

When is a crystal graph not crystallographic?

Olaf Delgado-Friedrichs

Order!Order? — Canberra 4 Dec 2019

When is a
crystal graph
not
crystallographic?

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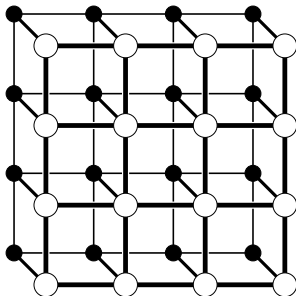
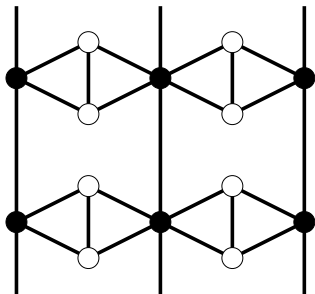
Too much
symmetry

Crystal nets

Crystallographic
groups

Tutte's barycentric
embedding

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.)*

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A crystalline material. What might be its atomic structure?

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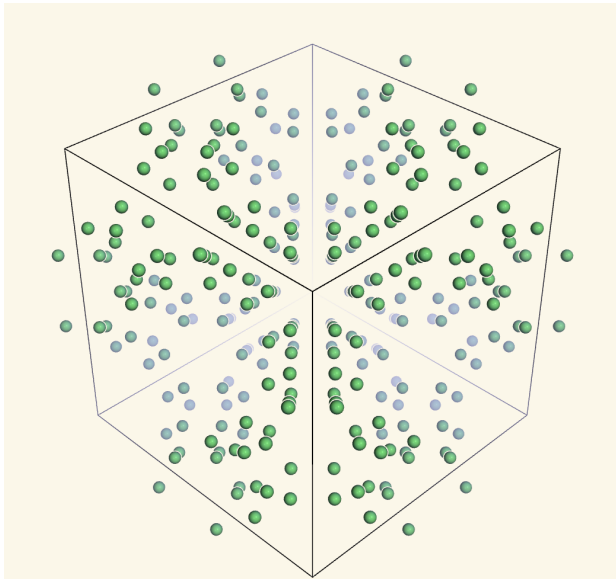
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X-ray crystallography produces something like this.

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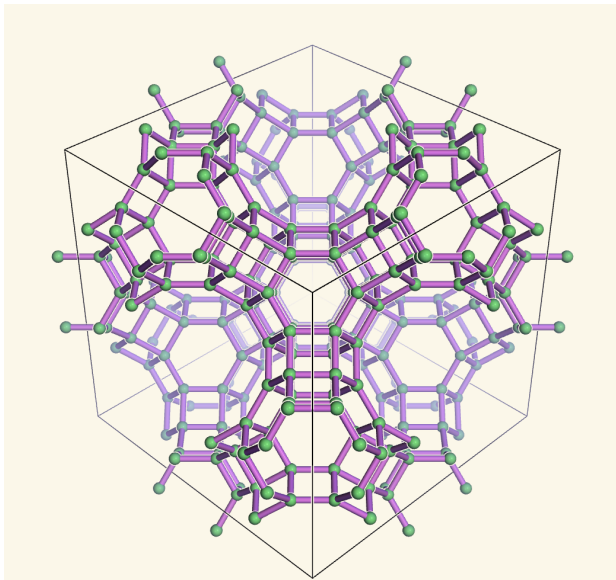
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Adding bonds (or ligands) yields a periodic graph or *net*.

