

When is a
crystal graph
not
crystallographic?

When is a crystal graph not crystallographic?

Olaf Delgado-Friedrichs

Order!Order? — Canberra 4 Dec 2019

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Crystal nets

Crystallographic
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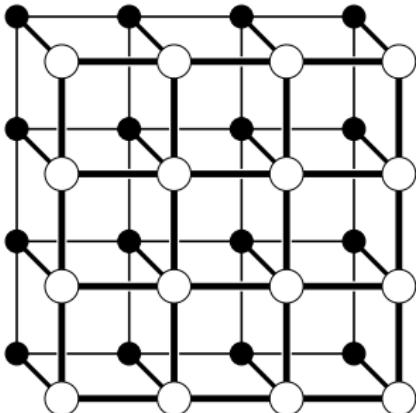
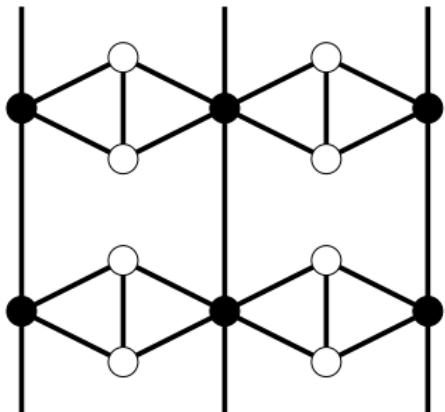
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More precisely: when its automorphism group is not a crystallographic space group.

*(Crystallographic nets and their quotient graphs,
W. E. Klee 2004.)*



A crystalline material. What might be its atomic structure?

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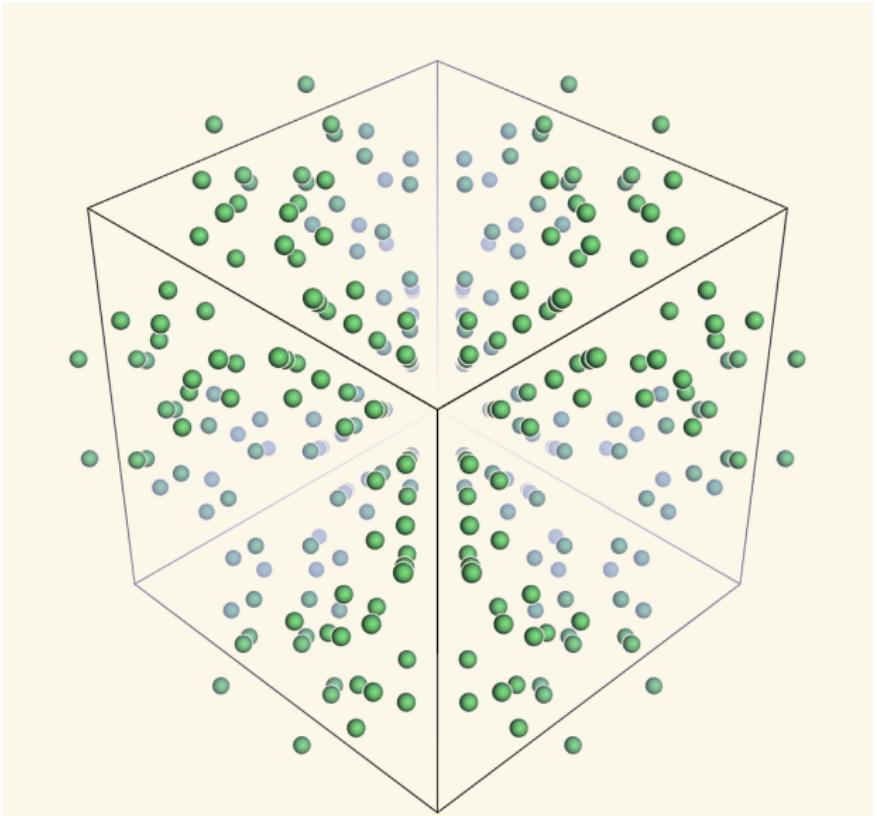
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X-ray crystallography produces something like this.

