

# When is a crystal graph not crystallographic?

Olaf Delgado-Friedrichs

Order!Order? — Canberra 4 Dec 2019

When is a  
crystal graph  
not  
crystallographic?

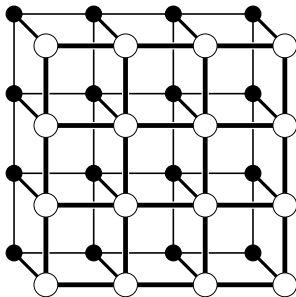
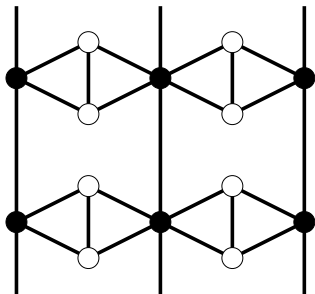
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Too much  
symmetry

Crystal nets

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?

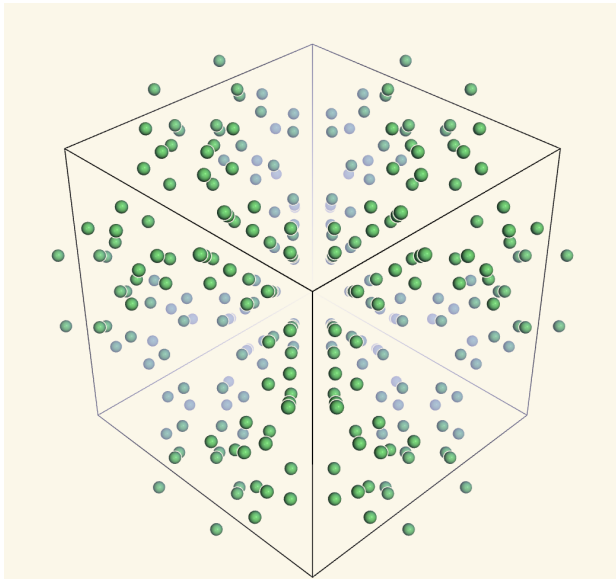
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X-ray crystallography produces something like this.

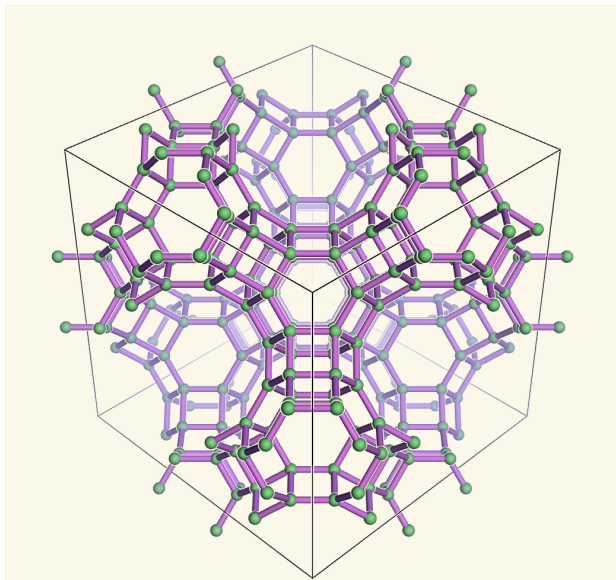
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Adding bonds (or ligands) yields a periodic graph or *net*.

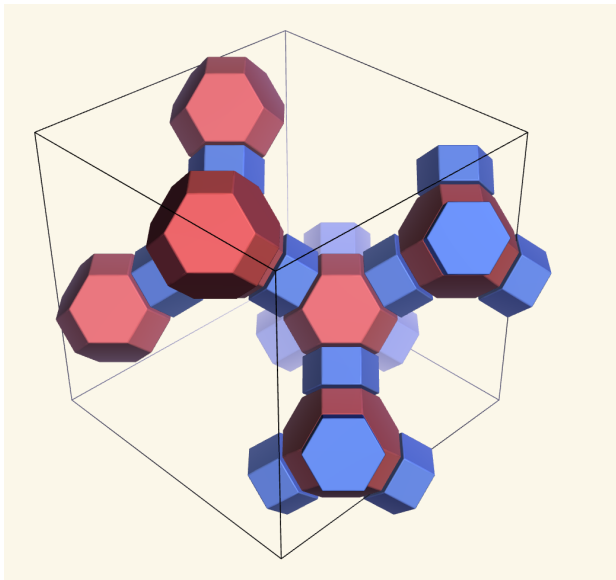
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Even richer structure from examining the cycle space.

