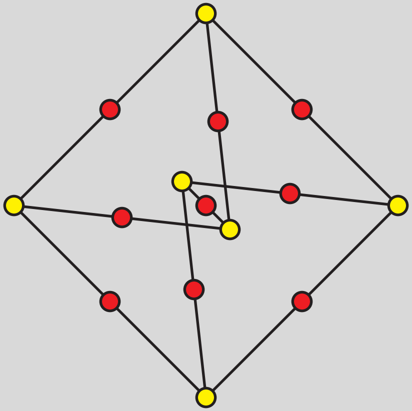
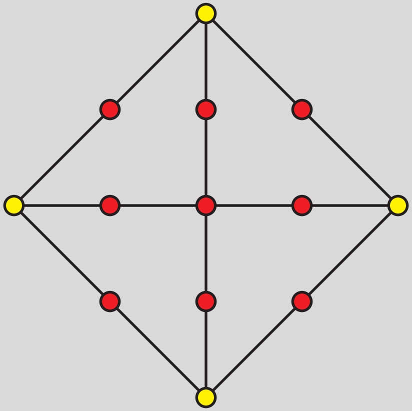
Geometric version of the gain graph



It's a geometric line graph!





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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 isometries of the geometry. Straightening Lemma for maps on the sphere [6].

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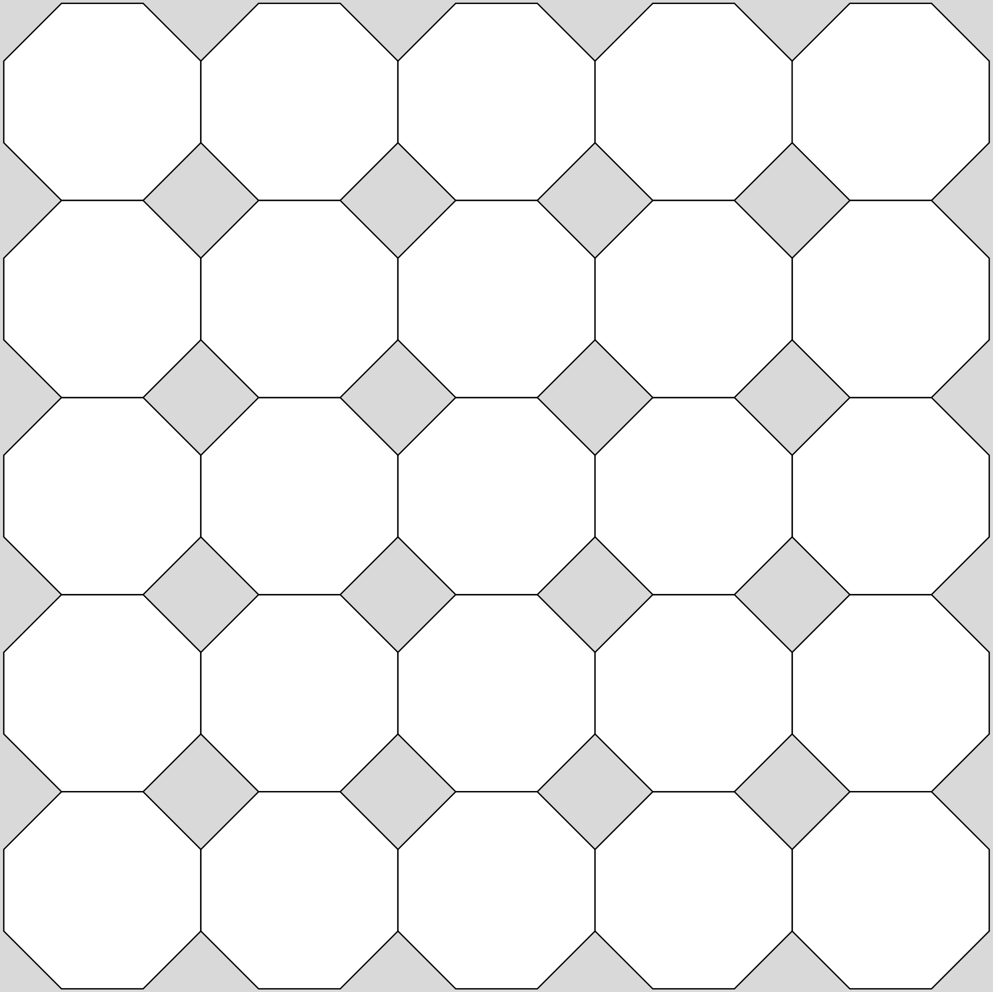
10. Vertex transitive 3-regular



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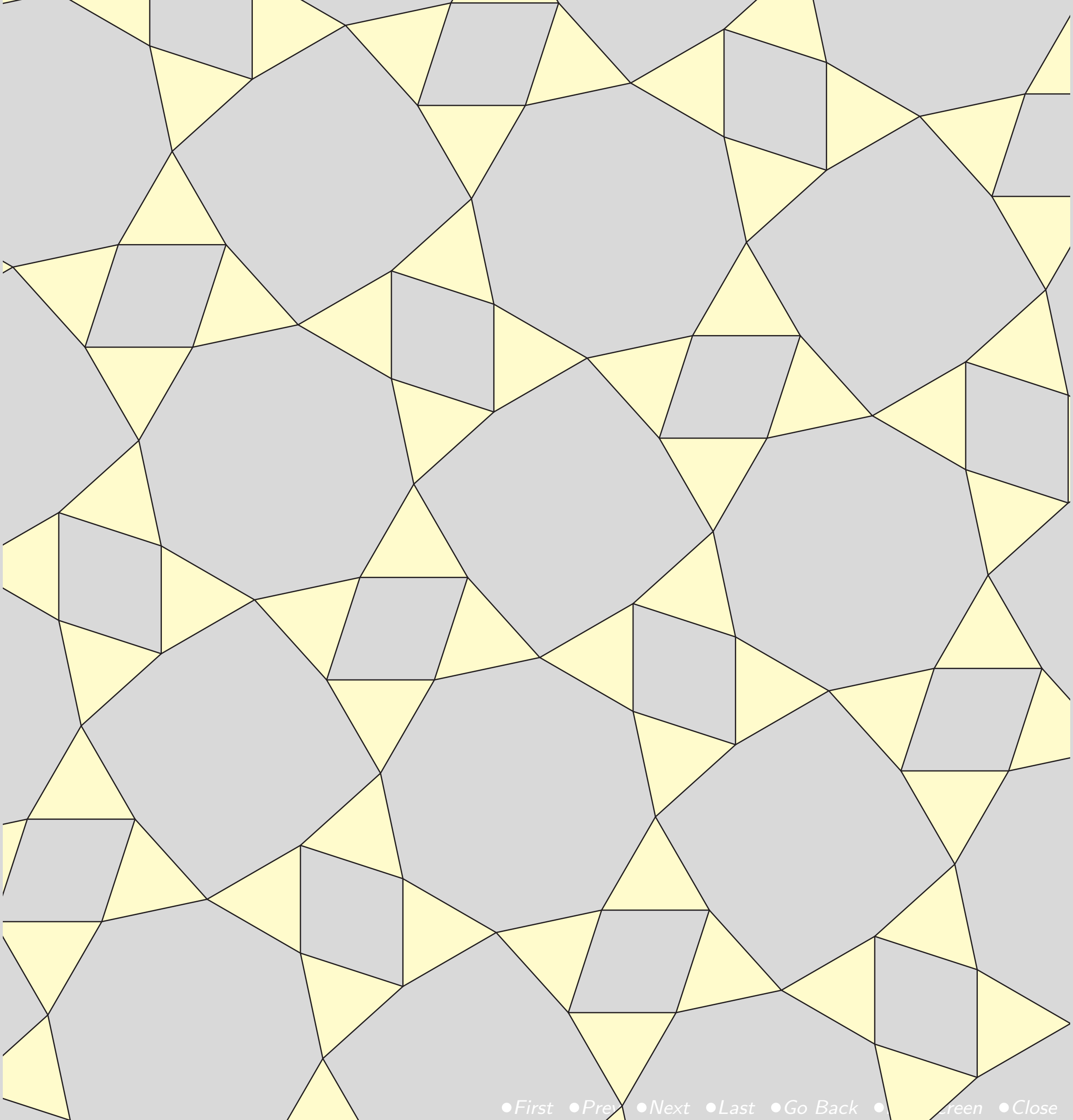

