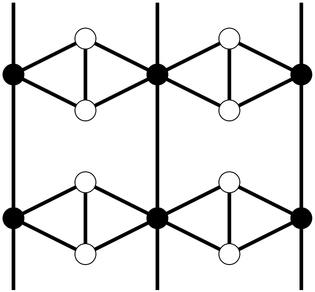
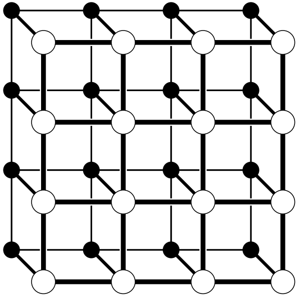
When is a crystal graph not crystallographic?

Olaf Delgado-Friedrichs

Order!Order? — Canberra 4 Dec 2019

Answer: when it has “too much symmetry”.

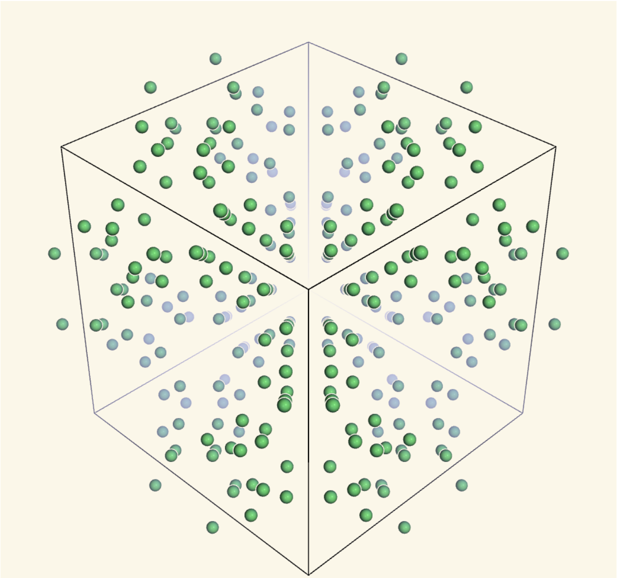




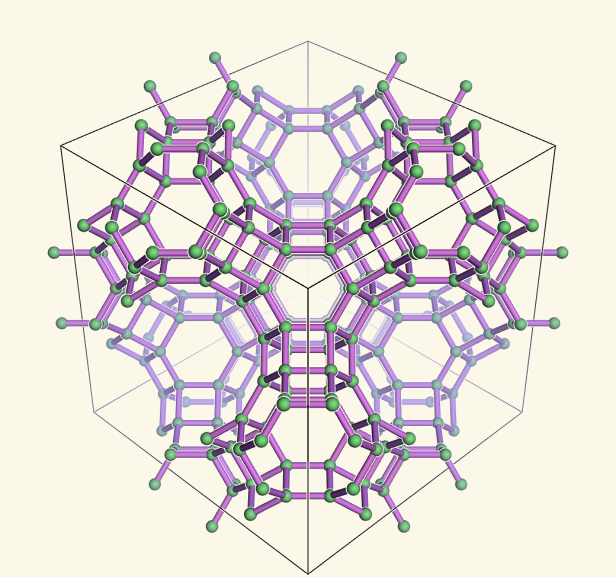
More precisely: when its automorphism group is not a crystallographic space group.

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

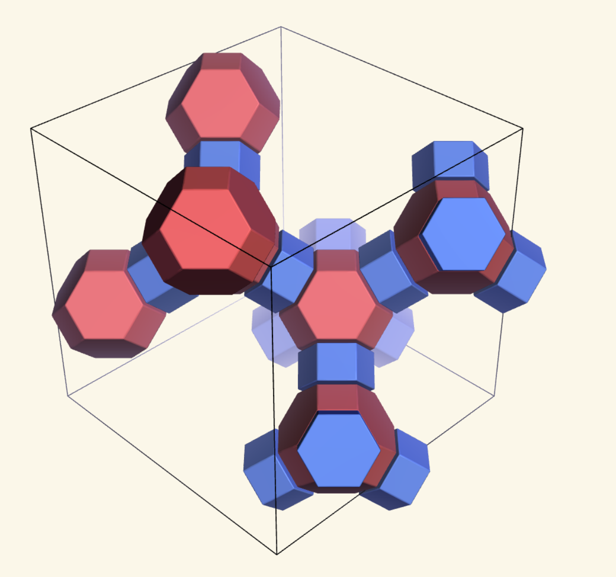
A crystalline material. What might be its atomic structure?



