

# When is a crystal graph not crystallographic?

Olaf Delgado-Friedrichs

Order!Order? — Canberra 4 Dec 2019

When is a  
crystal graph  
not  
crystallographic?

Olaf Delgado

Too much  
symmetry

Crystal nets

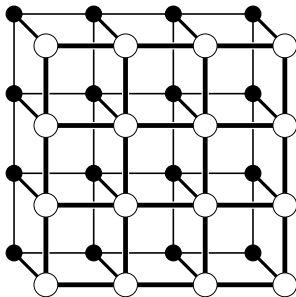
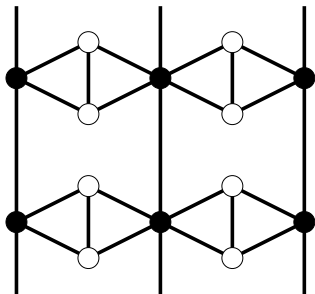
Crystallographic  
groups

Tutte's barycentric  
embedding

Unstable nets

Automorphisms to  
isometries

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.)*

When is a  
crystal graph  
not  
crystallographic?

Olaf Delgado

Too much  
symmetry

Crystal nets

Crystallographic  
groups

Tutte's barycentric  
embedding

Unstable nets

Automorphisms to  
isometries

When is a  
crystal graph  
not  
crystallographic?

Olaf Delgado

Too much  
symmetry

Crystal nets

Crystallographic  
groups

Tutte's barycentric  
embedding

Unstable nets

Automorphisms to  
isometries



A crystalline material. What might be its atomic structure?

When is a  
crystal graph  
not  
crystallographic?

Olaf Delgado

Too much  
symmetry

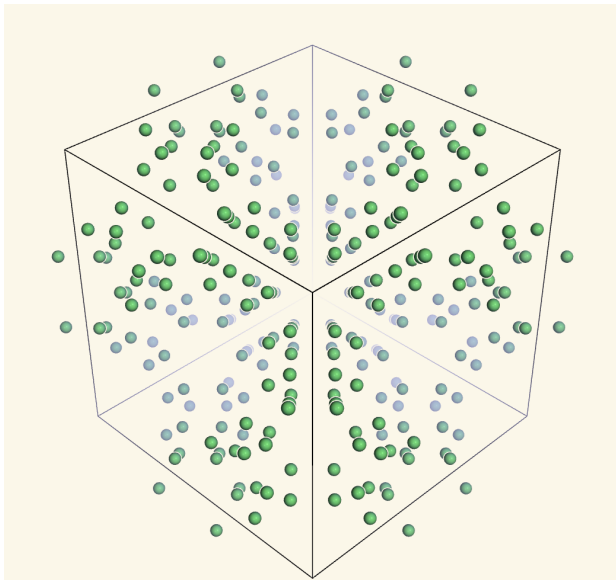
Crystal nets

Crystallographic  
groups

Tutte's barycentric  
embedding

Unstable nets

Automorphisms to  
isometries



X-ray crystallography produces something like this.

When is a  
crystal graph  
not  
crystallographic?

Olaf Delgado

Too much  
symmetry

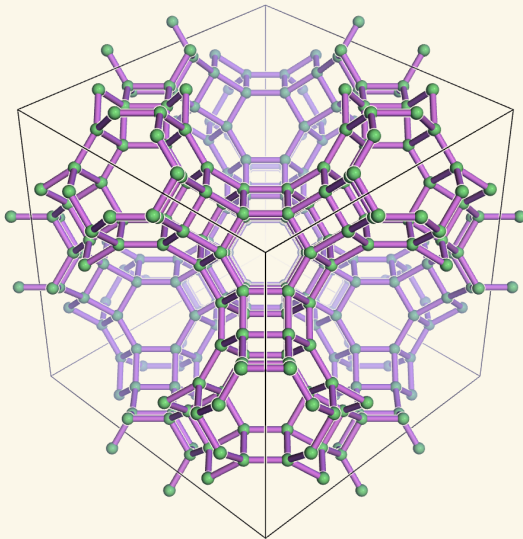
Crystal nets

Crystallographic  
groups

Tutte's barycentric  
embedding

Unstable nets

Automorphisms to  
isometries



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

When is a  
crystal graph  
not  
crystallographic?