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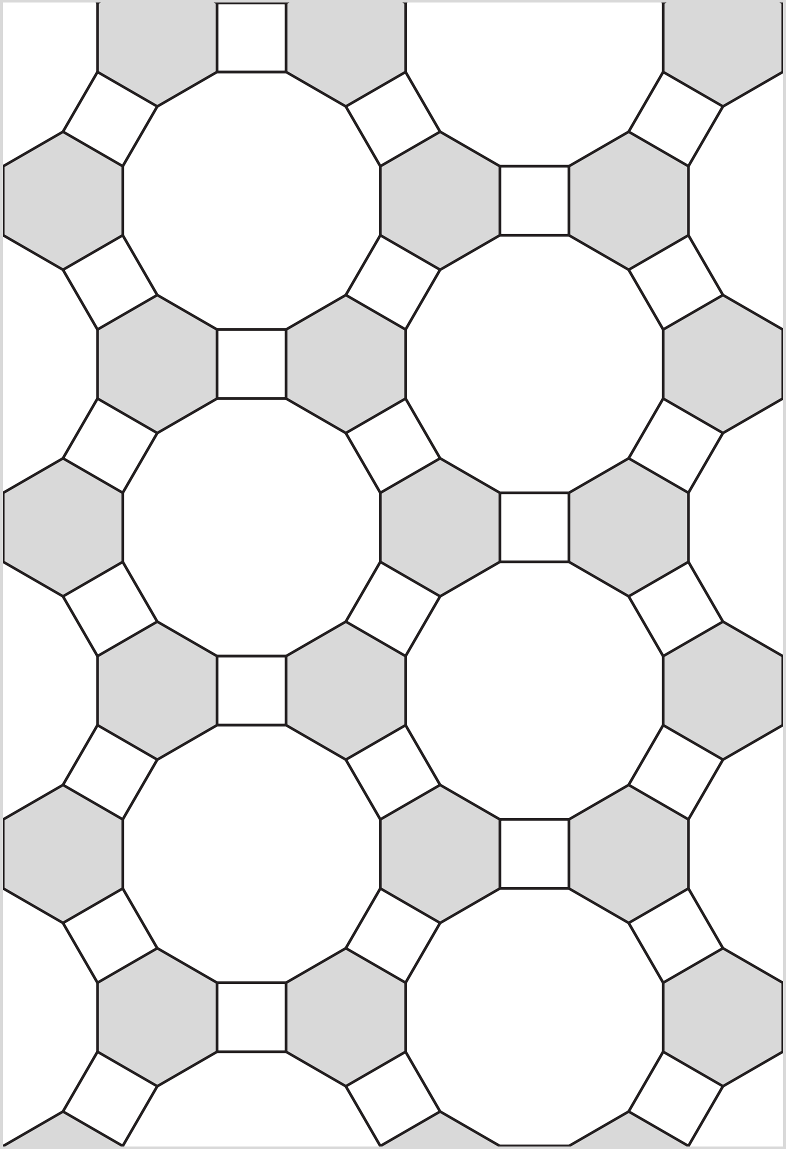

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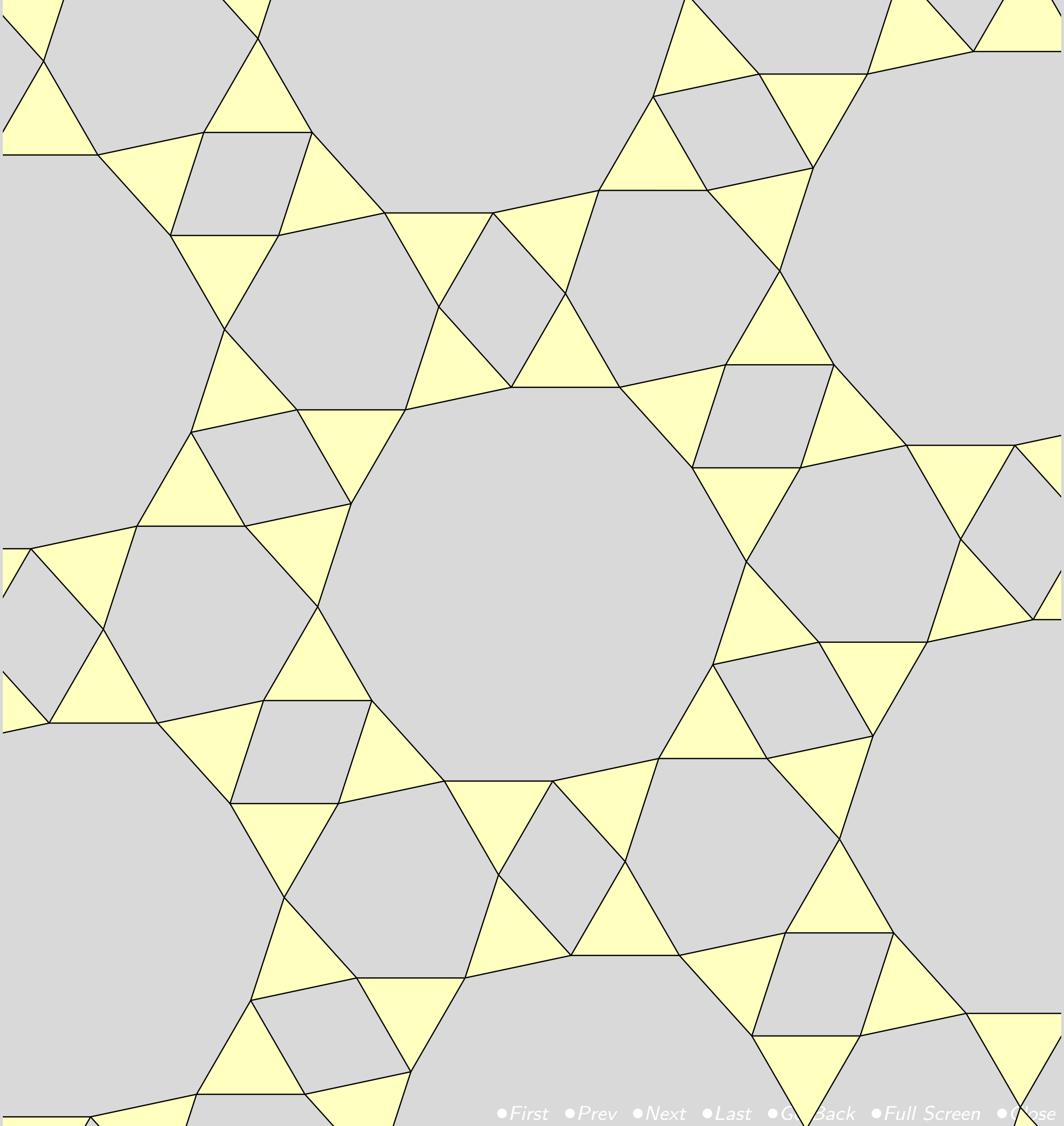

