

When is a
crystal graph
not
crystallographic?

When is a crystal graph not crystallographic?

Olaf Delgado-Friedrichs

Too much
symmetry

Crystal nets

Crystallographic
groups

Tutte's barycentric
embedding

Unstable nets

Automorphisms to
isometries

Order!Order? — Canberra 4 Dec 2019

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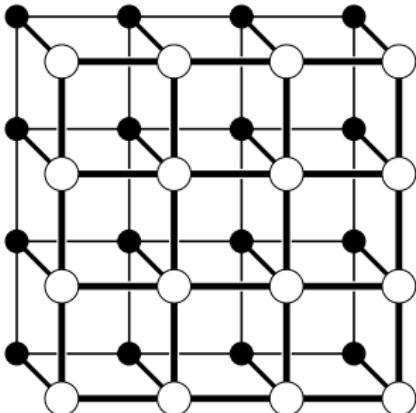
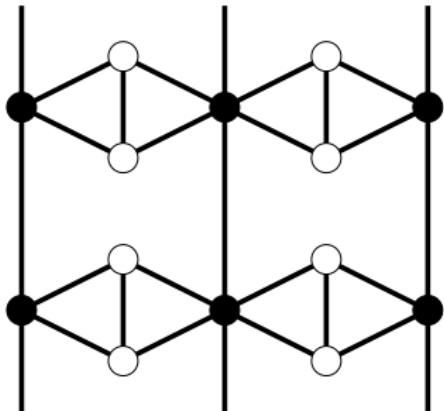
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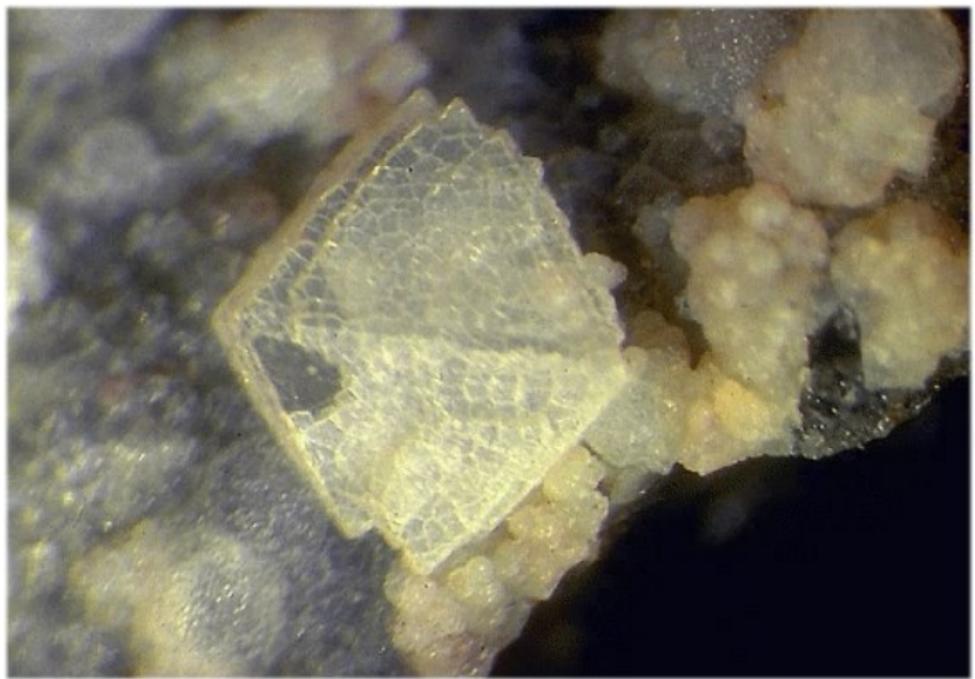
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Answer: when it has “too much symmetry”.



