# Nanocones

## A classification and generation result in chemistry

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# Outline



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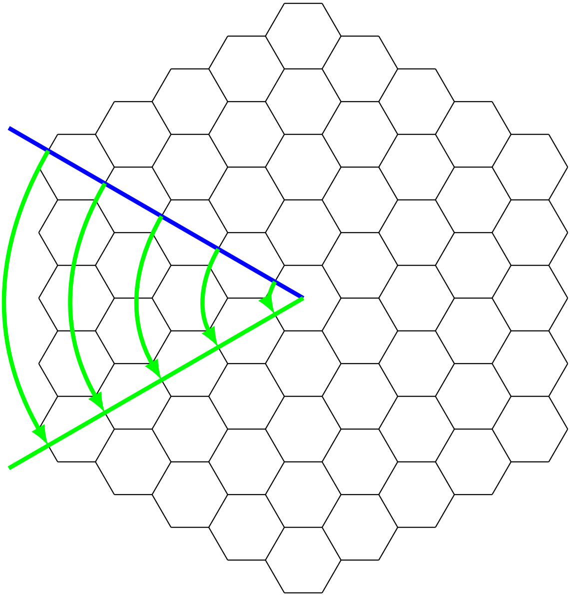
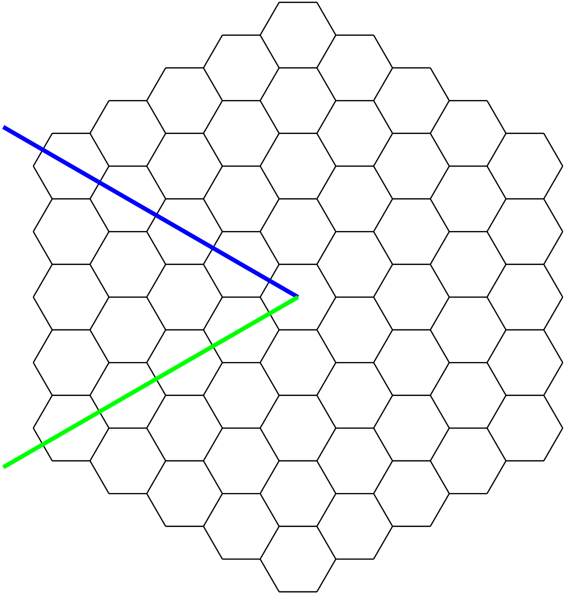
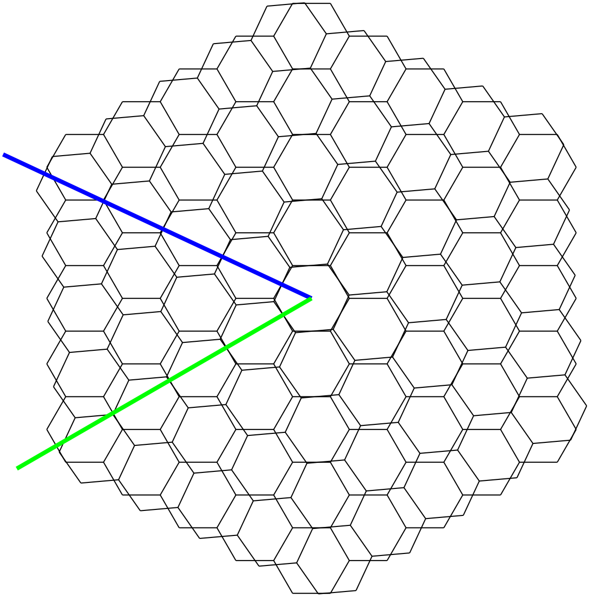
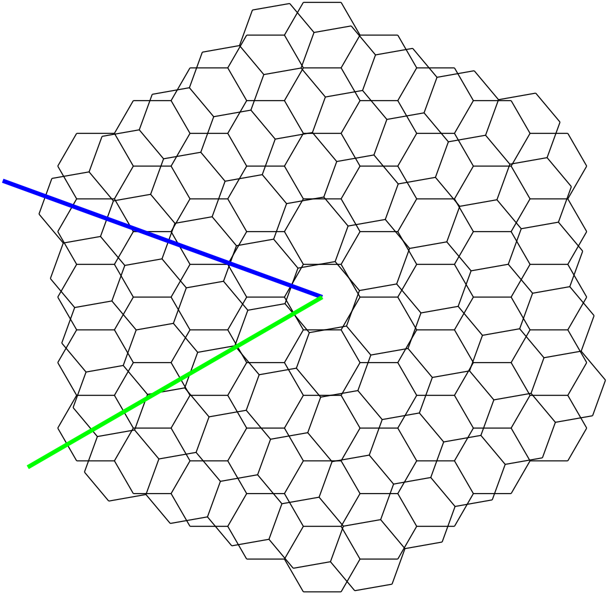
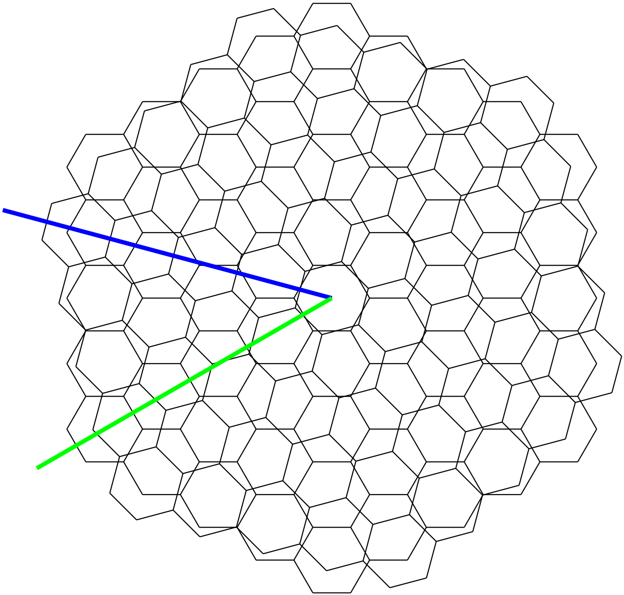
# Nón lá