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Finite Zeolites
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Holes in Zeolites
Motions
A geometric . . .
Vertex transitive . . .
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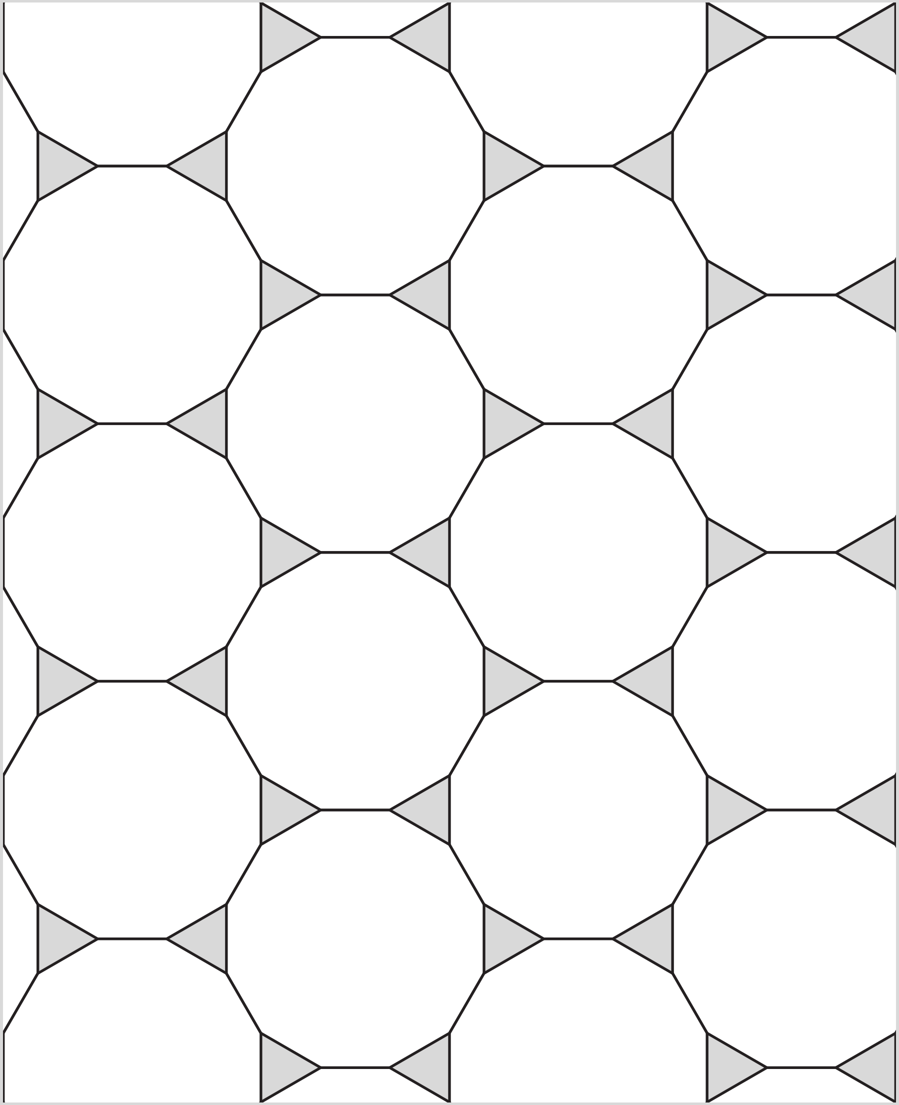

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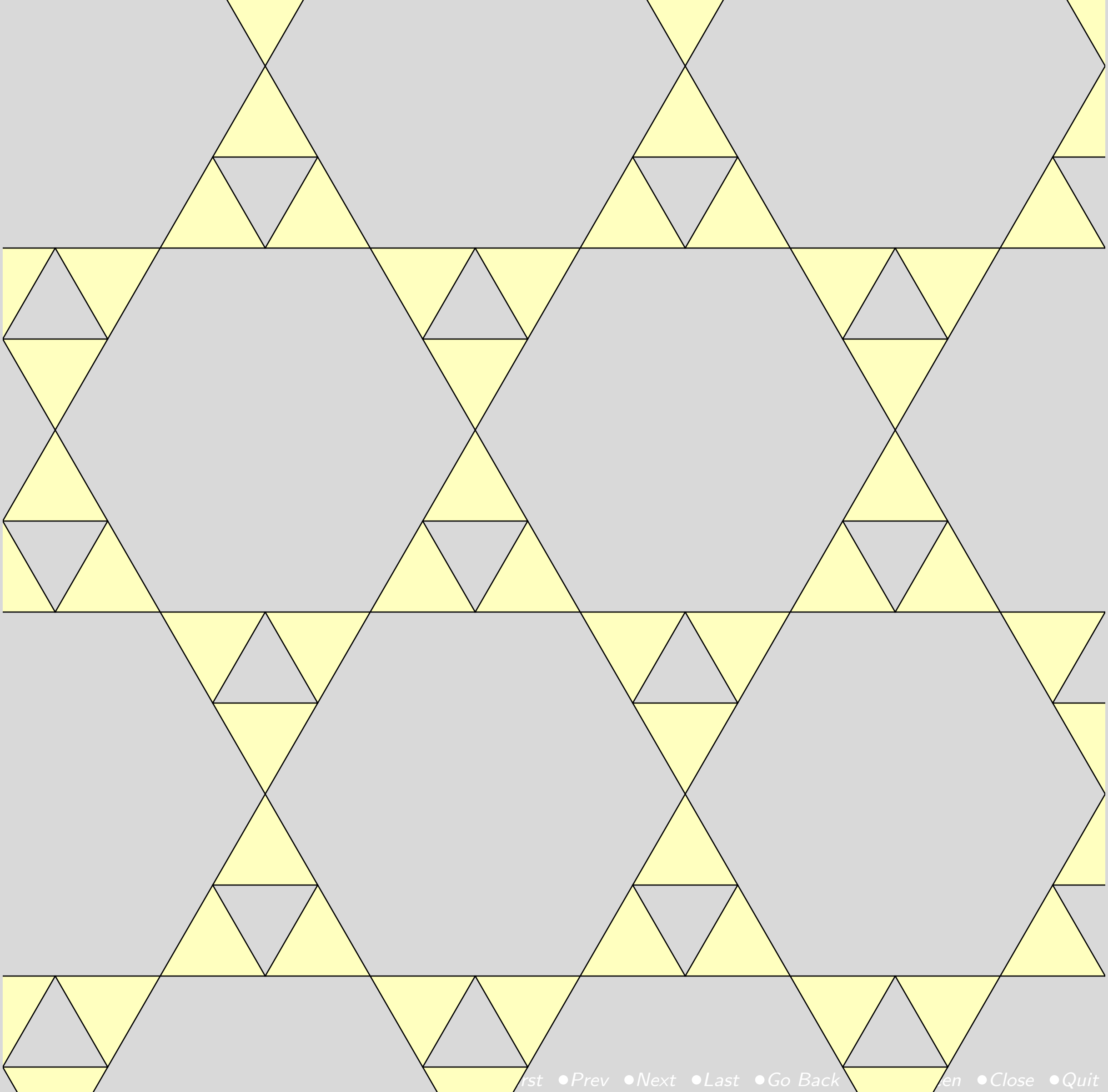

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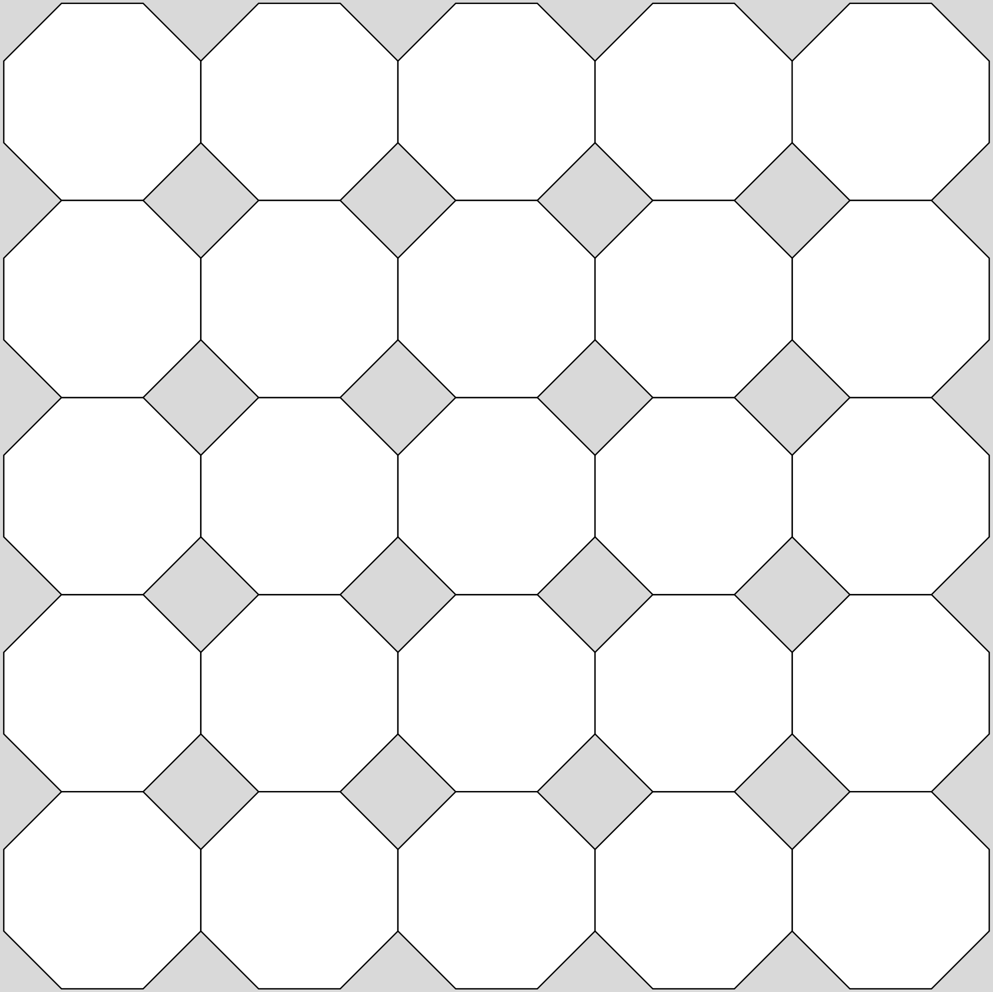