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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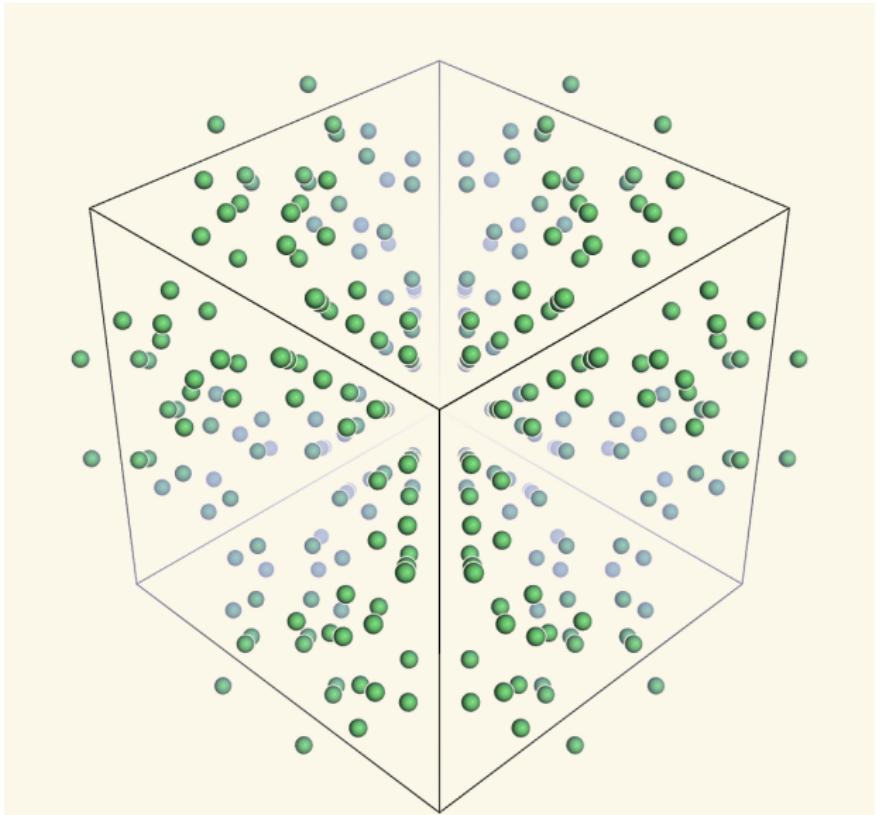
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X-ray crystallography produces something like this.

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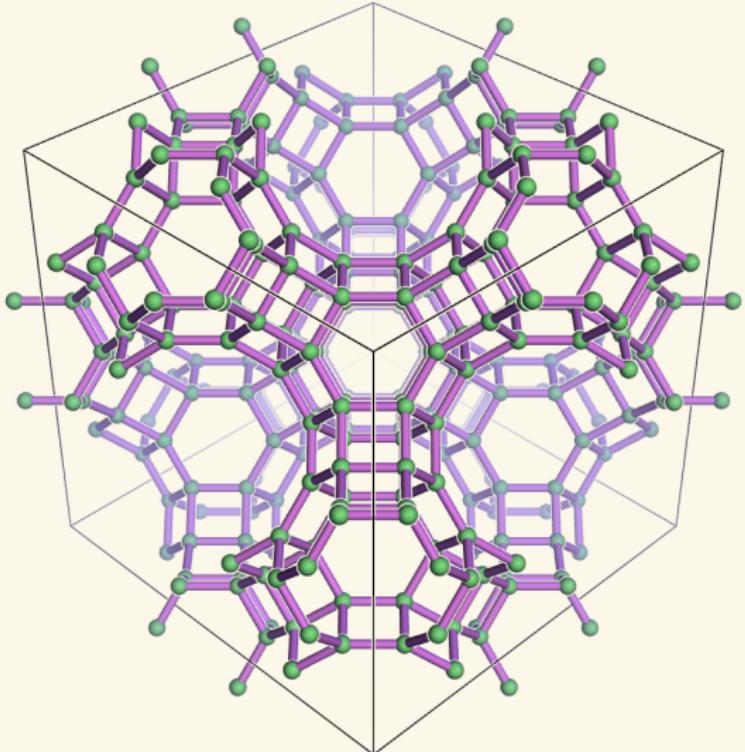
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Adding bonds (or ligands) yields a periodic graph or *net*.

