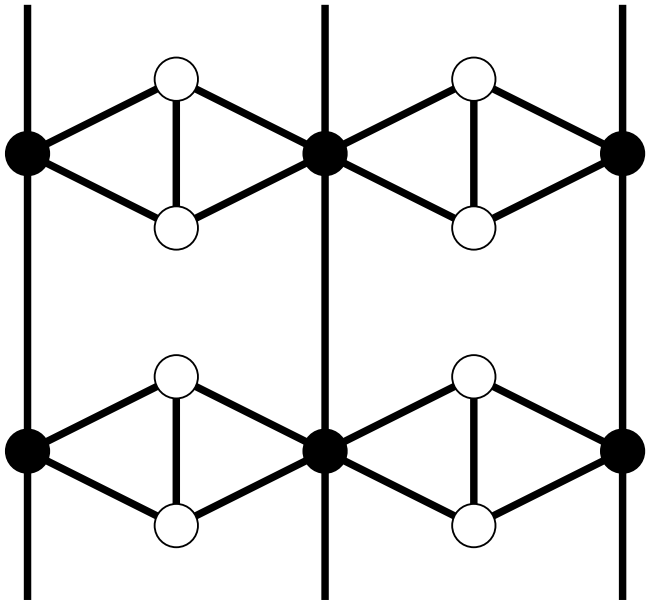
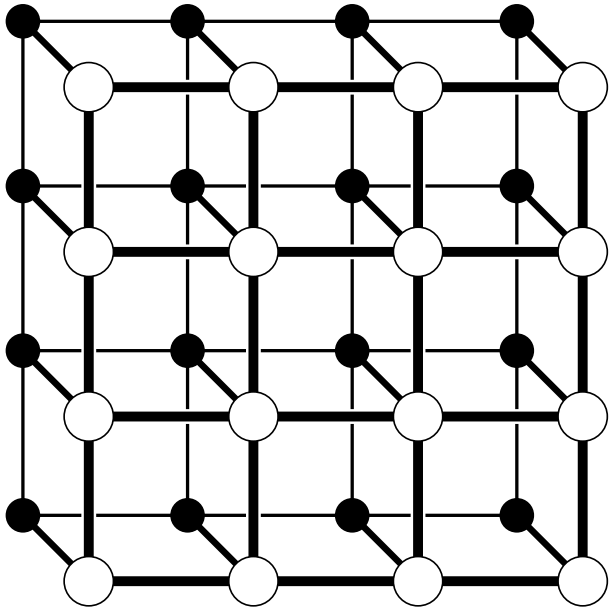
When is a crystal graph not crystallographic?

Olaf Delgado-Friedrichs

Order!Order? — Canberra 4 Dec 2019

Answer: when it has “too much symmetry”.

