Analyzing Periodic Nets via the Barycentre Construction

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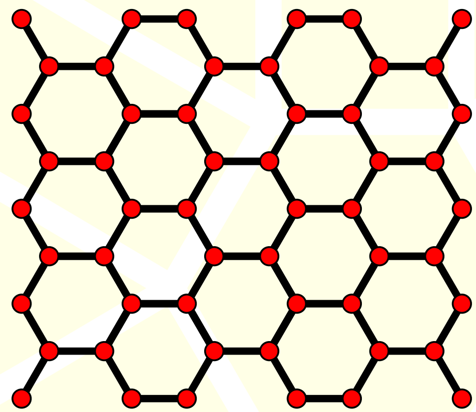
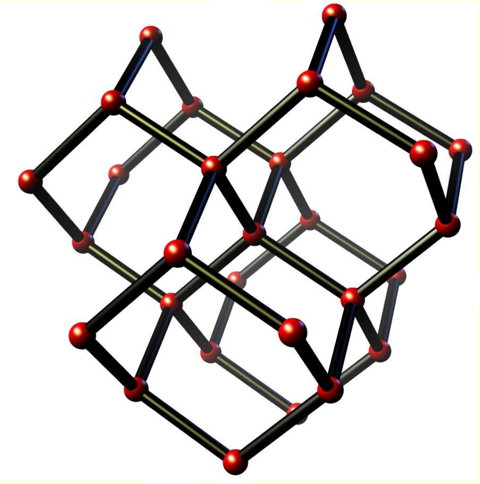
The Australian National University - Supercomputer Facility

Crystal topologies

Materials of the same chemical composition can have very different characteristics.

Goal: Describe their conformations qualitatively.





Potential applications:

- taxonomy
- structure recognition
- design of new materials

Topology?

The topology of an object conveys the aspects of its shape that are invariant under deformations.

- intrinsic topology — the structure itself
- ambient topology — its embedding into space

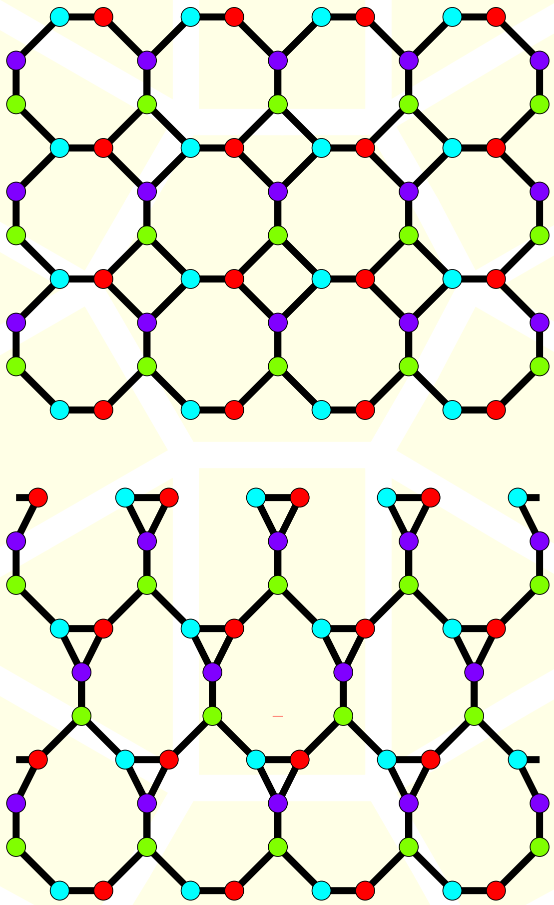
If we allow a knot to pass through itself, it can be turned into a circle. Its “knottedness” is not intrinsic.

Here, we will consider only intrinsic topology.

Conventions for today

- We will call periodic graphs also p-graphs or sometimes just graphs.
- If not mentioned otherwise, all graphs are connected.

The vector representation (1)



Two periodic graphs.

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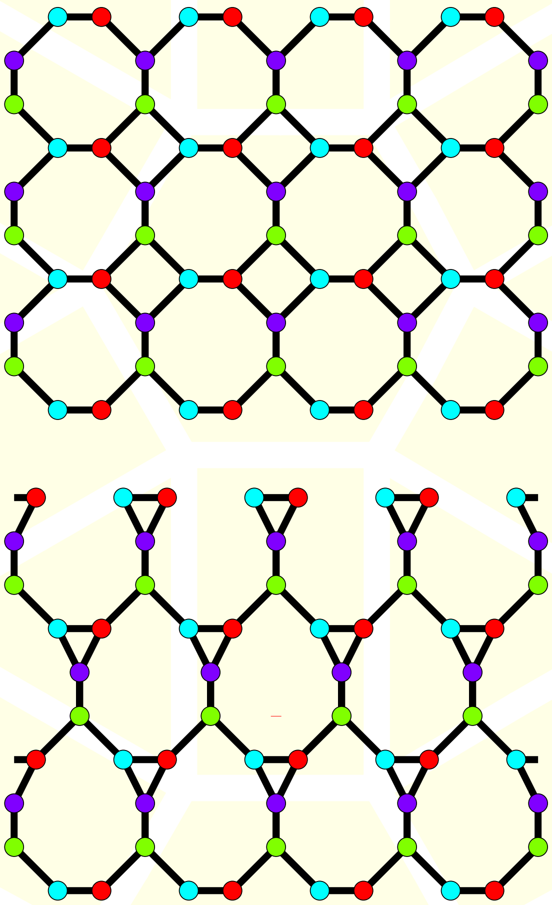

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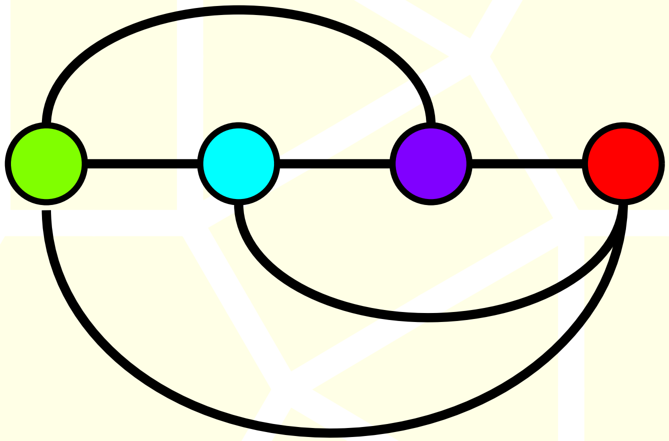
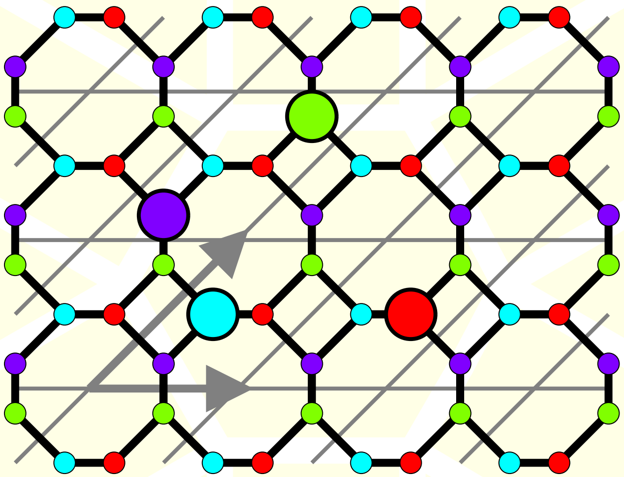


The same orbit graph.

The vector representation (2)



Choose vertex representatives and a coordinate system for translation vectors.