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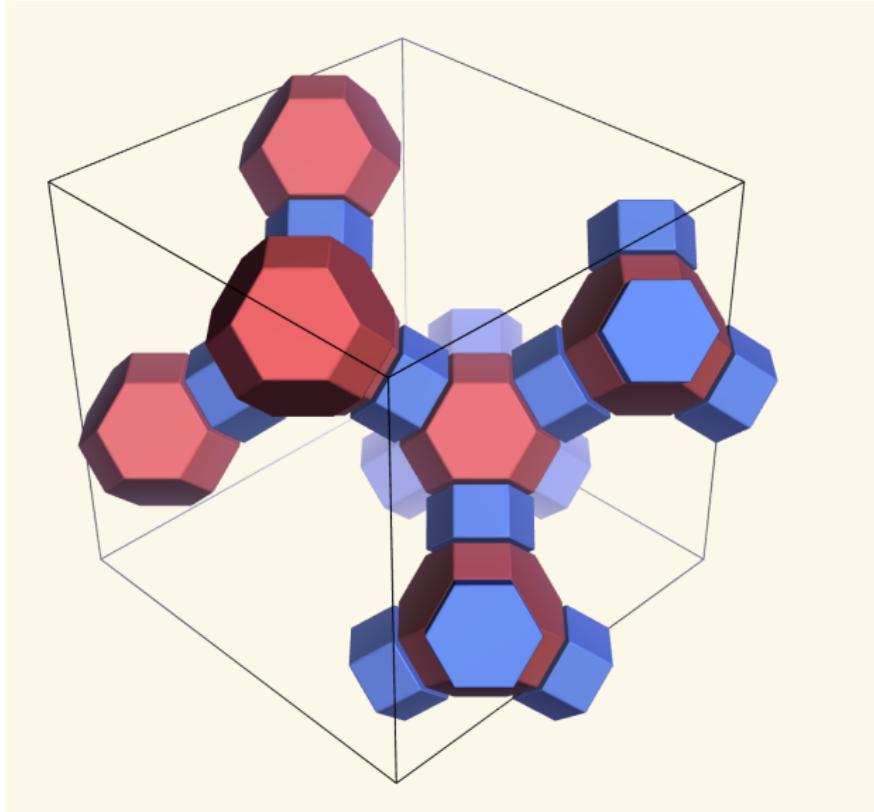
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Even richer structure from examining the cycle space.