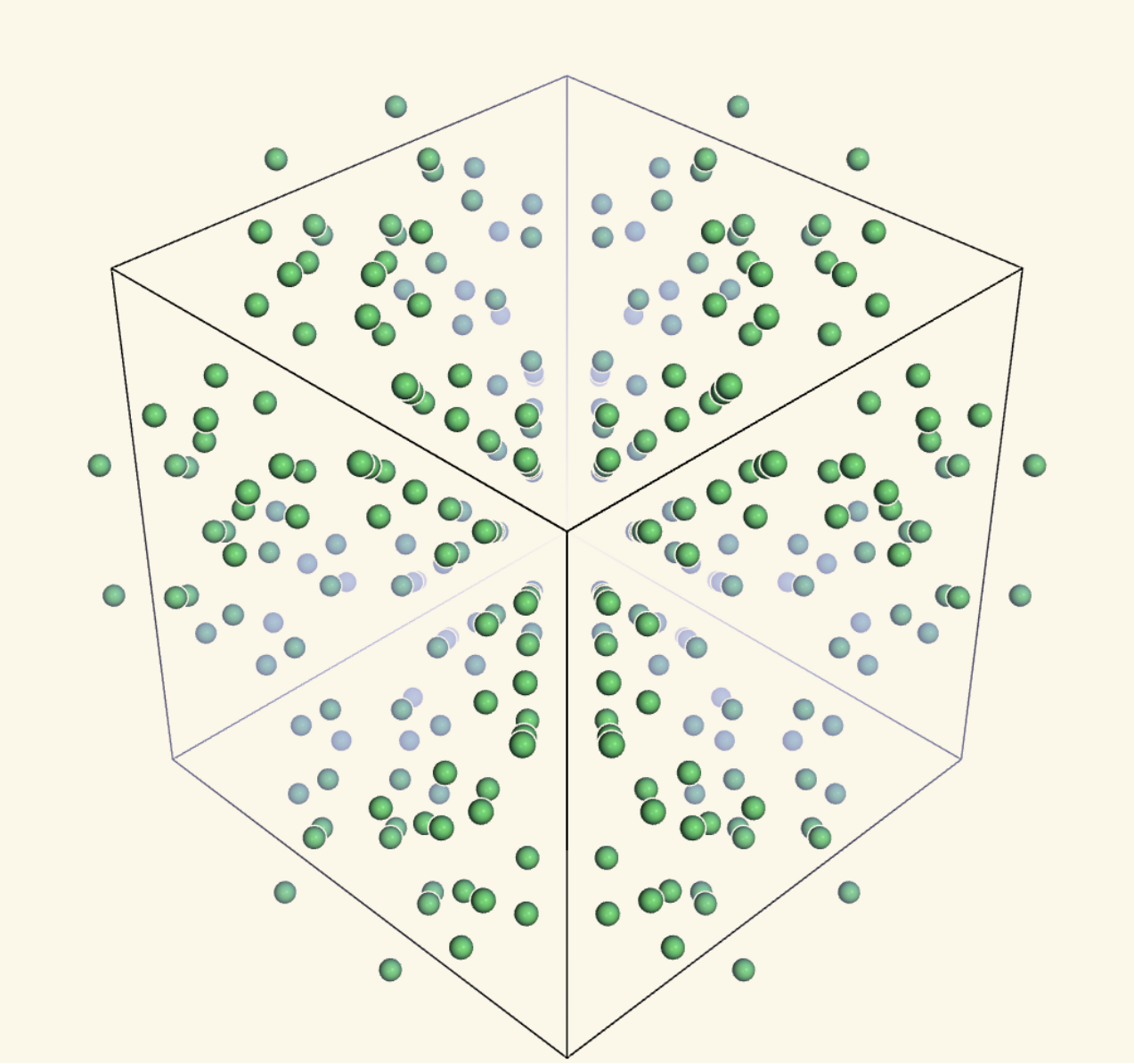




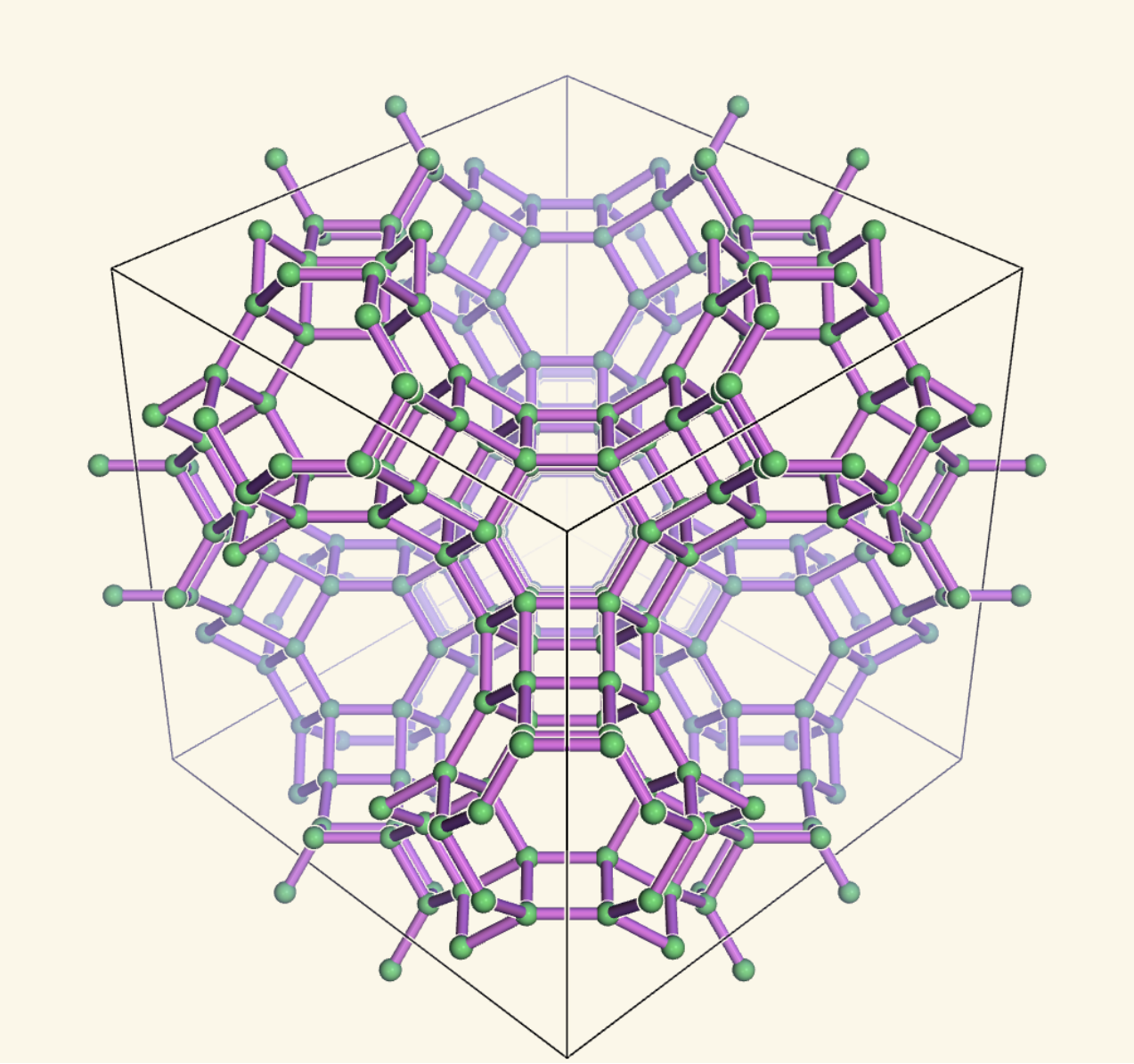
More precisely: when its automorphism group is not a crystallographic space group.

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

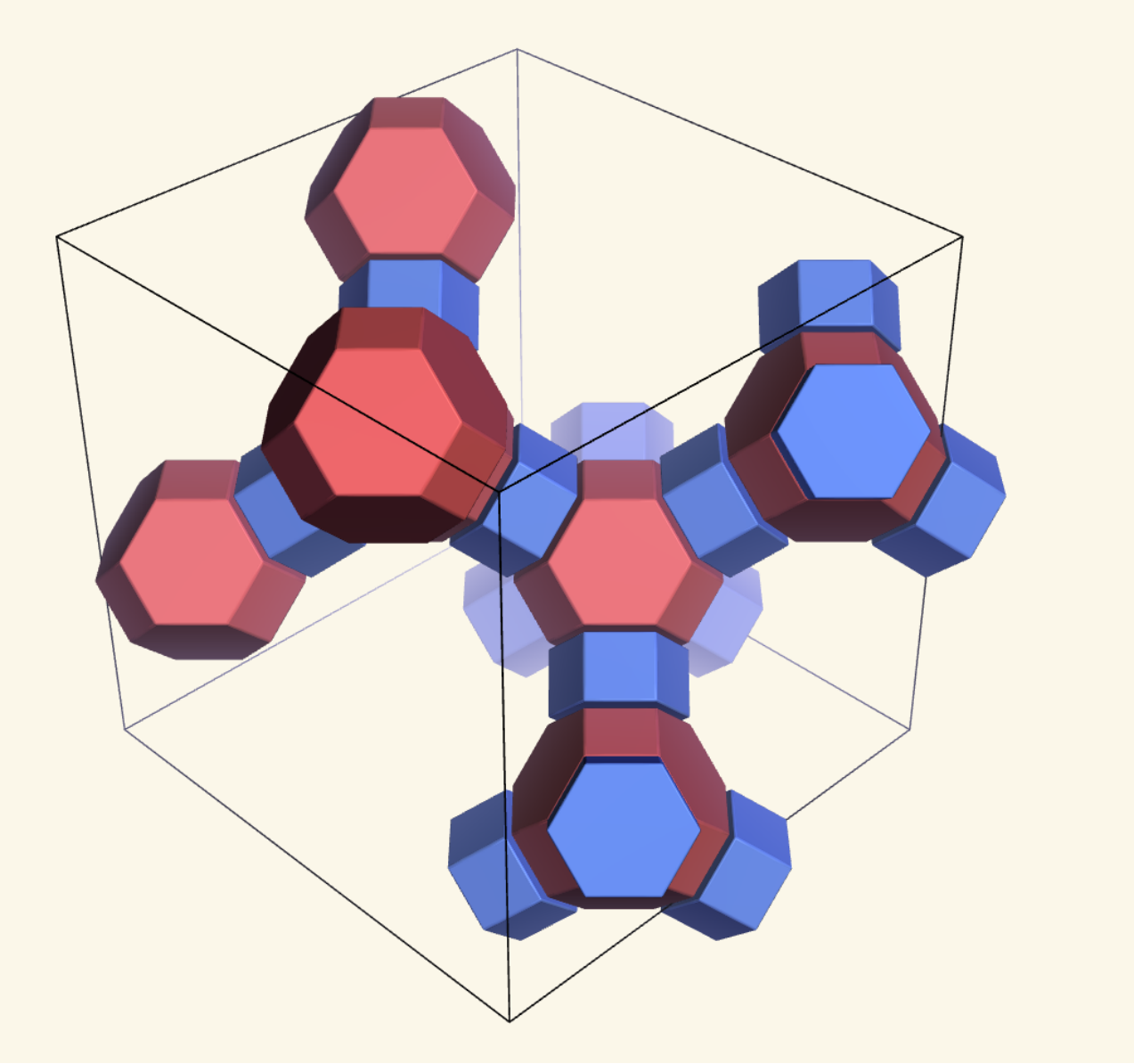
A crystalline material. What might be its atomic structure?