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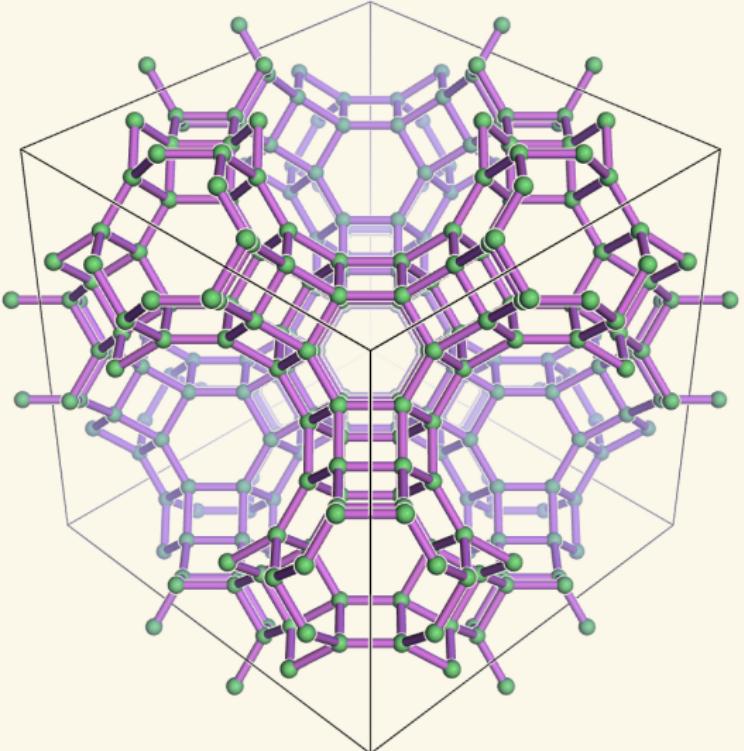
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Adding bonds (or ligands) yields a periodic graph or *net*.

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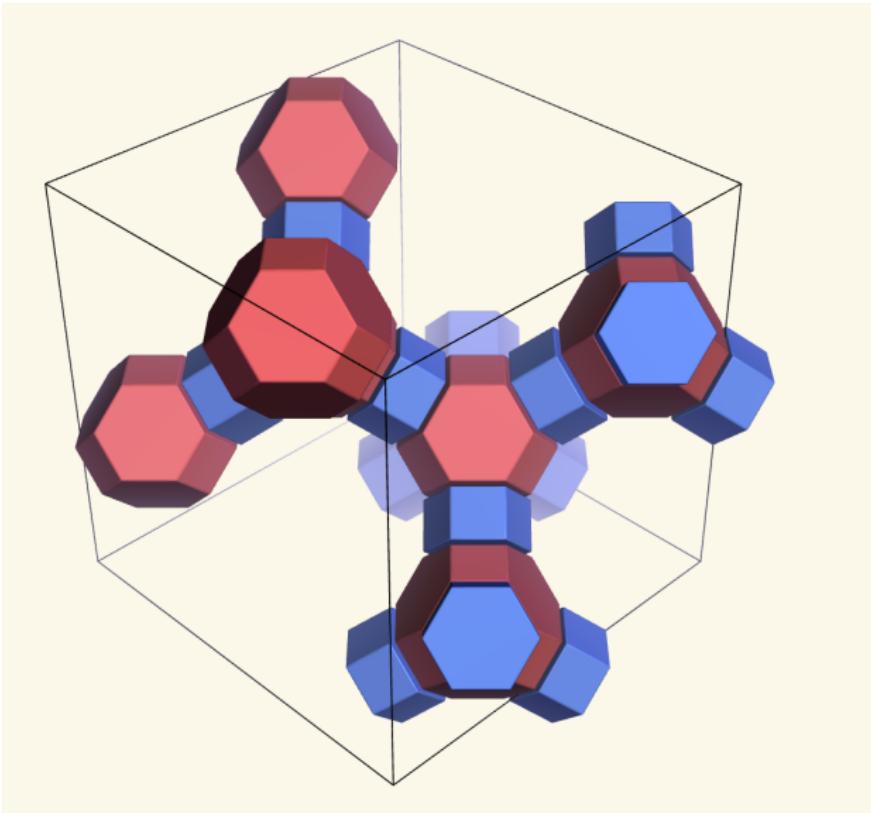
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Even richer structure from examining the cycle space.