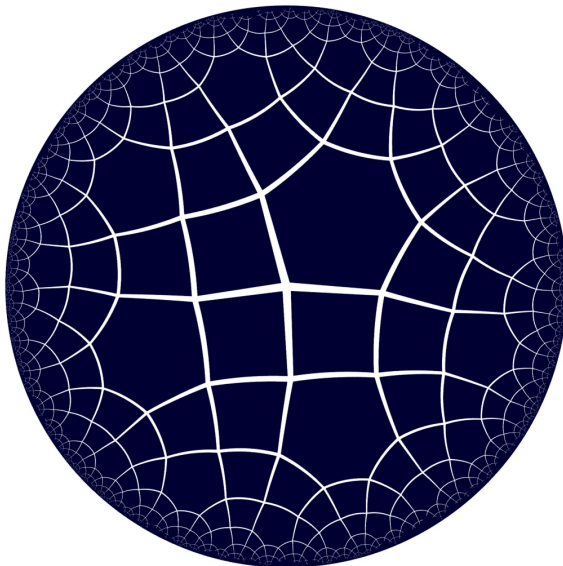
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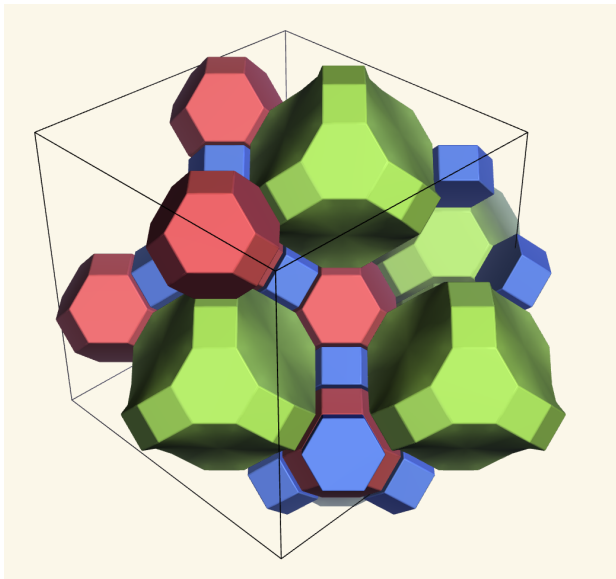
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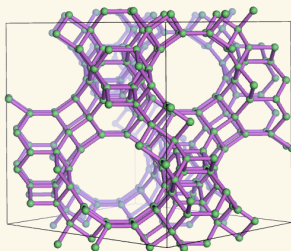
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A *net* is a connected, locally finite periodic graph.

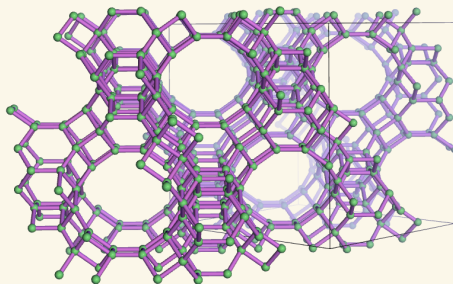
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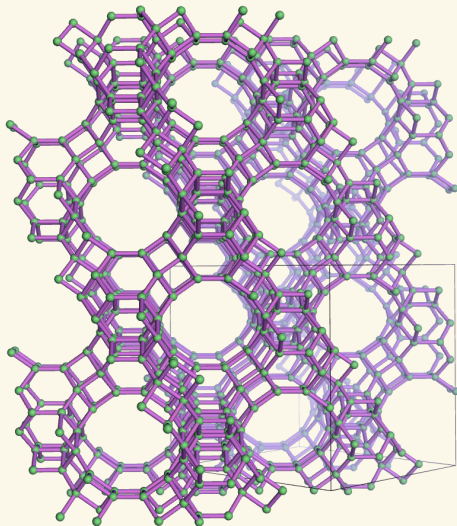
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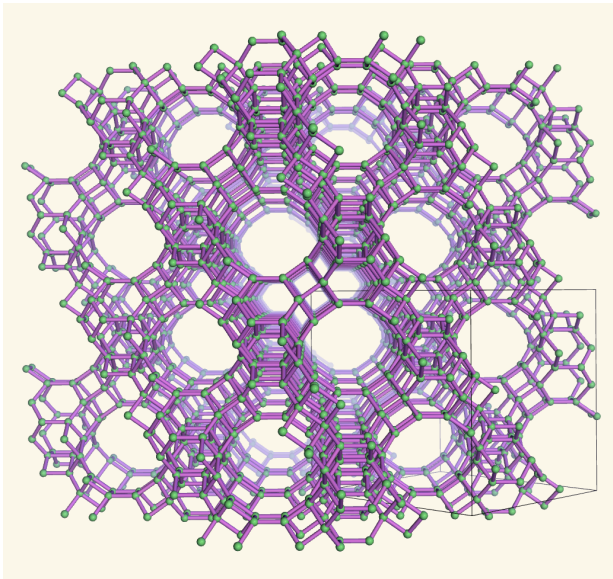
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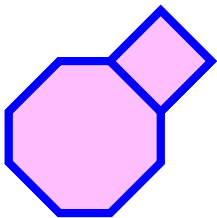
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A 2-dimensional net, which here also defined a tiling.

