

When is a  
crystal graph  
not  
crystallographic?

# When is a crystal graph not crystallographic?

Olaf Delgado

Too much  
symmetry

Crystal nets

Crystallographic  
groups

Tutte's barycentric  
embedding

Olaf Delgado-Friedrichs

Order!Order? — Canberra 4 Dec 2019

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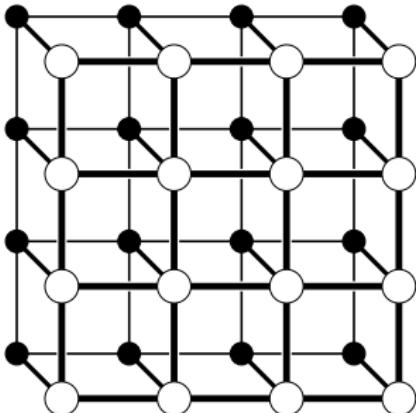
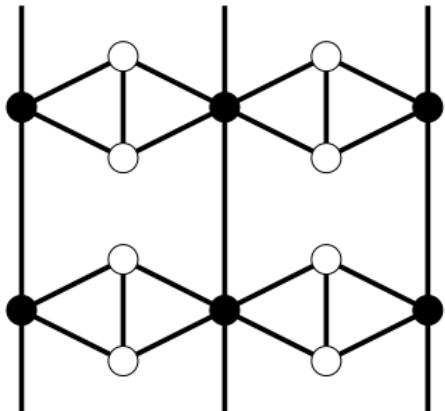
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Answer: when it has “too much symmetry”.



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?

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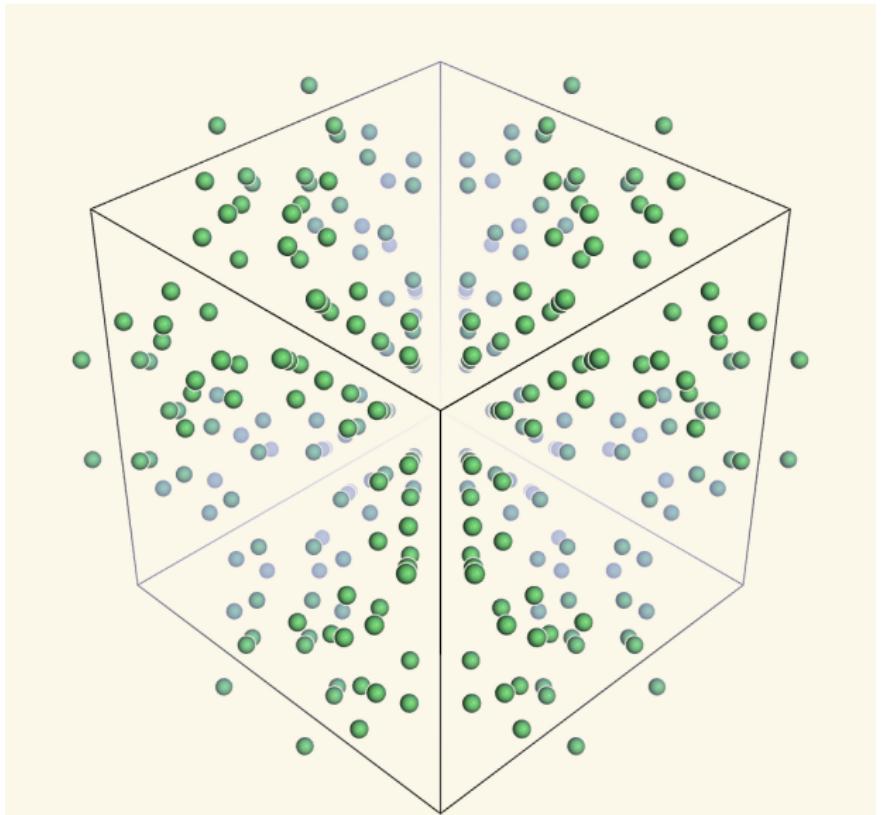
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X-ray crystallography produces something like this.