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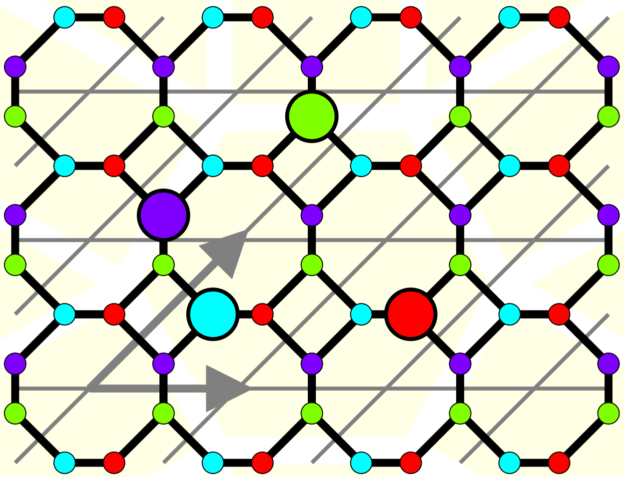
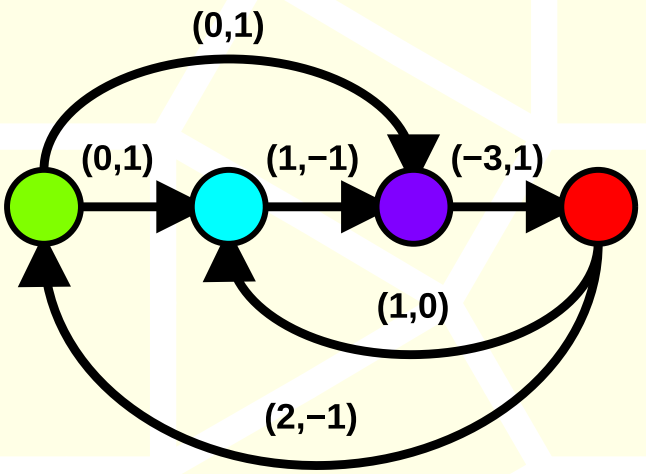
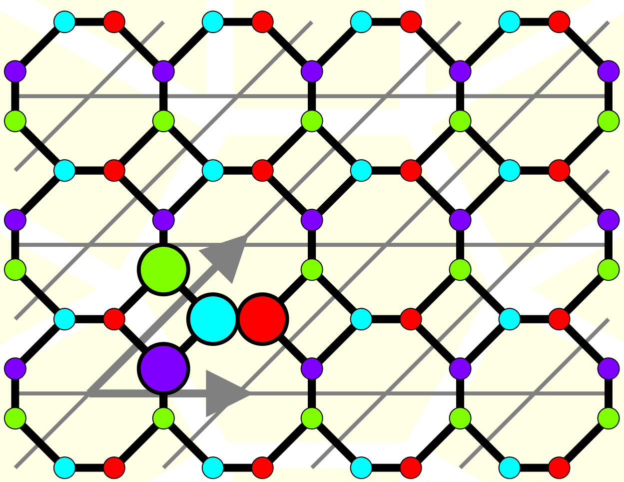




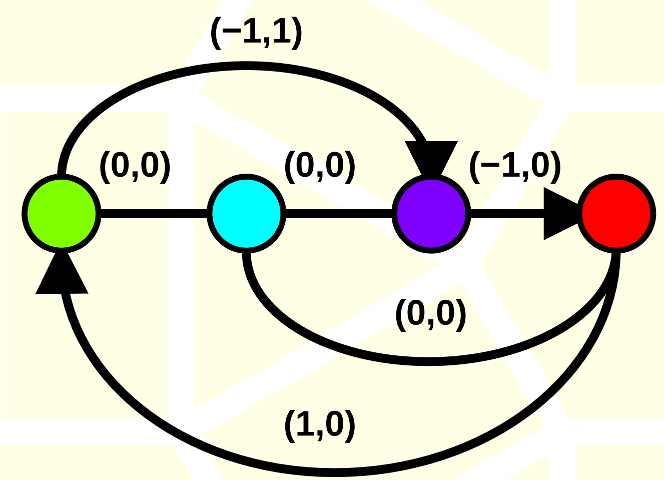
Choose vertex representatives and a coordinate system for translation vectors.

Choose directions for orbit graph edges and label with shift vectors.

The vector representation (2)

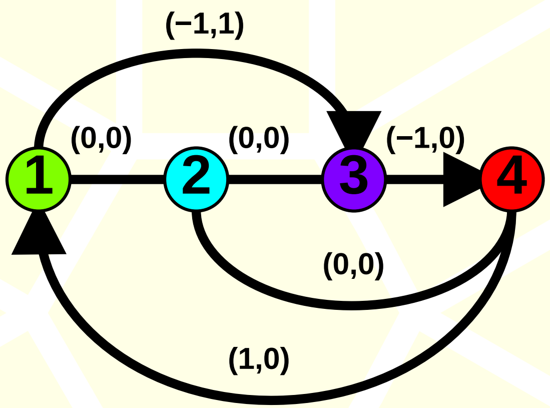


A “nicer” system of representatives.



The new edge labels.

The vector representation (3)



Assign vertex numbers.

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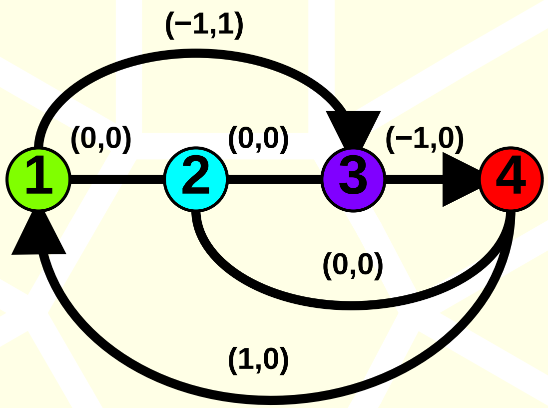

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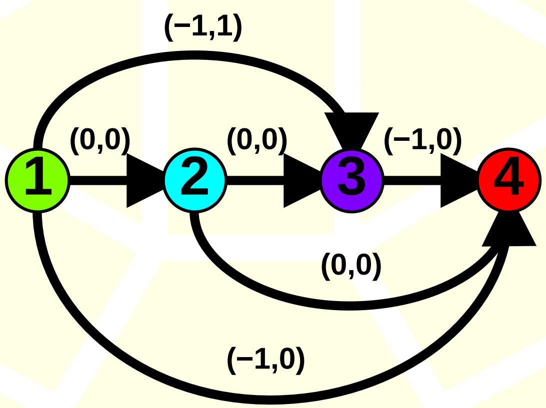

Normalize edges.

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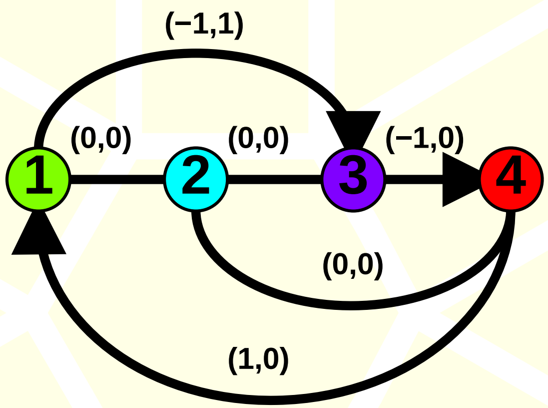

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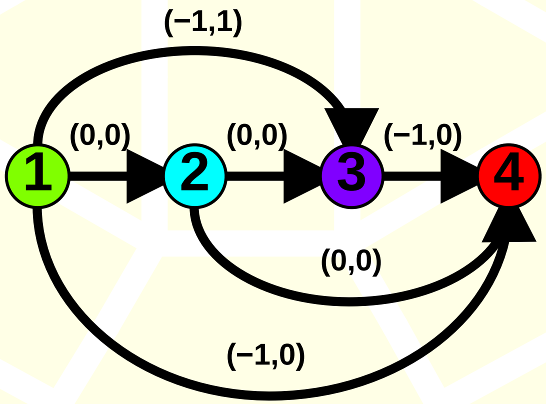
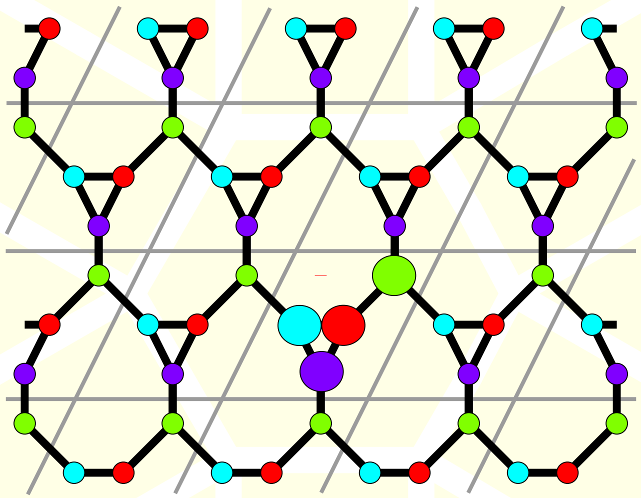


Normalize edges.

