When is a
crystal graph
not
crystallographic?

Olaf Delgado-Friedrichs

Order!Order? — Canberra 4 Dec 2019

Answer: when it has "too much symmetry".

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Crystal nets

Tutte's barycentric
embedding
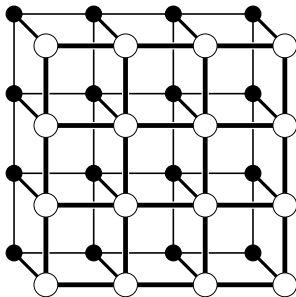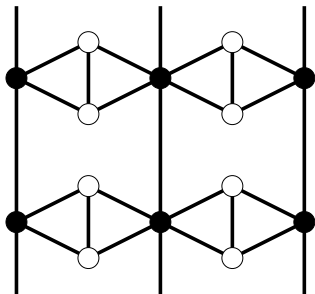
More precisely: when its automorphism group is not a
crystallographic space group.

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

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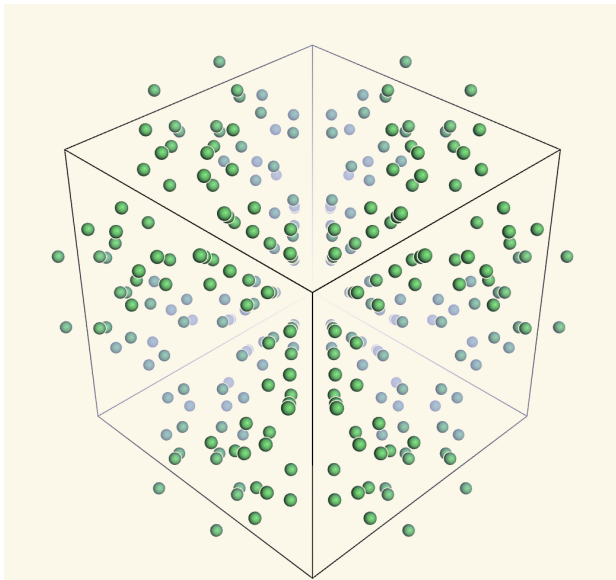A crystalline material. What might be its atomic structure?

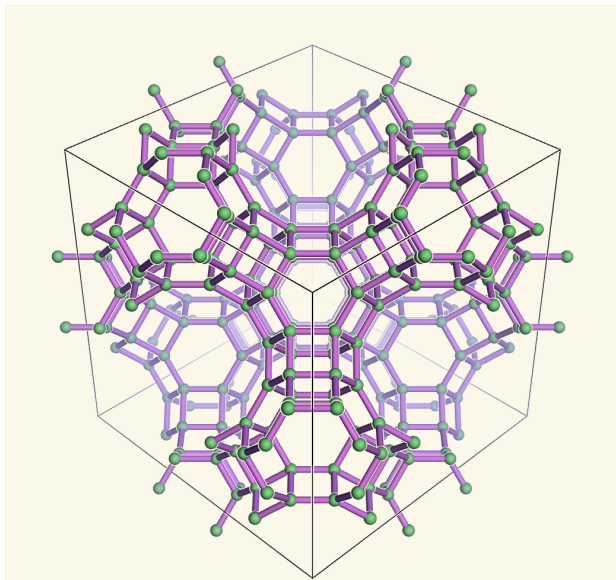X-ray crystallography produces something like this.

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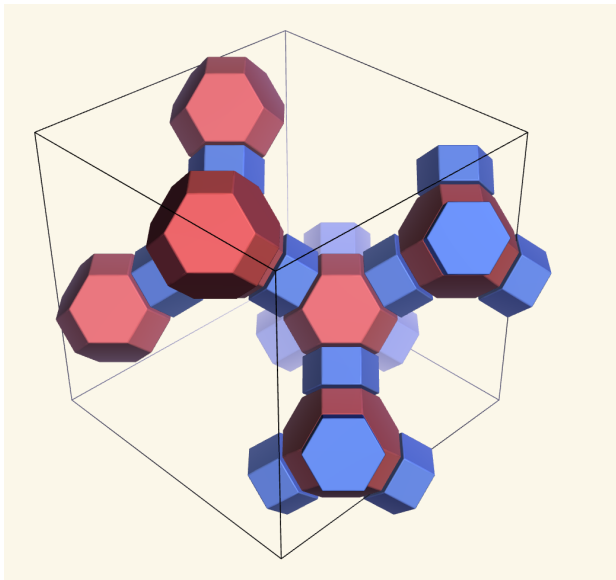Adding bonds (or ligands) yields a periodic graph or *net*.