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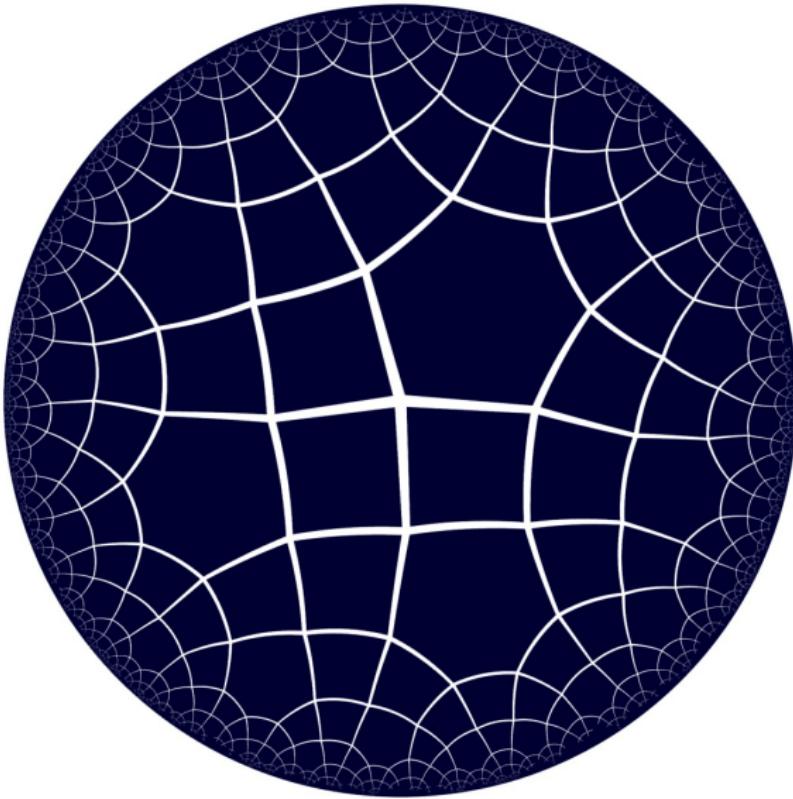
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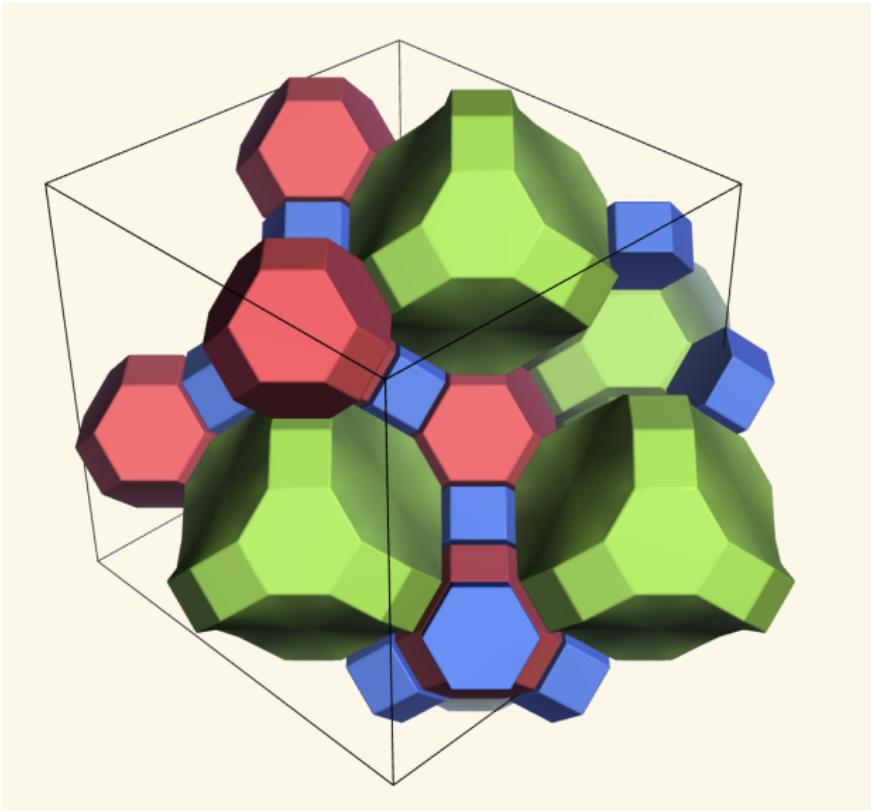
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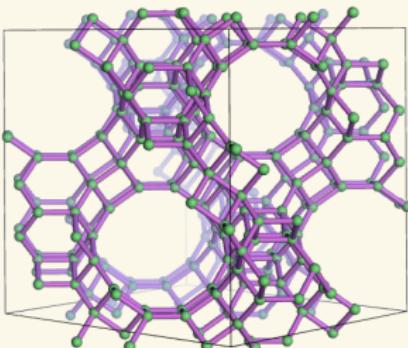
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A *net* is a (3-) connected, locally finite periodic graph.