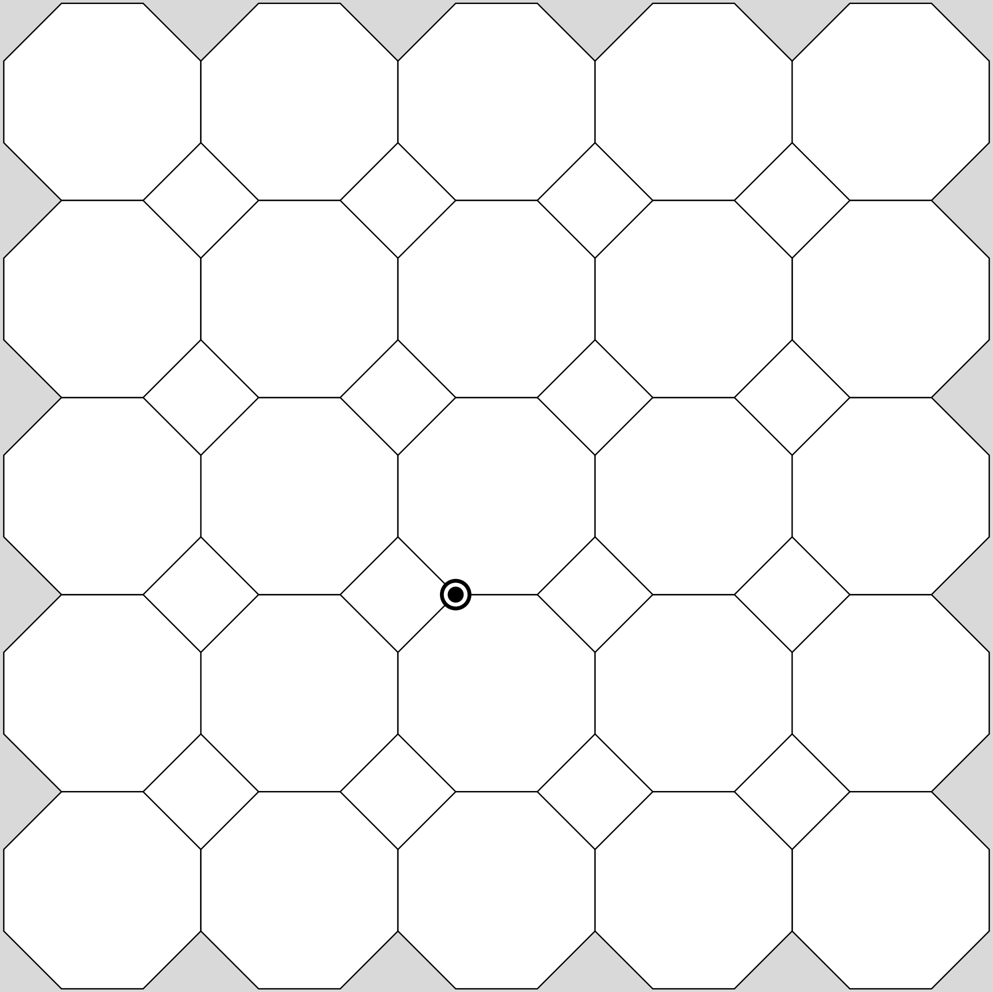

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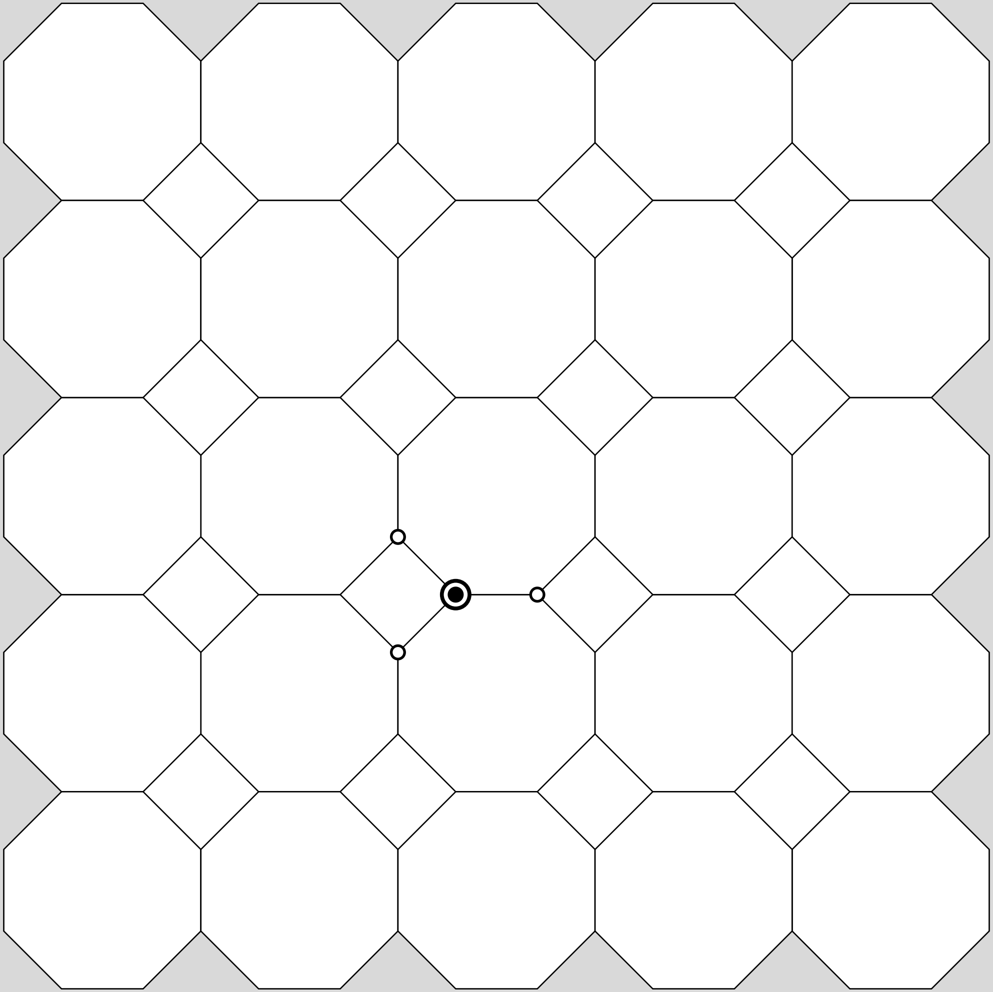

