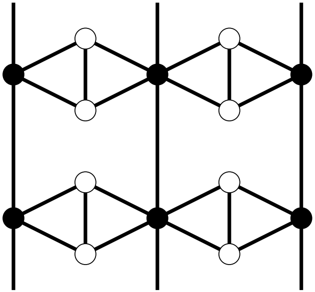
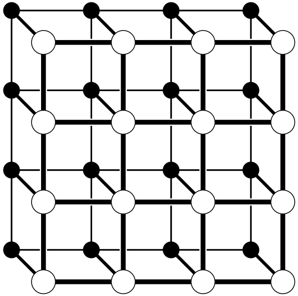
When is a crystal graph not crystallographic?

Olaf Delgado-Friedrichs

Order!Order? — Canberra 4 Dec 2019

Answer: when it has “too much symmetry”.

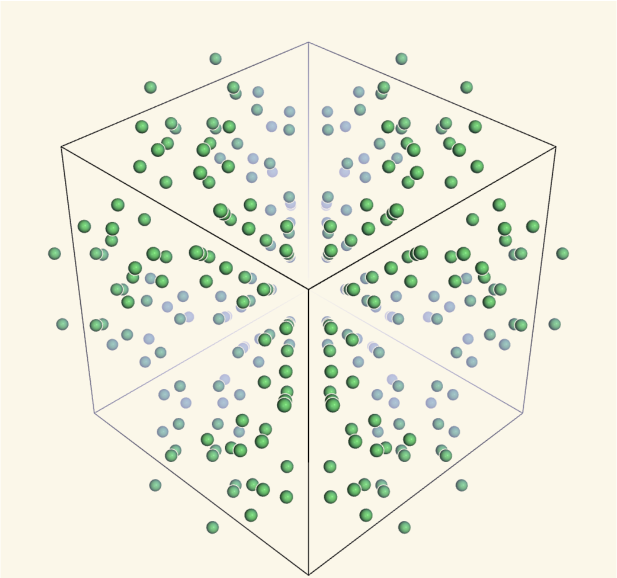




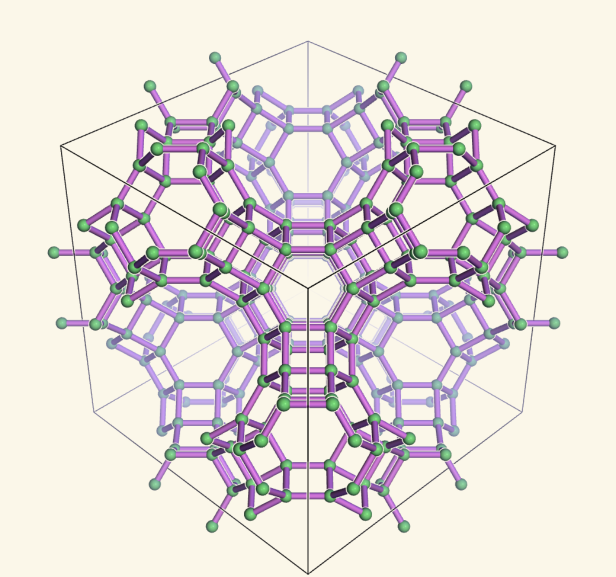
More precisely: when its automorphism group is not a crystallographic space group.

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

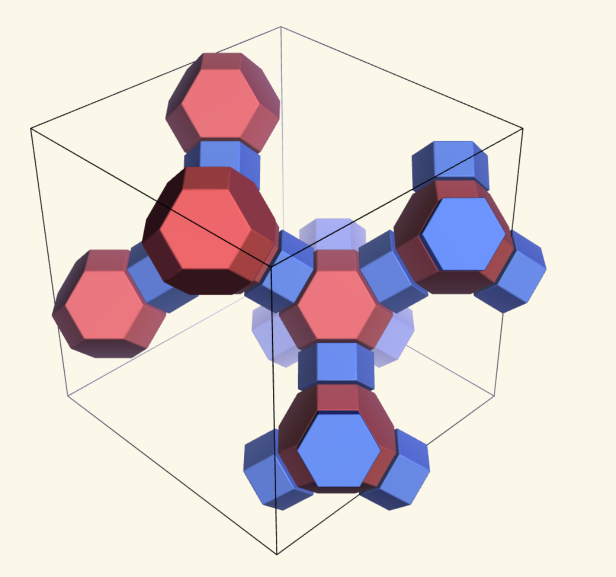
A crystalline material. What might be its atomic structure?