A (sorted) tabular representation:

1	2	0	0
1	3	-1	1
1	4	-1	0
2	3	0	0
2	4	0	0
3	4	-1	0

Now we see a difference



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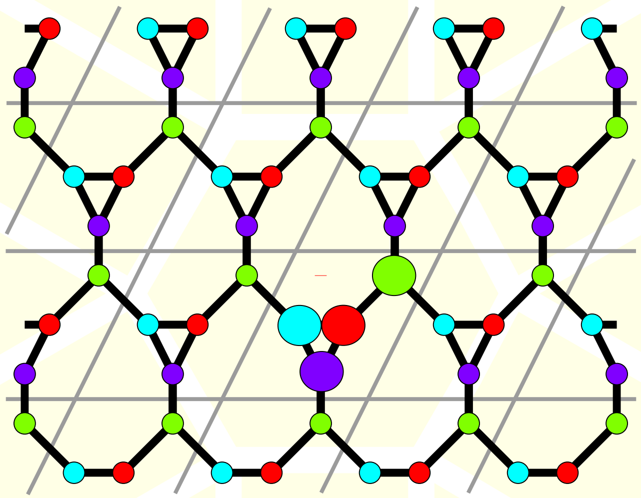

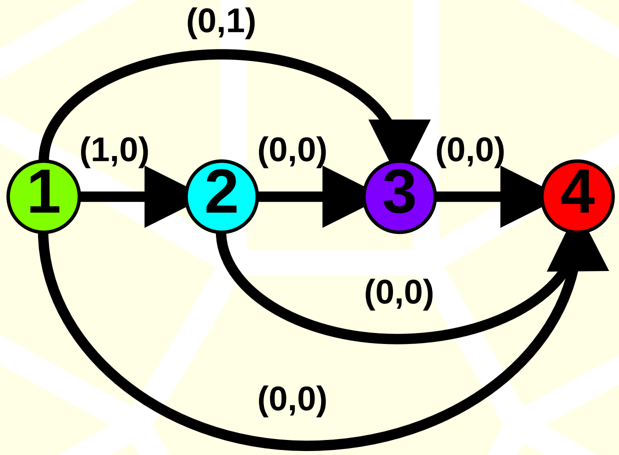

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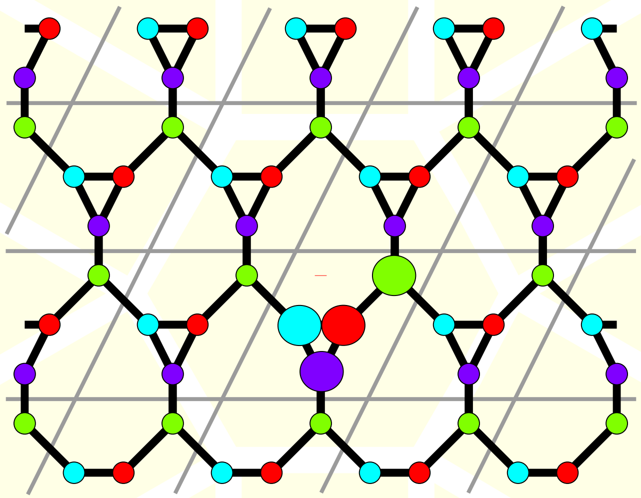

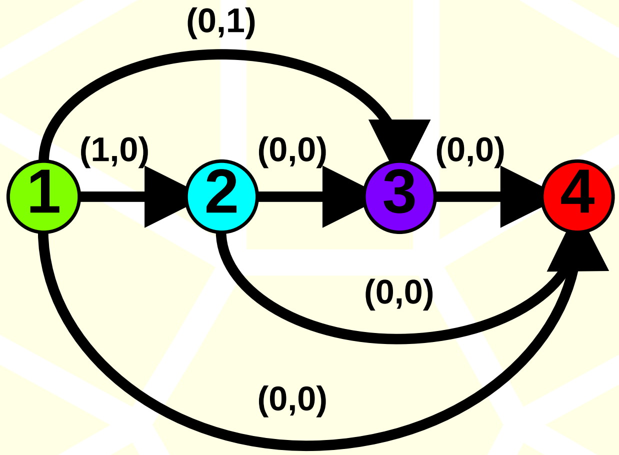

1	2	1	0
1	3	0	1
1	4	0	0
2	3	0	0
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3	4	0	0

But we have a problem

One of these things is not like the others...

1	2	0	1
1	3	0	1
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2	3	1	-1
2	4	-1	0
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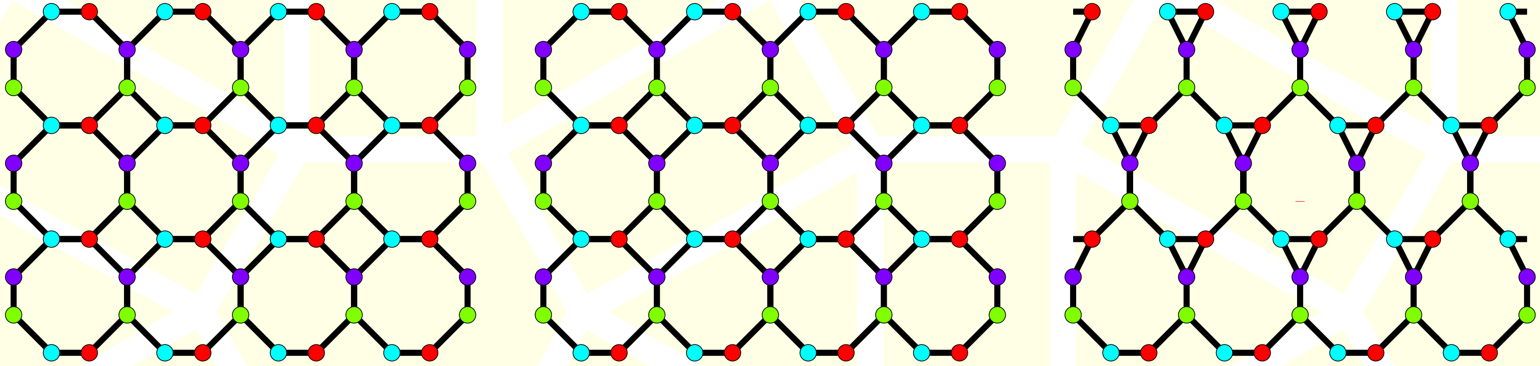

Some questions

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In the following, we will look at Systre's approach to these questions.

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In other words: an isomorphism can renumber the vertices of the orbit graph and change the coordinate system for the shift vectors.

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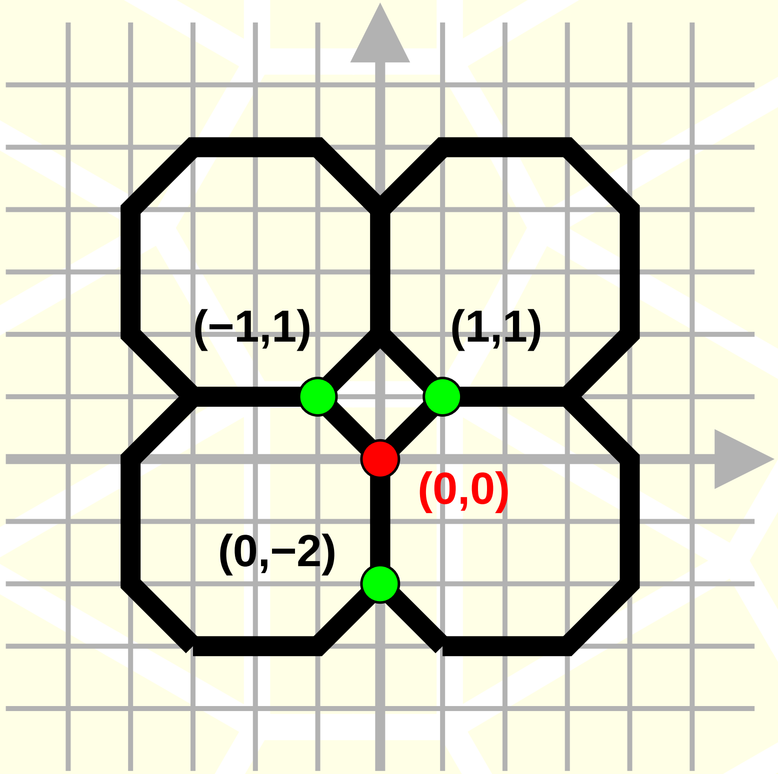
Important: Every symmetry of an embedded p-graph corresponds to an automorphism, but the reverse is not always true.

Barycentric drawings



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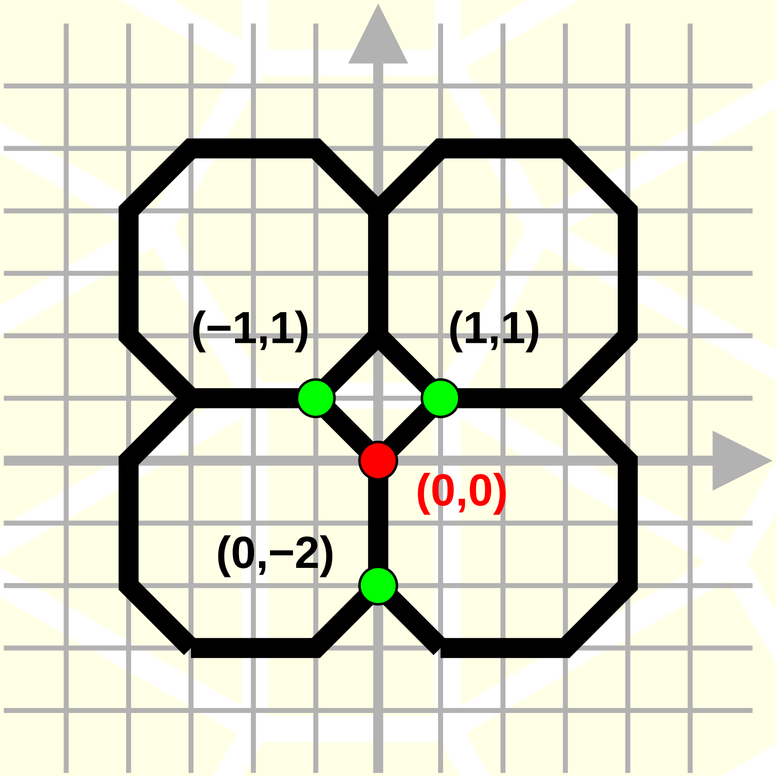