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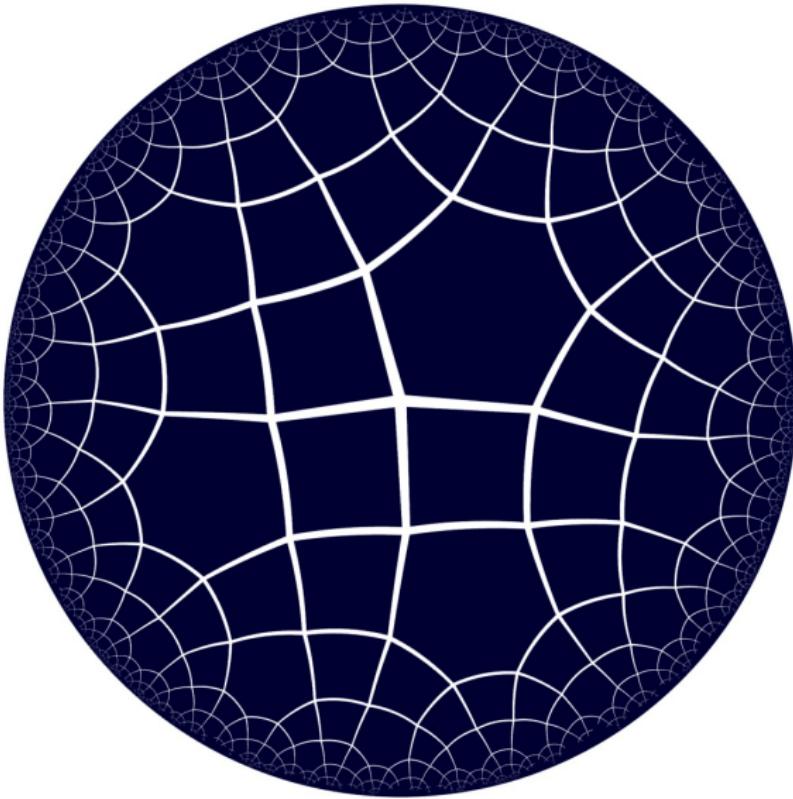
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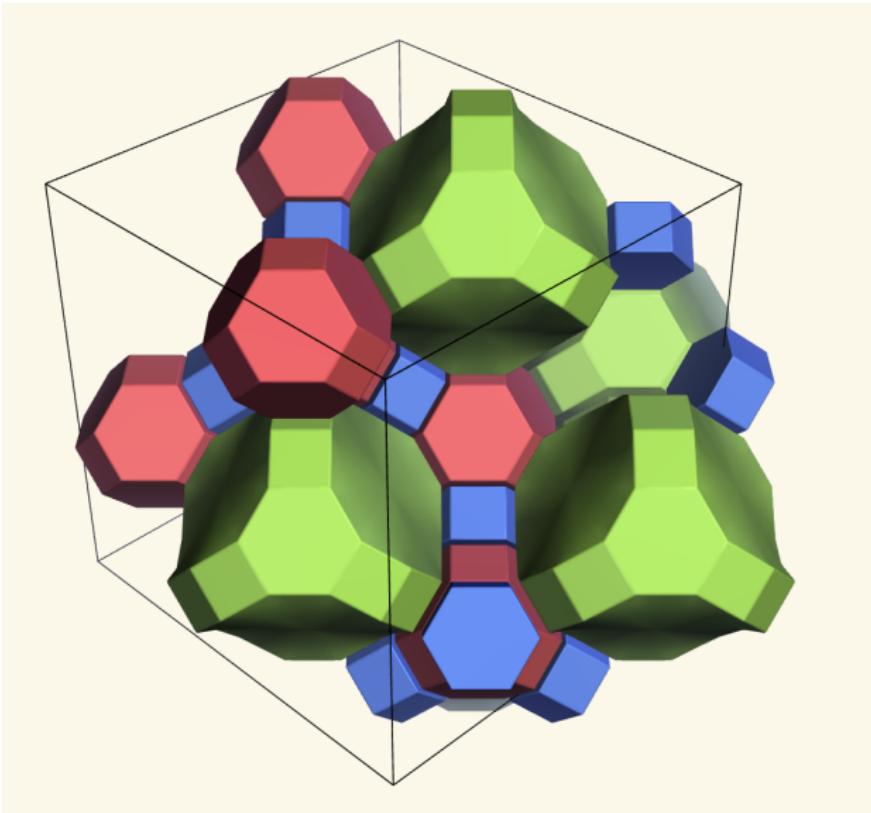
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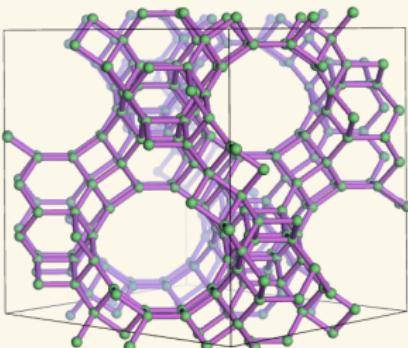
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A *net* is a (3-) connected, locally finite periodic graph.