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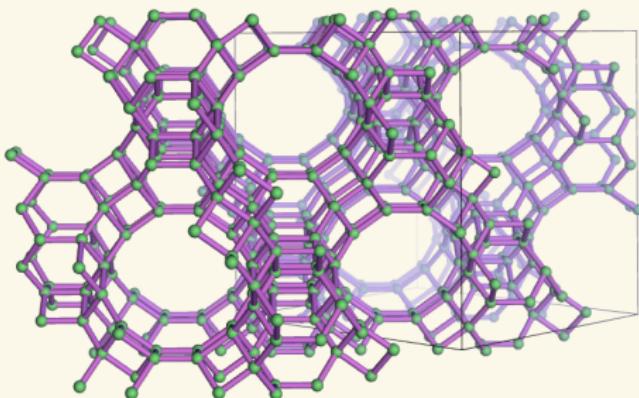
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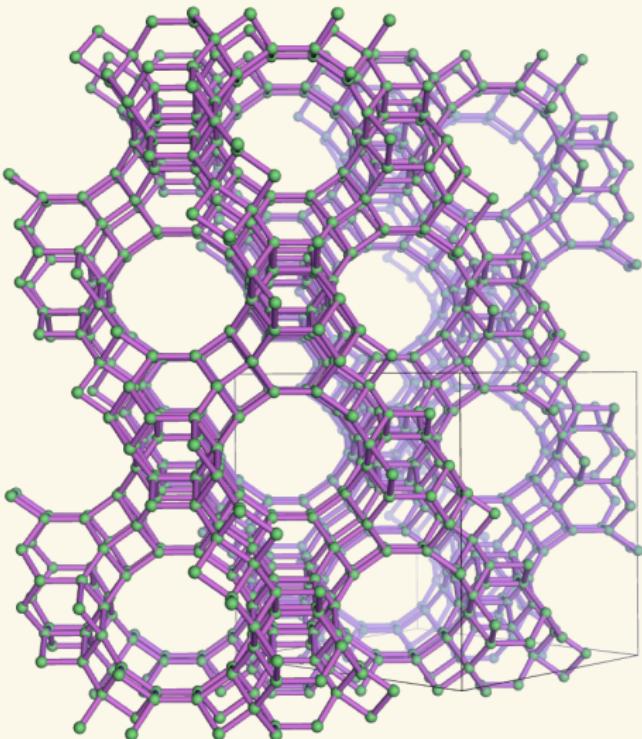
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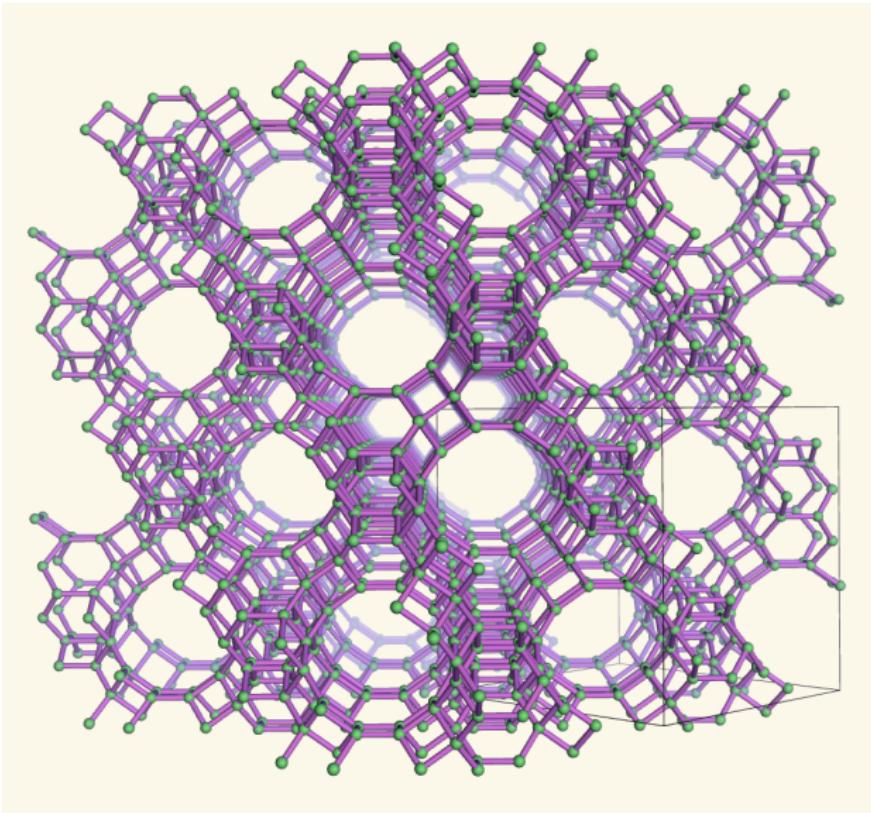
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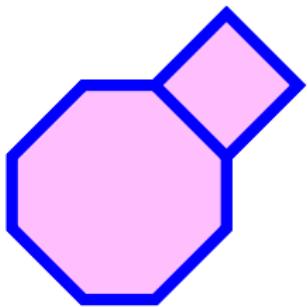
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A 2-dimensional net, which here also defines a tiling.