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$$\sum_{w \in N(v)} p(w) - p(v) = 0$$

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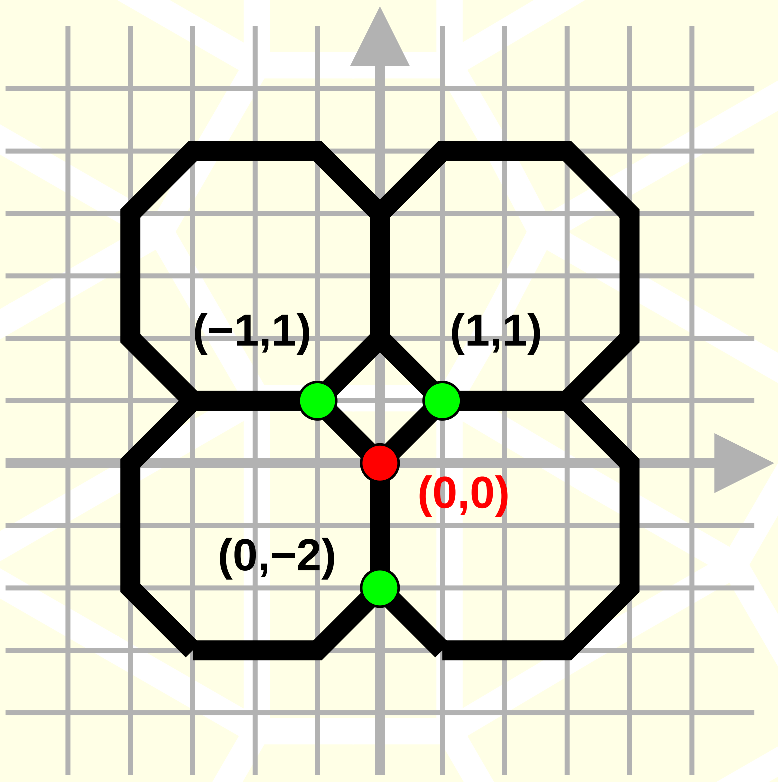

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where
$p(v) =$ position of v,
$N(v) =$ neighbors of v.

Tutte's idea
(for finite graphs)

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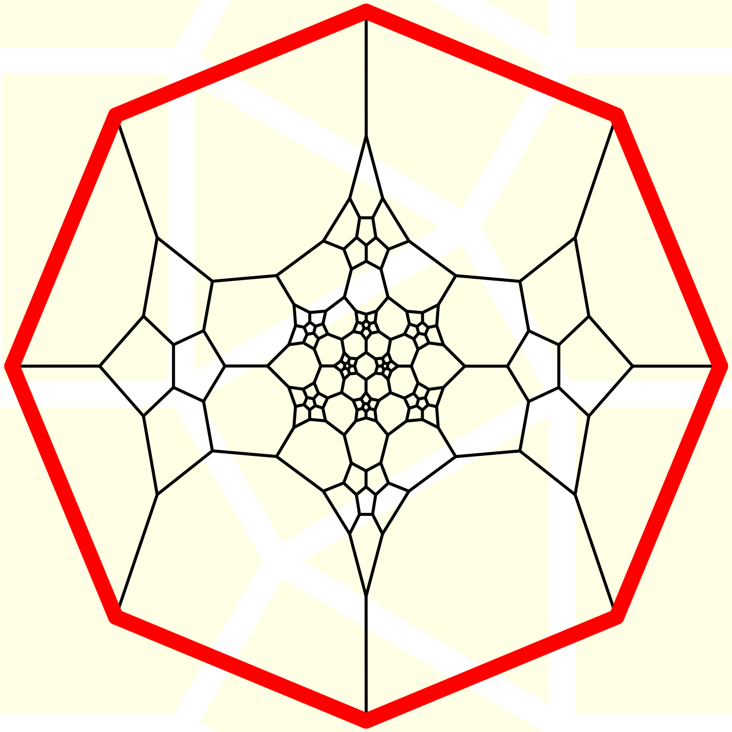

G planar, 3-connected
$\Rightarrow$ convex
planar drawing.

Periodic version

Theorem: Any proper choice of positions for one vertex and its translates gives rise to a unique barycentric placement.

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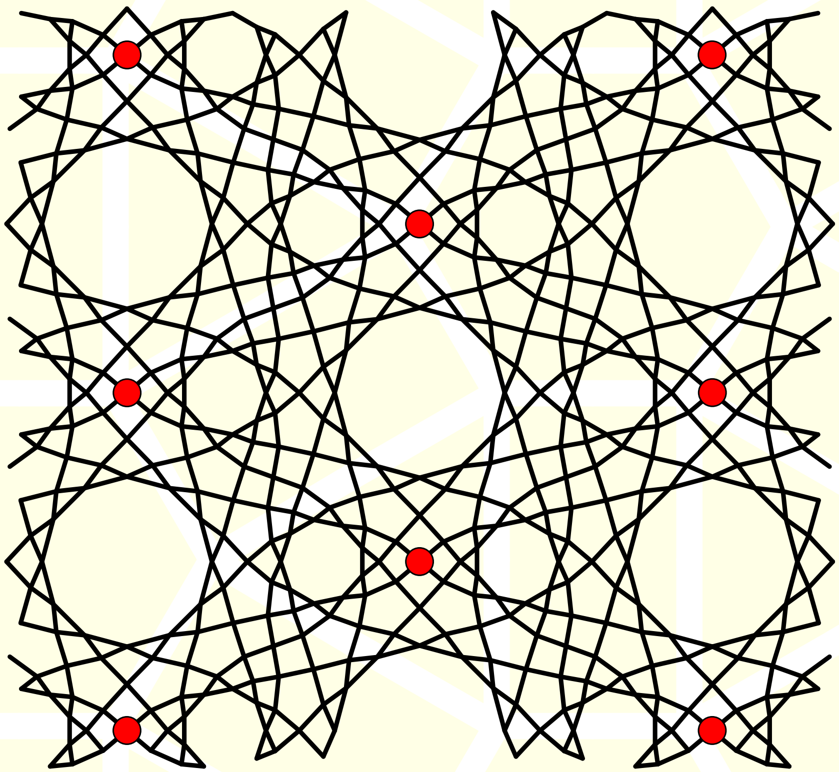
Consequence: All proper barycentric placements of a p-graph are “the same up to a choice of coordinate system.”



Uniqueness proof

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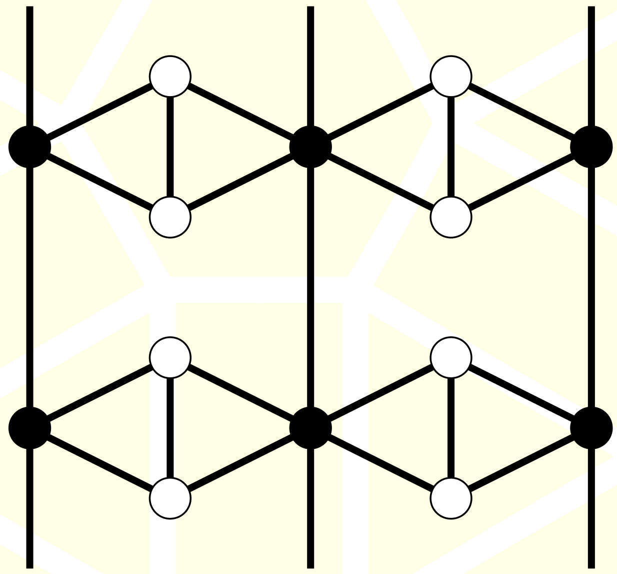
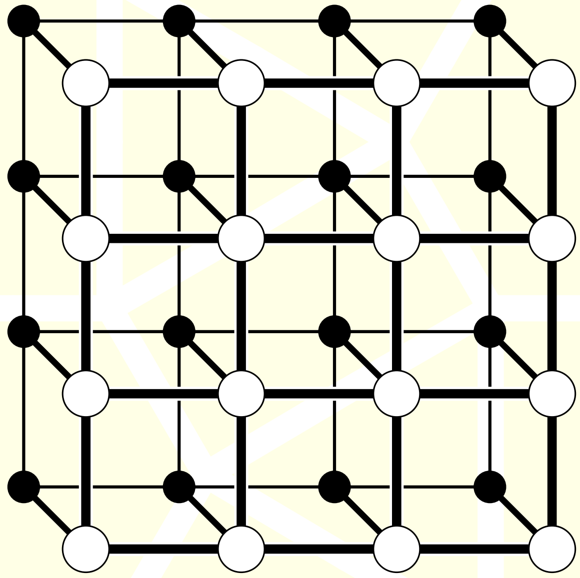
(This also shows that barycentric placement minimizes the square sum of edge lengths.)