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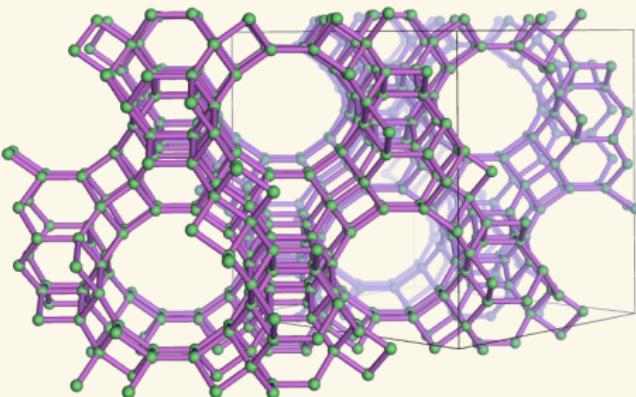
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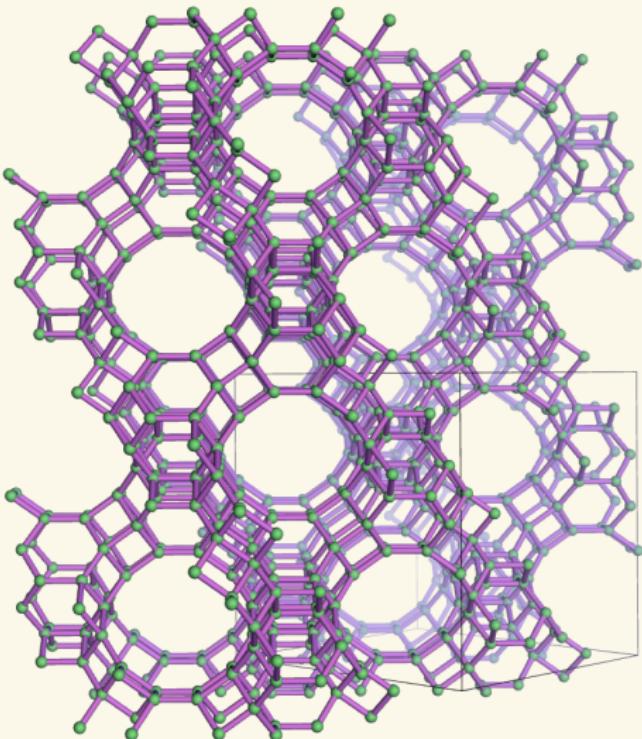
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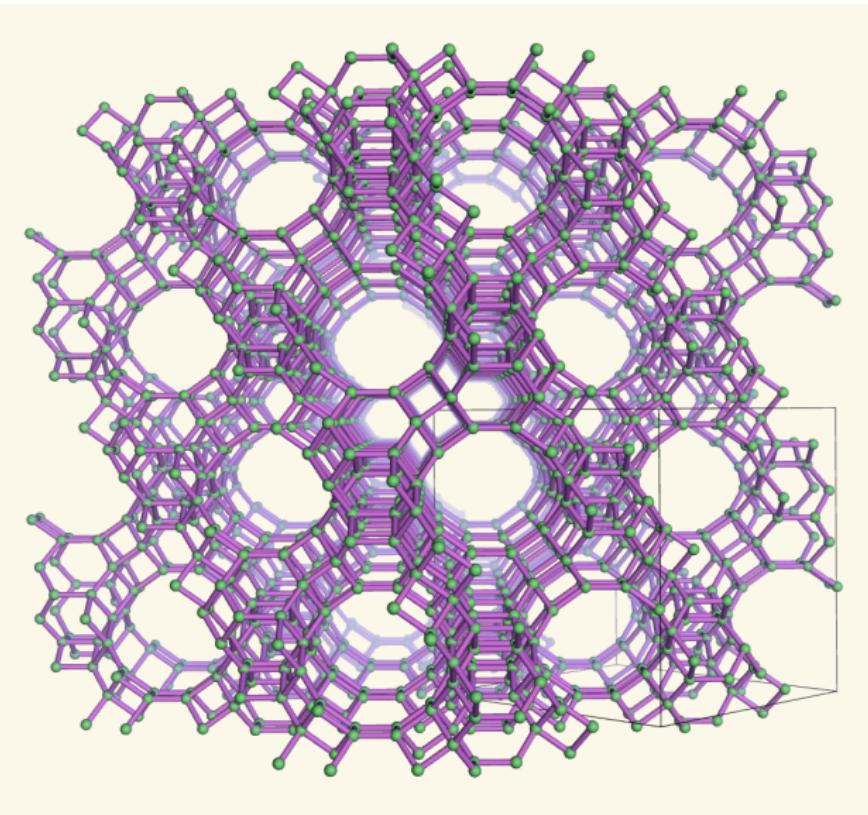
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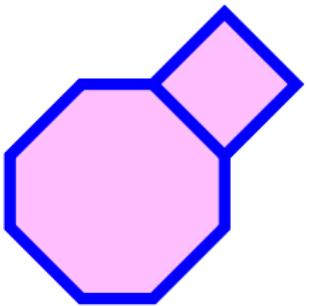
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A 2-dimensional net, which here also defines a tiling.