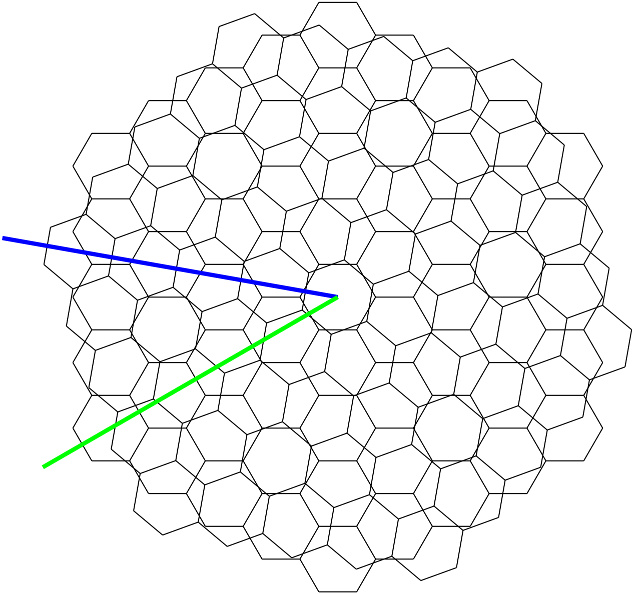


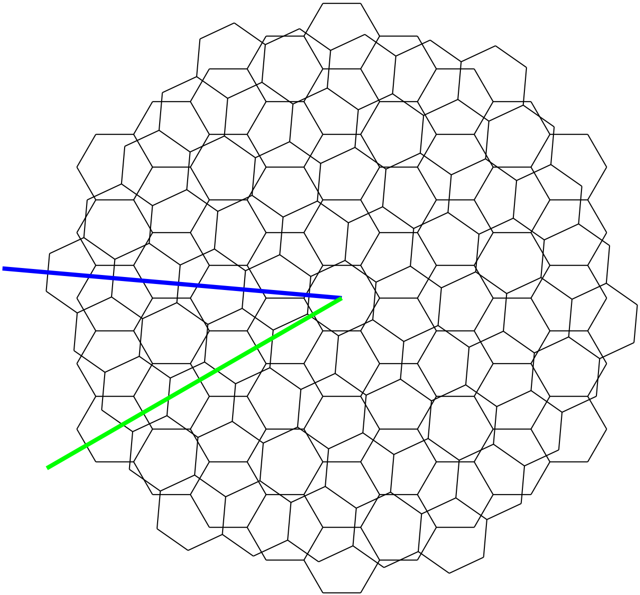


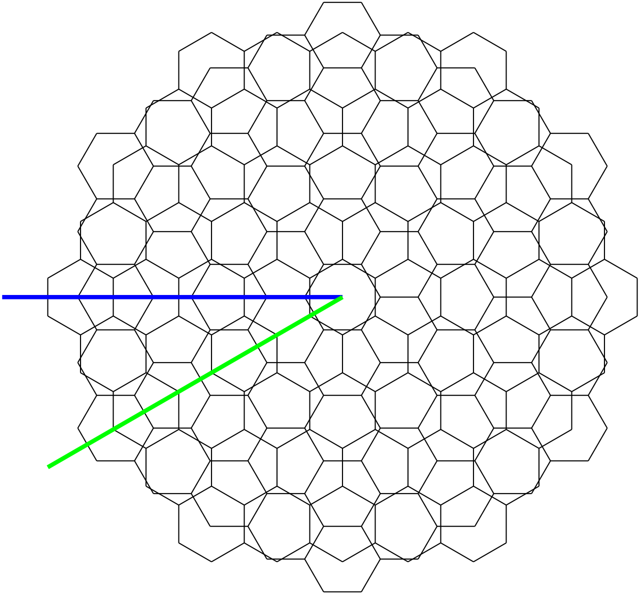


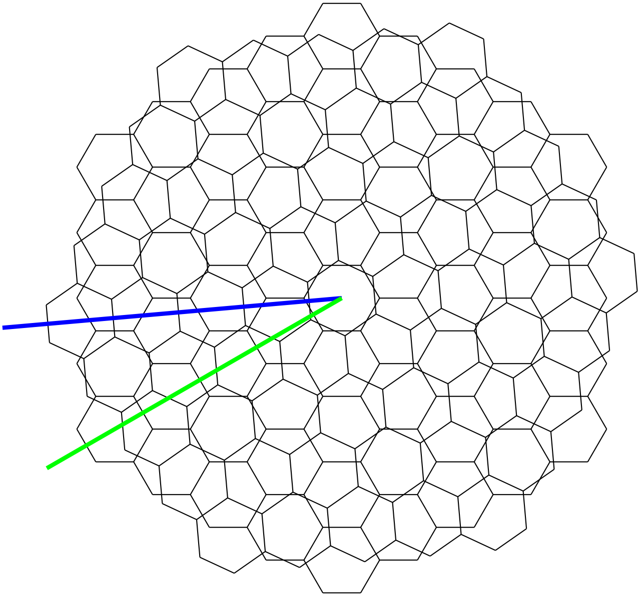


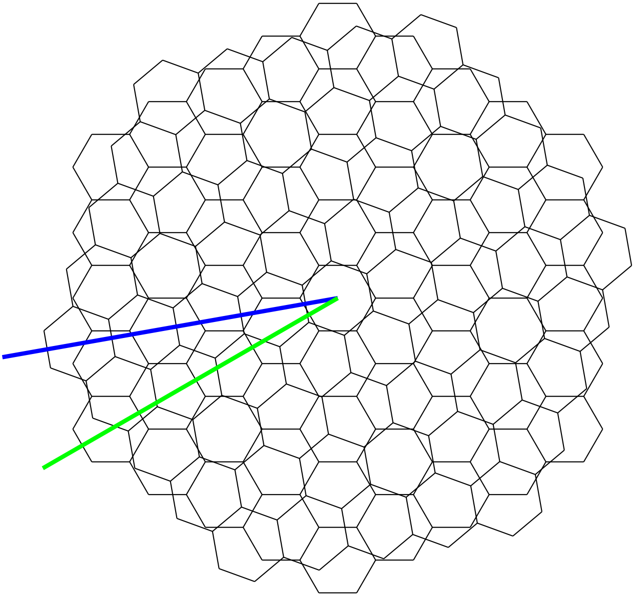


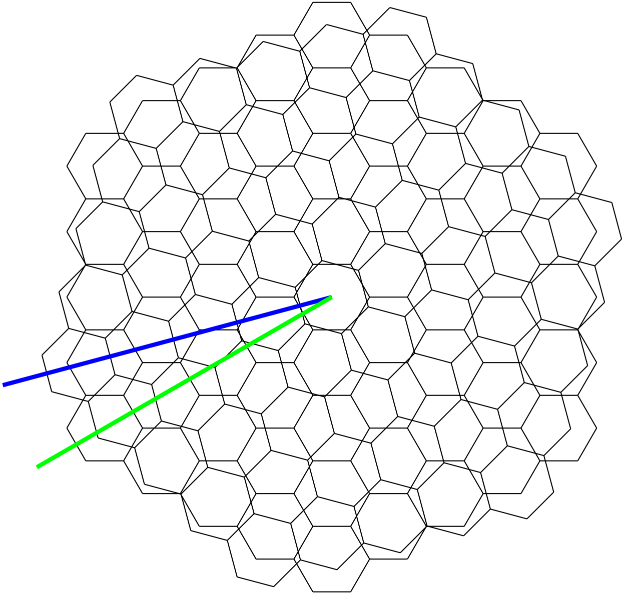


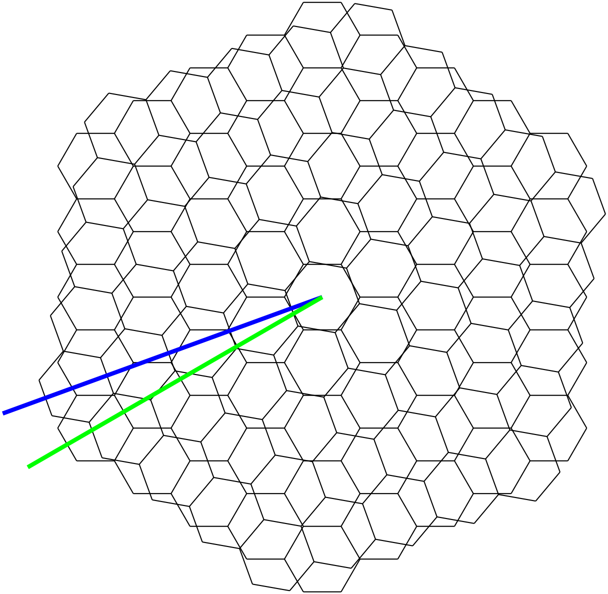


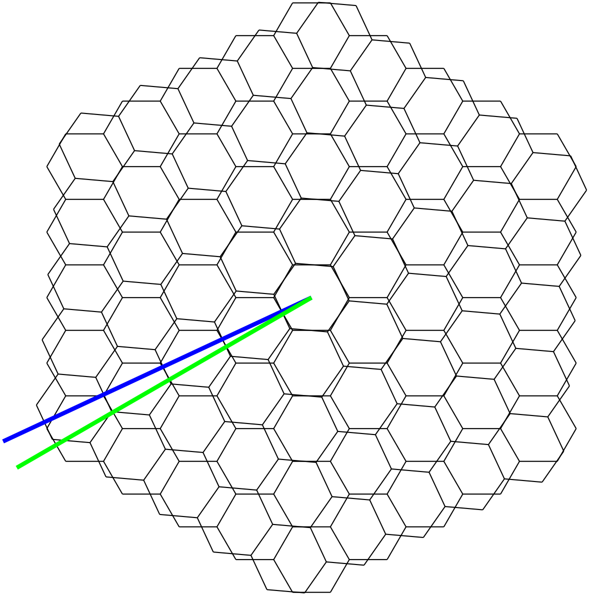