Caveat

Barycentric positions can “collide”:





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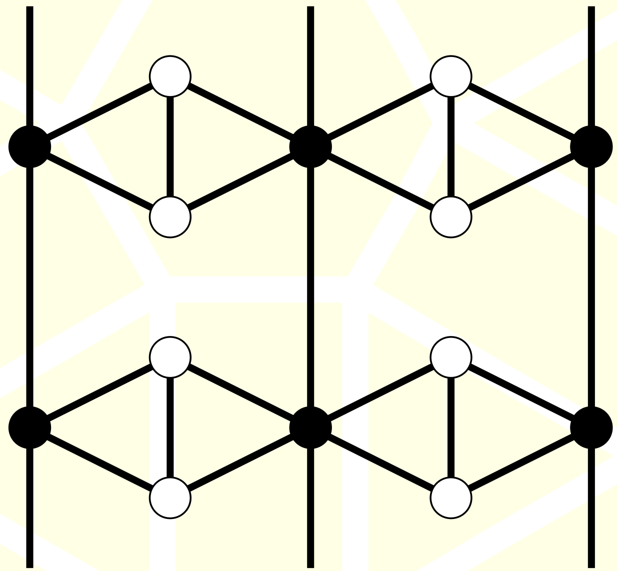

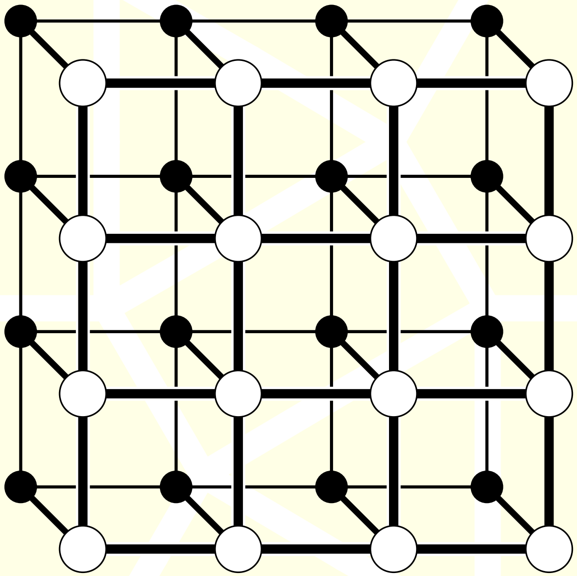

A p-graph without collisions is called stable — one without collisions of next-nearest neighbors is called locally stable.

Symmetries

- Uniqueness of barycentric placements $\Rightarrow$ each automorphism induces an (affine) symmetry.

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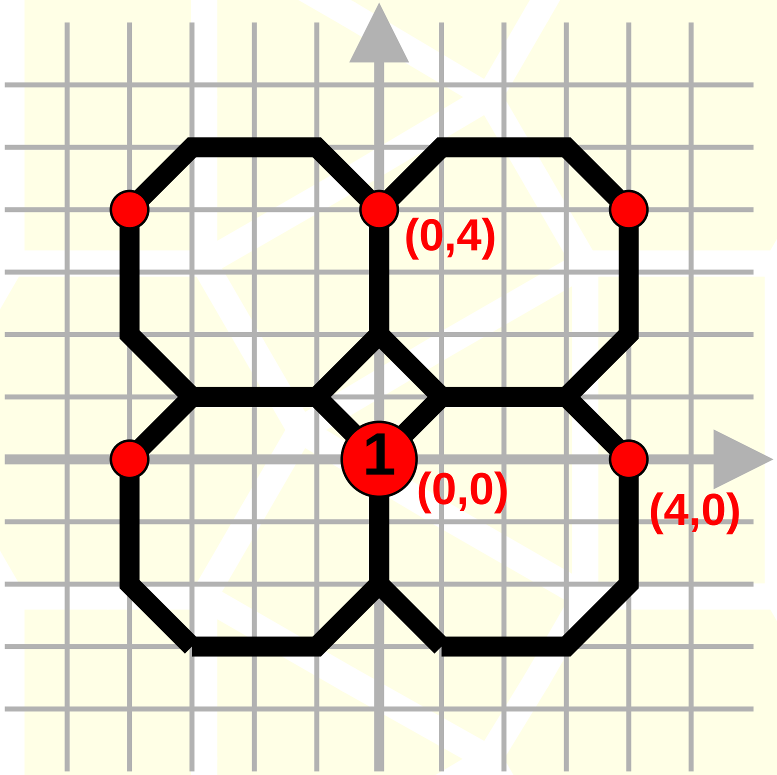
- For stable graphs, none of these symmetries is the identity.

$\Rightarrow$ A stable p-graph has an embedding in which every automorphism is realized as a symmetry.

Ordered traversals

For a locally stable periodic graph:

- Place a vertex and its translates.



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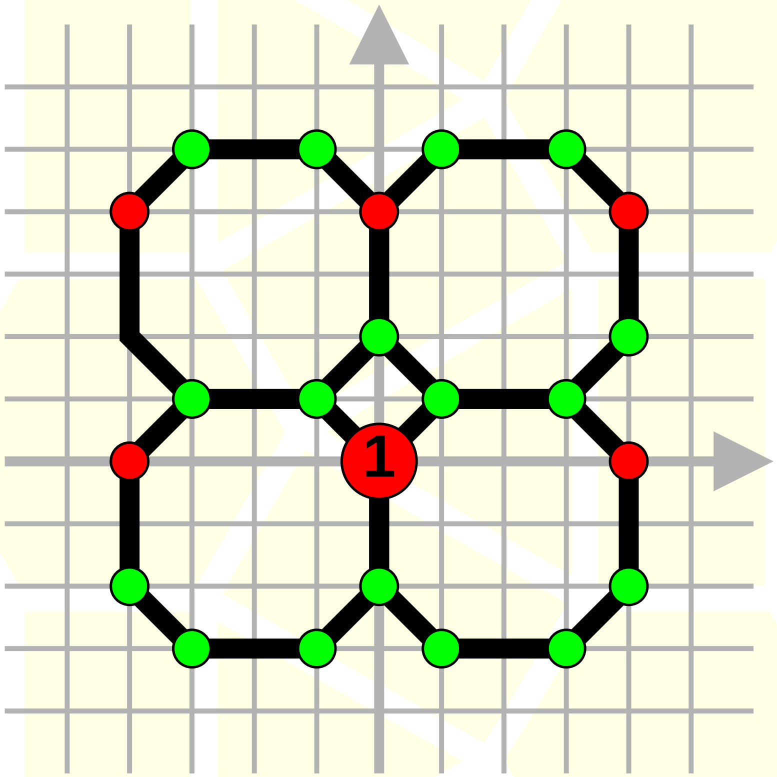

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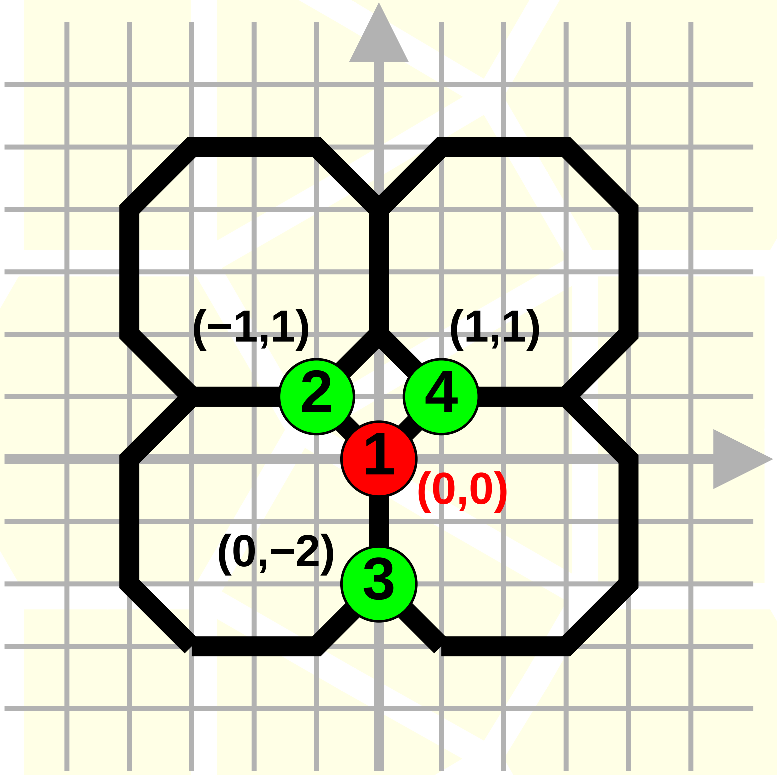