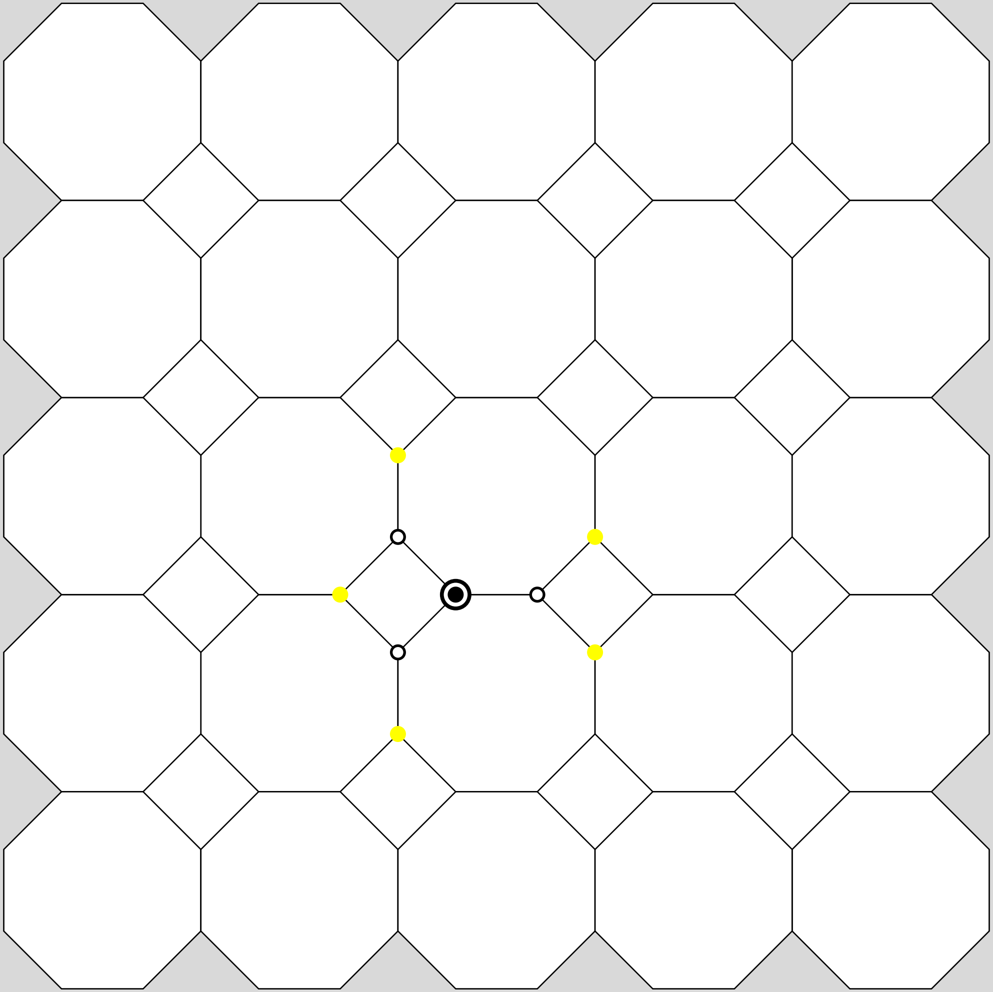

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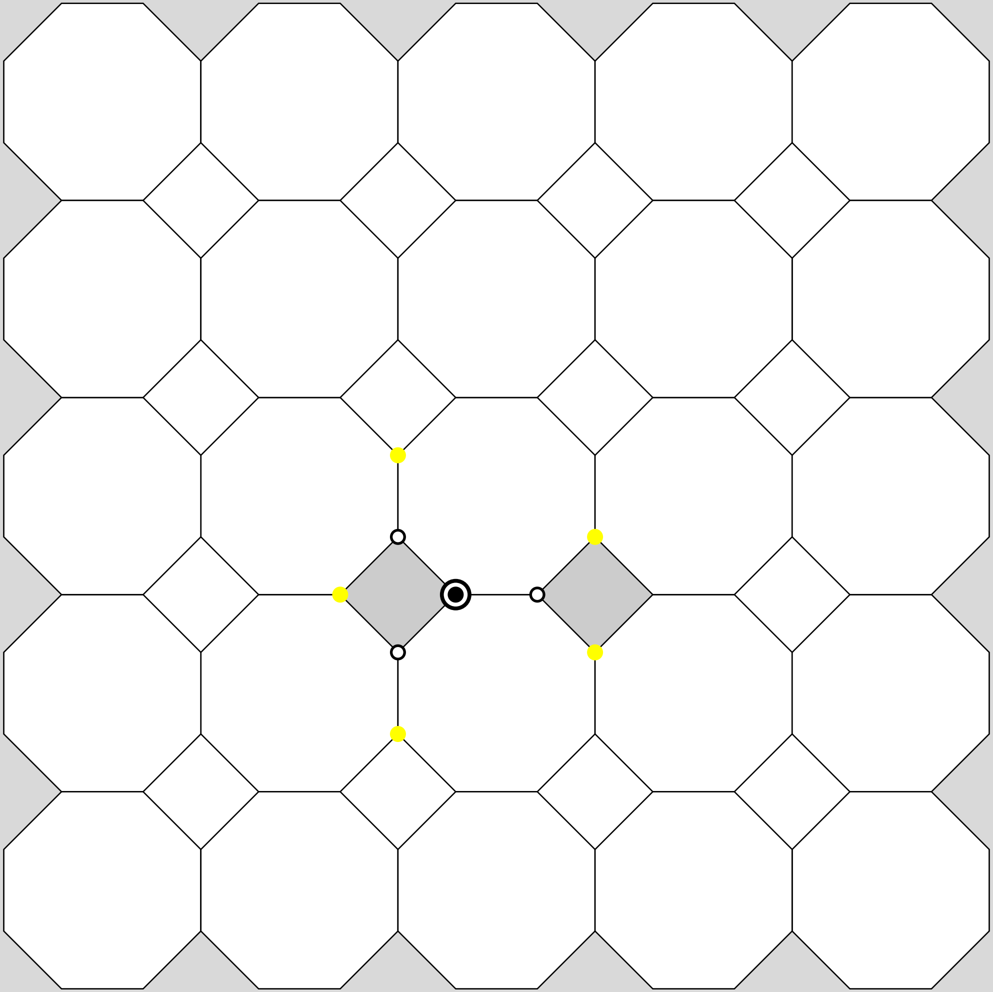

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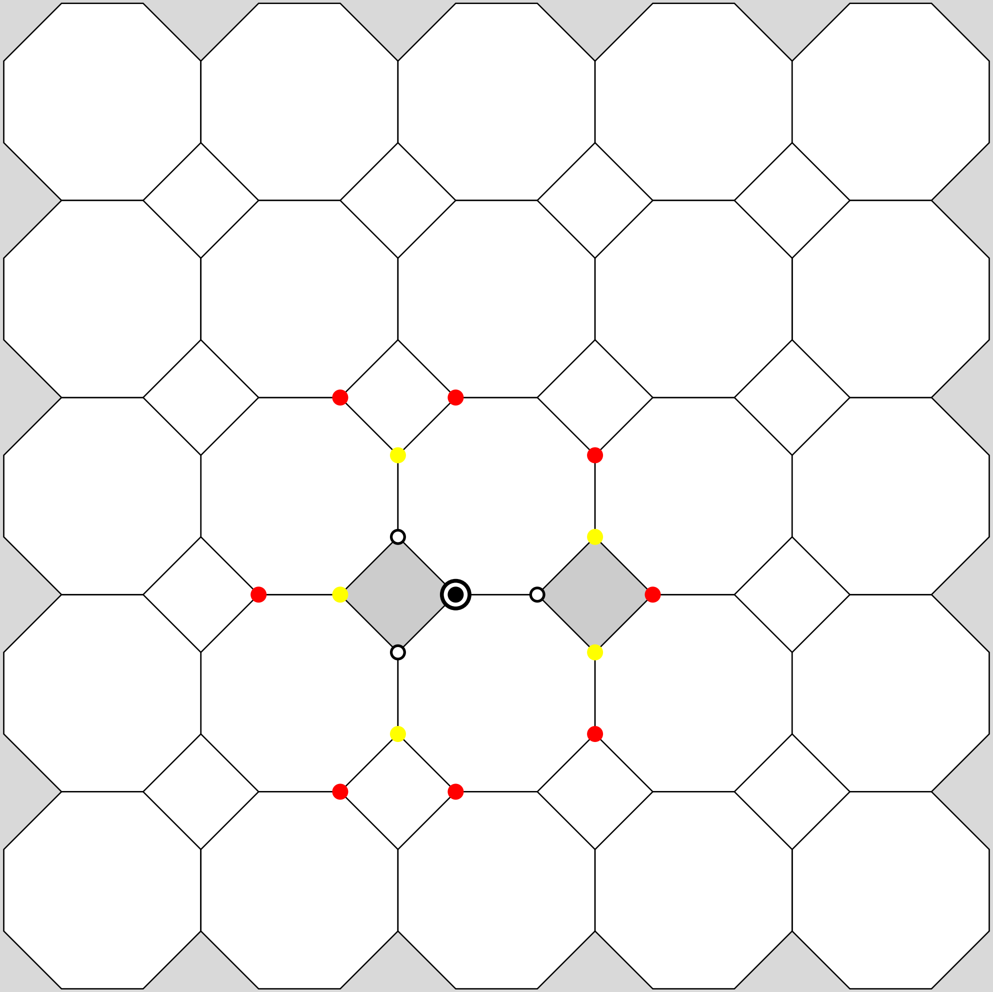