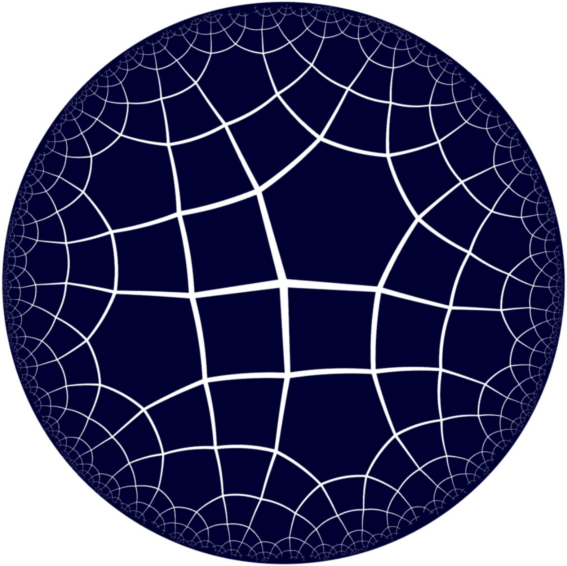
X-ray crystallography produces something like this.



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



Even richer structure from examining the cycle space.



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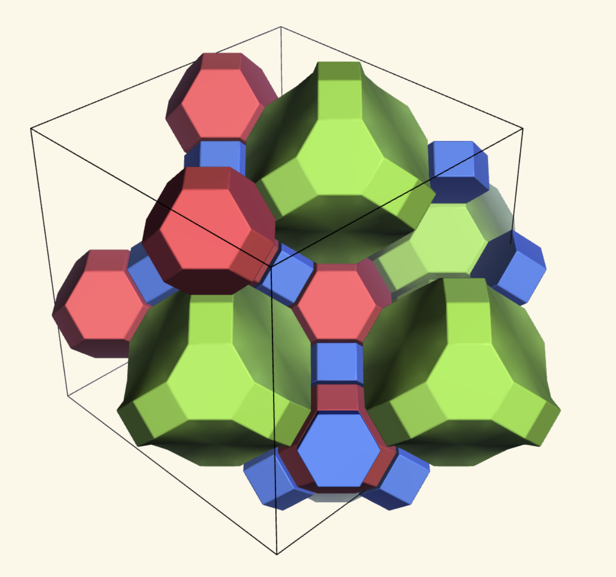