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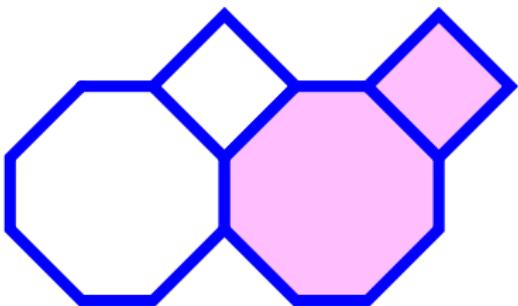
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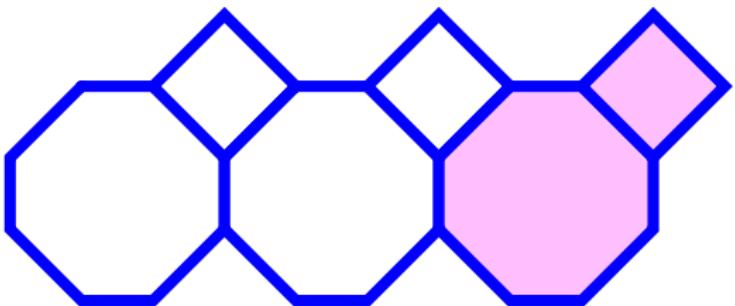
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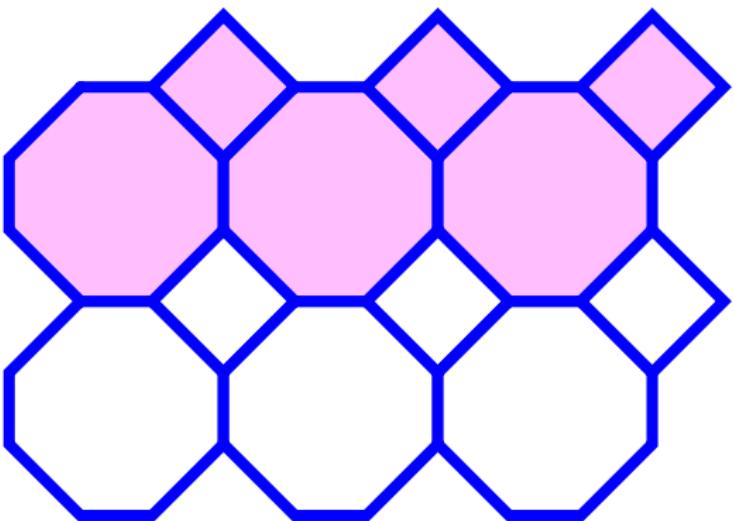