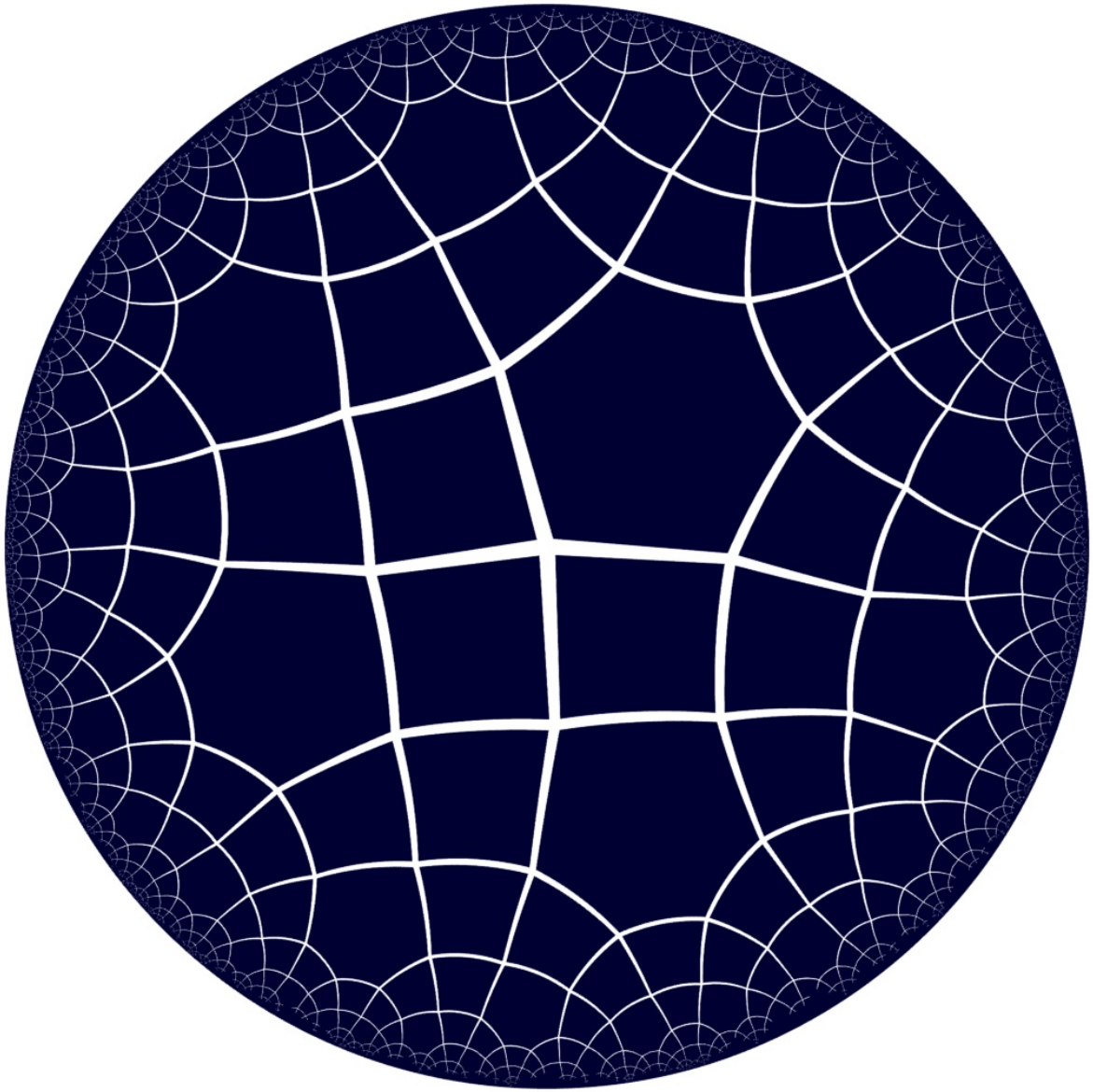
X-ray crystallography produces something like this.



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



Even richer structure from examining the cycle space.



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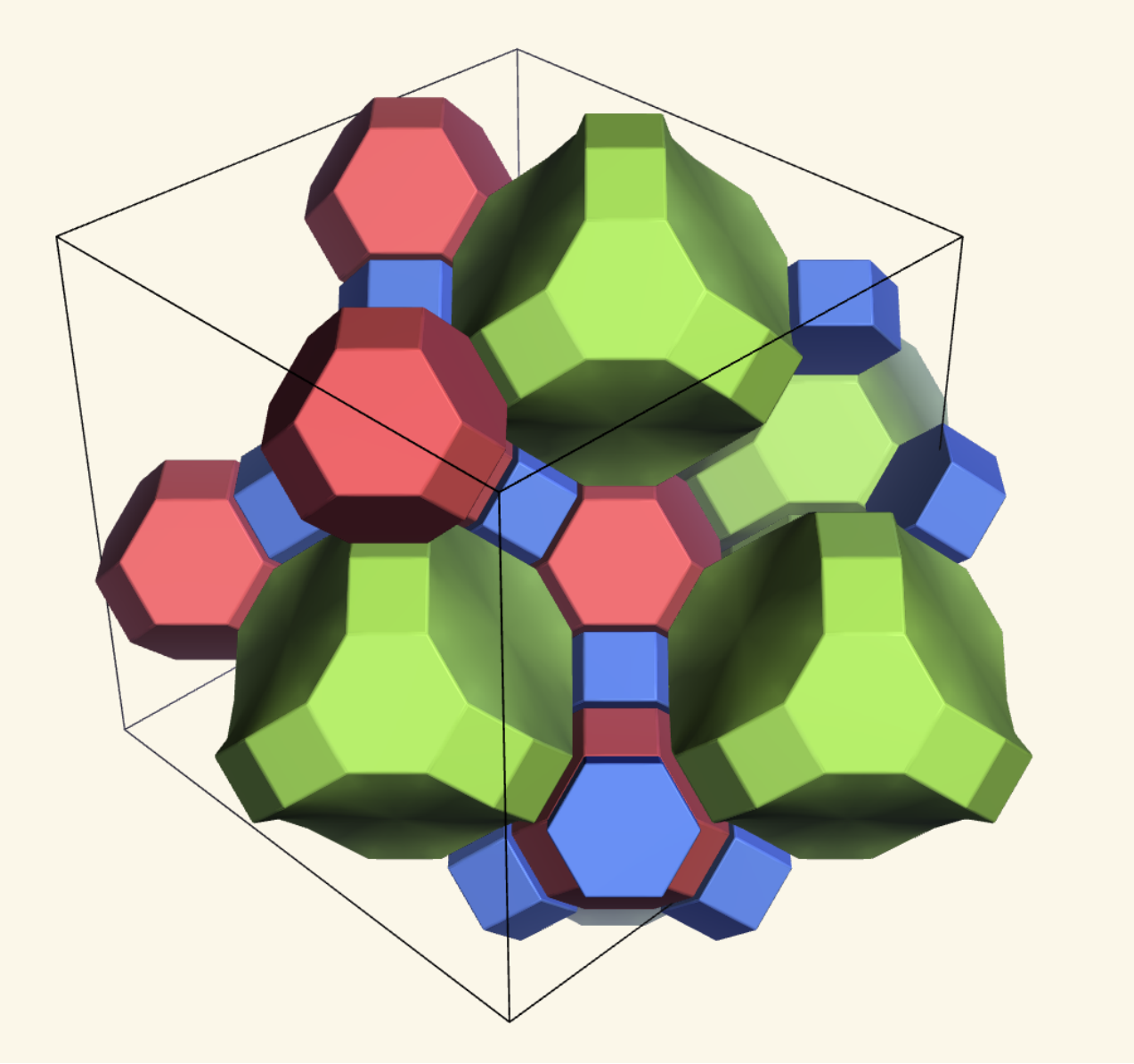