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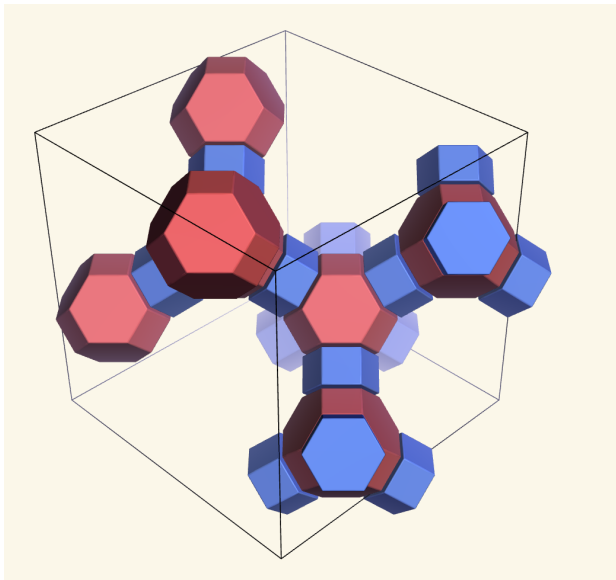
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Even richer structure from examining the cycle space.

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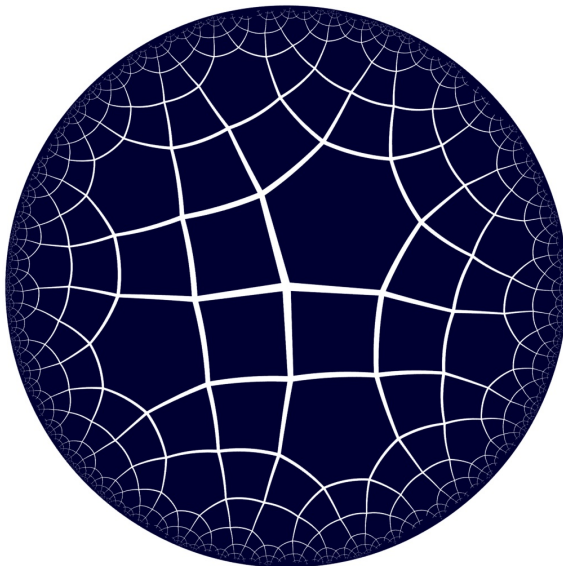
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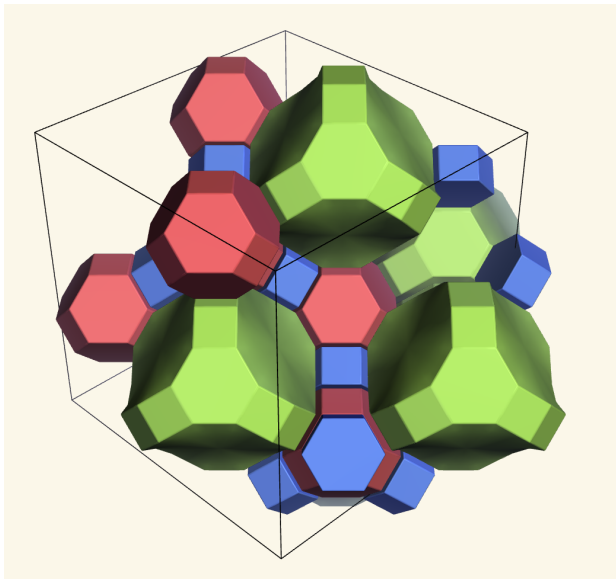
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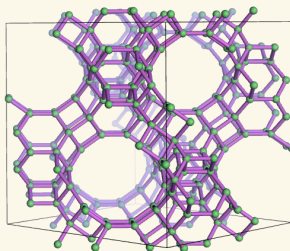
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A *net* is a (3-) connected, locally finite periodic graph.