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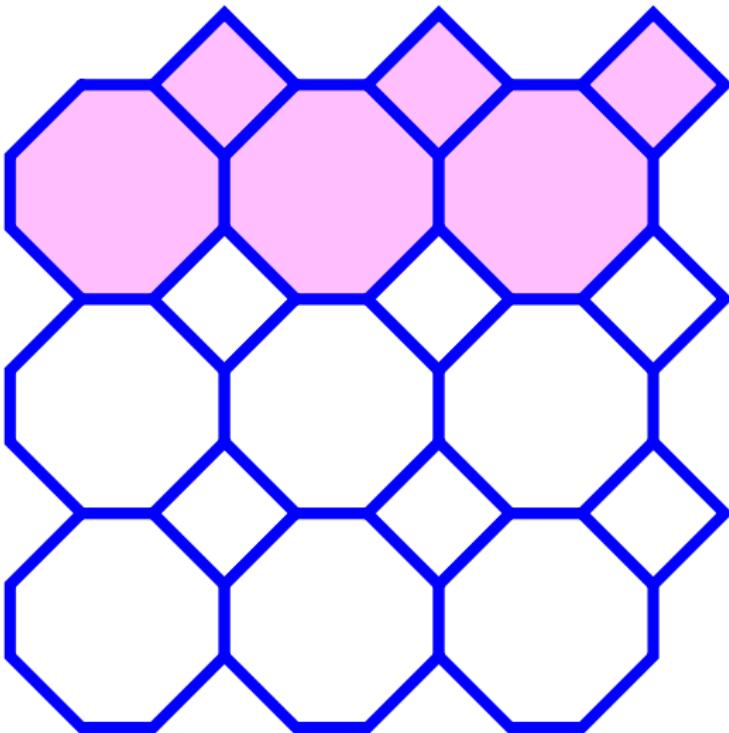
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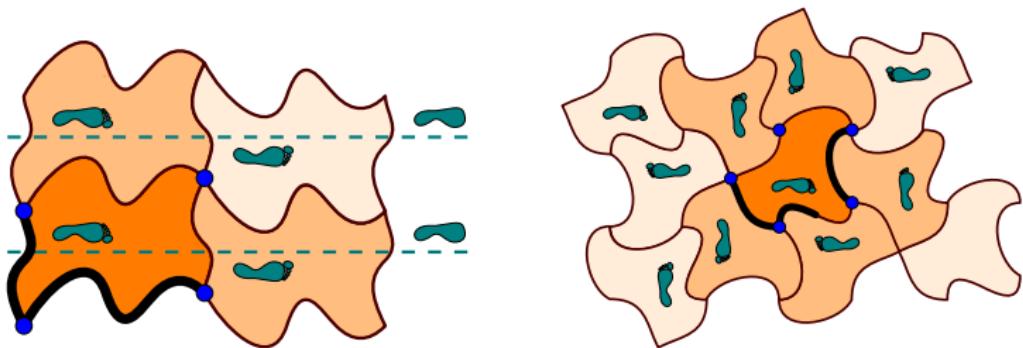
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A *crystallographic (space) group* is
a discrete group of motions in euclidean space
with a bounded fundamental domain.