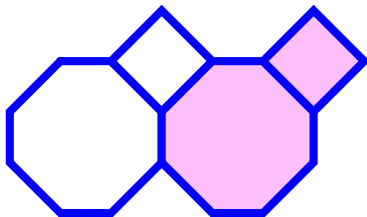
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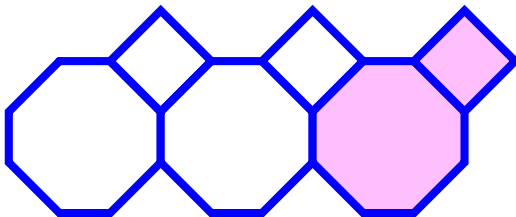
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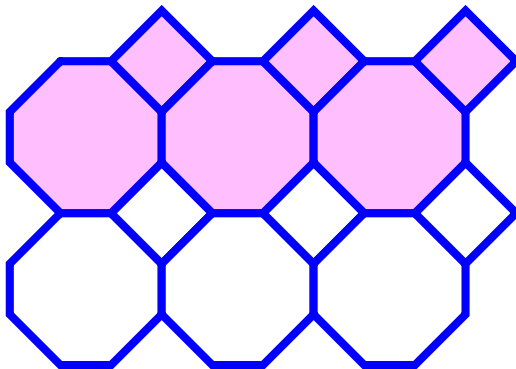
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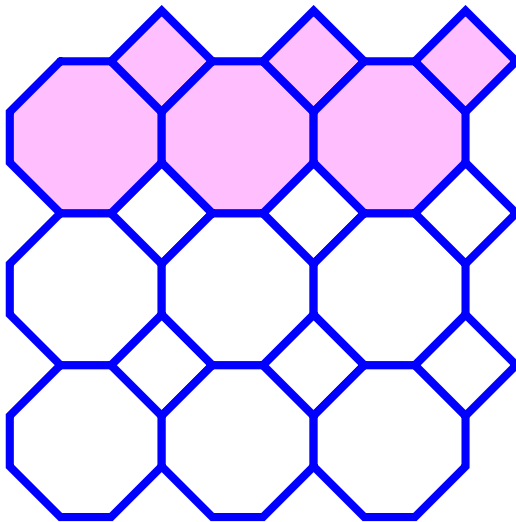
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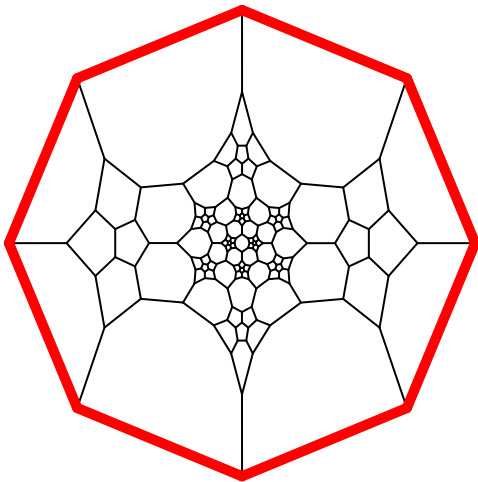
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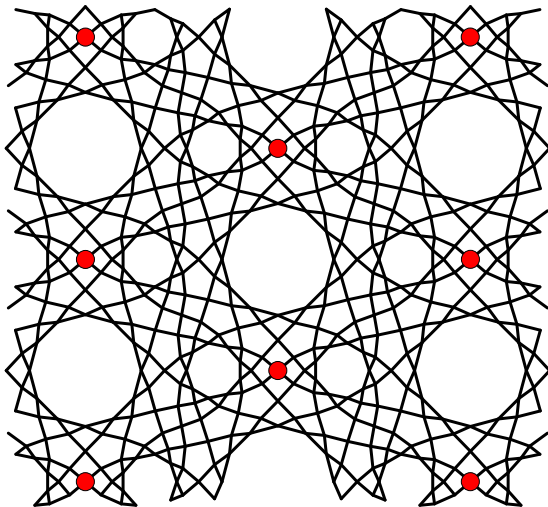
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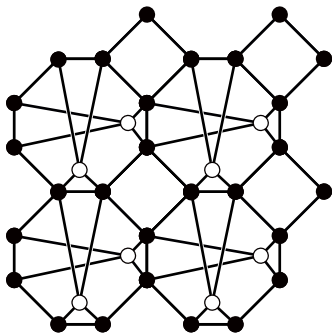
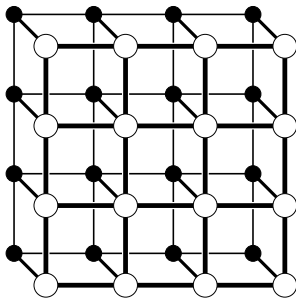
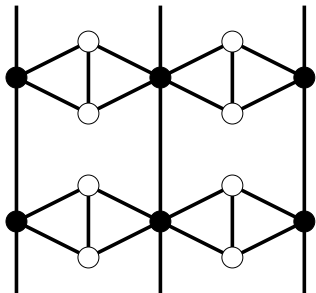
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