Nanocones

A classification result in chemistry

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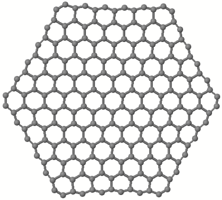
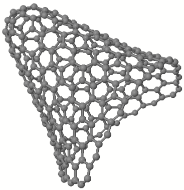
Carbon networks

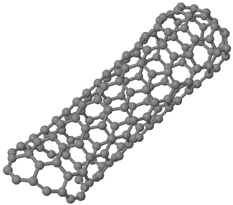
graphite



nanocone



nanotube

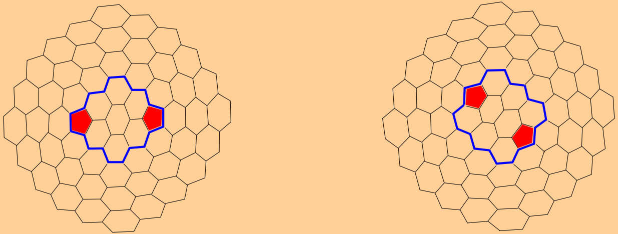


all structures infinite

Equivalent structures

Definition

Two infinite structures are called *equivalent* iff a finite part in both of them can be removed so that the (infinite) remainders are isomorphic.



Classification

graphite (0 pentagons)

unique structure – so 1 class only

cone with 1 pentagon

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nanotubes (6 pentagons)

infinitely many structures **and** infinitely many equivalence classes

a finite number of tubes in each class

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2 to 4 pentagons

infinitely many structures – 2 classes

5 pentagons

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First: D.J. Klein (2002)
independently C. Justus (2007)
Also some parts of what follows!

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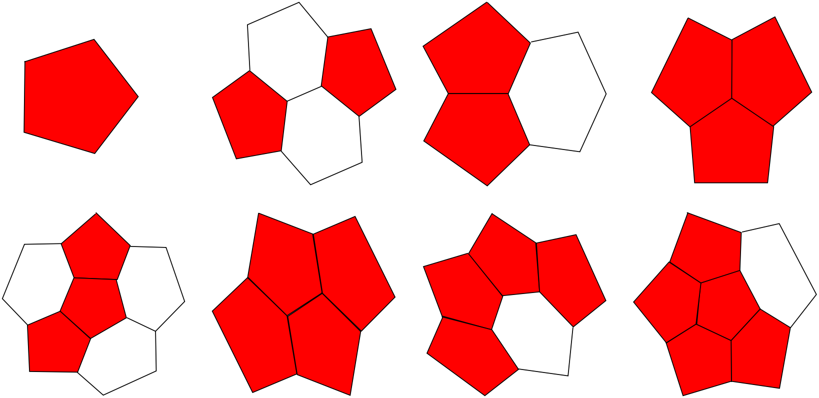

Why still another and independent proof?

- in fact the basic **very general** classification result is already from 1997 (Ludwig Balke)
- very easy (using Balke's result)
- very easy also for other structures – you could e.g. immediately work out the classes for square-cones or even cones of more complicated periodic structures

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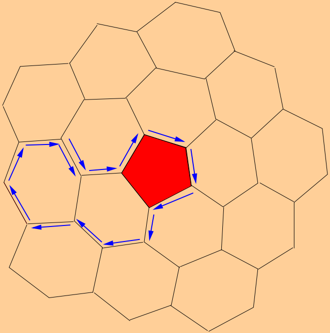
Theorem (L. Balke (1997) rephrased for these circumstances)

A disordered periodic tiling is up to equivalence characterized by

- *the periodic tiling $\mathcal{T}$ that is disordered (the hexagonal lattice in this case)*
- *a* winding number *(can be neglected here)*
- *a conjugacy class of an automorphism in the symmetry group of $\mathcal{T}$*

Take **any** closed path around the disorder.



Here: llrrrlrrlrrrr.

Follow the **same** path llrrrlrrlrrrr in the lattice

A counterclockwise rotation by 60 degrees.

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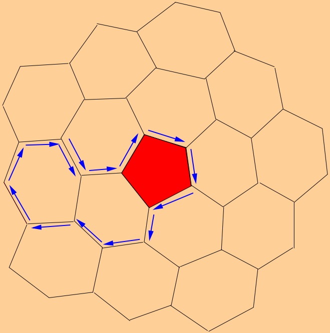

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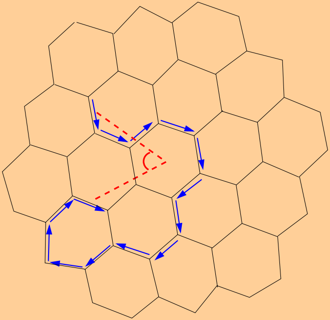
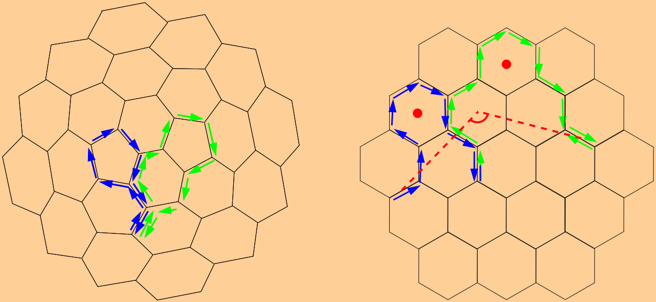


A counterclockwise rotation by 60 degrees.