Crystallographic groups are just the ones that generate
unbounded, discrete point patterns.

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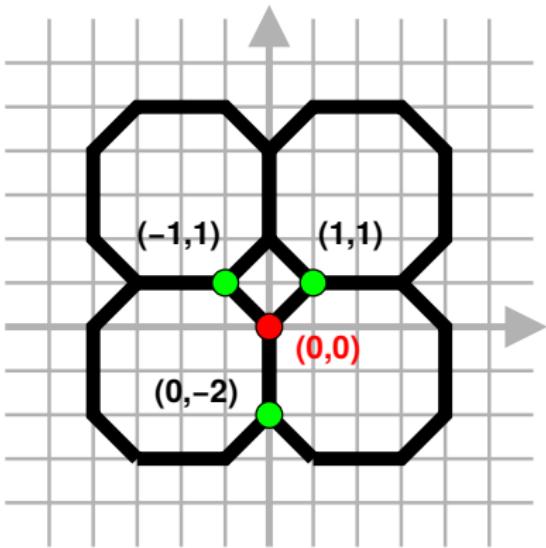
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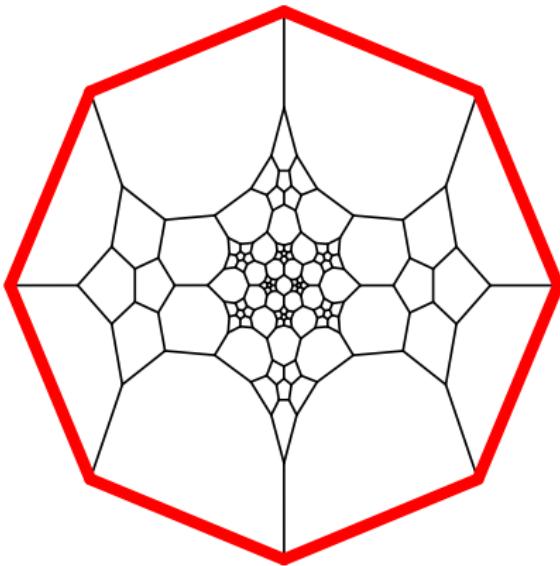


Place a vertex v in the *barycenter* of its neighbors:

$$\sum_{w \in \text{Neighbors}(v)} \text{position}(w) - \text{position}(v) = 0$$

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For polyhedral graphs, this ensures convex drawings.
(How to draw a graph, W. T. Tutte 1963.)

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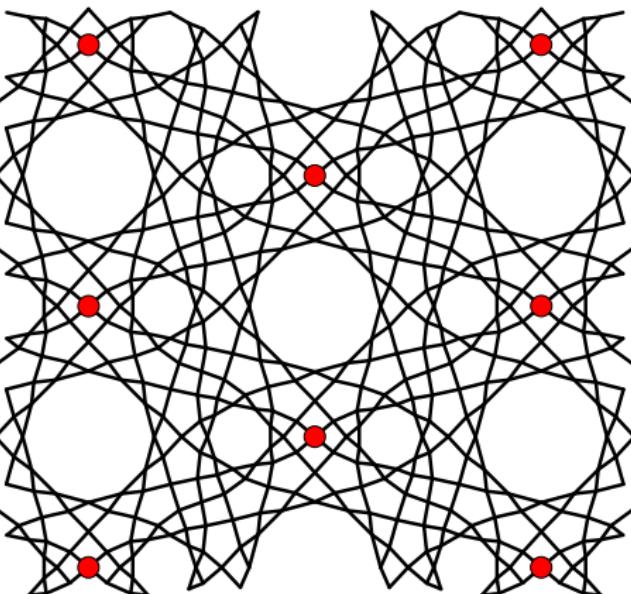
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The solution is then unique, so all periodic barycentric placements are the same up to affine transformations.

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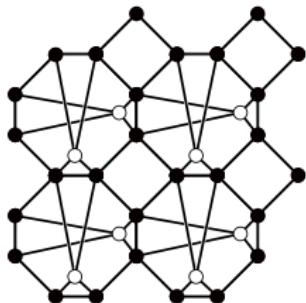
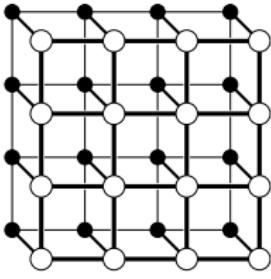
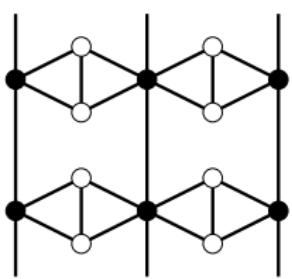
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Two non-crystallographic and one crystallographic net,
all unstable.

But can non-crystallographic nets be stable?