Olaf Delgado

Too much  
symmetry

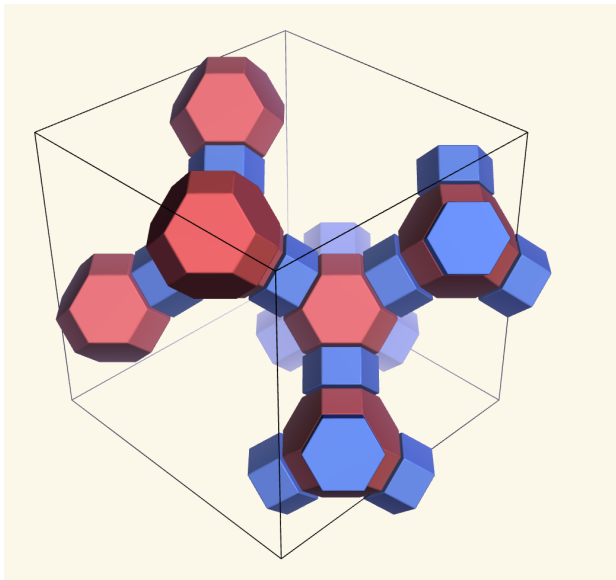
Crystal nets

Crystallographic  
groups

Tutte's barycentric  
embedding

Unstable nets

Automorphisms to  
isometries



Even richer structure from examining the cycle space.

When is a  
crystal graph  
not  
crystallographic?

Olaf Delgado

Too much  
symmetry

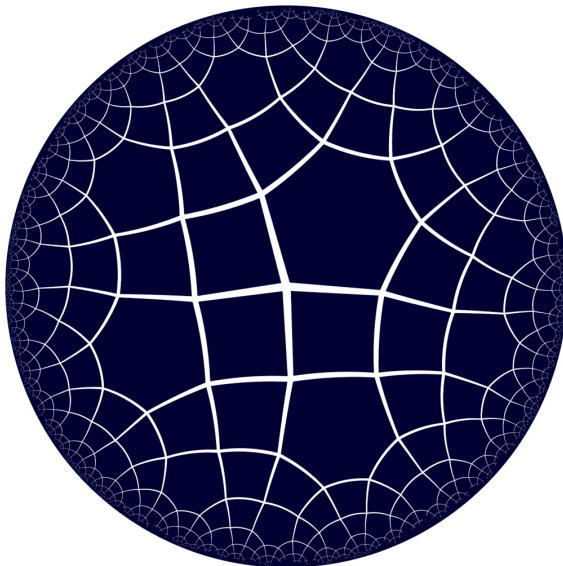
Crystal nets

Crystallographic  
groups

Tutte's barycentric  
embedding

Unstable nets

Automorphisms to  
isometries



Even richer structure from examining the cycle space.

When is a  
crystal graph  
not  
crystallographic?

Olaf Delgado

Too much  
symmetry

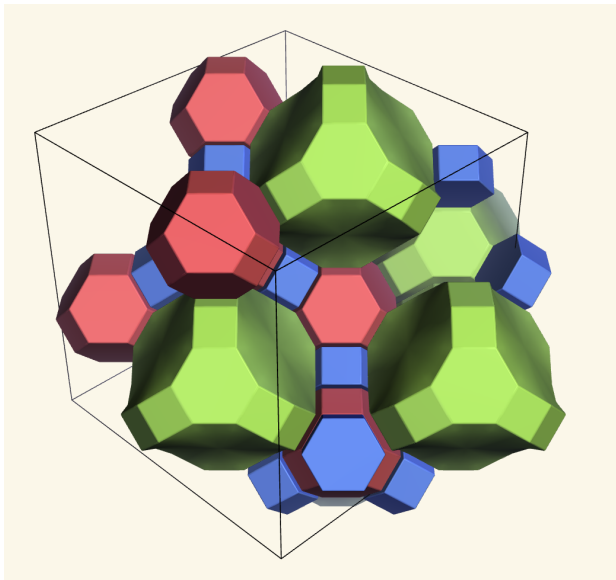
Crystal nets

Crystallographic  
groups

Tutte's barycentric  
embedding

Unstable nets

Automorphisms to  
isometries



Even richer structure from examining the cycle space.