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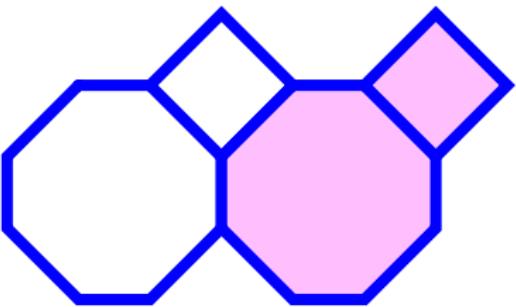
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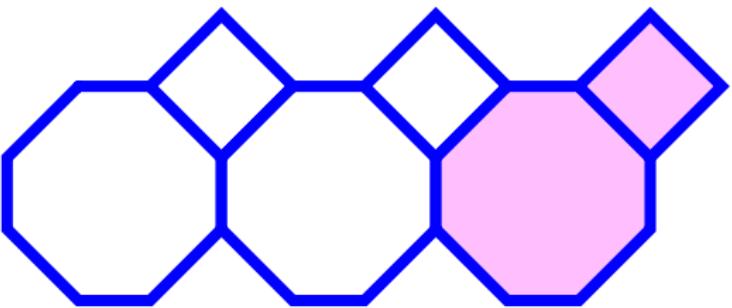
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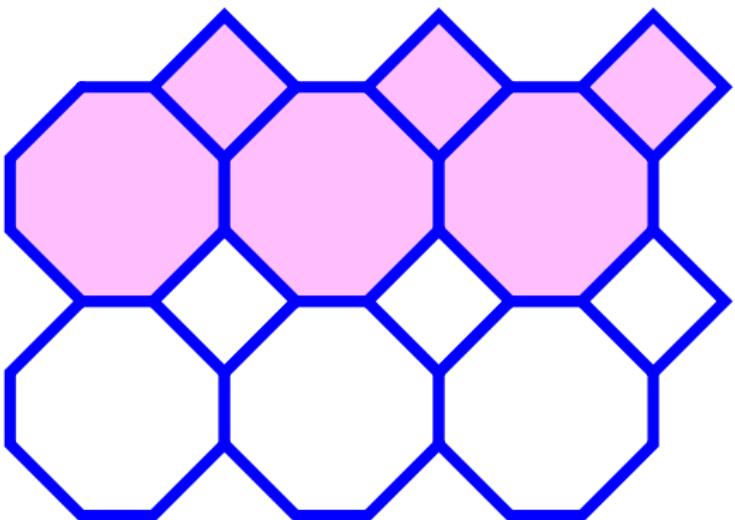
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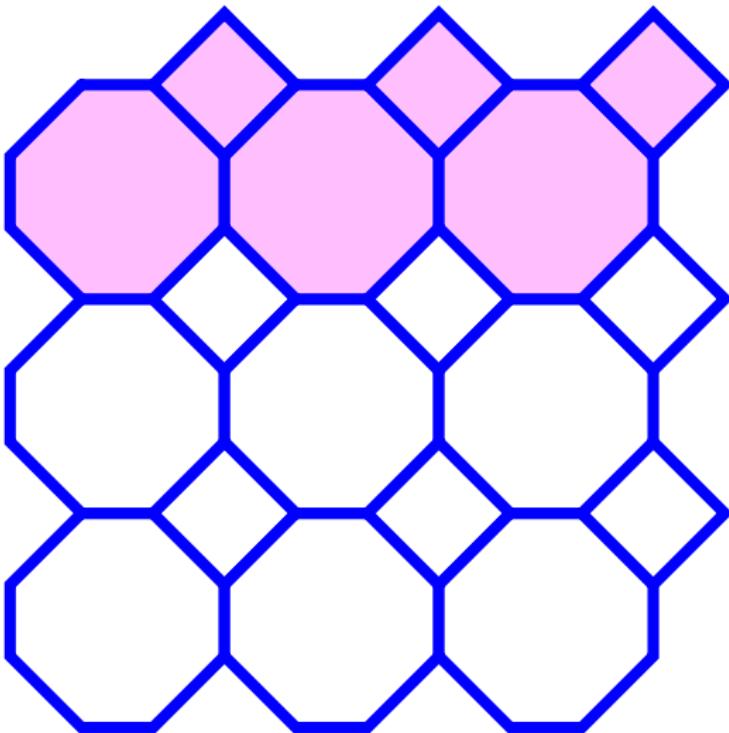
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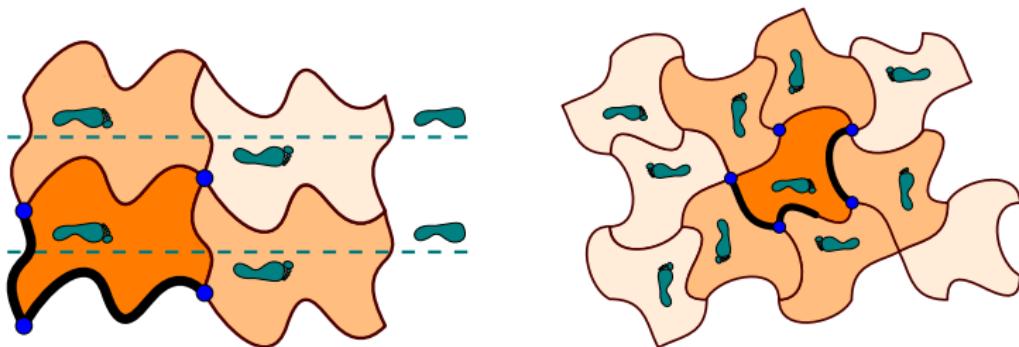
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Crystallographic groups are just the ones that generate
unbounded, discrete point patterns.