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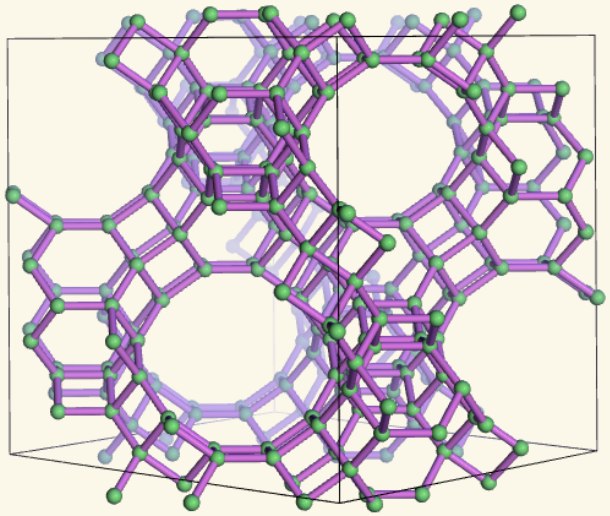
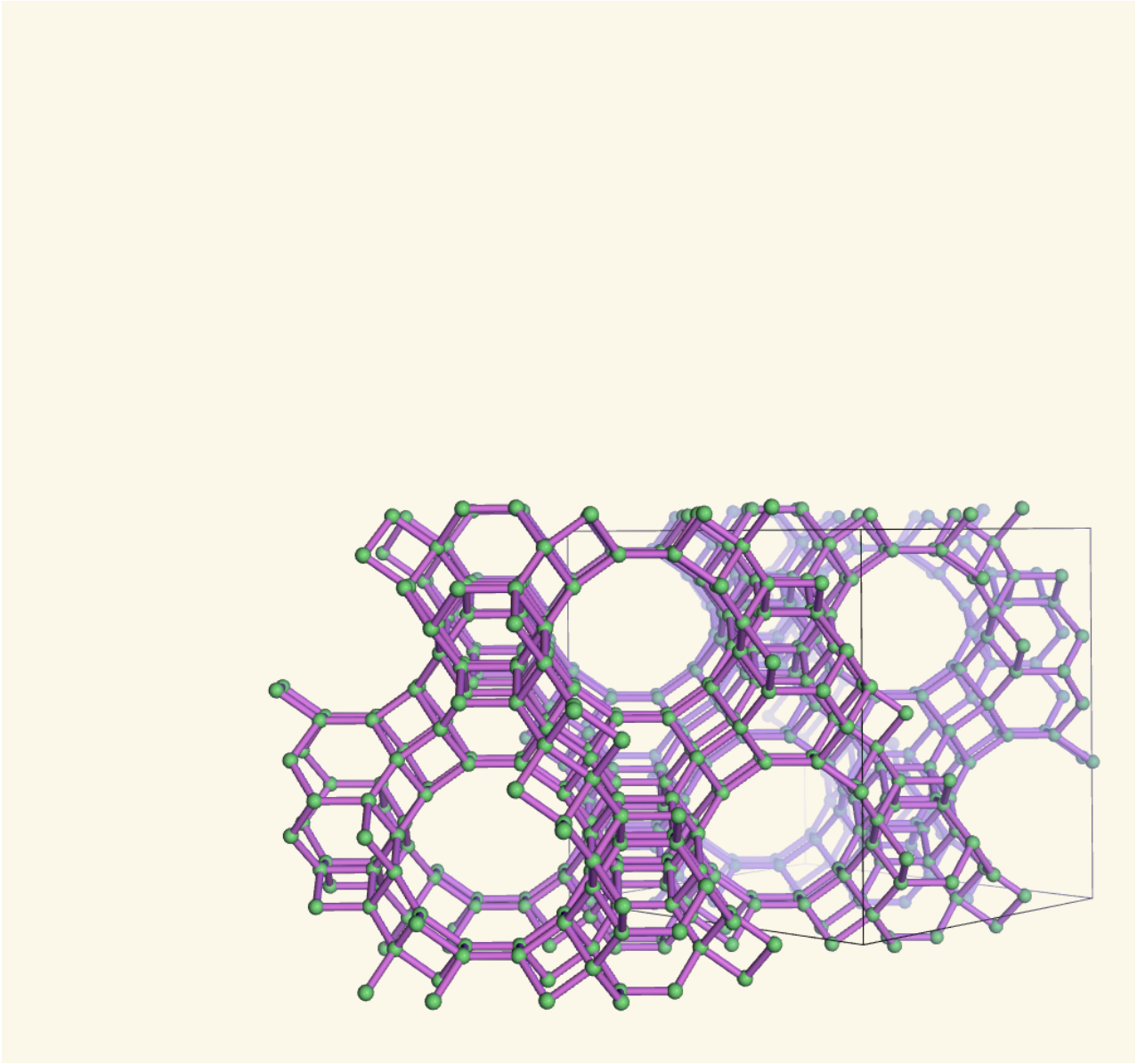


A *net* is a (3-) connected, locally finite periodic graph.