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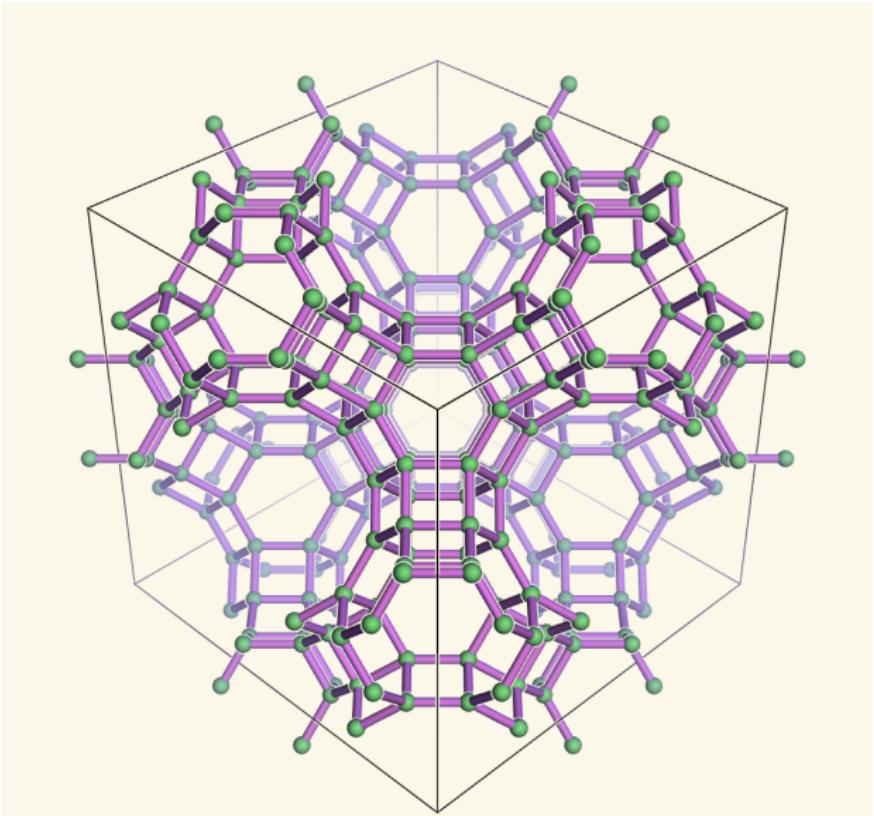
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Adding bonds (or ligands) yields a periodic graph or *net*.

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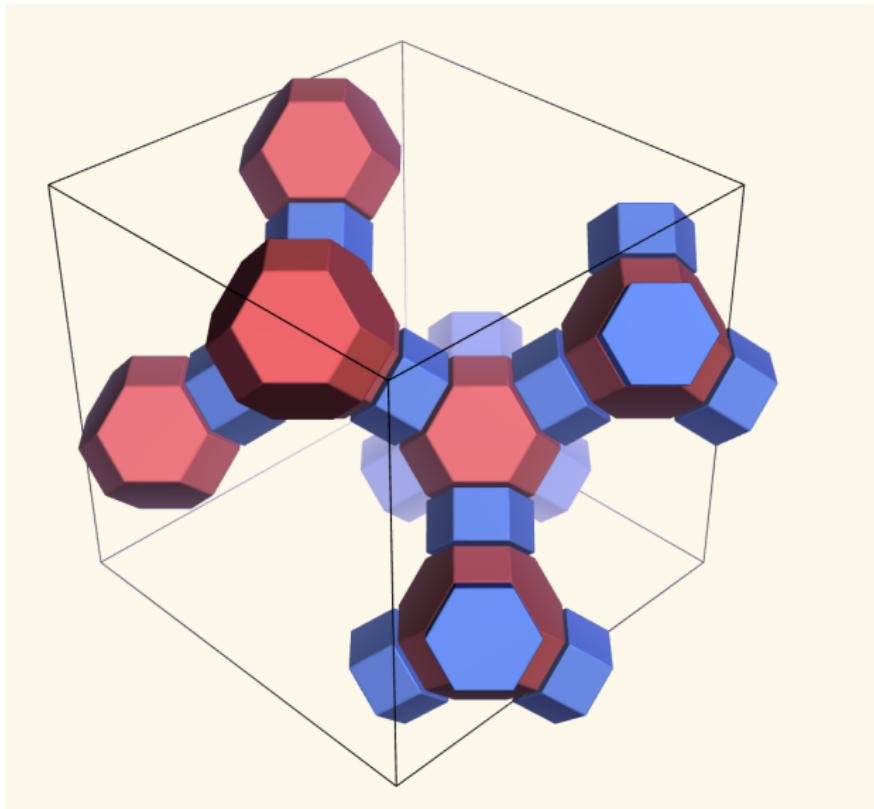
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Even richer structure from examining the cycle space.