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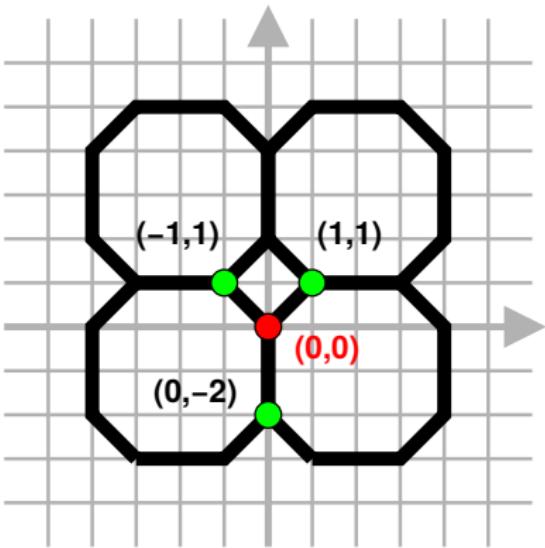
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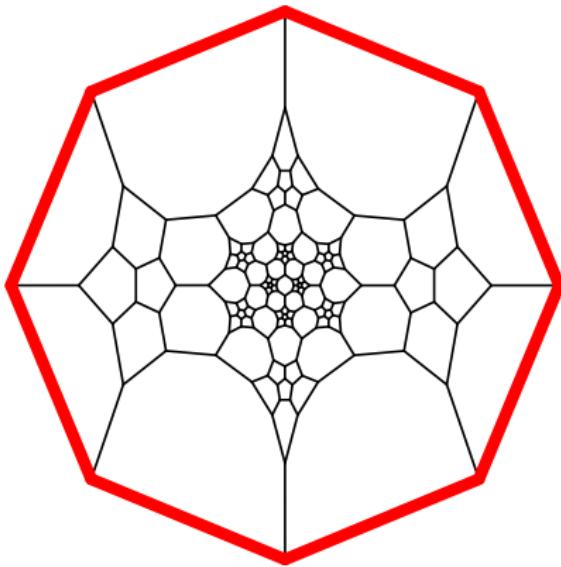


Place a vertex v in the *barycenter* of its neighbors:

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

For finite graphs, prescribe a convex outer face.