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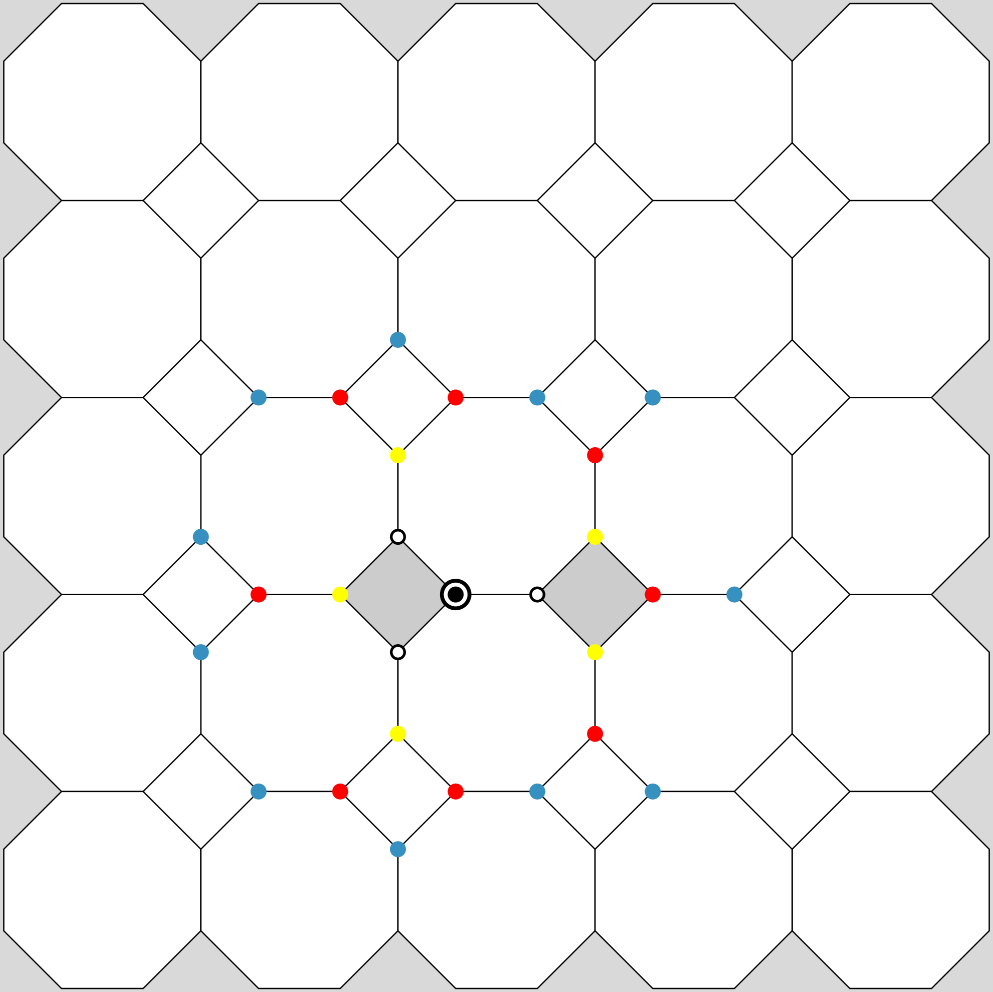

May be pinned isostatically [8].

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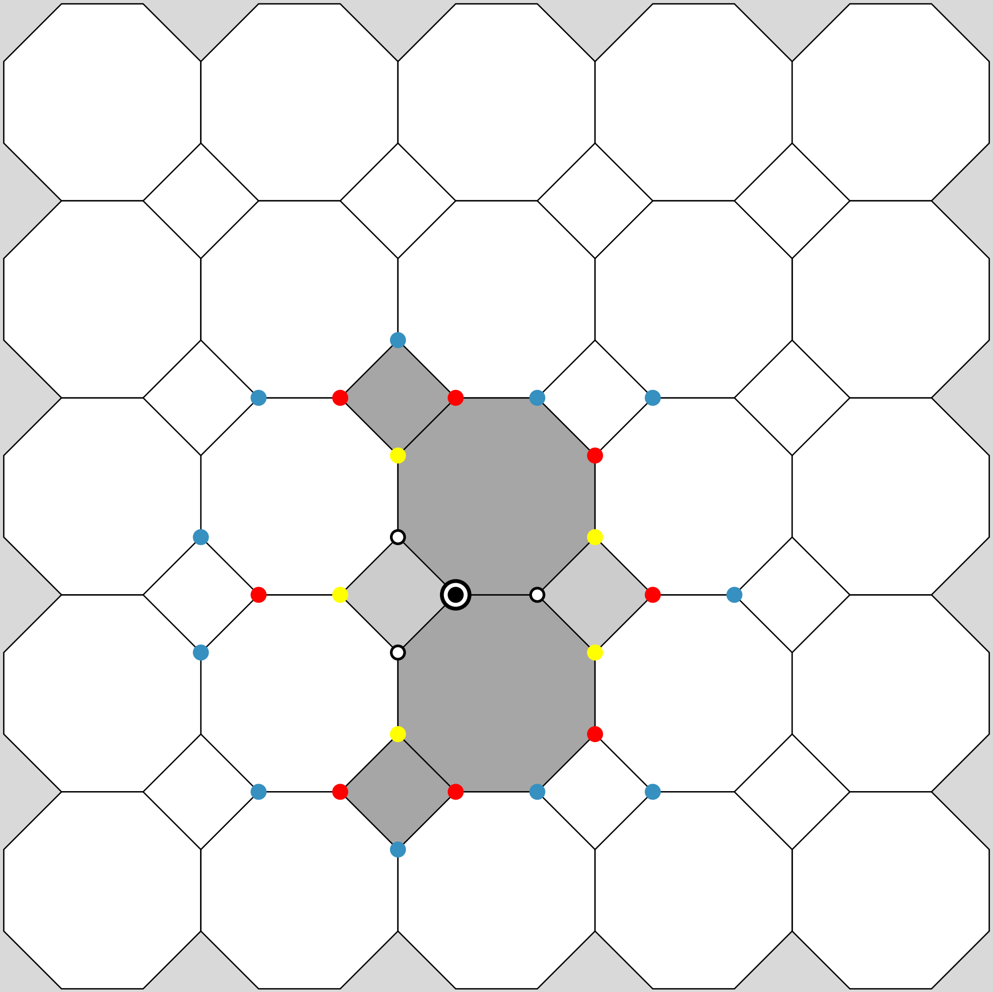

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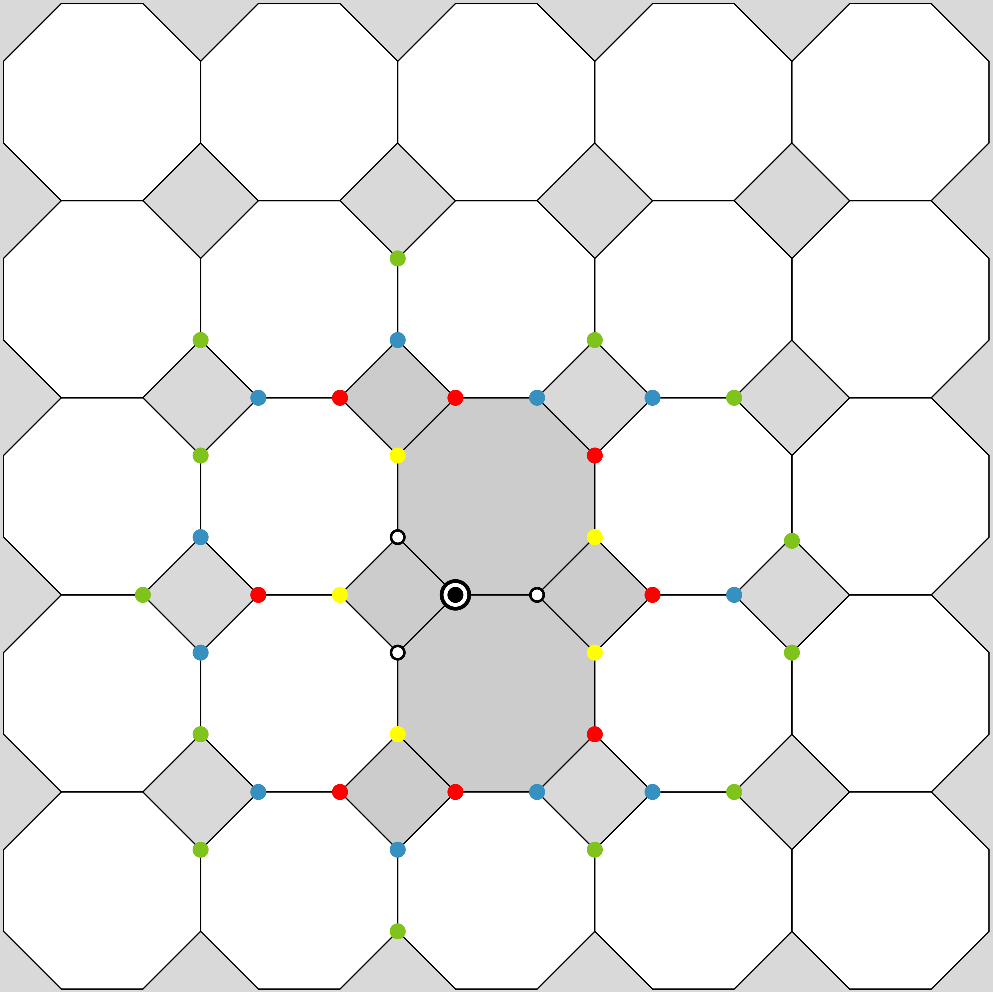