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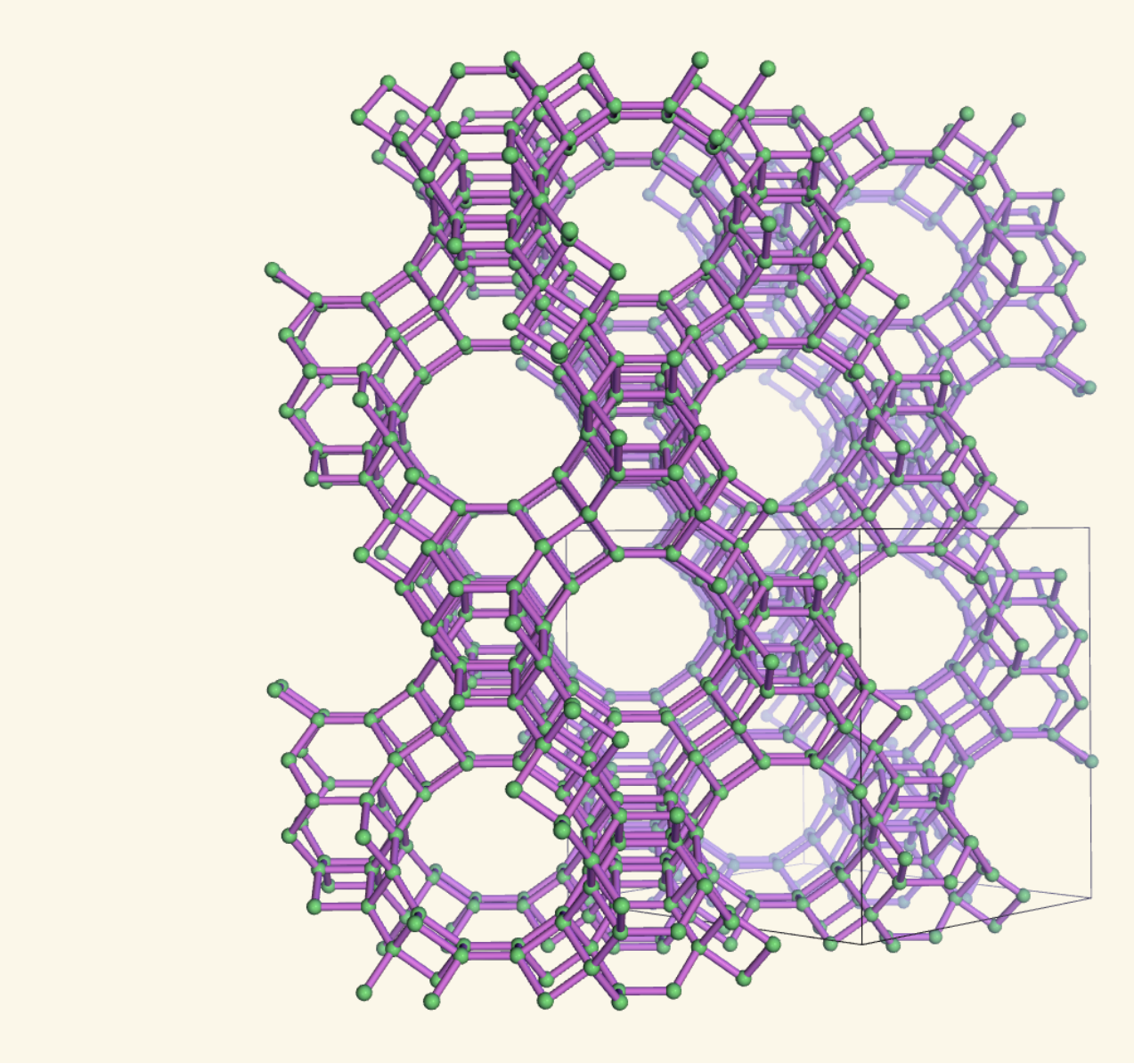

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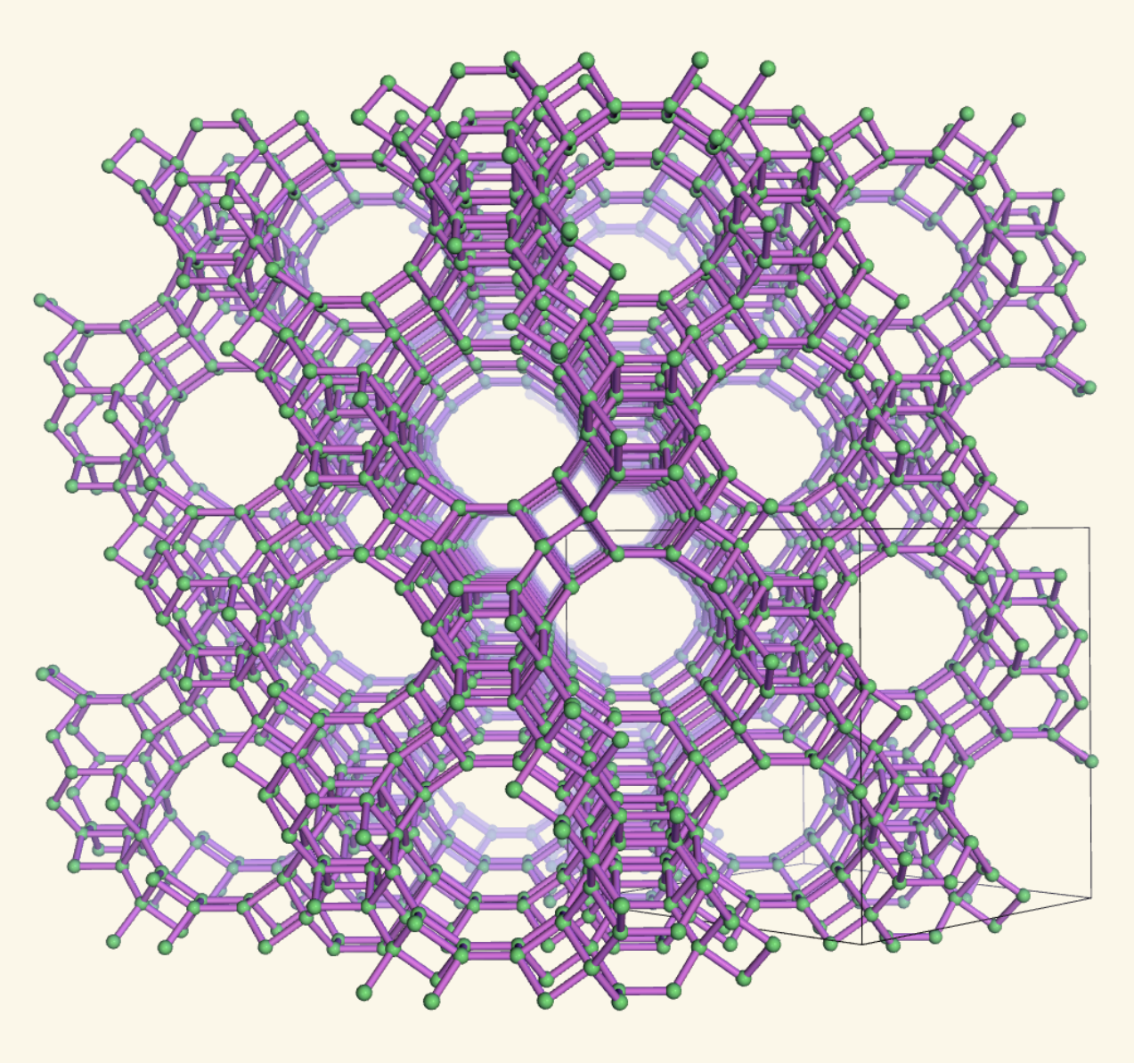