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

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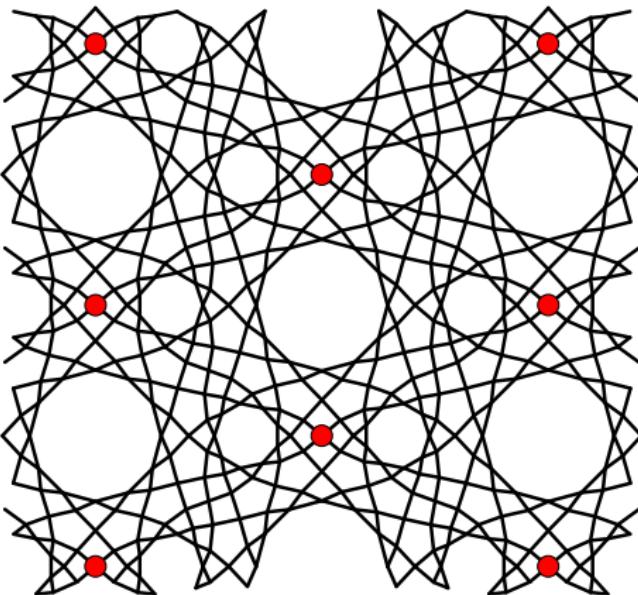
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The solution is then unique, so all periodic barycentric placements are the same up to affine transformations.

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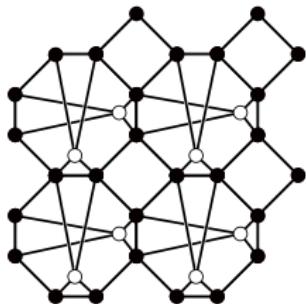
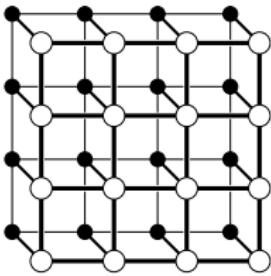
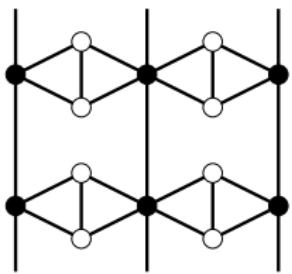
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An *unstable* net is one with
colliding barycentric vertex positions.



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

But can non-crystallographic nets be stable?

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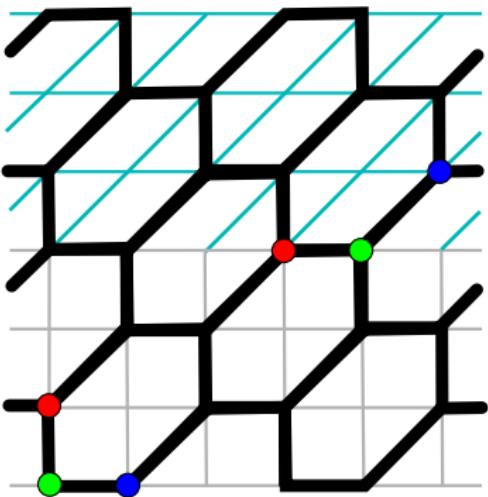
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Define $\alpha_\varphi: \mathbb{R}^n \rightarrow \mathbb{R}^n$ affine with $\alpha_\varphi(p(v_i)) = p(\varphi(v_i))$ for just enough vertices $v_i \in V(G)$ to make it unique.

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

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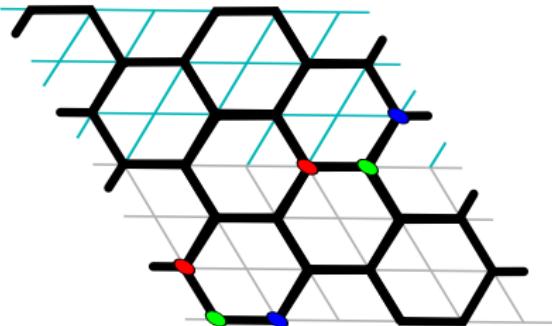
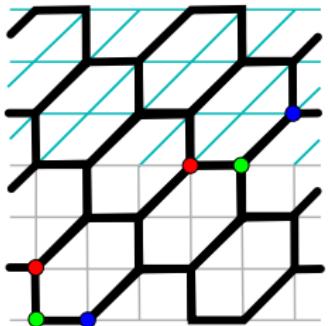
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Because we have finitely many edge lattices, there can up to translations only be finitely many such α_φ .



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.