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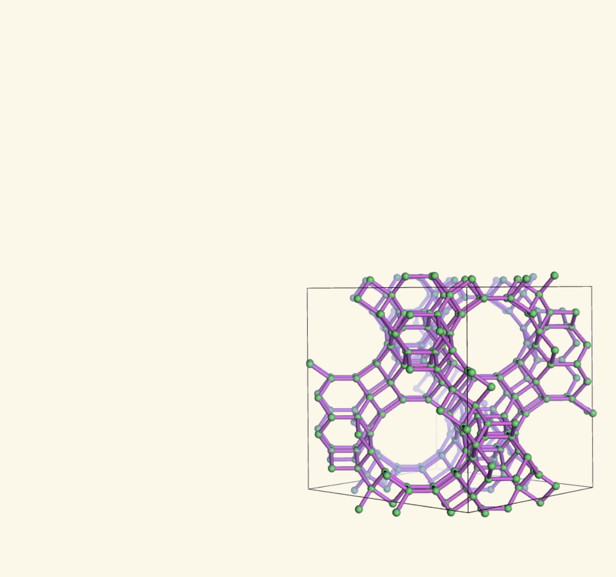
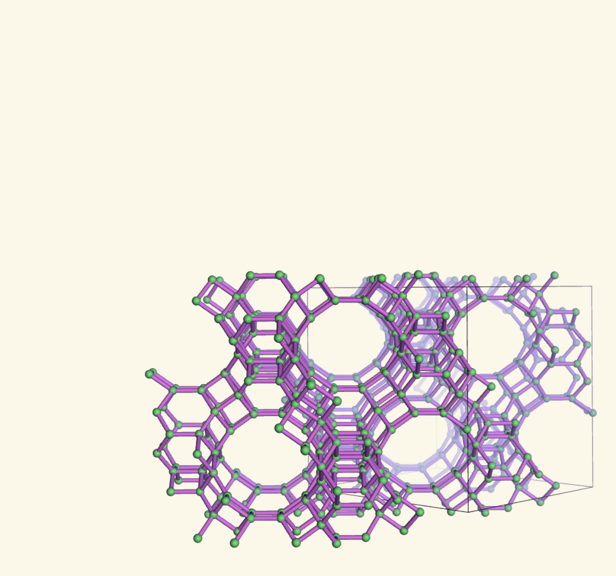


A *net* is a (3-) connected, locally finite periodic graph.



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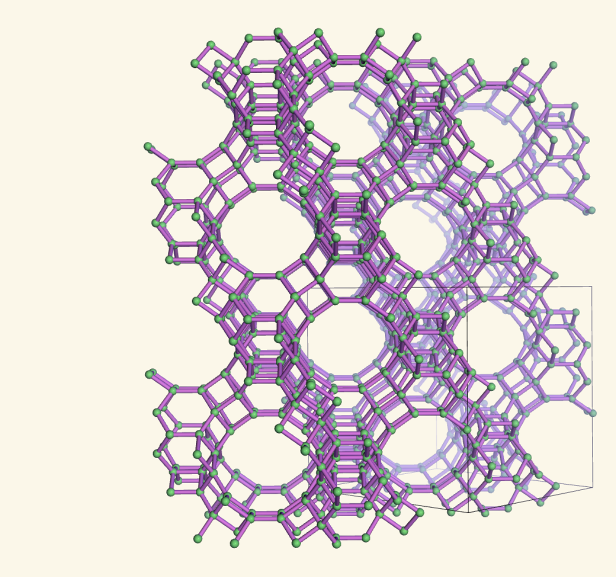

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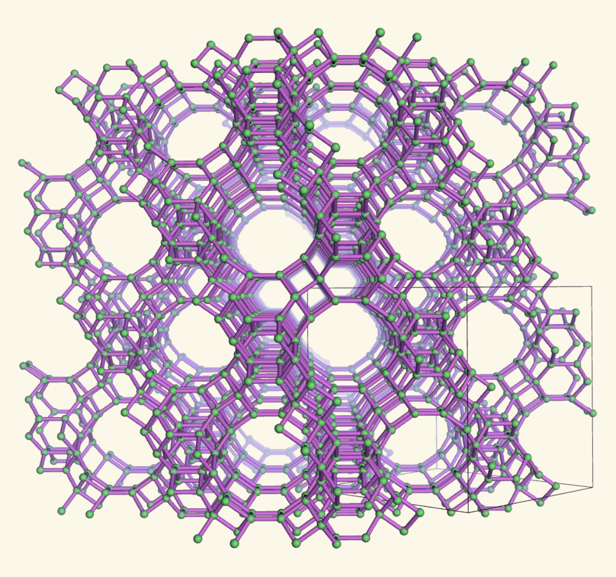

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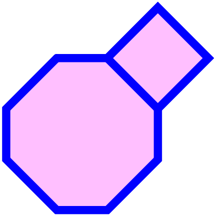
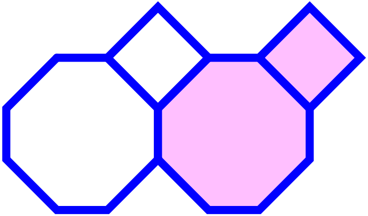


A 2-dimensional net, which here also defines a tiling.