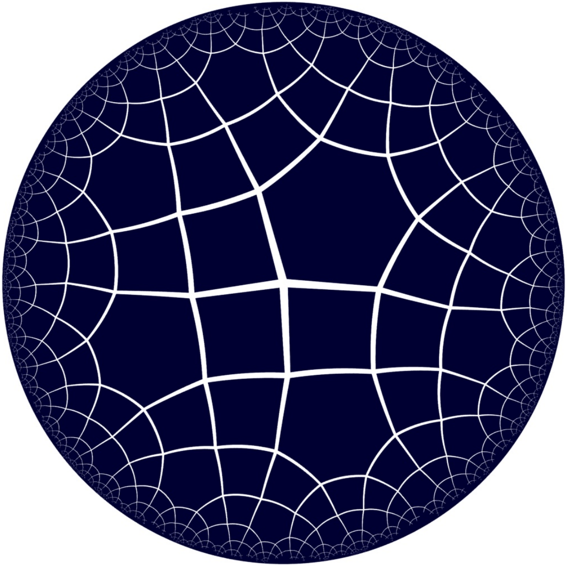
X-ray crystallography produces something like this.



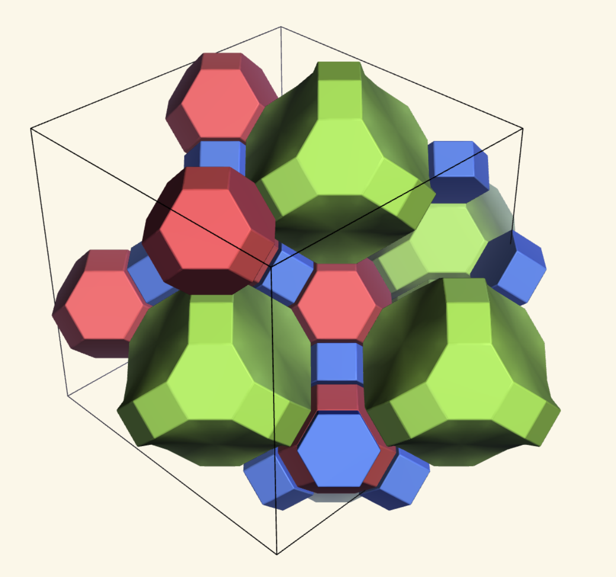
Adding bonds (or ligands) yields a periodic graph or *net*.



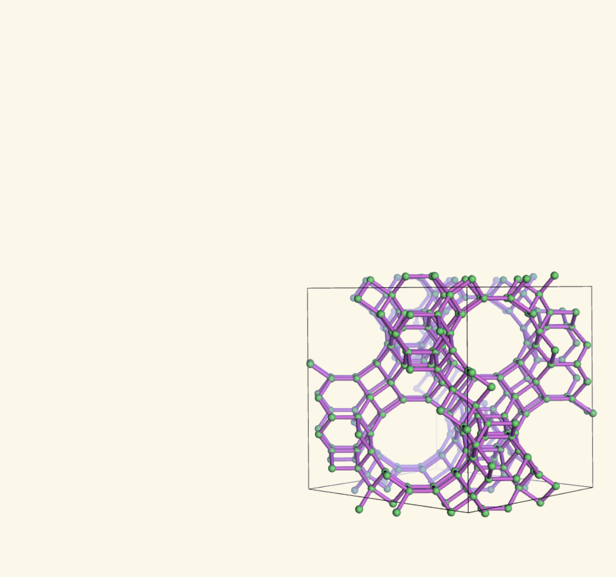
We can discover further structure in this graph . . .