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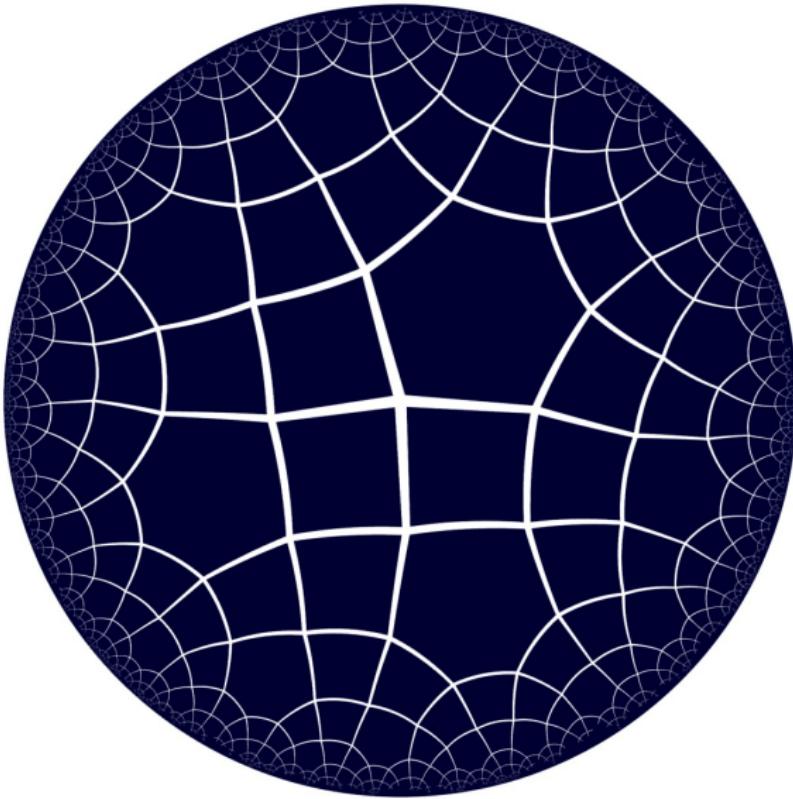
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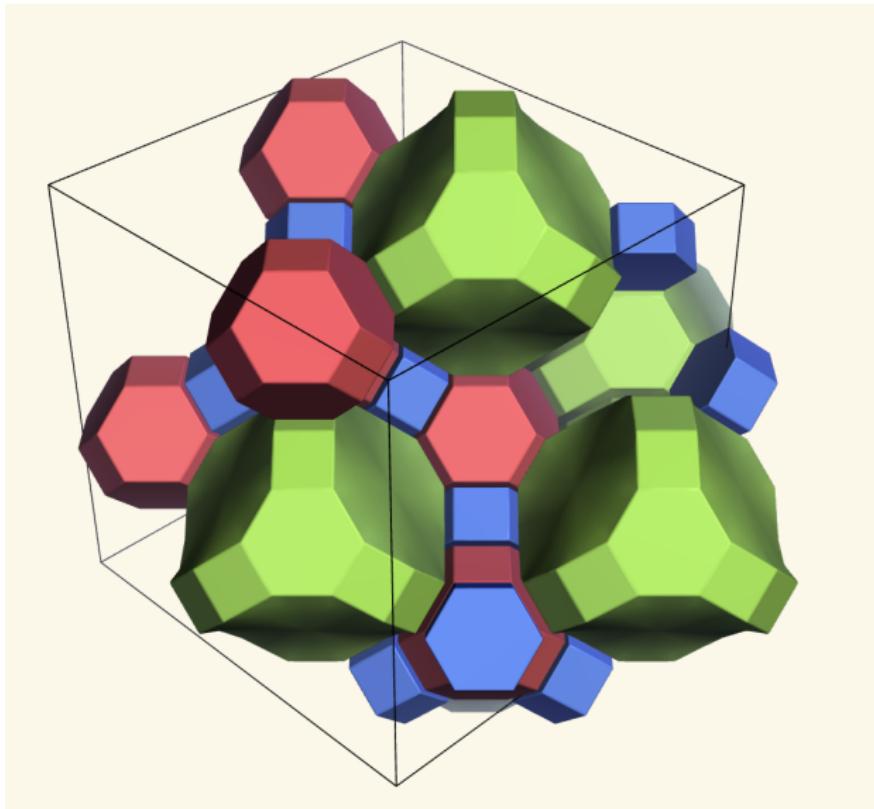
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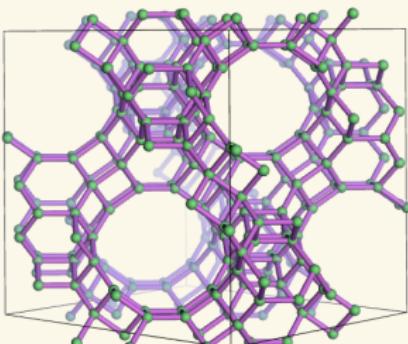
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A *net* is a connected, locally finite periodic graph.