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Even richer structure from examining the cycle space.
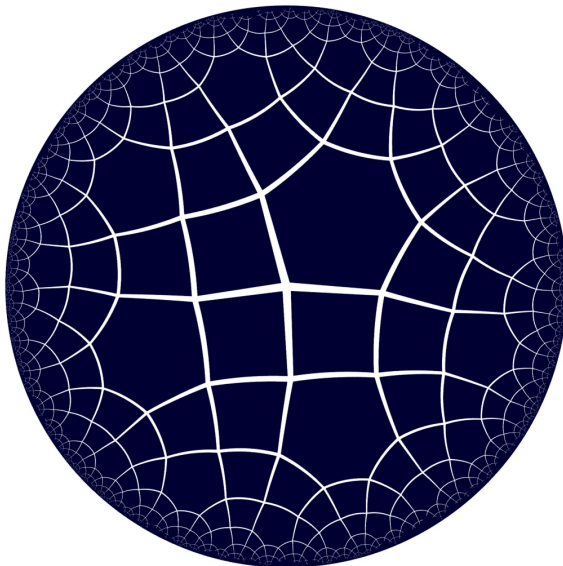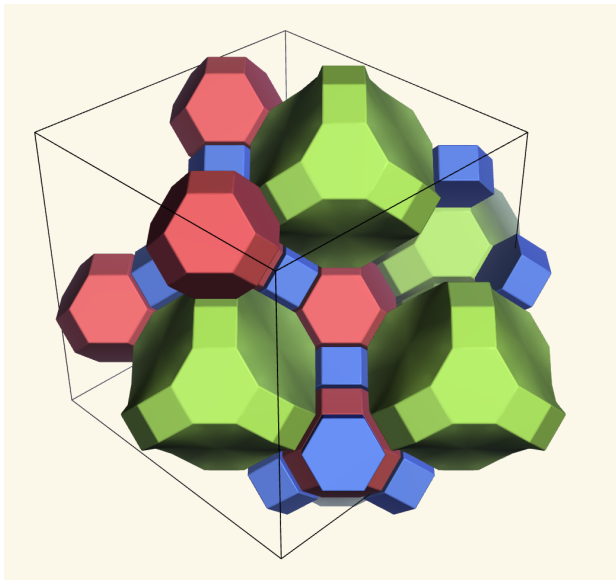
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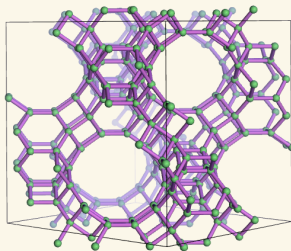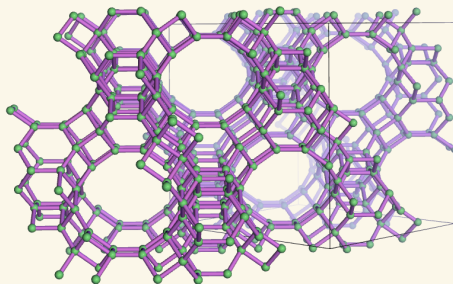Even richer structure from examining the cycle space.

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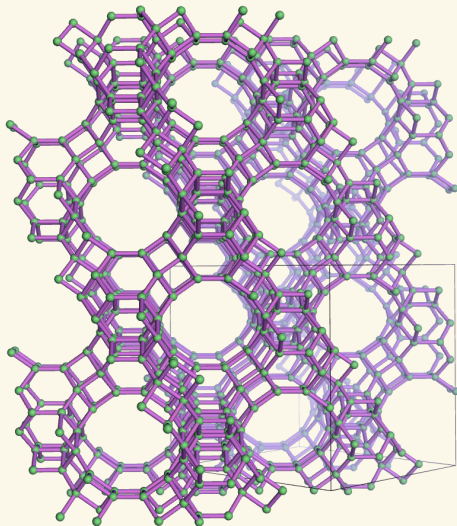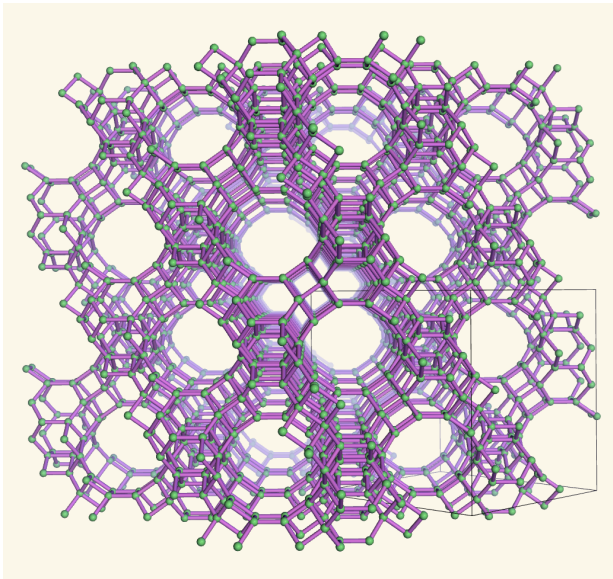Crystal nets

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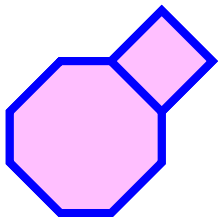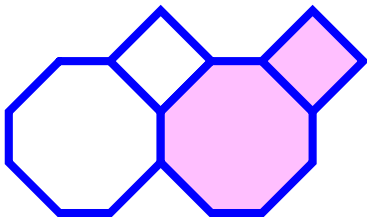A *net* is a connected, locally finite periodic graph.