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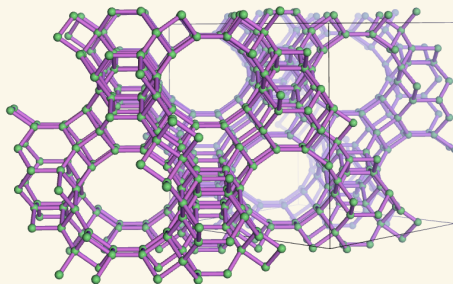
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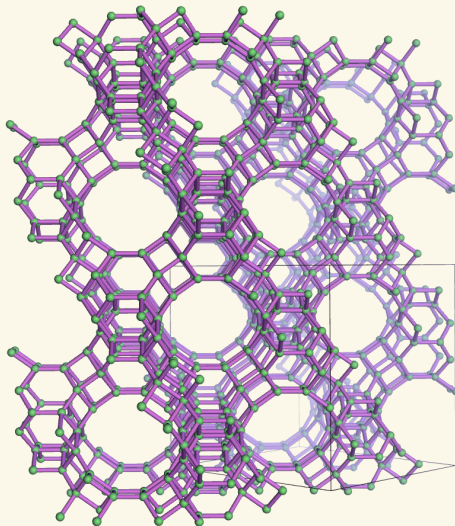
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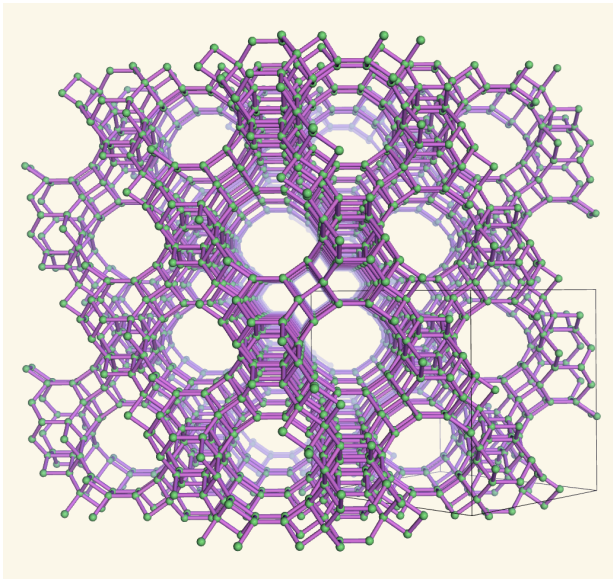
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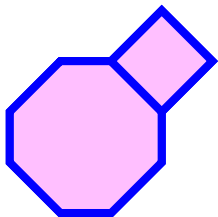
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A 2-dimensional net, which here also defines a tiling.

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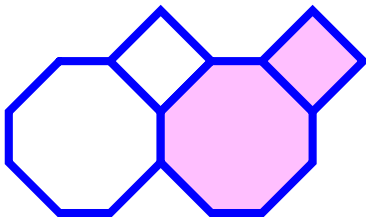
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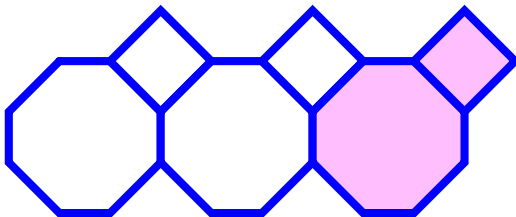
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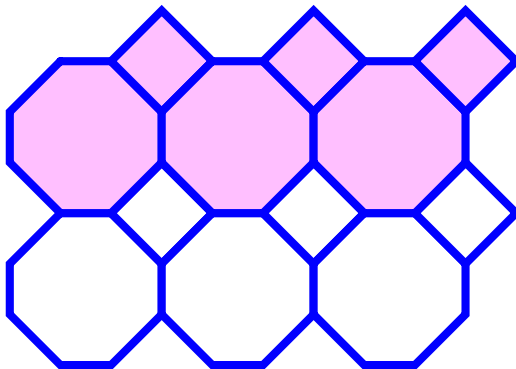
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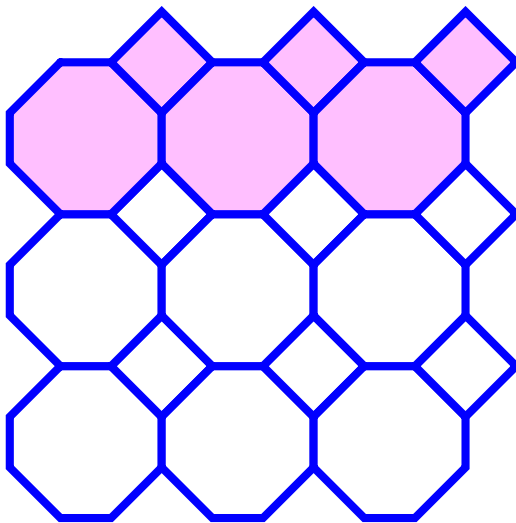
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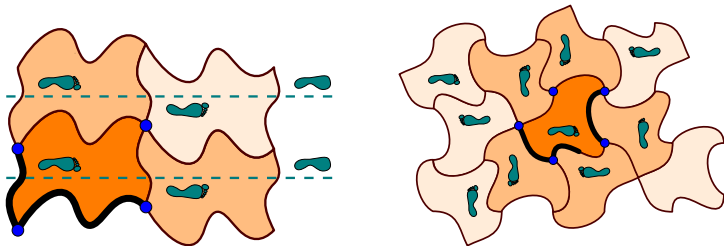
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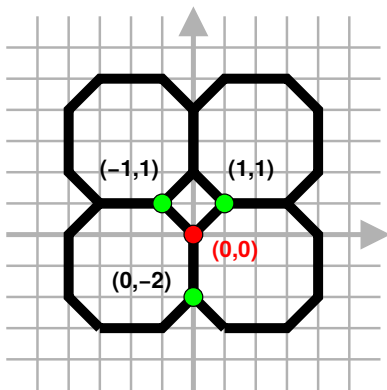
A 2-dimensional net, which here also defines a tiling.

