Olaf Delgado-Friedrichs

Order!Order? — Canberra 4 Dec 2019

When is a crystal graph not crystallographic?

Olaf Delgado

Too much symmetry

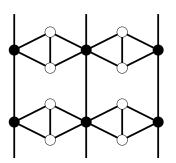
Crystal nets

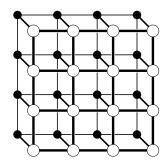
rystallographic roups

utte's barycentric embedding

Instable nets

Answer: when it has "too much symmetry".





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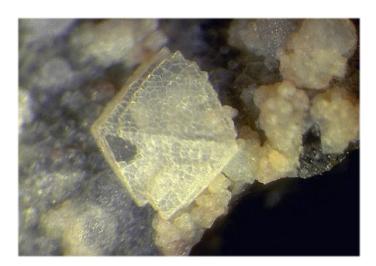
futte's barycentric embedding

Instable net

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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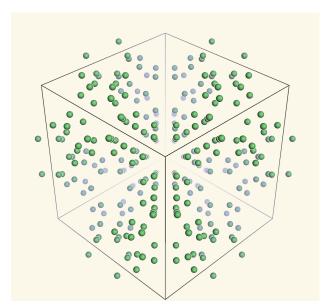
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X-ray crystallography produces something like this.

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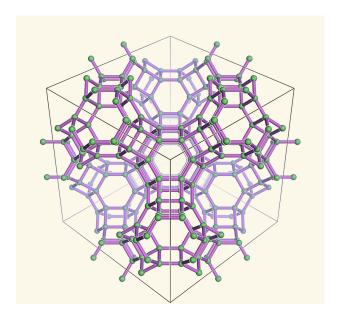
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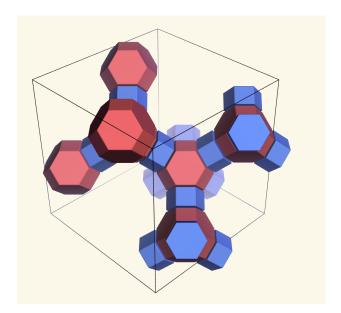
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Adding bonds (or ligands) yields a periodic graph or net.





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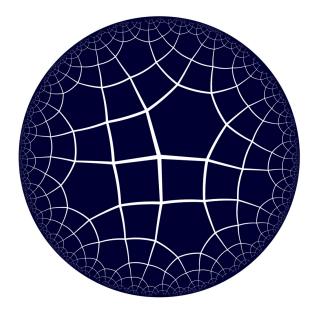
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Even richer structure from examining the cycle space.





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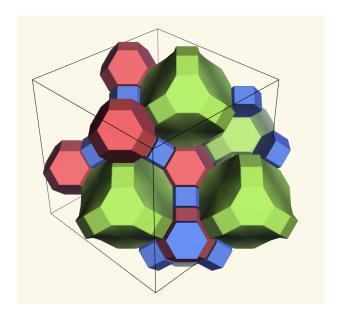
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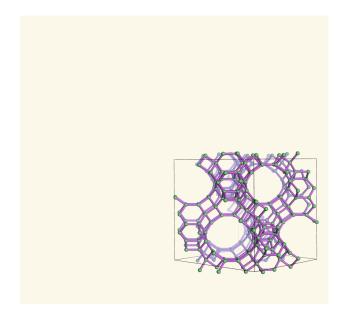
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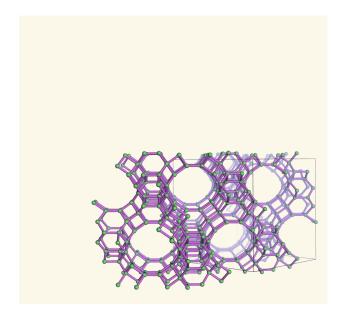
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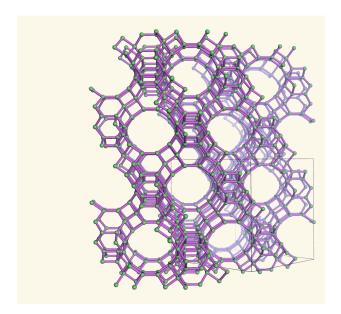
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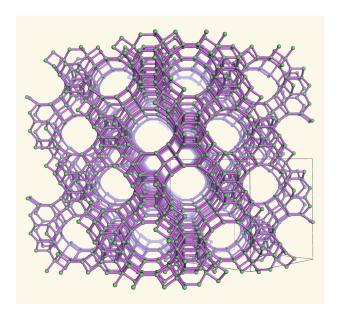
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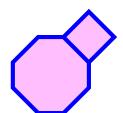
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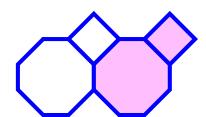
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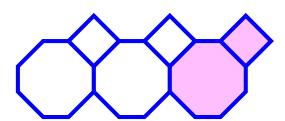
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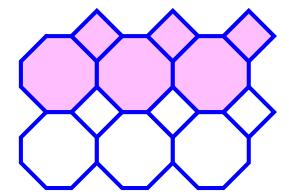
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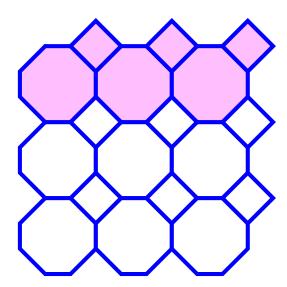




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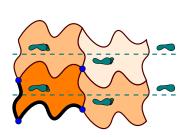
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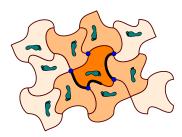
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A crystallographic (space) group is a discrete group of motions in euclidean space with a bounded fundamental domain.





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

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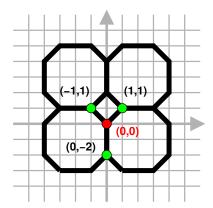
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Tutte's idea for drawing graphs "nicely":



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

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

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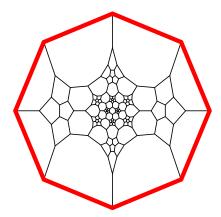
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For finite graphs, prescribe a convex outer face.



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

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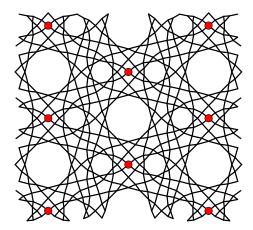
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For periodic graphs, prescribe a vertex lattice.



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

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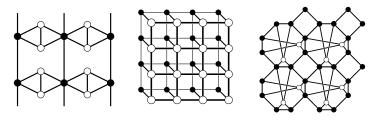
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An *unstable* net is one with colliding barycentric vertex positions.



Two non-crystallographic and one crystallographic net, all unstable.

But can non-crystallographic nets be stable?

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