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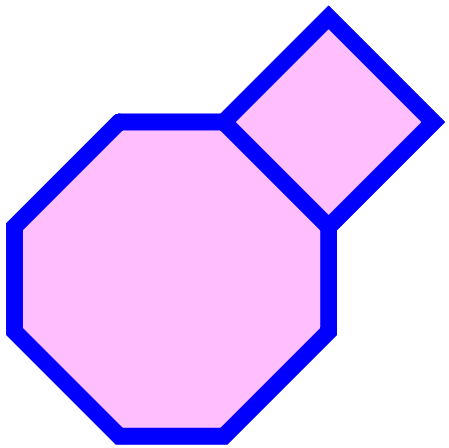
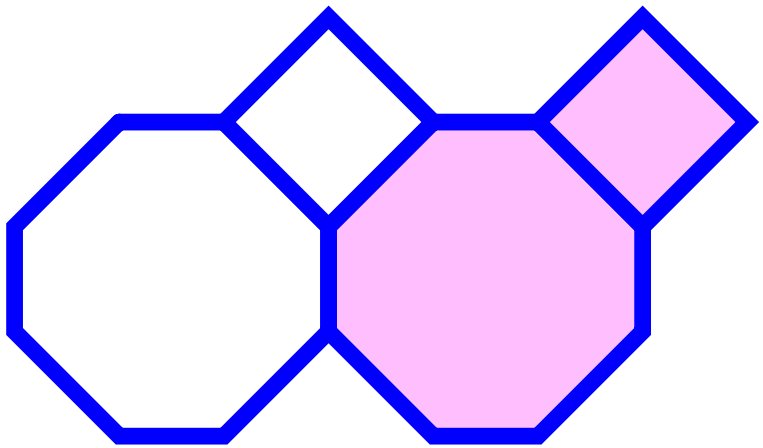


A 2-dimensional net, which here also defines a tiling.



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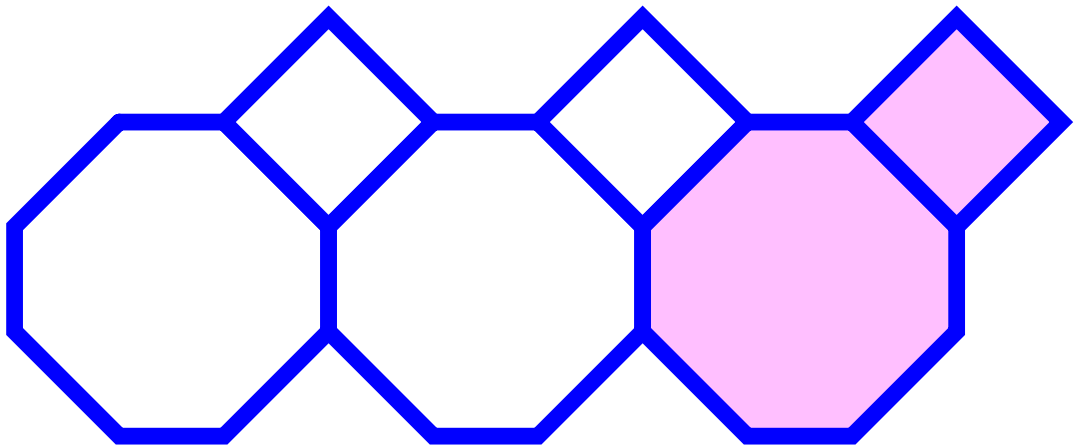

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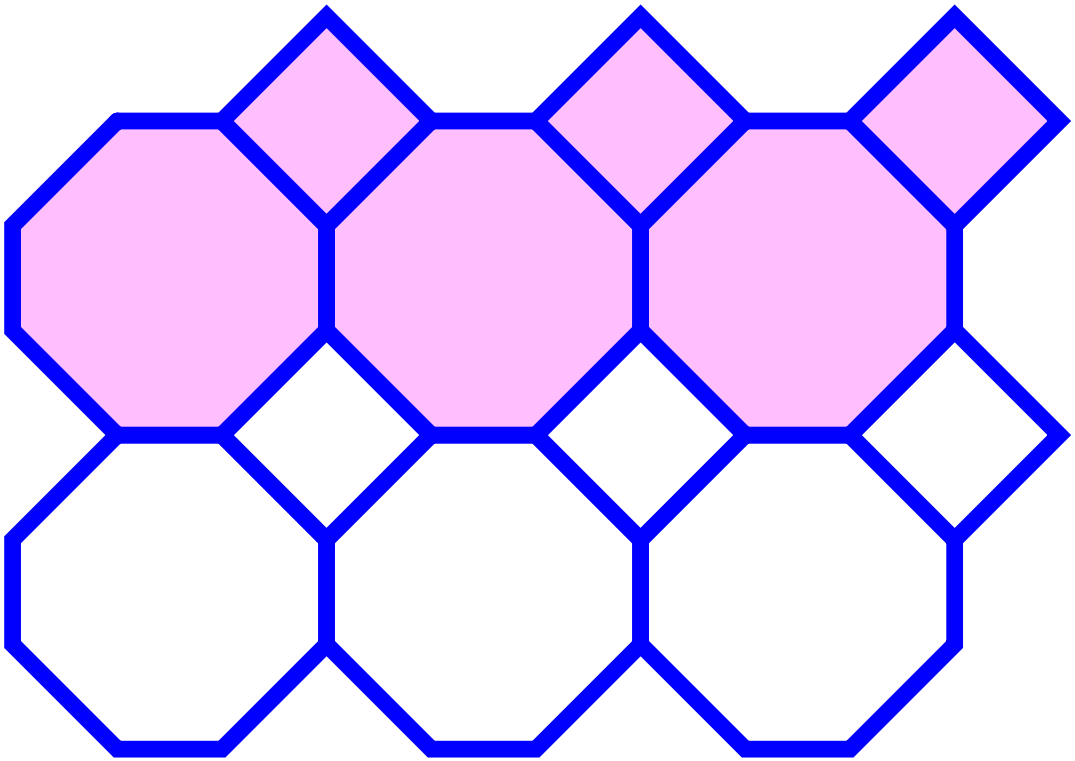