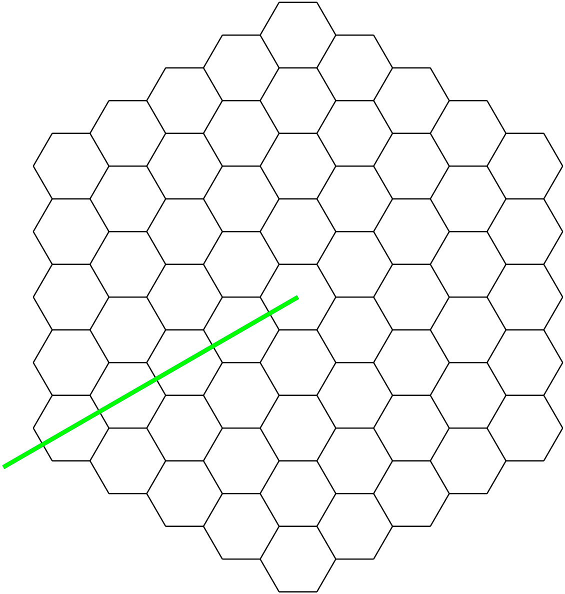


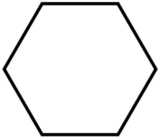


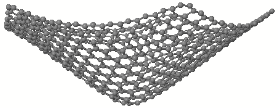


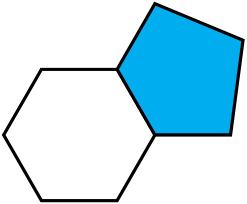


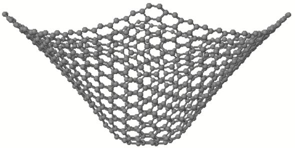


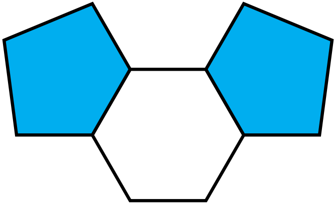


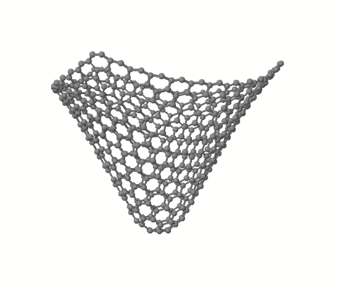


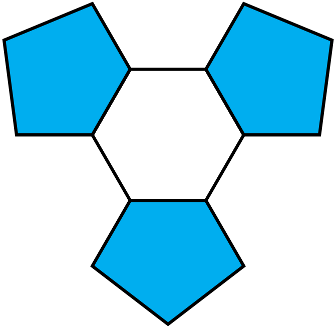