When is a  
crystal graph  
not  
crystallographic?

Olaf Delgado

Too much  
symmetry

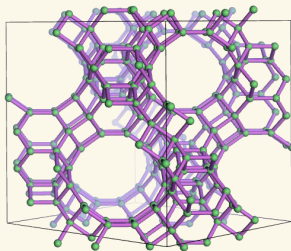
Crystal nets

Crystallographic  
groups

Tutte's barycentric  
embedding

Unstable nets

Automorphisms to  
isometries



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

When is a  
crystal graph  
not  
crystallographic?

Olaf Delgado

Too much  
symmetry

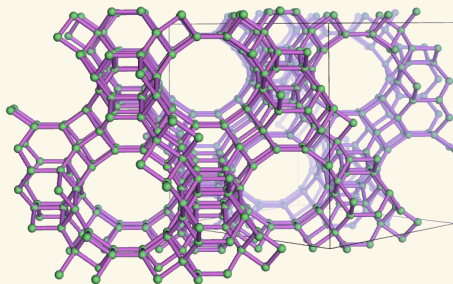
Crystal nets

Crystallographic  
groups

Tutte's barycentric  
embedding

Unstable nets

Automorphisms to  
isometries



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

When is a  
crystal graph  
not  
crystallographic?

Olaf Delgado

Too much  
symmetry

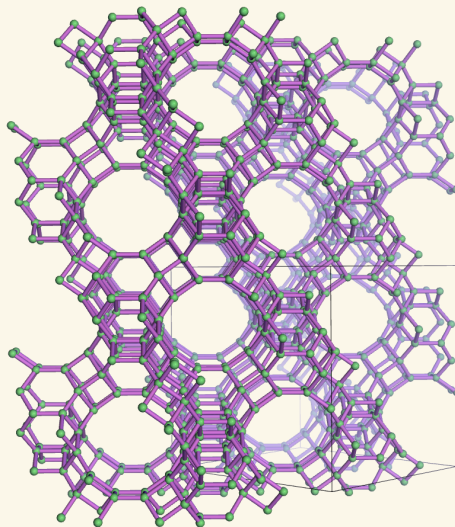
Crystal nets

Crystallographic  
groups

Tutte's barycentric  
embedding

Unstable nets

Automorphisms to  
isometries



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

When is a  
crystal graph  
not  
crystallographic?

Olaf Delgado

Too much  
symmetry

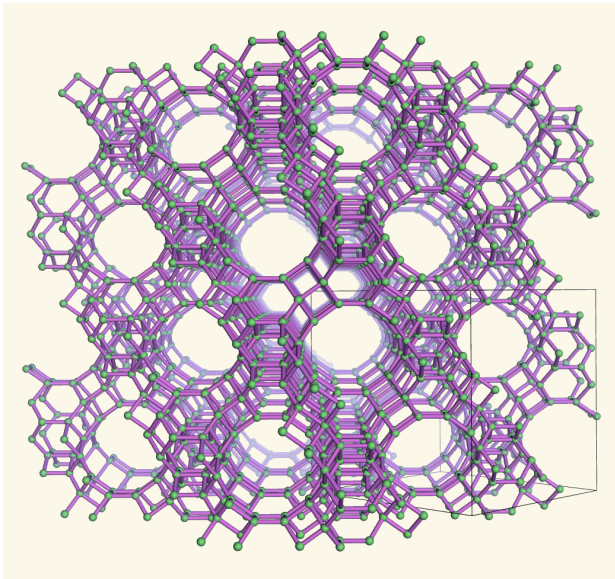
Crystal nets

Crystallographic  
groups

Tutte's barycentric  
embedding

Unstable nets

Automorphisms to  
isometries



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

When is a  
crystal graph  
not  
crystallographic?