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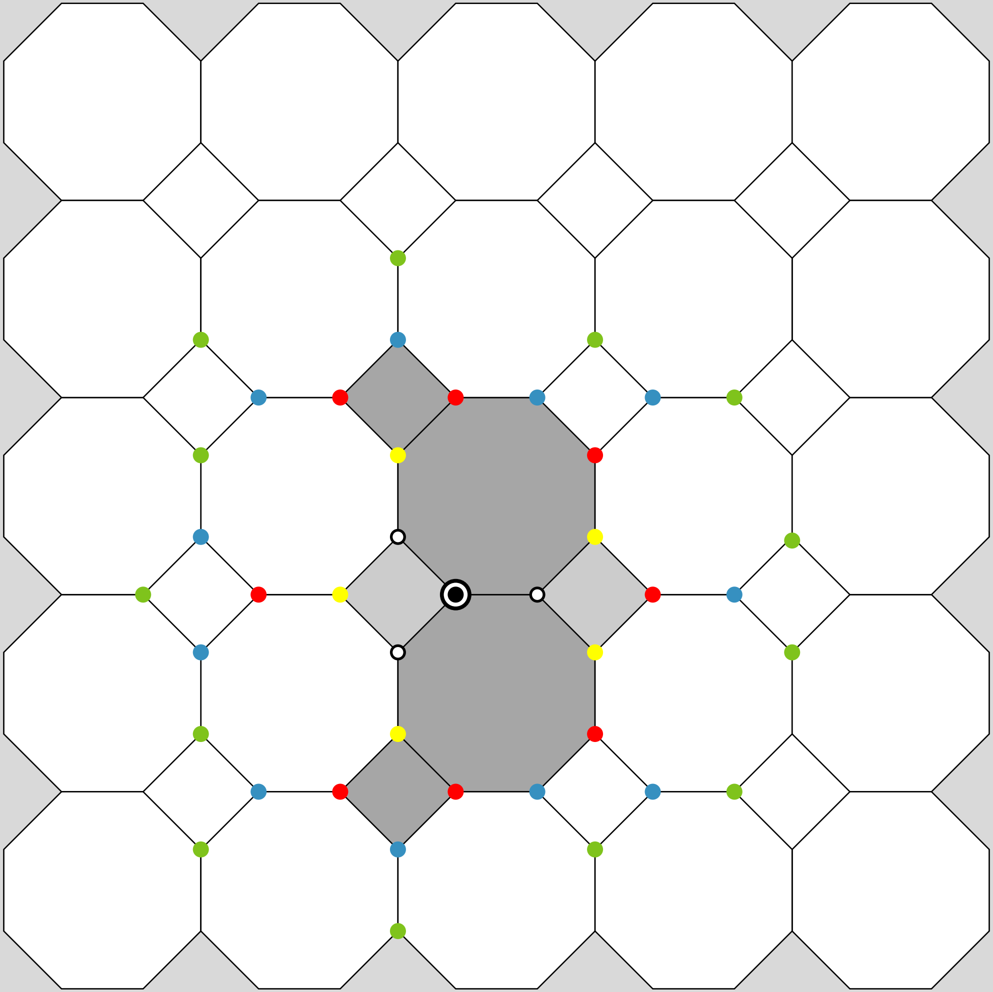

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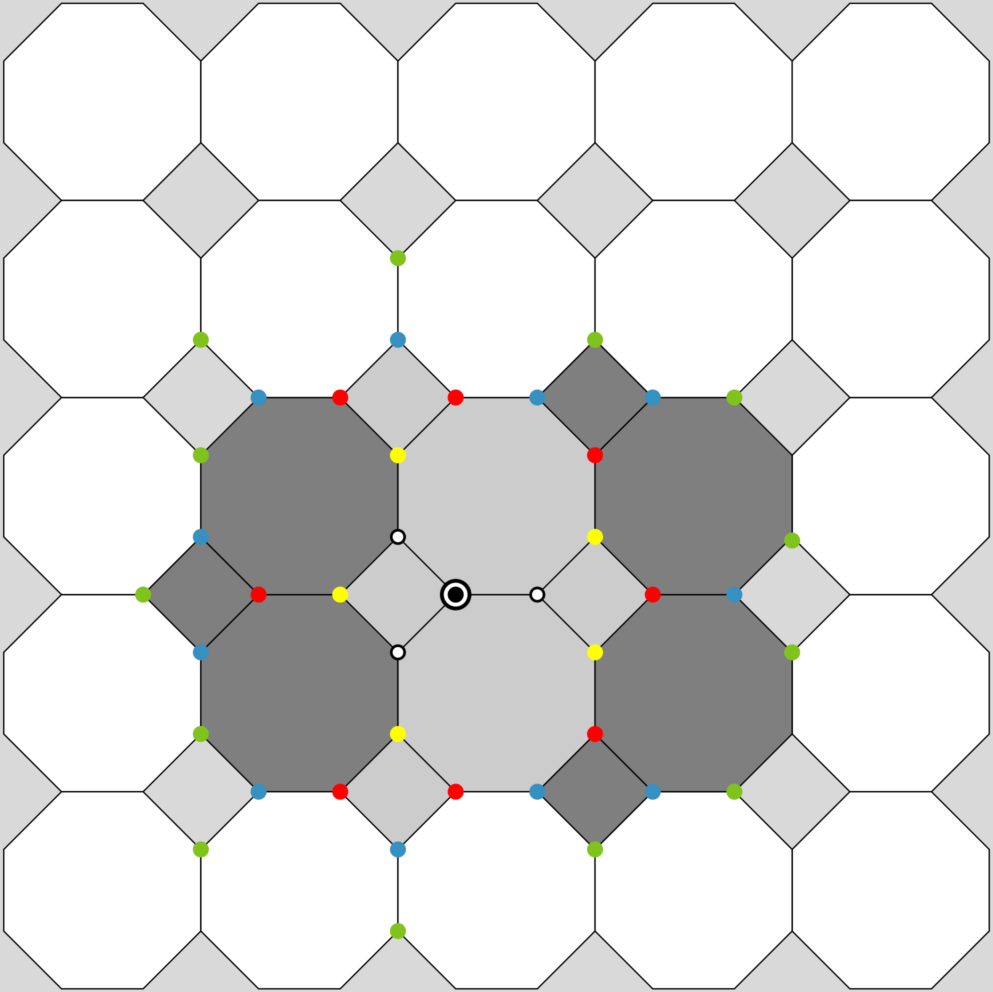

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11. Open Problems

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

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

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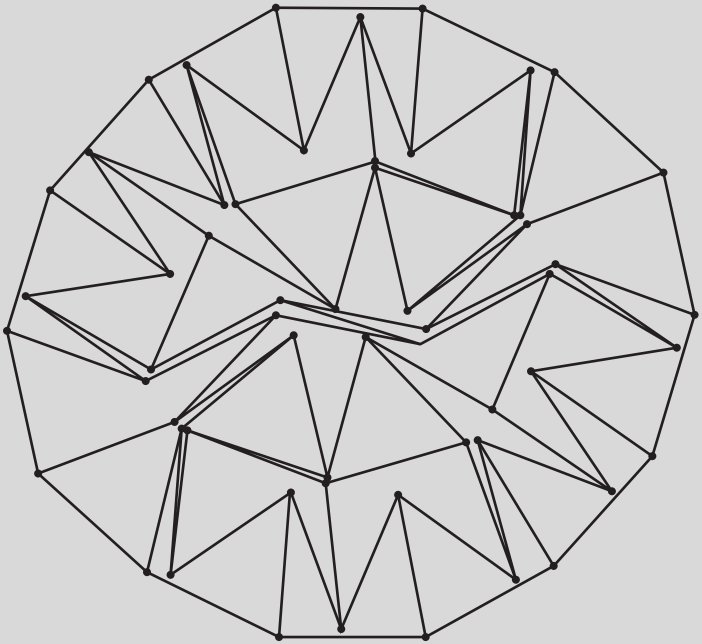
Do there exist finite non-interpenetrating zeolites with unit distance plane non-rigid realizations?