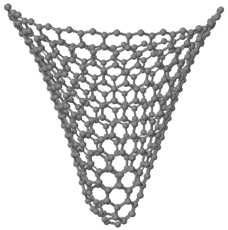


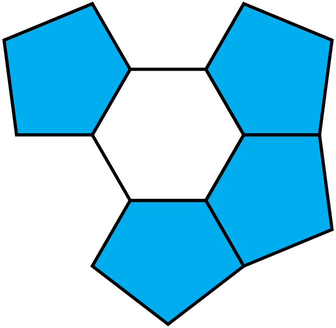


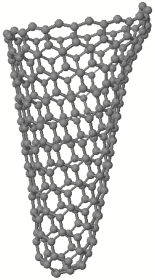


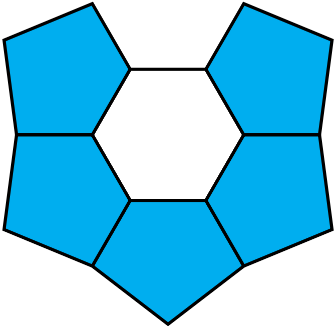


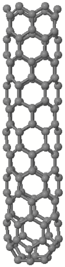


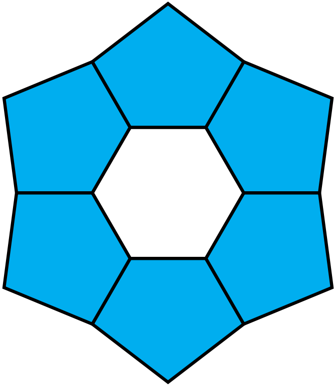






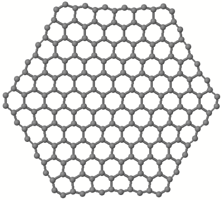




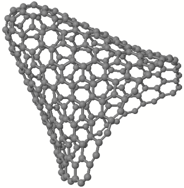


# Carbon networks

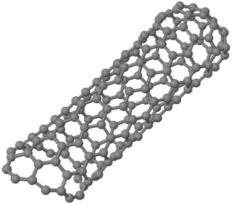
graphene



nanocone



nanotube



all structures infinite

# Definition

## Nanocone (graph)

A nanocone (graph) is an infinite, cubic, 3-connected, plane graph with $1 \leq p \leq 5$ pentagonal faces and all remaining faces hexagonal.