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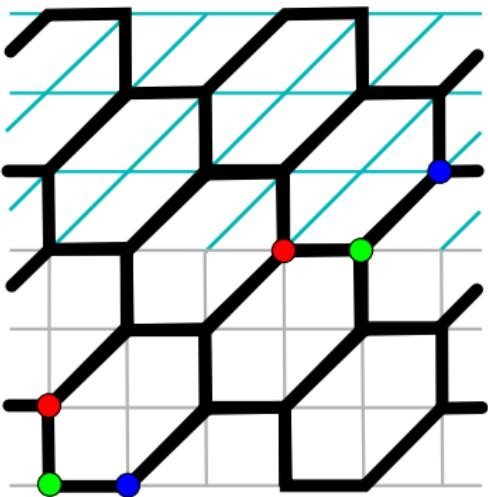
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Define affine map $\alpha_\varphi: \mathbb{R}^n \rightarrow \mathbb{R}^n$ with $\alpha_\varphi(p(v_i)) = p(\varphi(v_i))$
for just enough vertices $v_i \in V(G)$ to make it unique.

If p and $p \circ \varphi$ are periodic, then $\alpha_\varphi \circ p = p \circ \varphi$ everywhere.

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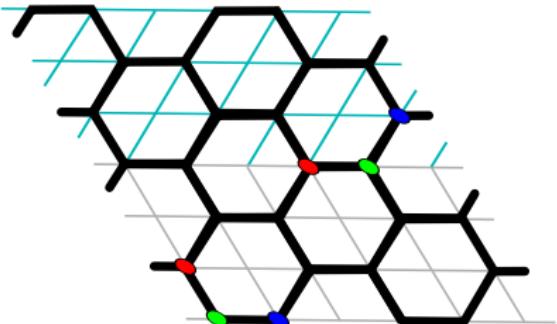
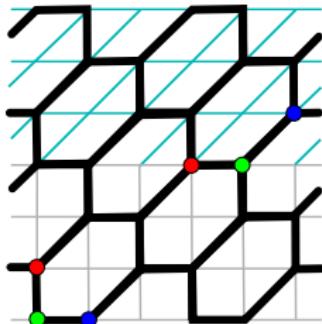
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Because we have finitely many edge lattices, there can up to translations only be finitely many such α_φ .



By a standard trick (averaging the inner product), we can turn them all into rigid motions, a.k.a. isometries.

Thus $\varphi \mapsto \alpha_\varphi$ defines a group homomorphism that maps $\text{Aut}(G)$ onto a crystallographic group.

If G is stable, the kernel must be trivial.

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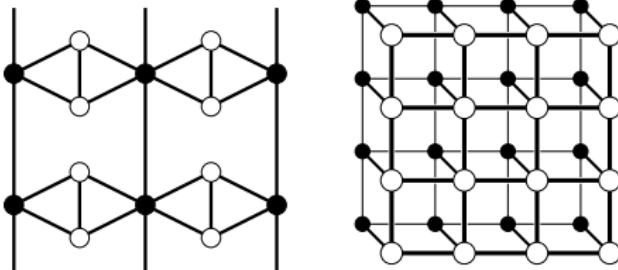
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How could p be periodic, but not $p \circ \varphi$?



For an abstract graph G , we must explicitly pick a translation group $T \leq \text{Aut}(G)$.

If G is not crystallographic, T is not unique and we can have $\varphi T \varphi^{-1} \neq T$.

But p was only constructed to be periodic with respect to T , not necessarily $\varphi T \varphi^{-1}$.

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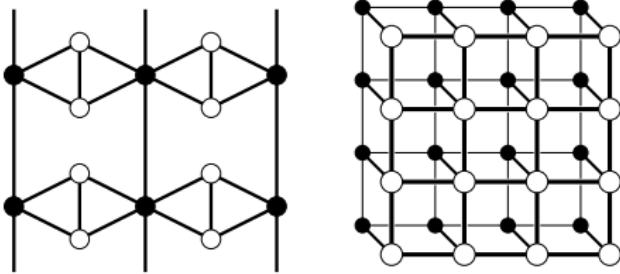
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Possible ways forward:

- Show uniqueness of barycentric placements under weaker conditions.
- Construct the homomorphism onto a crystallographic group without requiring α_φ to be a global match.
- Learn more about the structure of non-crystallographic nets (c.f. work by Eon and Moreira de Oliveira).

That's all folks!

Further reading:

Delgado-Friedrichs 2005, Moreira de Oliveira & Eon 2011, 2013, 2014, 2018

Slides:

<http://gavrog.org/order-order.pdf>

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