Ordered traversals

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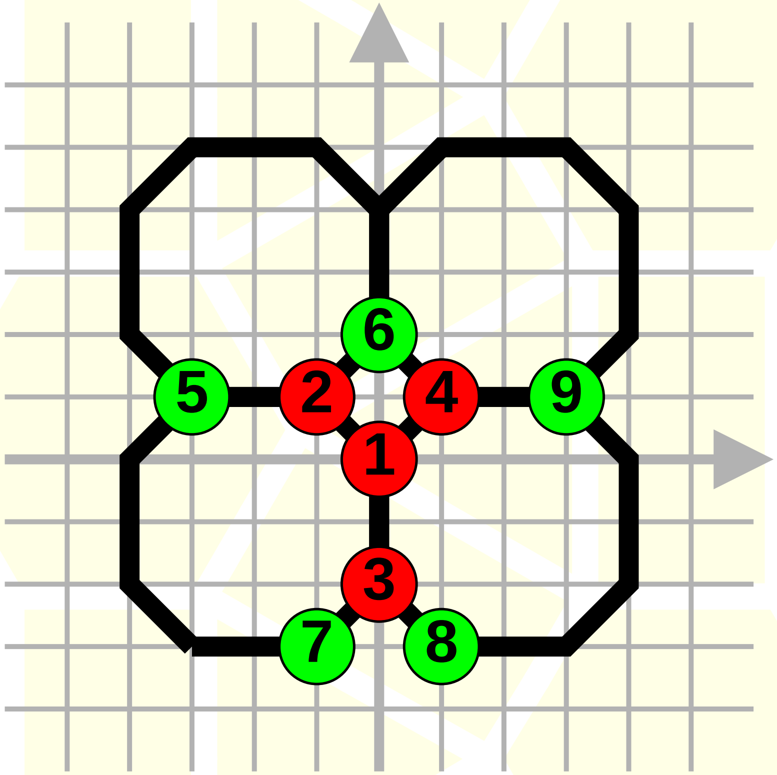
- Do a breadth first traversal, using position for sorting.
- Vertex order only depends on initial step.



Finding isomorphisms

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- Guess a linear map (matrix) that maps positions for A with origin at v to positions for B with origin at w.

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- Pick a vertex v of A and guess its image w in B.
- Guess a linear map (matrix) that maps positions for A with origin at v to positions for B with origin at w.
- Use an ordered traversal to see if the guesses were correct.

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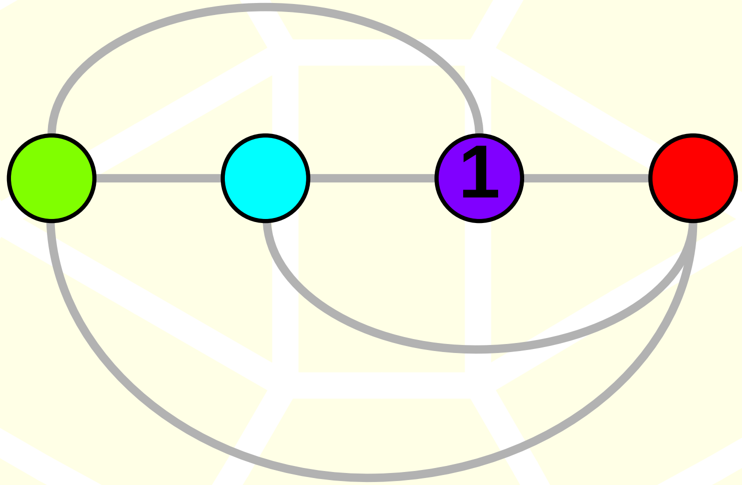
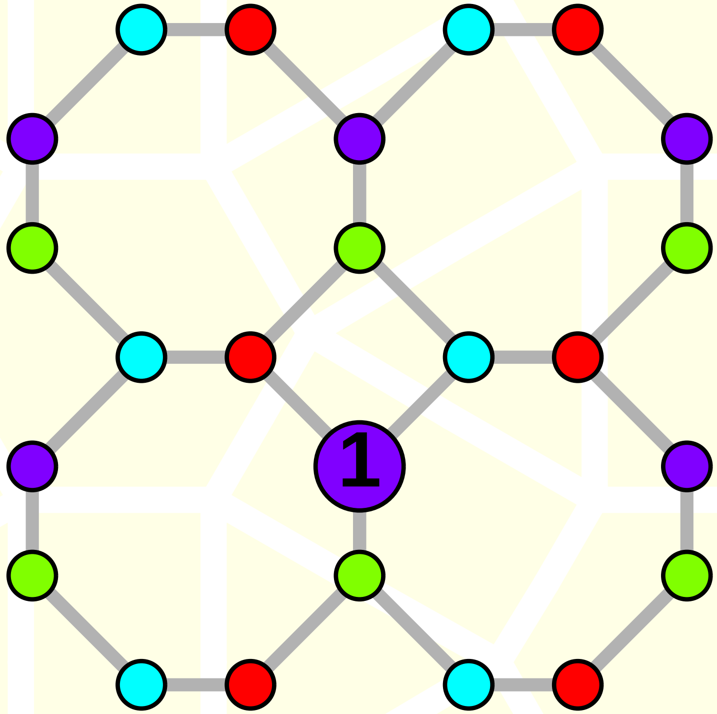
- $\Rightarrow$ very fast isomorphism testing.
- Idea: generate a small characteristic collection of representations and pick the lexicographically smallest.
- By characteristic collection we mean one that does not depend on the way the graph was originally written.

Labelling the orbit graph

Mimik an ordered traversal on the unlabelled orbit graph; use the first vertex of each set of translates as that set's representative:





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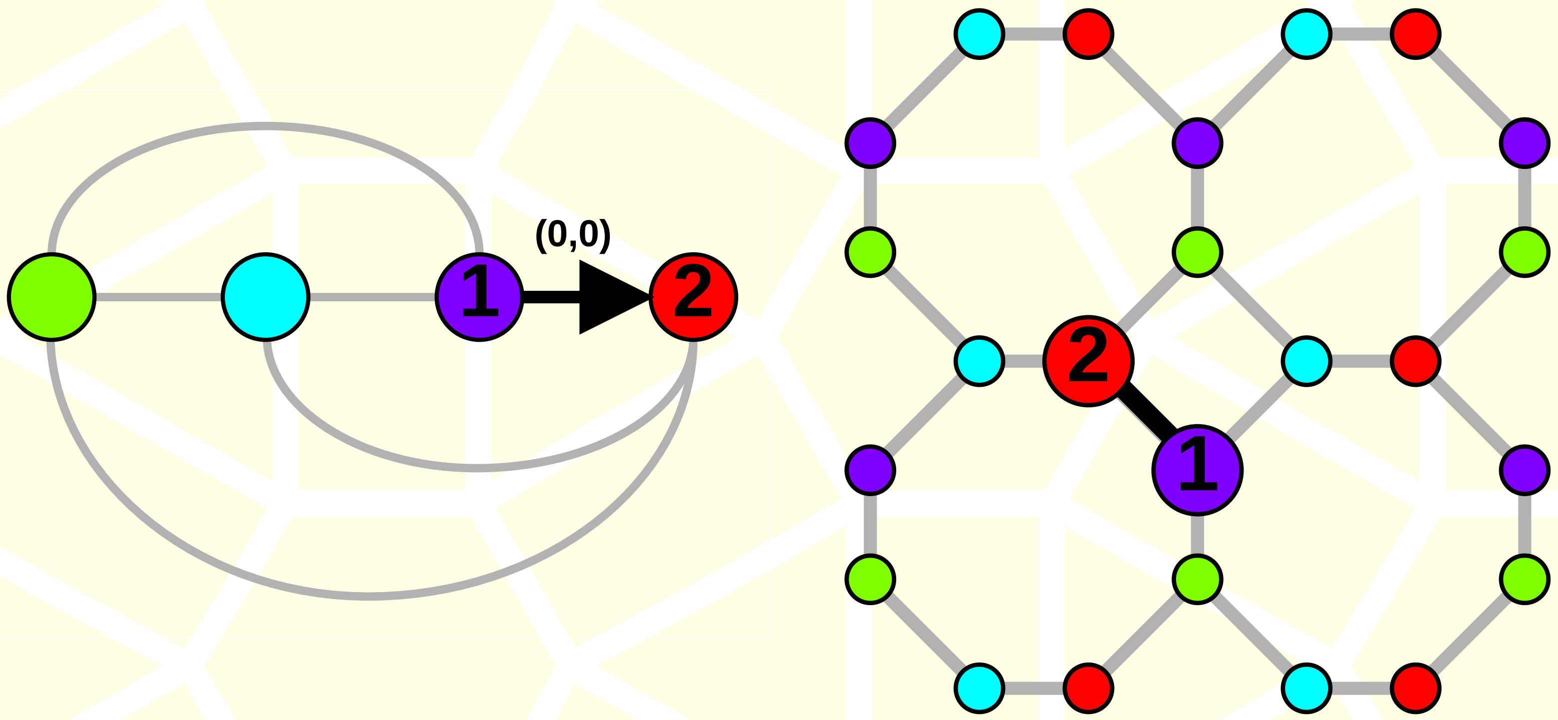