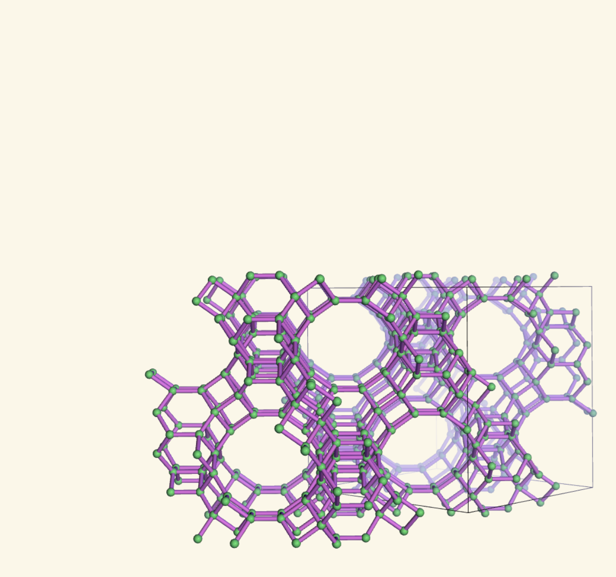
... which could lead us into the hyperbolic plane ...



…or towards a complete partitioning of space.



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



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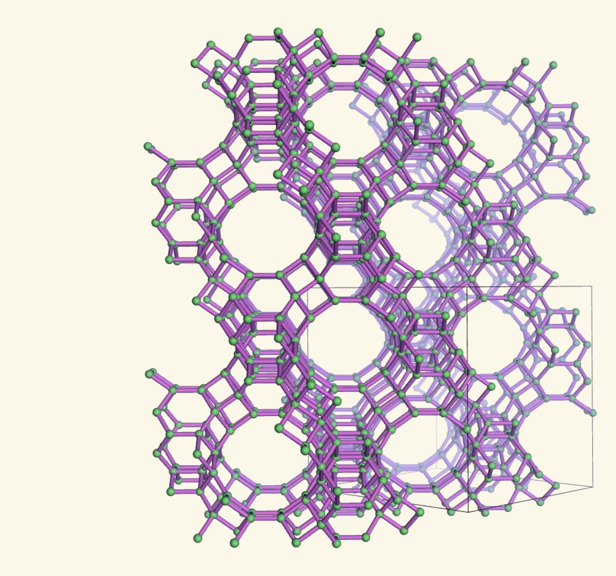

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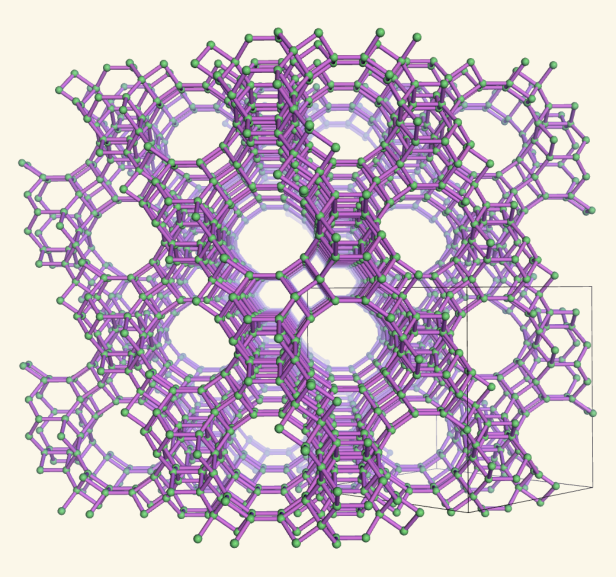

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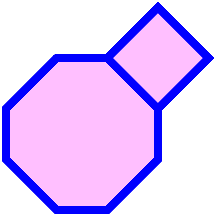
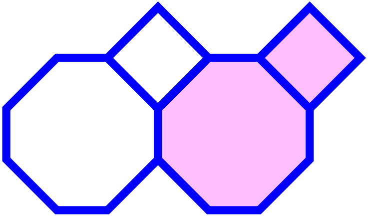


A 2-dimensional net, which happens to be planar.