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



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:

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

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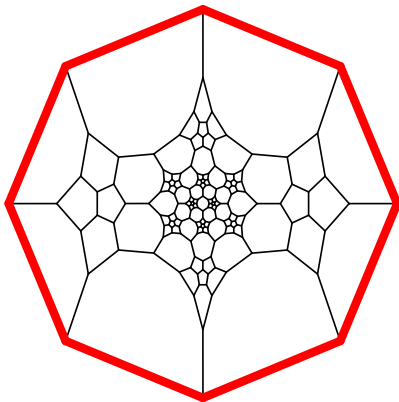
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For finite graphs, prescribe a convex outer face.



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

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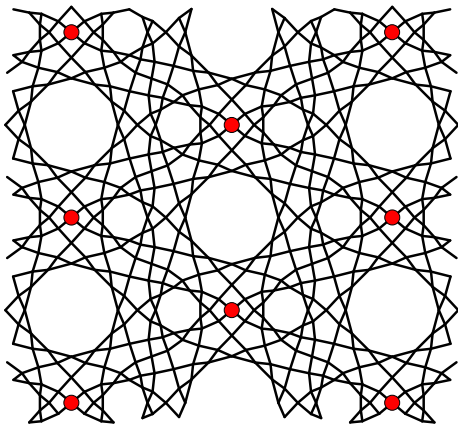
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For periodic graphs, prescribe a vertex lattice.



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

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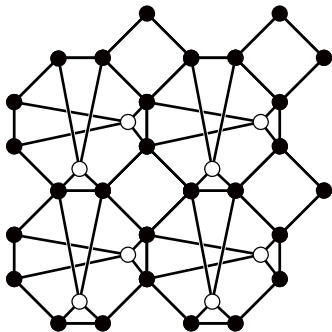
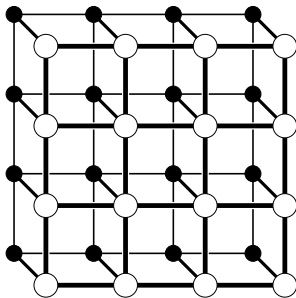
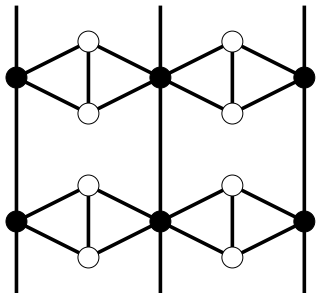
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