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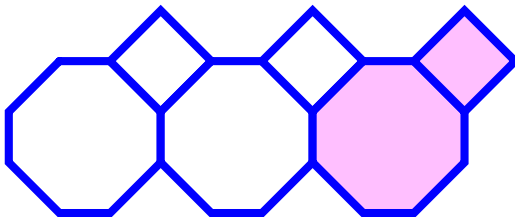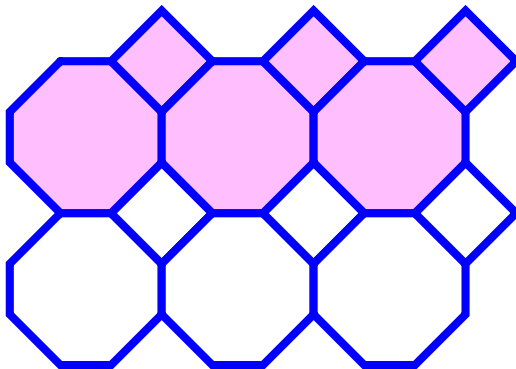
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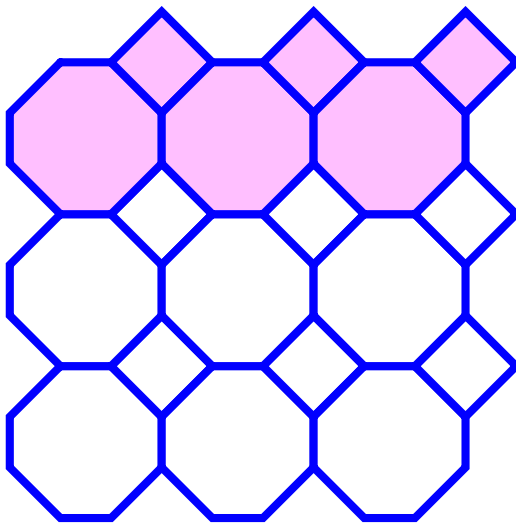A 2-dimensional net, which here also defines a tiling.

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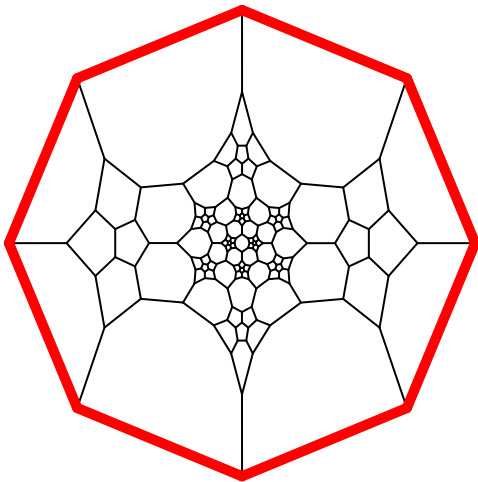A 2-dimensional net, which here also defines a tiling.
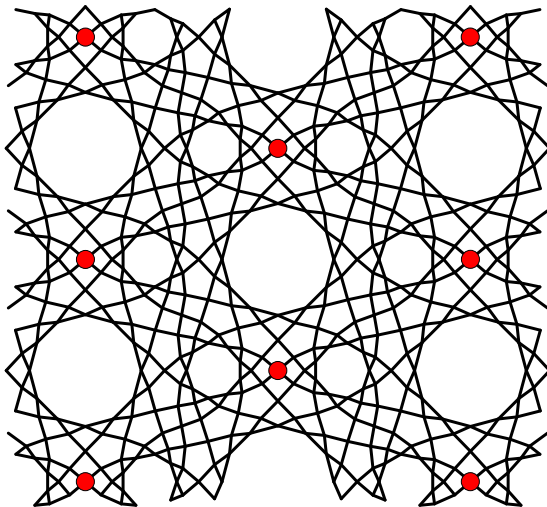
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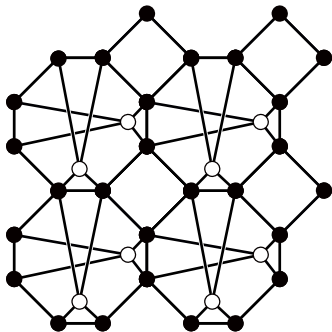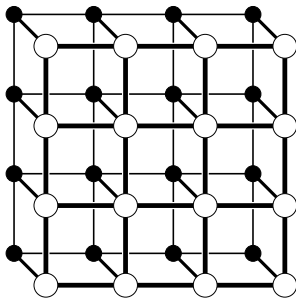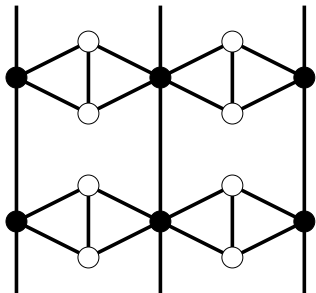not
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