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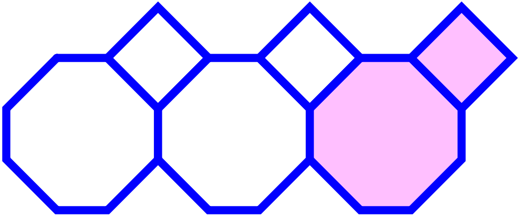

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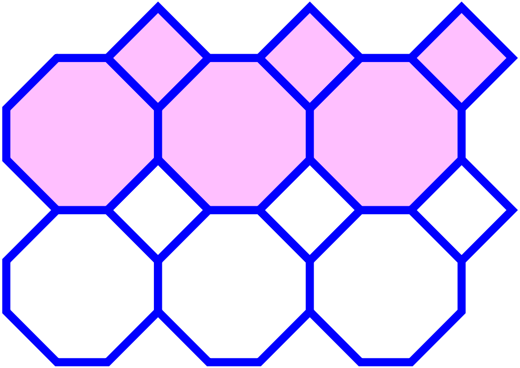

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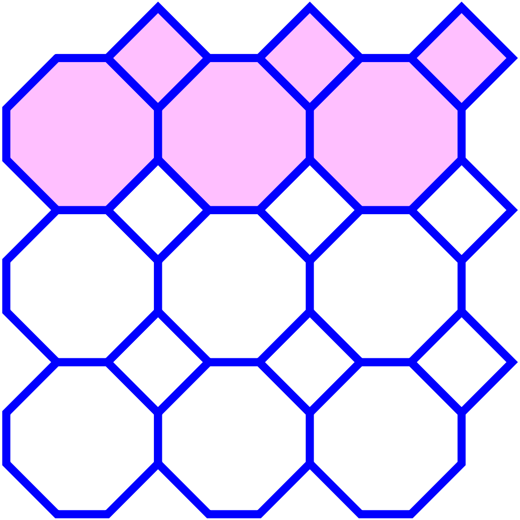
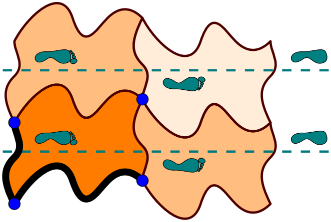
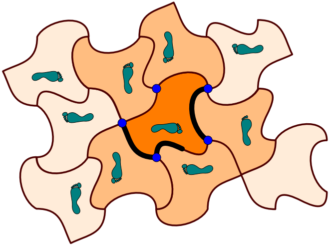


A 2-dimensional net, which happens to be planar.

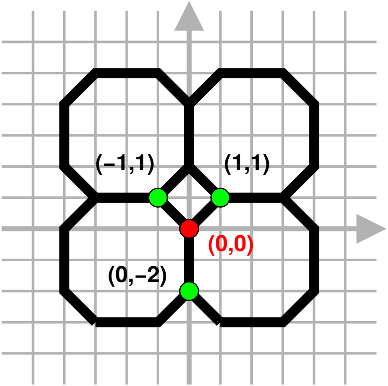
A *crystallographic (space) group* is
a discrete group of motions in euclidean space
with a bounded fundamental domain.