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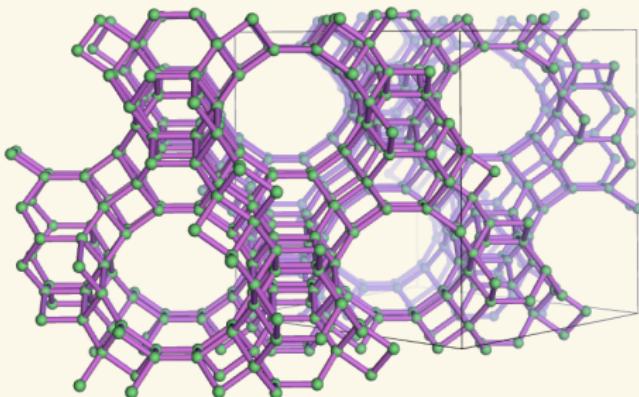
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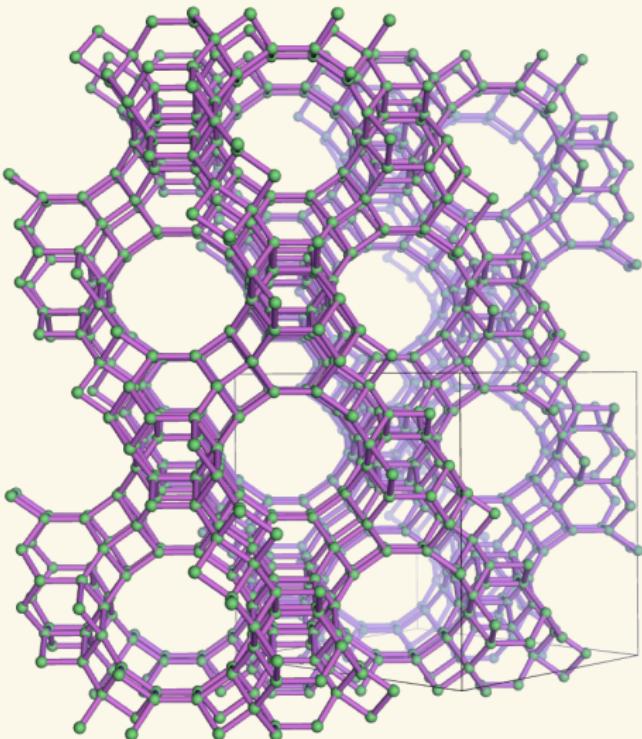
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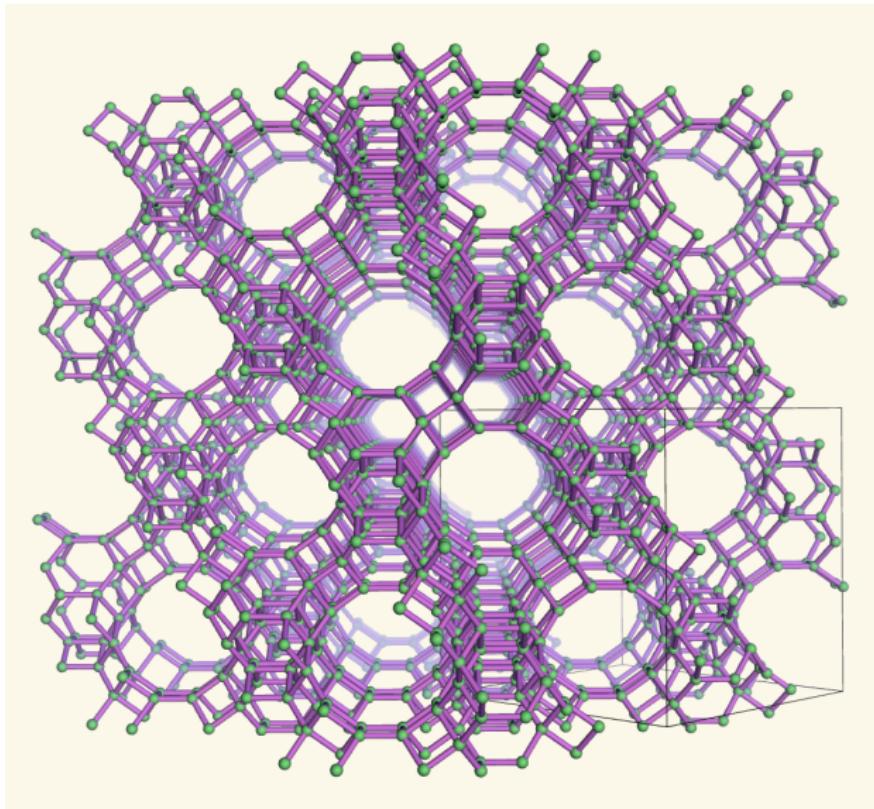
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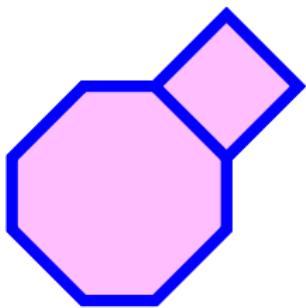
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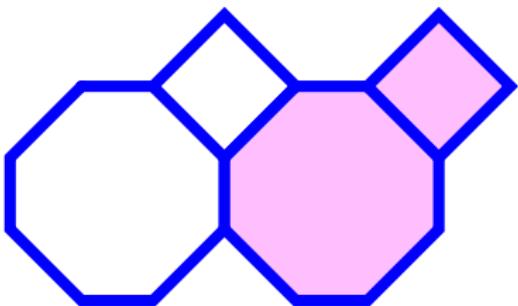
A 2-dimensional net, which here also defines a tiling.