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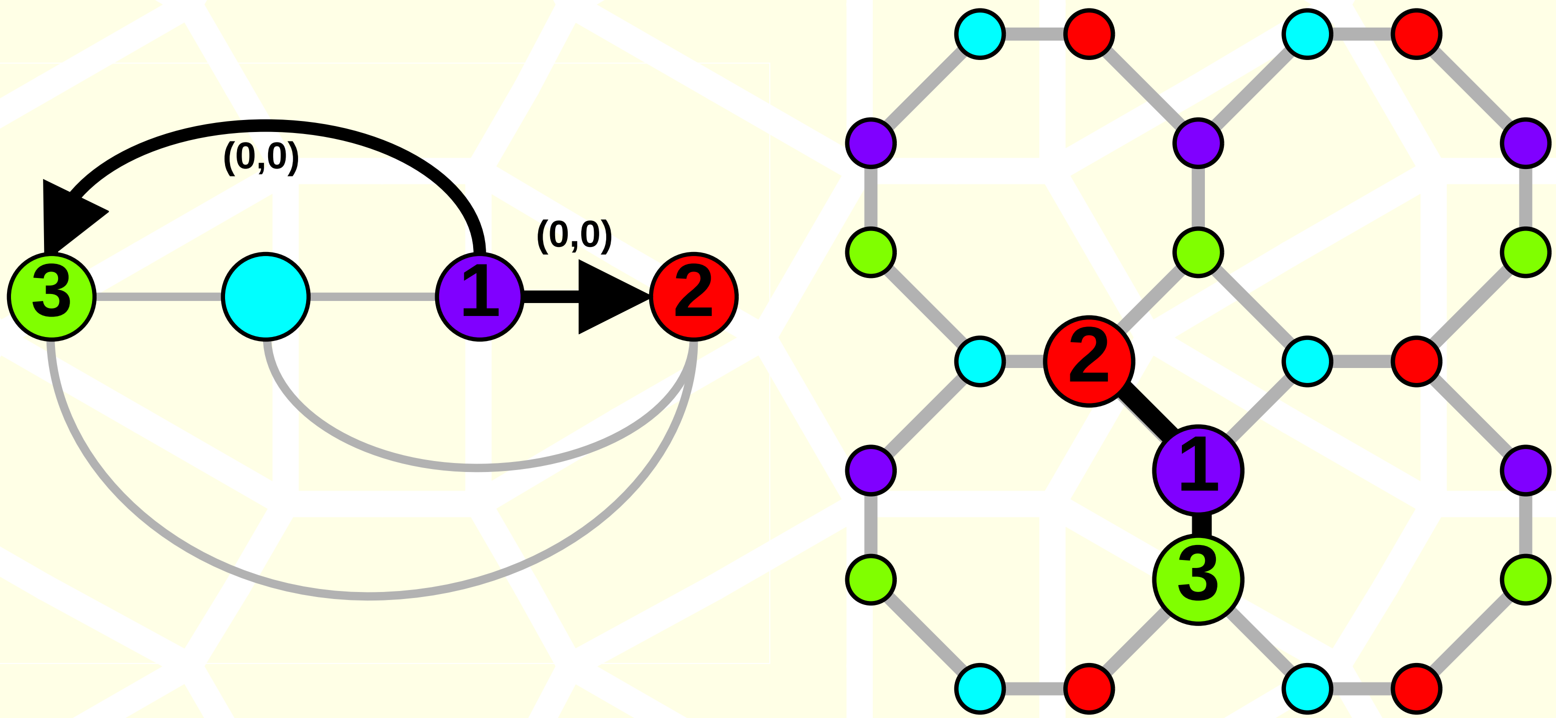

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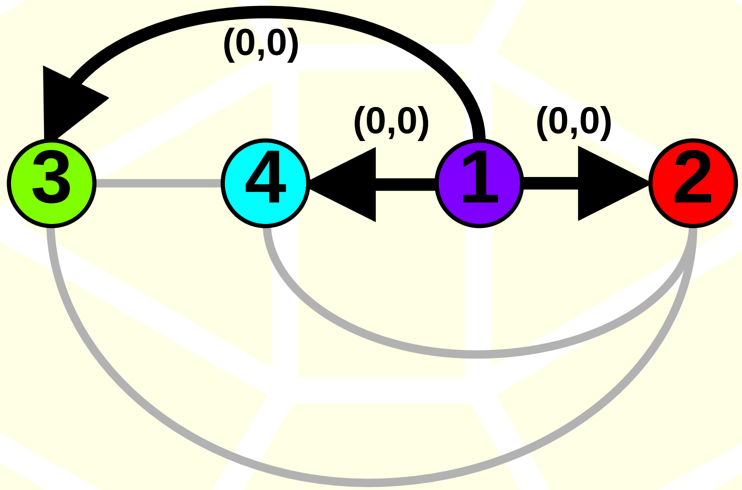

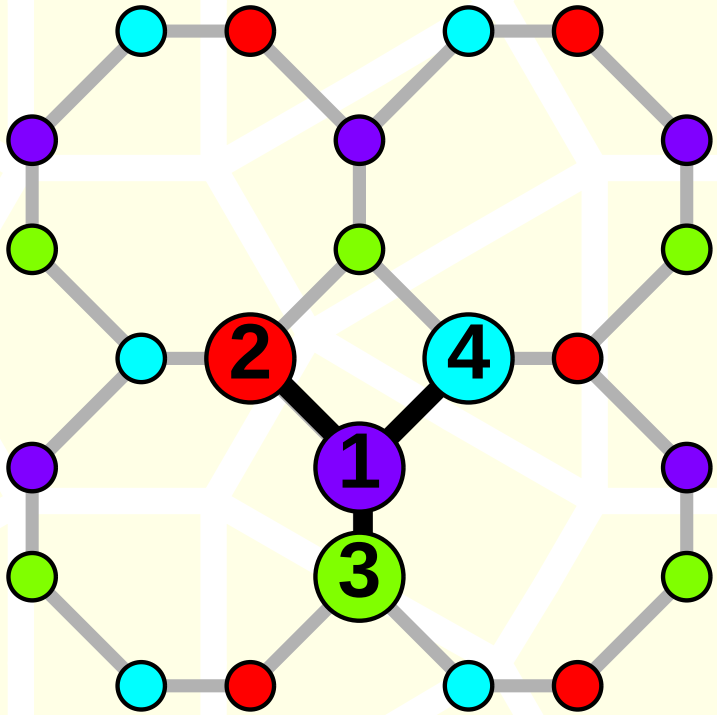

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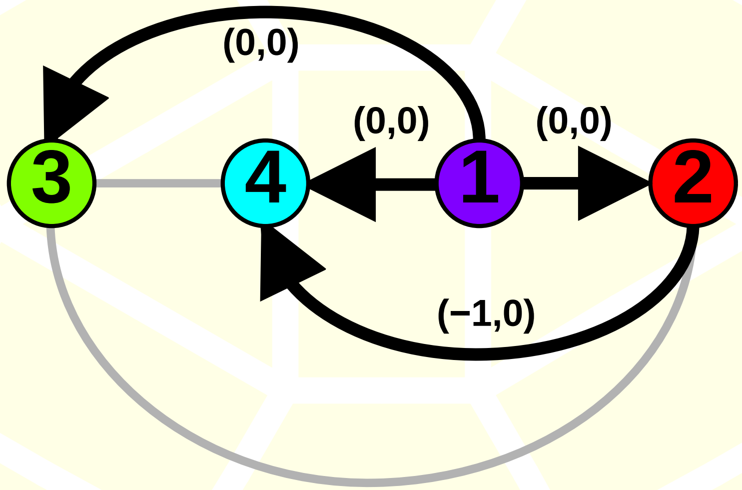

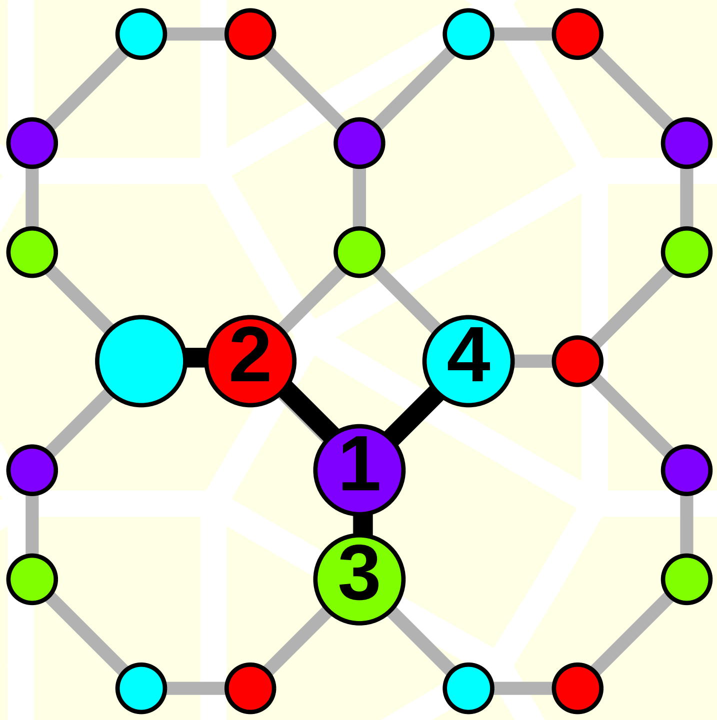

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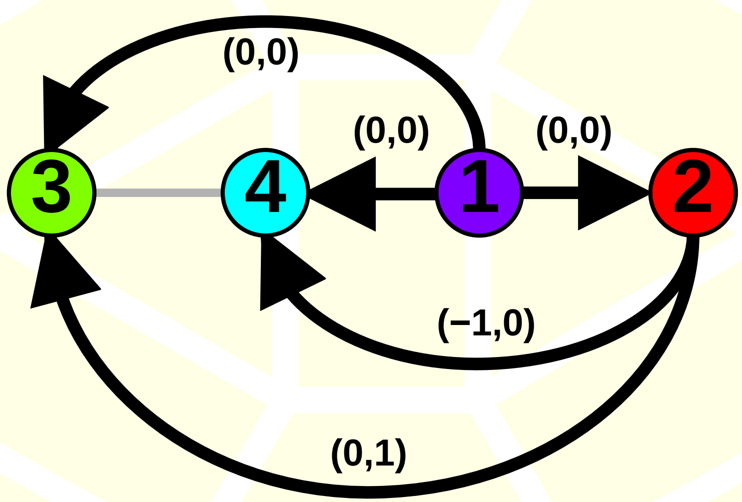