Rigidity properties of the line graph? Unit distance realization?

Line graphs of unit distance graphs

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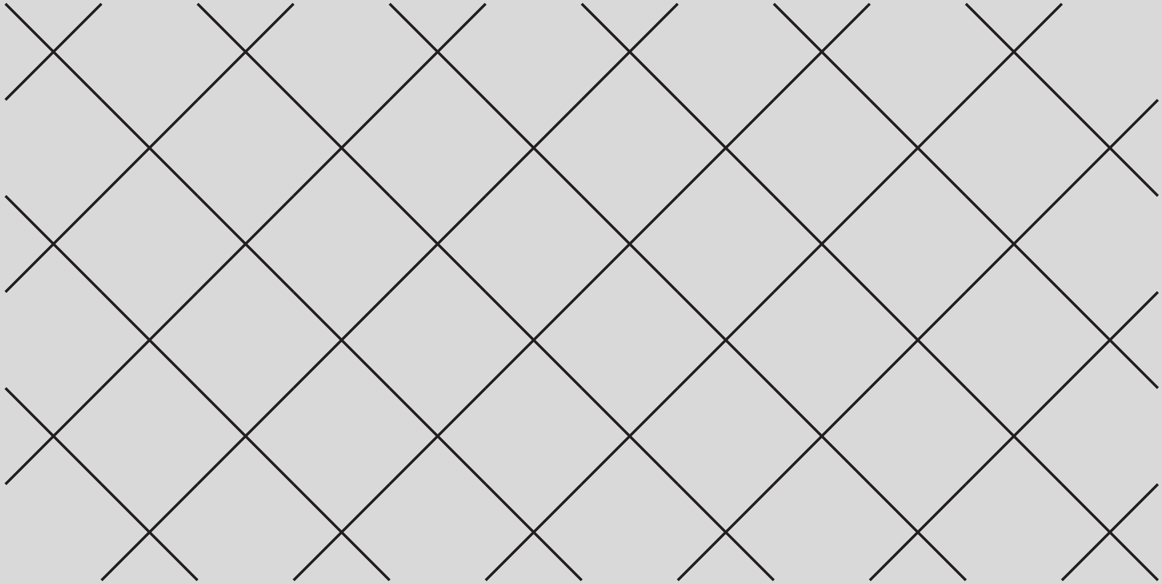
Line graphs of unit distance graphs



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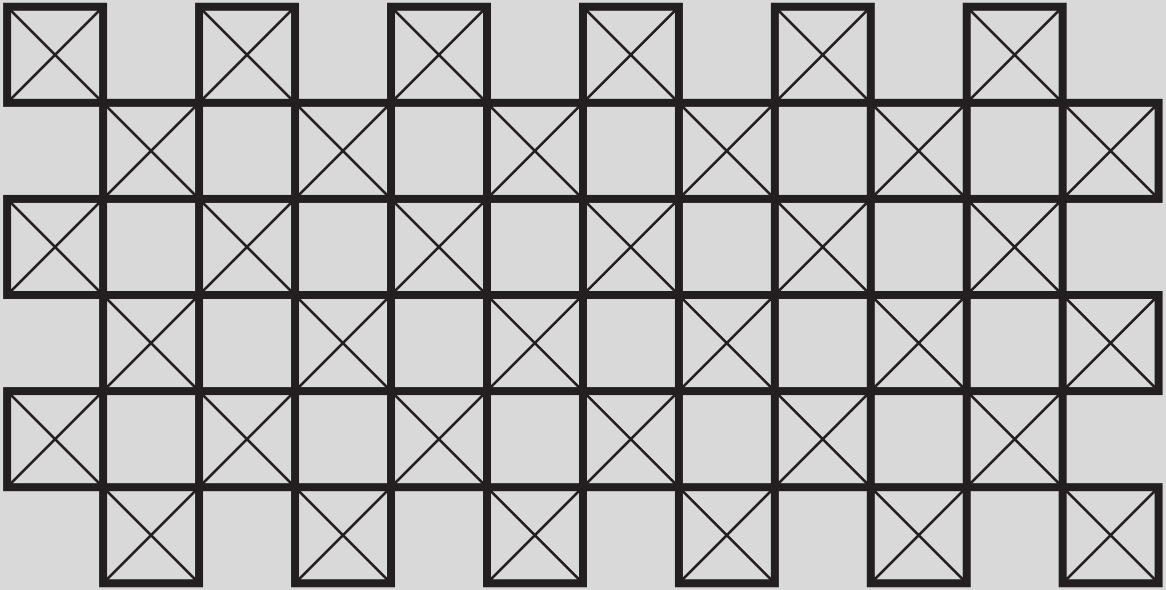

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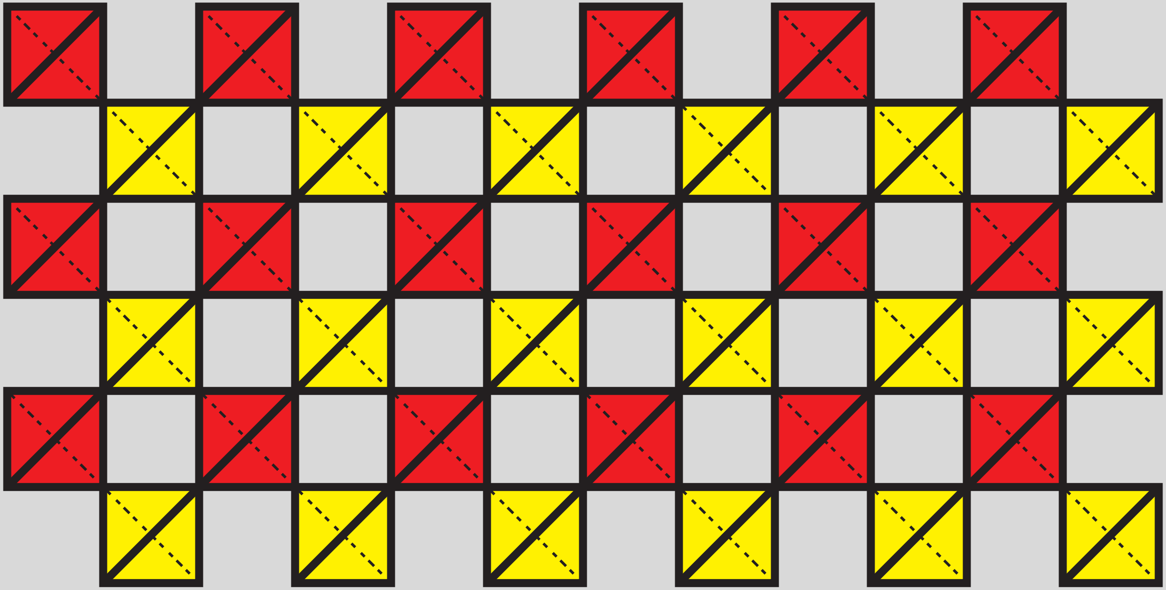

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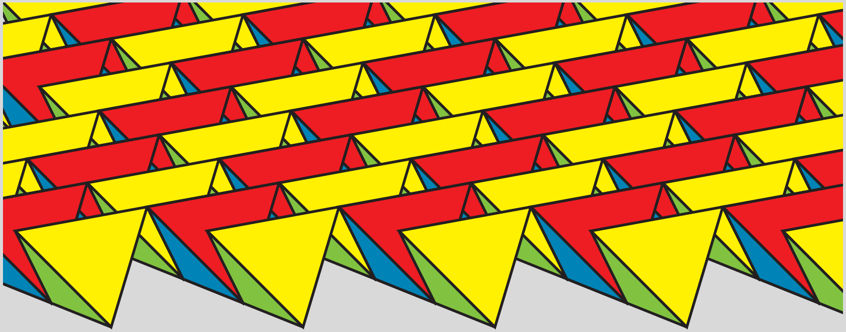

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Line graphs of line graphs?

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Design nano lentils and prove their realization

Mildred Dresselhaus (*née* Spiewak; November 11, 1930 – February 20, 2017), known as the “queen of carbon science”

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