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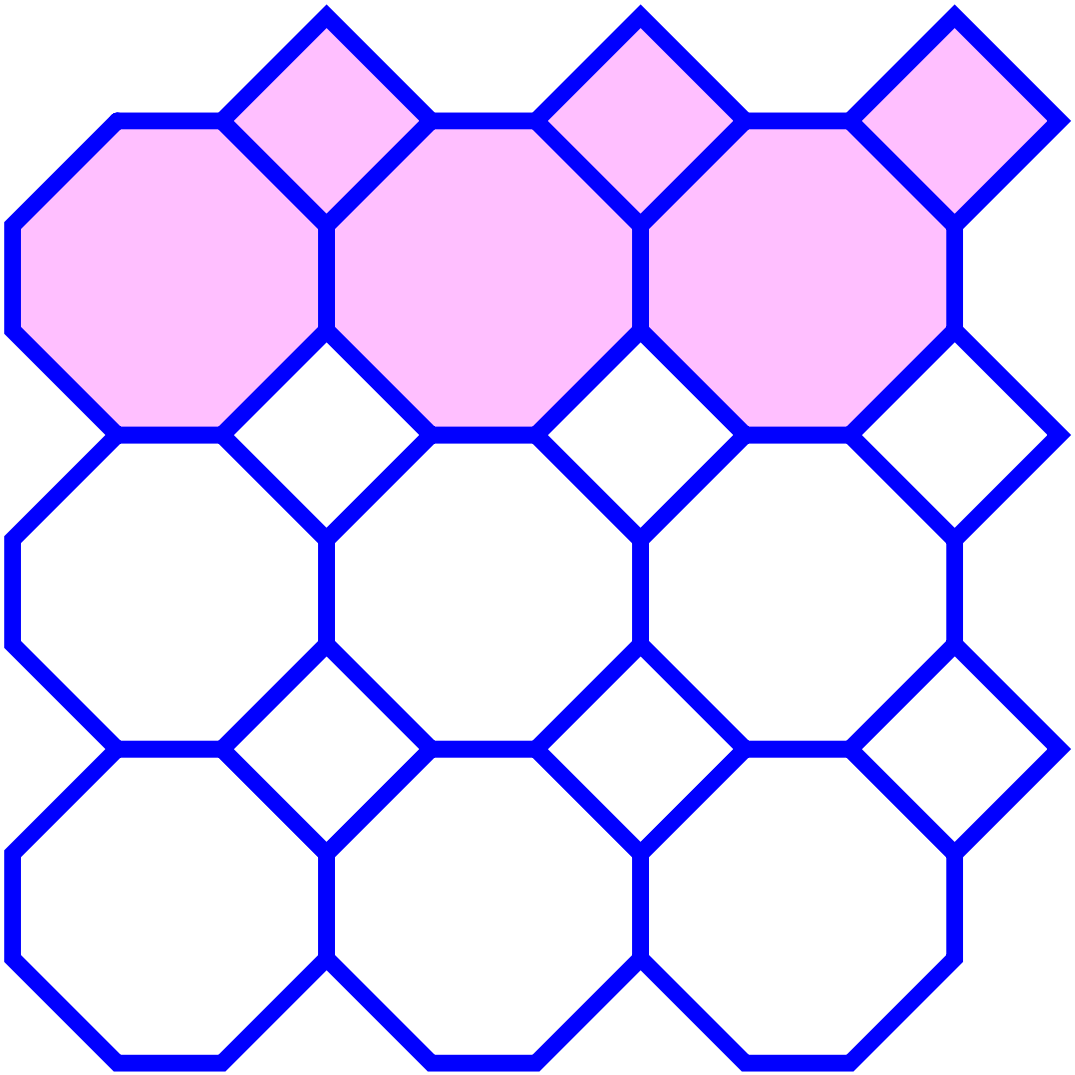

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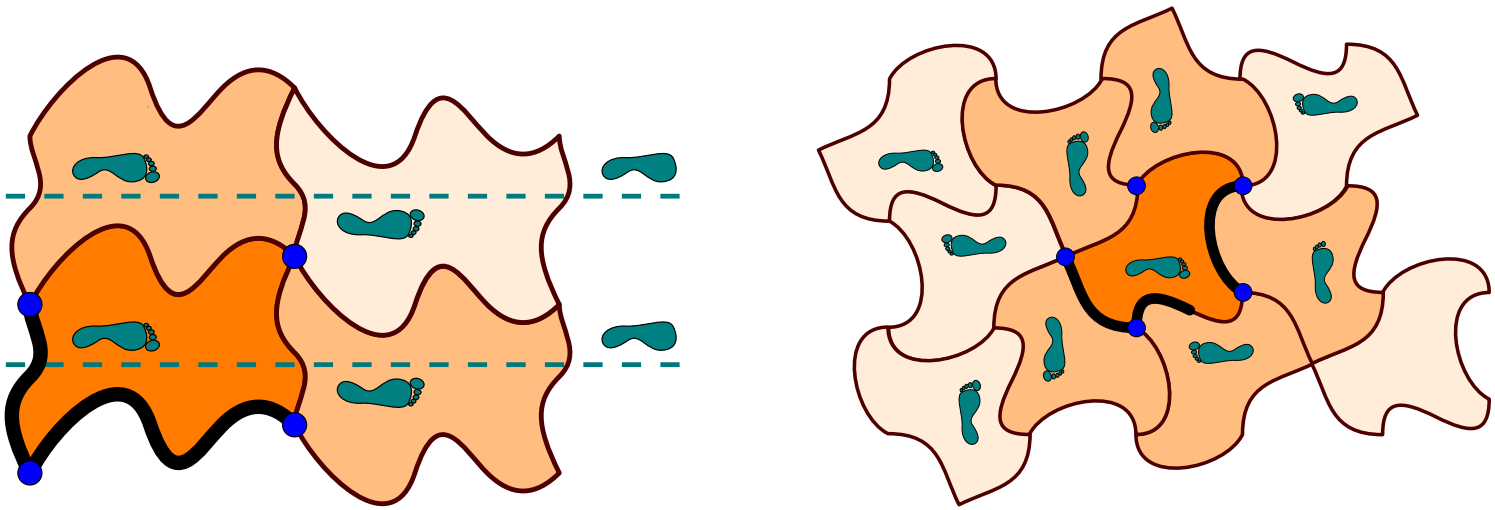
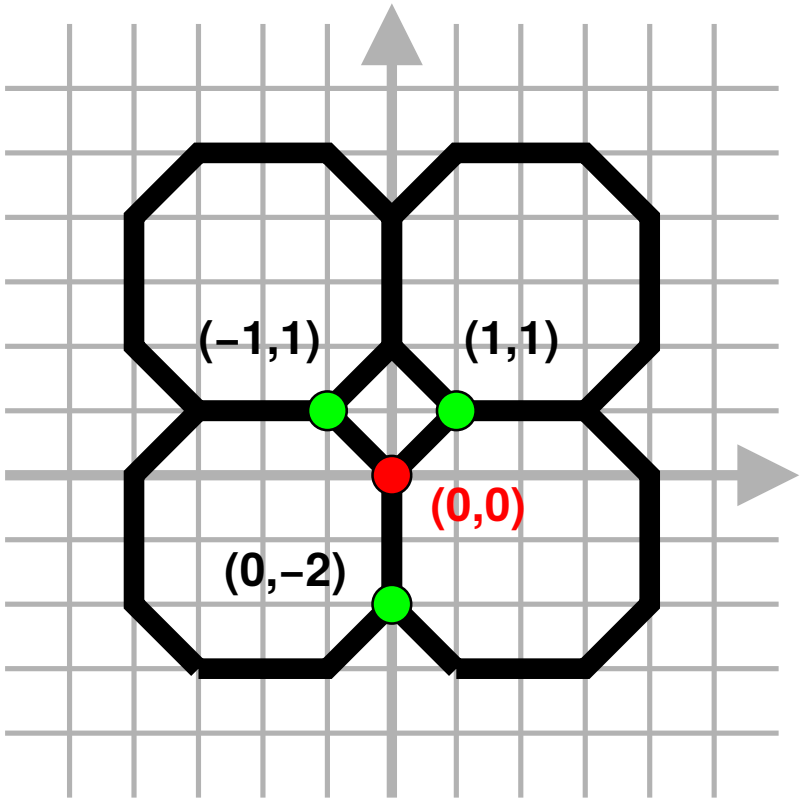
A *crystallographic (space) group* is a discrete group of motions in euclidean space with a bounded fundamental domain.