Olaf Delgado

Too much  
symmetry

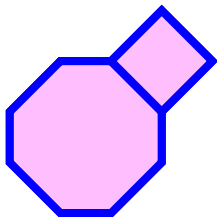
Crystal nets

Crystallographic  
groups

Tutte's barycentric  
embedding

Unstable nets

Automorphisms to  
isometries



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

When is a  
crystal graph  
not  
crystallographic?

Olaf Delgado

Too much  
symmetry

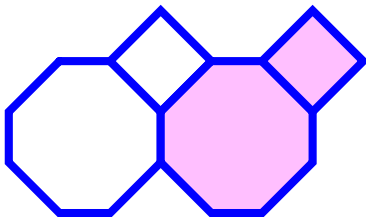
Crystal nets

Crystallographic  
groups

Tutte's barycentric  
embedding

Unstable nets

Automorphisms to  
isometries



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

When is a  
crystal graph  
not  
crystallographic?

Olaf Delgado

Too much  
symmetry

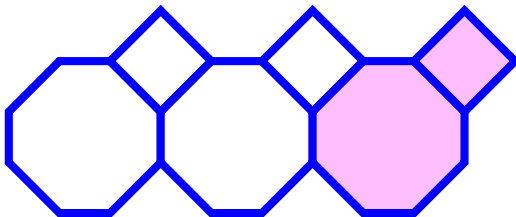
Crystal nets

Crystallographic  
groups

Tutte's barycentric  
embedding

Unstable nets

Automorphisms to  
isometries



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

When is a  
crystal graph  
not  
crystallographic?

Olaf Delgado

Too much  
symmetry

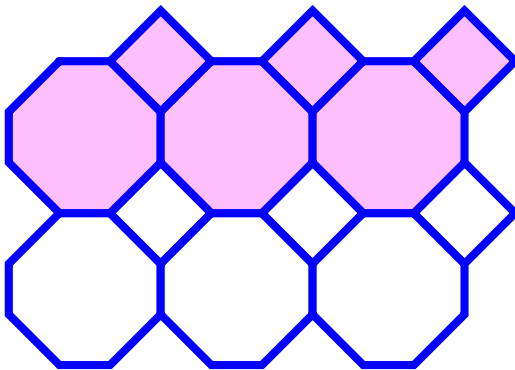
Crystal nets

Crystallographic  
groups

Tutte's barycentric  
embedding

Unstable nets

Automorphisms to  
isometries



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



When is a  
crystal graph  
not  
crystallographic?

Olaf Delgado

Too much  
symmetry

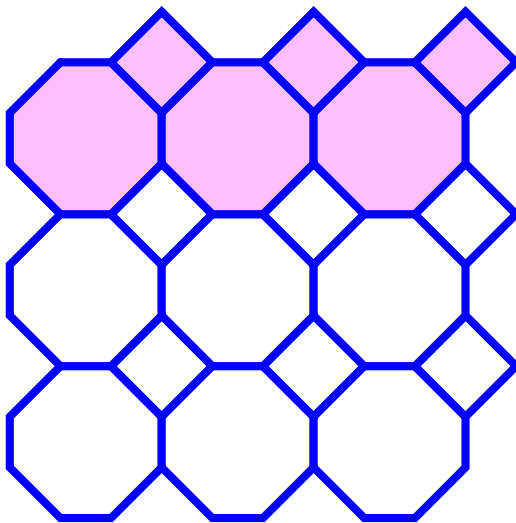
Crystal nets

Crystallographic  
groups

Tutte's barycentric  
embedding

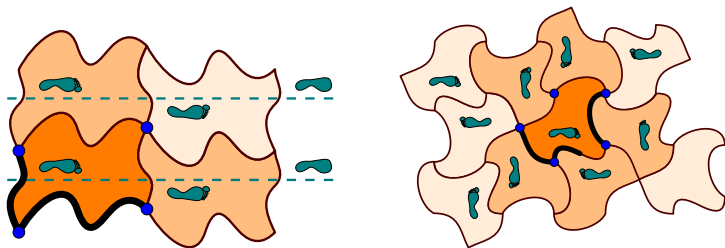
Unstable nets

Automorphisms to  
isometries



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.