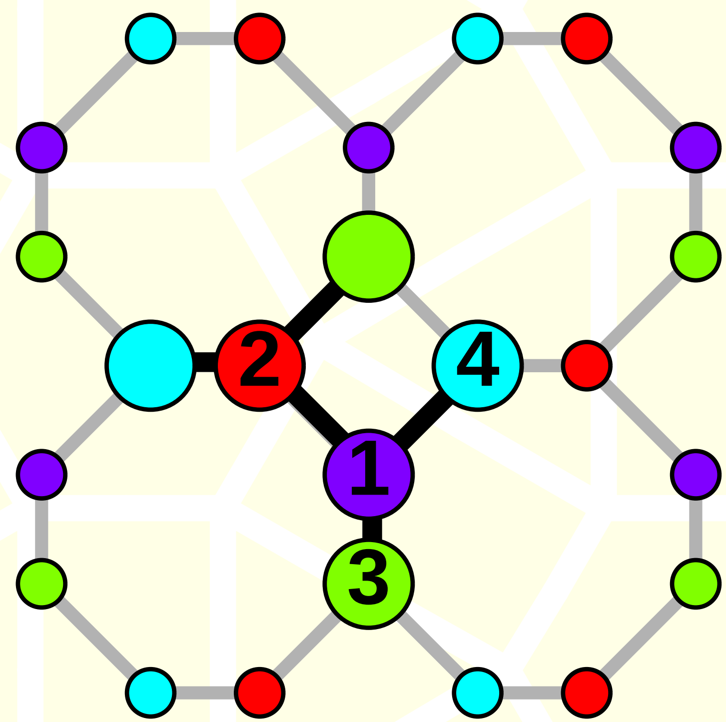

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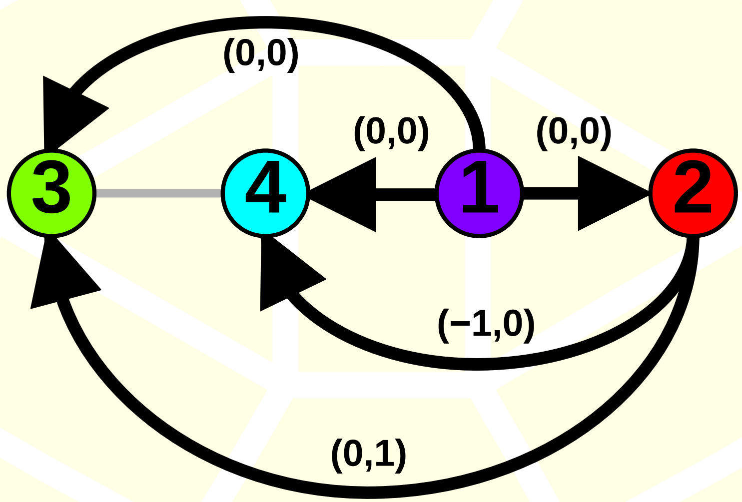

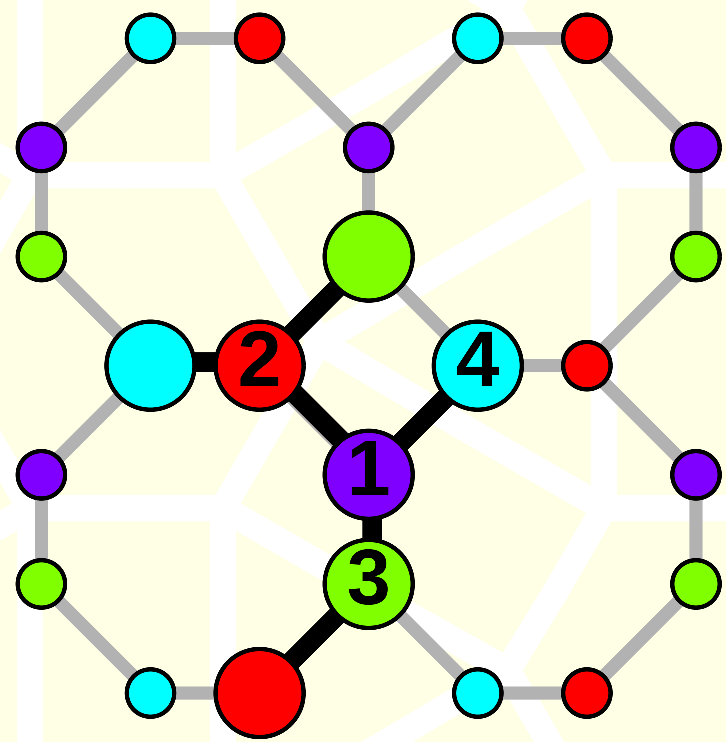

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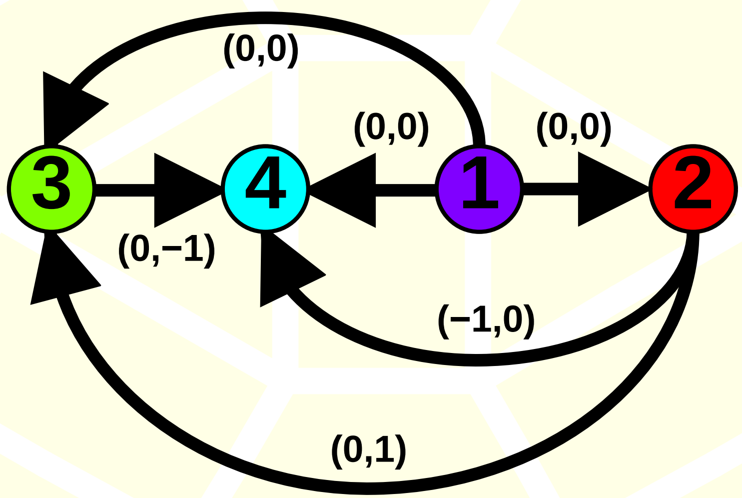

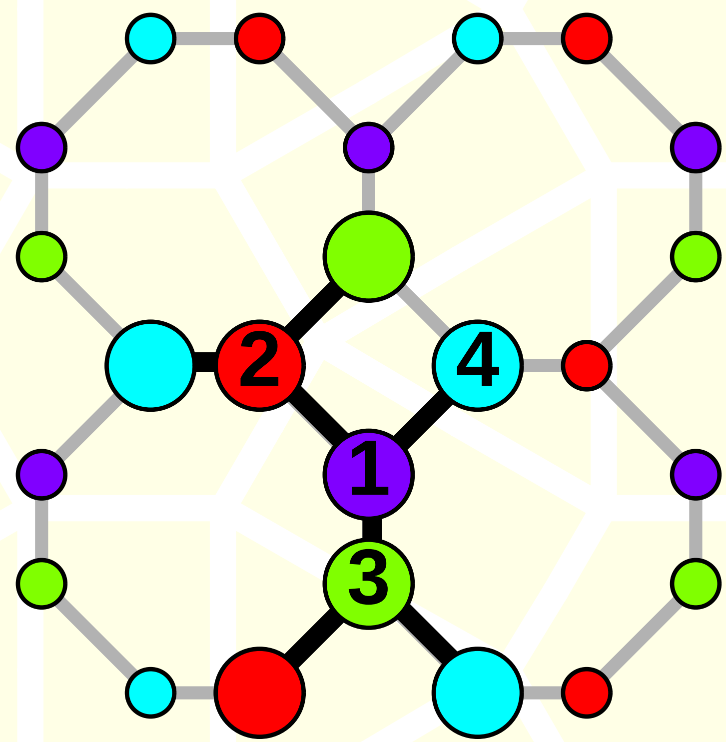

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- $\Rightarrow$ the isomorphism problem for locally stable p-graphs is in P.

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But: for non-stable p-graphs, barycentric placements might still help us reduce these problems to the finite case.

Thanks for your attention!

Software is available at

www.gavrog.org