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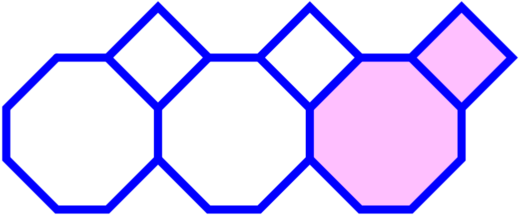

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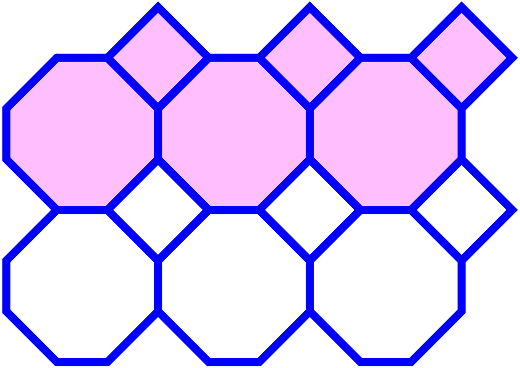

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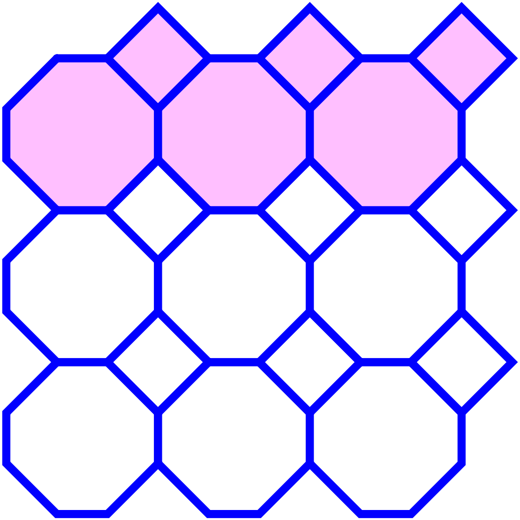
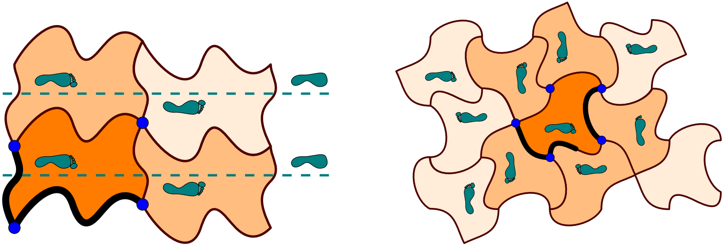


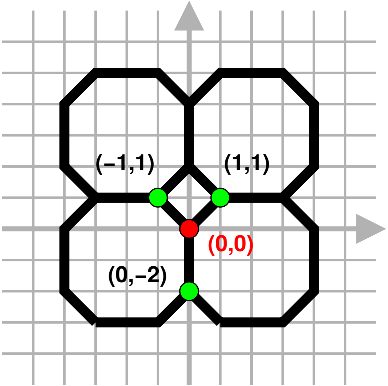
A 2-dimensional net, which here also defines a tiling.

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.