# Classification of cones

## History

First: D. Klein and A. Balaban (2002,2006)

# Why a new classification?

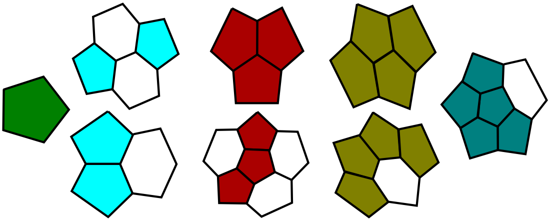
- an application of an abstract classification result of disordered tilings by L. Balke (1997)
- very easy (using Balke's result)
- very easy also for other structures – you could, e.g., immediately work out the classes for quadrangle cones or even cones of more complicated periodic structures

# Outline

# Classification

## Summary

- Infinite number of nanocones
- 8 (infinite) classes based on cone body



# Classification

**graphene (0 pentagons)**

unique structure – so 1 class only

**cone with 1 pentagon**

unique structure – so 1 class only

**nanotubes (6 pentagons)**

infinitely many structures **and** infinitely many equivalence classes
a finite number of tubes in each class

# Classification of cones

**cone with 1 pentagon**

unique structure – 1 class

**2 to 4 pentagons**

infinitely many structures – 2 classes

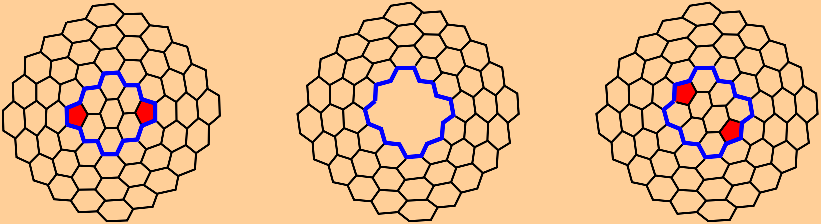
**5 pentagons**

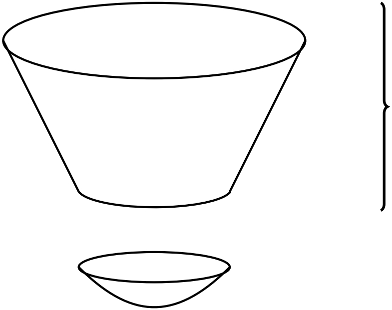
infinitely many structures – 1 class

# Equivalent structures

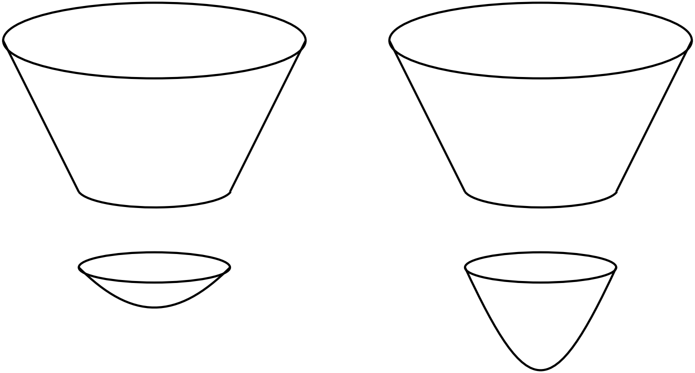
## Definition

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

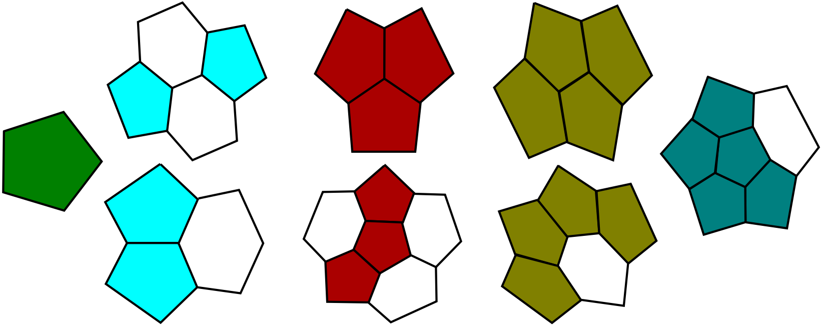




isomorphic cone body ⇒ equivalent



Each cone is equivalent to exactly one of the following cones (only caps shown)