The path around two pentagons corresponds to the product of two paths – the rotation corresponds to the product of two rotations by 60 degrees.



This allows to determine possible equivalence classes.

Example: 3 pentagons

There are two such conjugacy classes in the symmetry group:

- rotation around the center of an edge
- rotation around the center of a face.

So two candidate classes.

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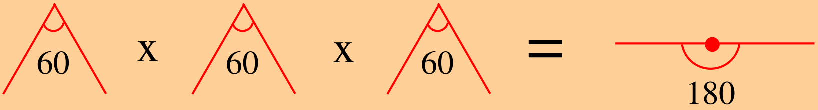

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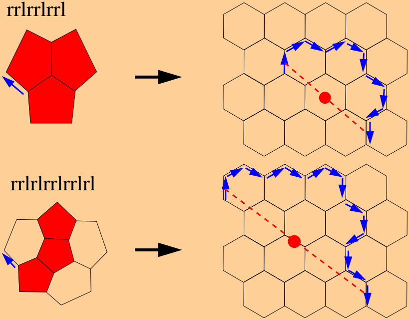
Both classes exist for 3 pentagons



Balke: proof of existence for **general** disorders – not necessarily of the form needed here.

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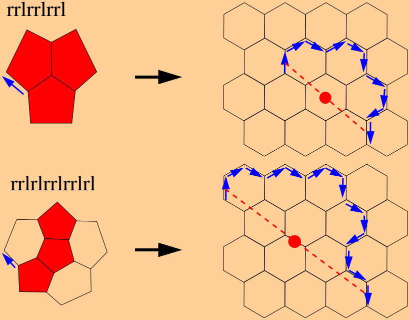

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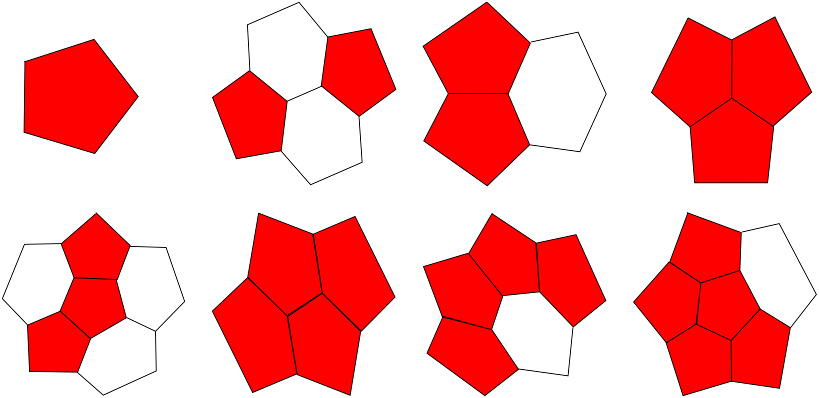

Further classification

In the equivalence classes for nanotubes the region with the pentagons is bounded – the parameters of the class allow to compute upper bounds for this *disordered region*!

Aim

Take the localization of the defects also into account for cones. Classify by innermost paths of a certain form.

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Definitions

Assume $2 \leq p \leq 5$ fixed.

Definition

A closed path of the form $((lr)^m r)^{6-p}$ (for some m) is called a symmetric path (for p and m).

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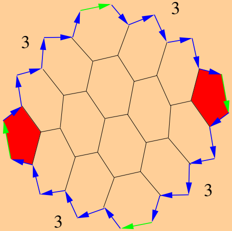
"symmetric" conepath



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Note: always $6 - p$ edges with two times right

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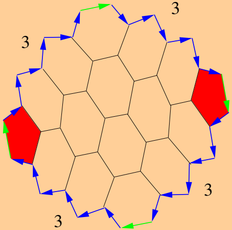

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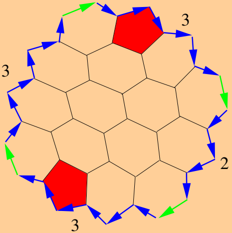

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Definitions

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A closed path in a cone is called a conepath if it is symmetric or nearsymmetric, shares an edge with a pentagon and has only hexagons in its exterior.

Finer classification of cones

Theorem

- *In every cone there is a* **unique** *cone path.*

  unless $p = 2$ *and there is an nearsymmetric conepath.*
  In this case there are exactly two isomorphic conepaths with isomorphic interior.

Finer classification of cones

Theorem

So there is a 1-1 correspondence between caps (interiors of cone paths) and cones.

Note

The corresponding result does not hold for nanotubes.