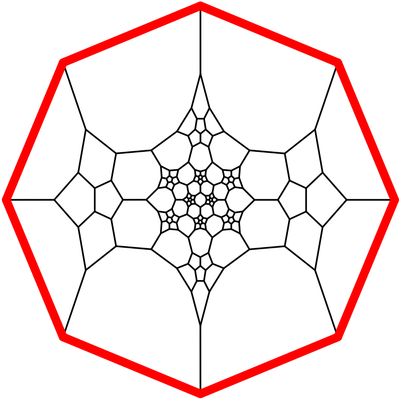
Tutte's idea for drawing graphs "nicely":



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

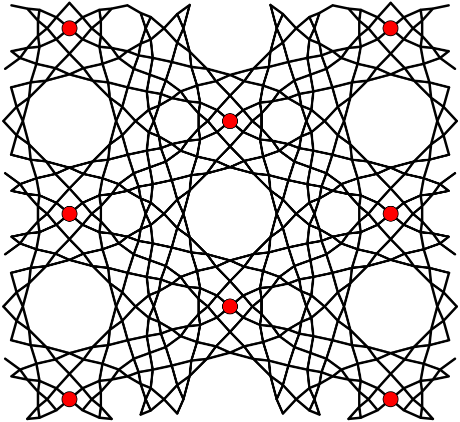
$$\sum_{w \in Neighbors(v)} position(w) - position(v) = 0$$

For finite graphs, prescribe a convex outer face.



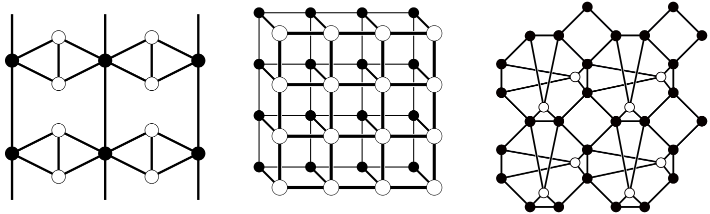
For polyhedral graphs, this ensures convex drawings.
(*How to draw a graph,* W. T. Tutte 1963.)

For periodic graphs, prescribe a vertex lattice.



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

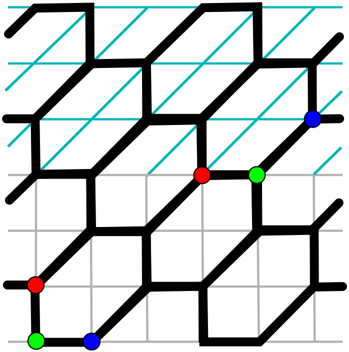
An *unstable* net is one with colliding barycentric vertex positions.



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

But can non-crystallographic nets be stable?

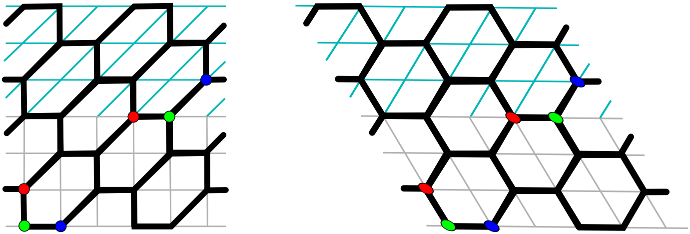
If $p\colon G \to \mathbb{R}^n$ is barycentric and $\varphi\colon G \to G$ an automorphism, then $p \circ \varphi$ is also barycentric.



Define $\alpha_\varphi\colon \mathbb{R}^n \to \mathbb{R}^n$ 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.

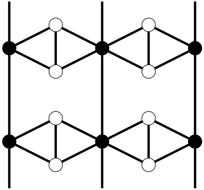
Because we have finitely many edge lattices, there can up to translations only be finitely many such α_φ.

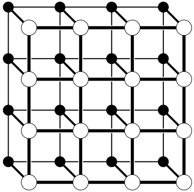


By a standard trick (averaging the inner product), we can turn them all into rigid motions, a.k.a. isometries.

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

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





For an abstract graph G, we have to explicitly pick a translation group $T \leq \mathrm{Aut}(G)$. If G is not crystallographic, T is not unique and we can have $\varphi T \varphi^{-1} \neq T$.

If we can show that α_φ can be defined on some vertex sublattice with respect to T, everything is good.

How can we exclude rogue automorphisms that mess up all the sublattices, no matter how large?