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

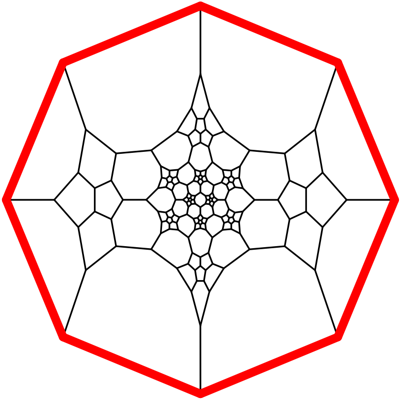
Tutte's idea for drawing graphs "nicely":



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

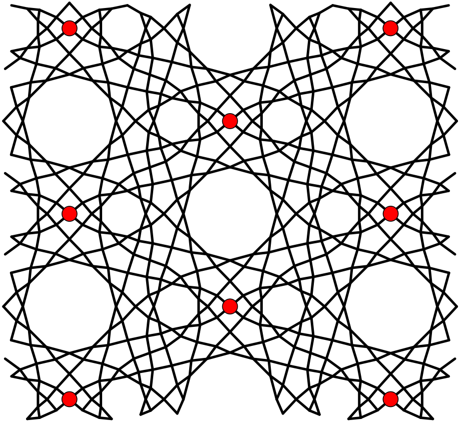
$$\sum_{w \in Neighbors(v)} position(w) - position(v) = 0$$

For finite graphs, prescribe a convex outer face.



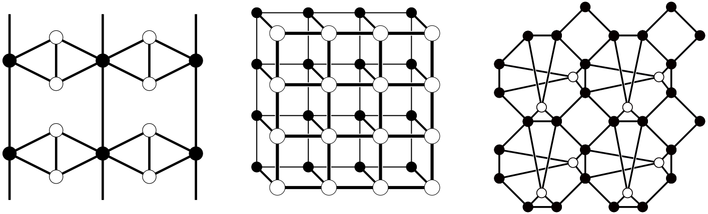
For polyhedral graphs, this ensures convex drawings.
(*How to draw a graph,* W. T. Tutte 1963.)

For periodic graphs, prescribe a vertex lattice.



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

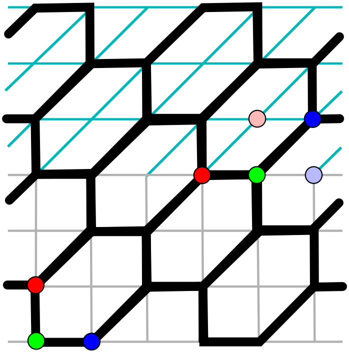
An *unstable* net is one with colliding barycentric vertex positions.



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

But can non-crystallographic nets be stable?

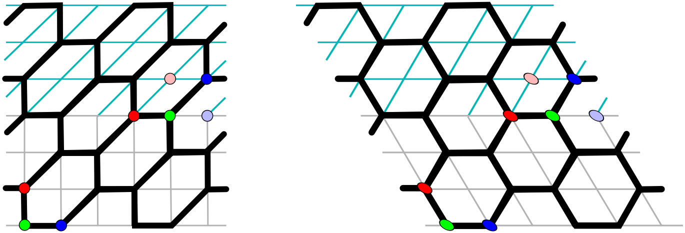
If $p\colon G \to \mathbb{R}^n$ is barycentric and $\varphi\colon G \to G$ an automorphism, then $p \circ \varphi$ is also barycentric.



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

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

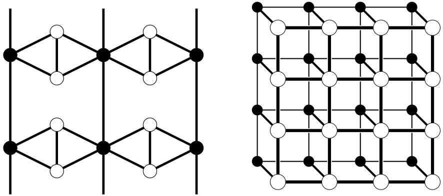


By a standard trick (averaging the inner product), we can turn them all into rigid motions, a.k.a. isometries.

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

If G is stable, the kernel must be trivial.

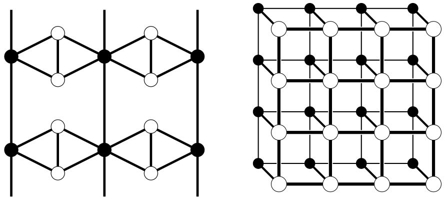
How could p be periodic, but not $p \circ \varphi$?



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

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

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



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`