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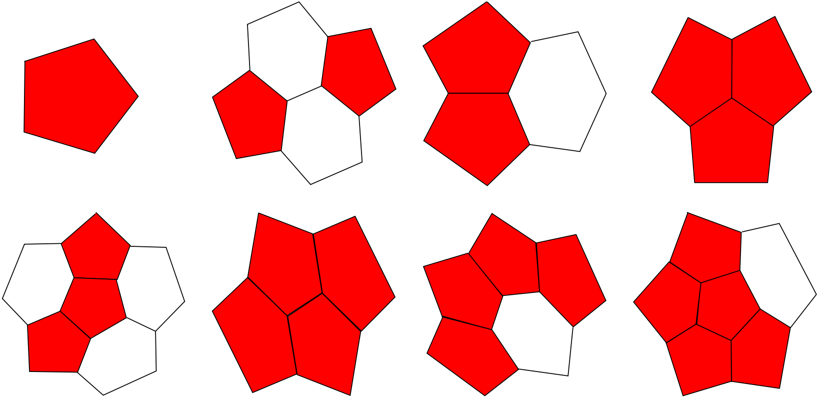
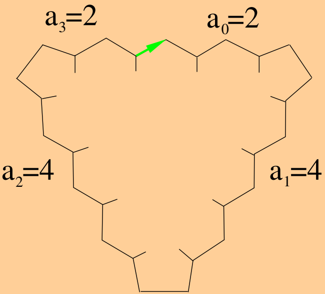
Sketch of the existence proof

Each cone is equivalent to exactly one of the following cones



Sketch of the uniqueness proof

cone



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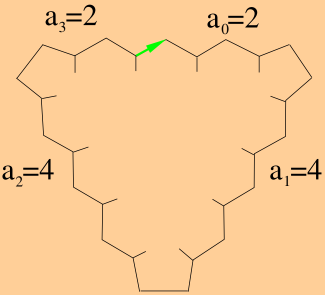
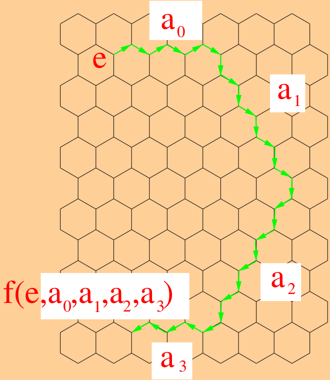


graphite lattice



Sketch of the uniqueness proof

Method

- if two conepaths exist, they are of the same *type* and share and edge e
- following the two paths in the lattice from the same starting edge gives the same endedge – so $f(e, a_0, \ldots, a_k) = f(e, a'_0, \ldots, a'_k)$
- solve the equations for the different possible variables a_i

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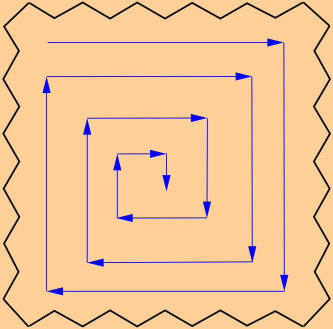
Construction of cone caps

Easy: conecaps are pseudo-convex and therefore have an inner spiral



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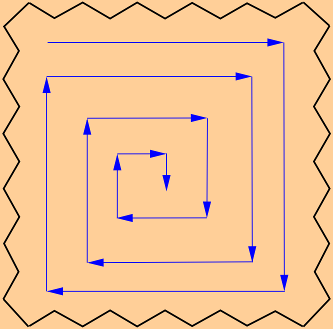

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Construction of cone caps with two pentagons

All possible positions of the pentagons can be computed directly!

Idea

knowing the center of the rotation given by the boundary, one pentagon determines the position of the other

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symmetric cones with two pentagons: $\lceil \frac{m+1}{2} \rceil$
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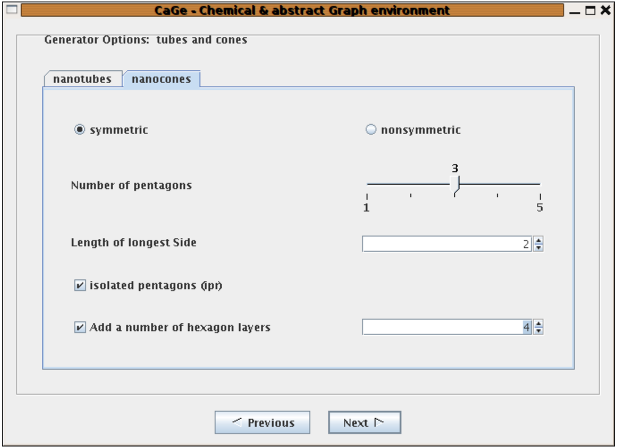
Some results

Example: 3 pentagons, symmetric conepath

sidelength	number cones	min atoms	max atoms
5	18	58	82
10	124	163	261
15	387	318	542
20	915	523	921
25	1.757	778	1.402
30	3.039	1.083	1.981
35	4.793	1.438	2.662
40	7.164	1.843	3.441
45	10.162	2.298	4.322
50	13.955	2.803	5.301

CaGe

The program can be used inside the environment CaGe:



http://caagt.ugent.be/CaGe