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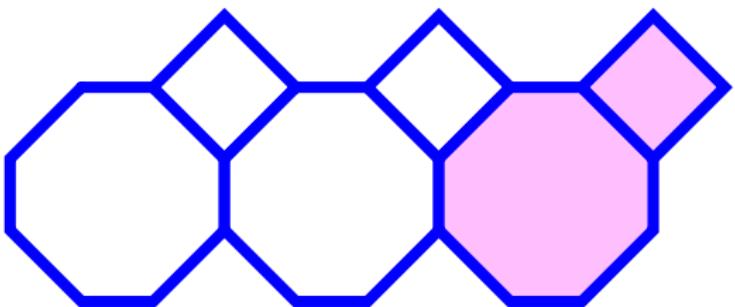
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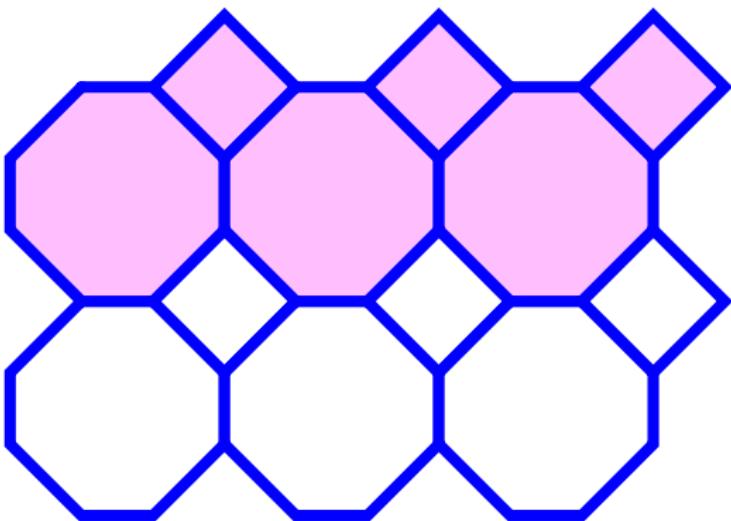
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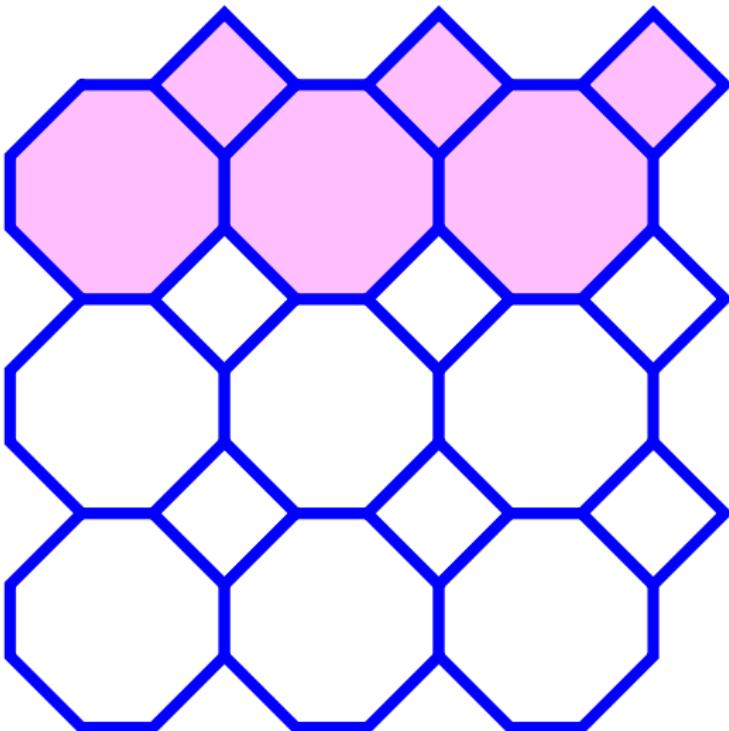
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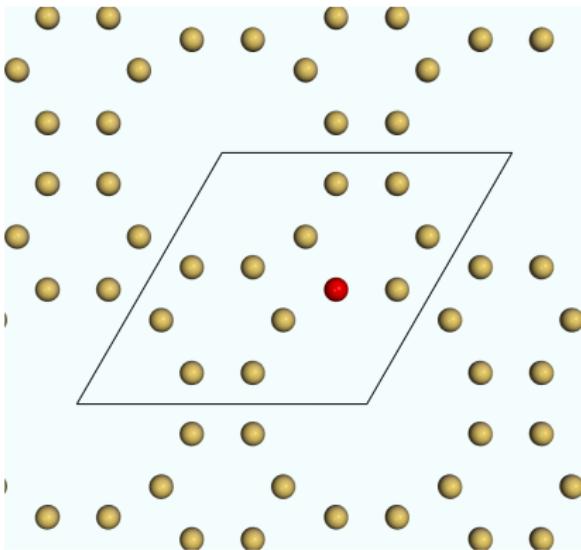