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

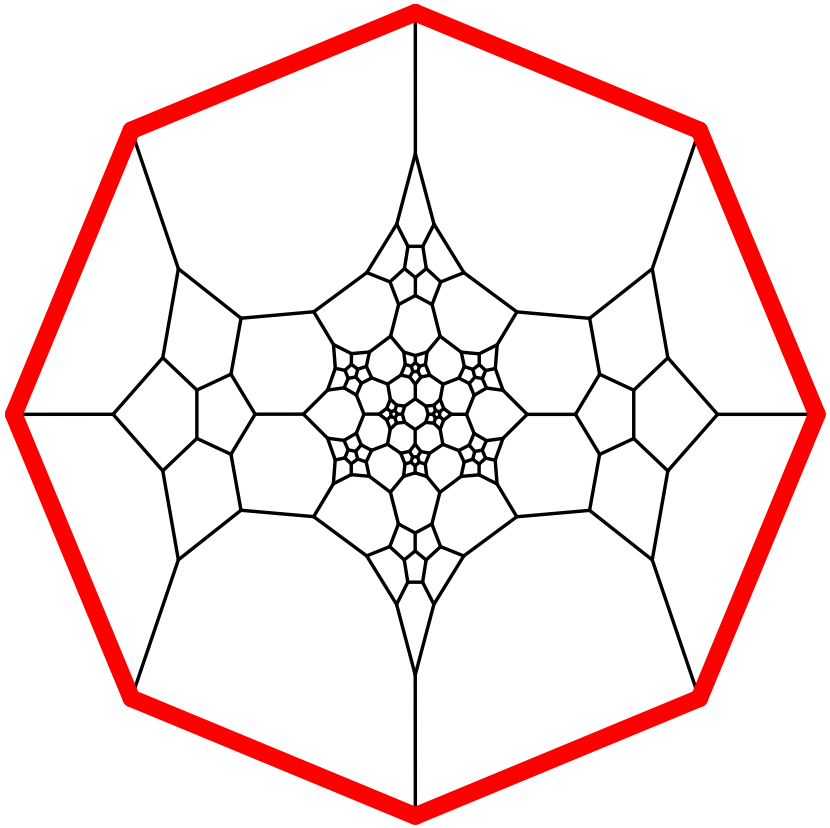
Tutte's idea for drawing graphs "nicely":



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

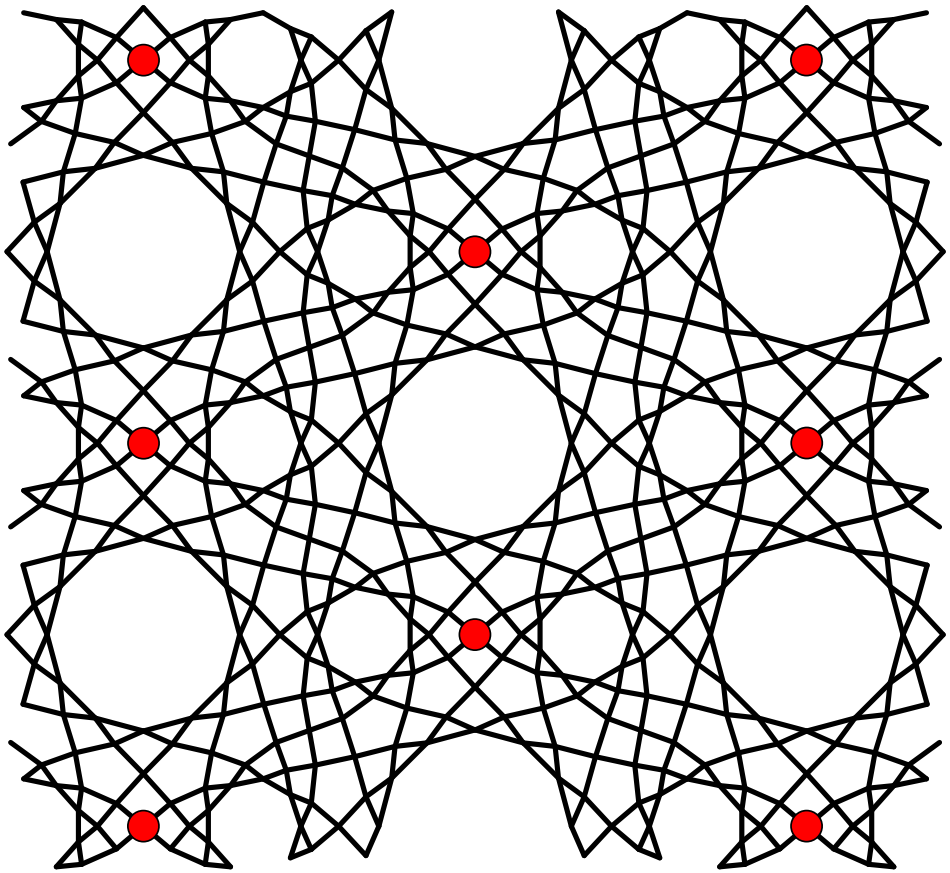
$$\sum_{w \in Neighbors(v)} position(w) - position(v) = 0$$

For finite graphs, prescribe a convex outer face.



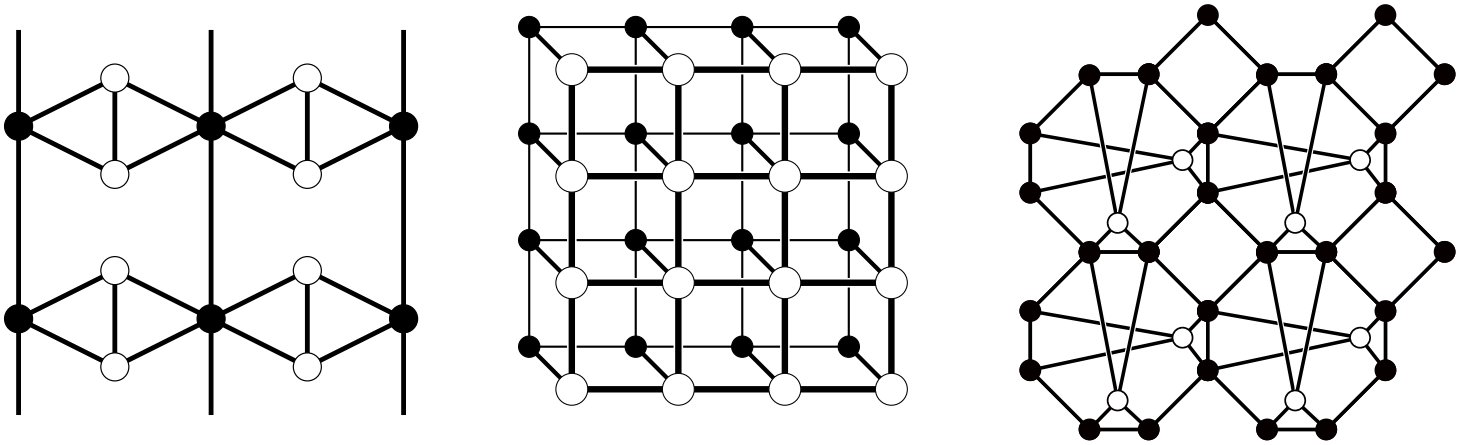
For polyhedral graphs, this ensures convex drawings.
(*How to draw a graph,* W. T. Tutte 1963.)

For periodic graphs, prescribe a vertex lattice.



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?