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

Too much  
symmetry

Crystal nets

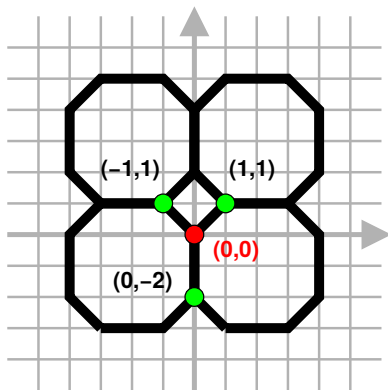
Crystallographic  
groups

Tutte's barycentric  
embedding

Unstable nets

Automorphisms to  
isometries

Tutte's idea for drawing graphs “nicely”:



When is a  
crystal graph  
not  
crystallographic?

Olaf Delgado

Too much  
symmetry

Crystal nets

Crystallographic  
groups

Tutte's barycentric  
embedding

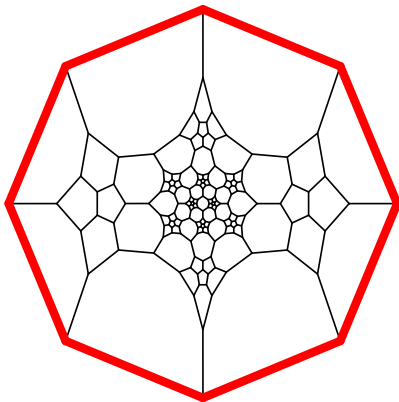
Unstable nets

Automorphisms to  
isometries

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

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

For finite graphs, prescribe a convex outer face.



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

When is a  
crystal graph  
not  
crystallographic?

Olaf Delgado

Too much  
symmetry

Crystal nets

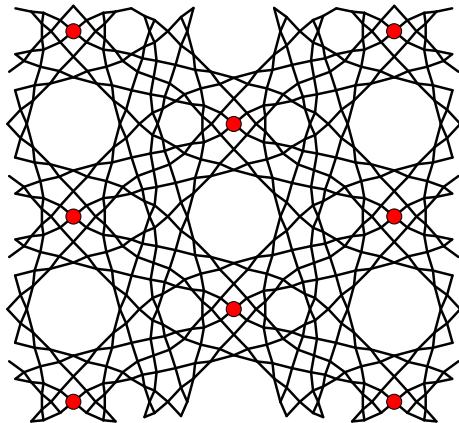
Crystallographic  
groups

Tutte's barycentric  
embedding

Unstable nets

Automorphisms to  
isometries

For periodic graphs, prescribe a vertex lattice.



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

When is a  
crystal graph  
not  
crystallographic?

Olaf Delgado

Too much  
symmetry

Crystal nets

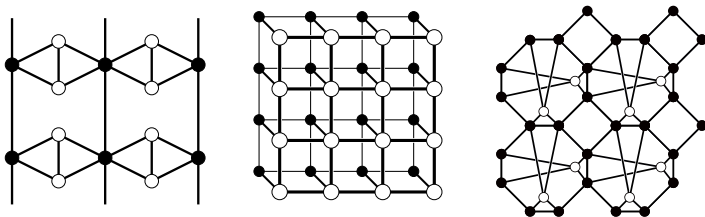
Crystallographic  
groups

Tutte's barycentric  
embedding

Unstable nets

Automorphisms to  
isometries

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?

Too much  
symmetry

Crystal nets

Crystallographic  
groups

Tutte's barycentric  
embedding

Unstable nets

Automorphisms to  
isometries

When is a  
crystal graph  
not  
crystallographic?

Olaf Delgado

Too much symmetry

## Crystal nets

## Crystallographic groups

Tutte's barycentric embedding

## Unstable nets

## Automorphisms to isometries