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These are just the groups that generate unbounded,  
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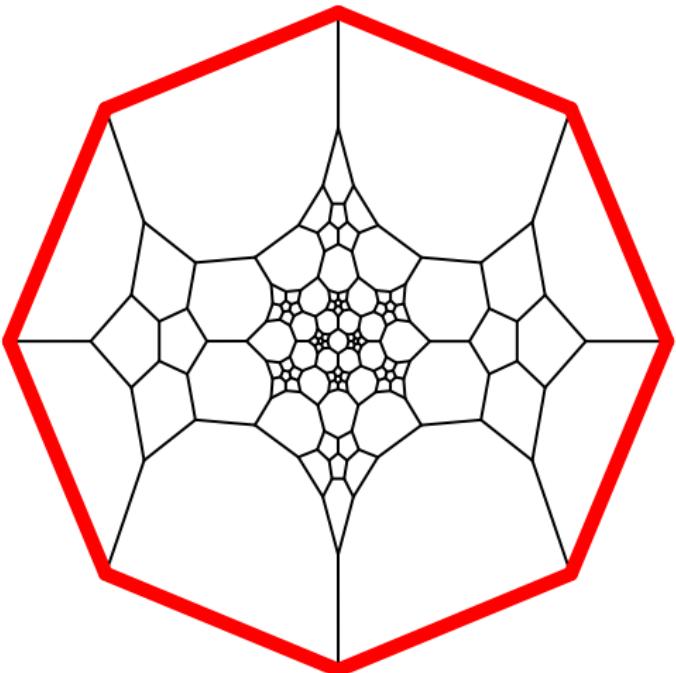
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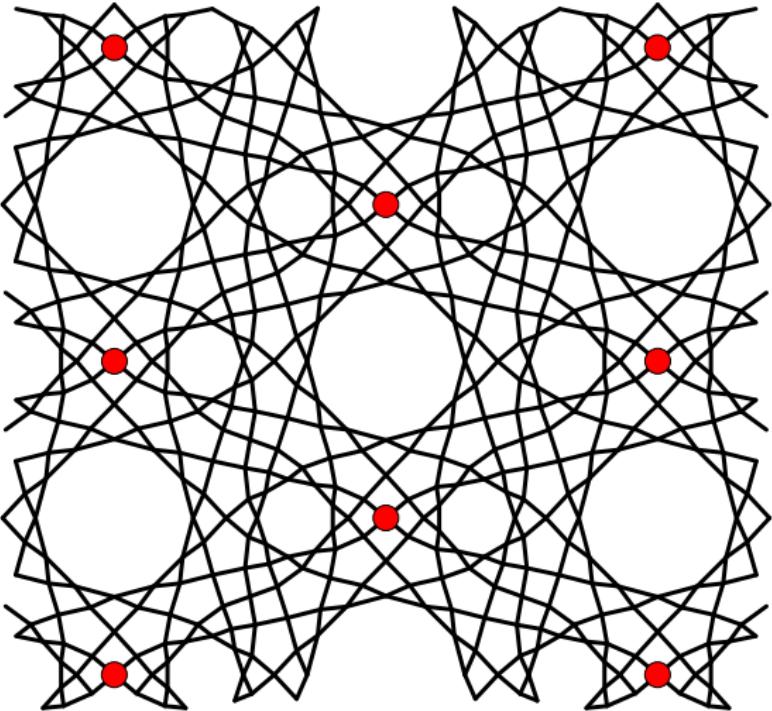
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