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

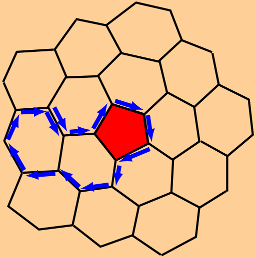
*A disordered periodic tiling is up to equivalence characterized by*

- *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 $\mathcal{T}$ (rotations of $p \times 60$ degrees)*

**Theorem**

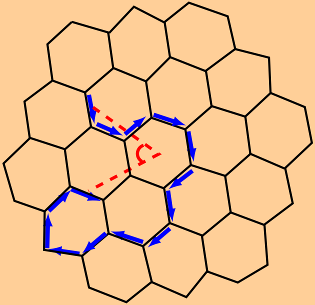
Two nanocones are equivalent if and only if they correspond to the same conjugacy class of rotations in the symmetry group of the hexagonal lattice.

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



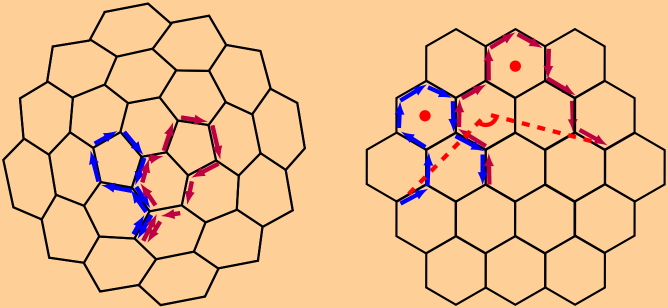
Here: llrrrlrrlrrrr.

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



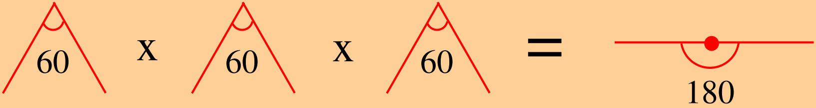
A counterclockwise rotation by 60 degrees.

- Following two paths after each other corresponds to product of rotation.
- Following two paths after each other is equivalent to following one path around both disorders.



This allows to determine possible equivalence classes.

## Example: 3 pentagons

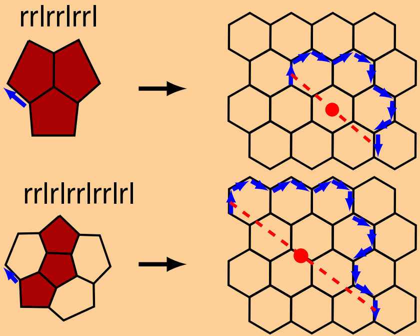



There are two 180 degrees rotation conjugacy classes in the symmetry group of the hexagonal lattice:

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

So two candidate classes.

## Both classes exist for 3 pentagons



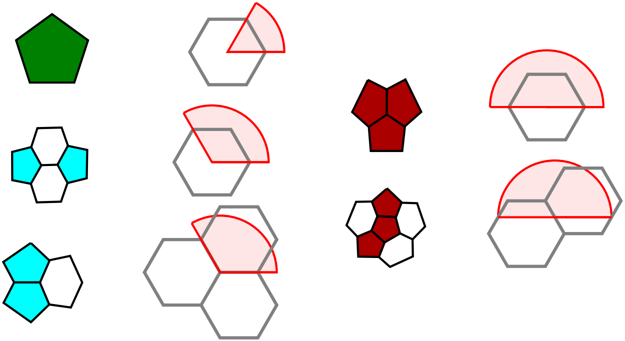

Balke: proof of existence for **general** disorders – not necessarily of the form needed here.

# Conjugacy classes of rotations

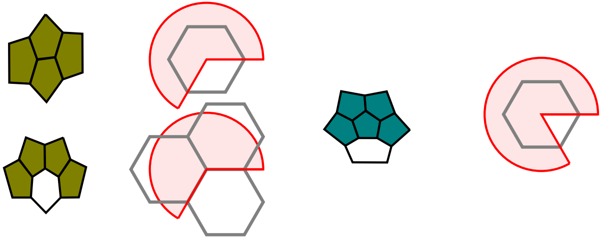
There are 8 conjugacy classes of rotations of $p \times 60$ degrees counterclockwise with $1 \leq p \leq 5$:

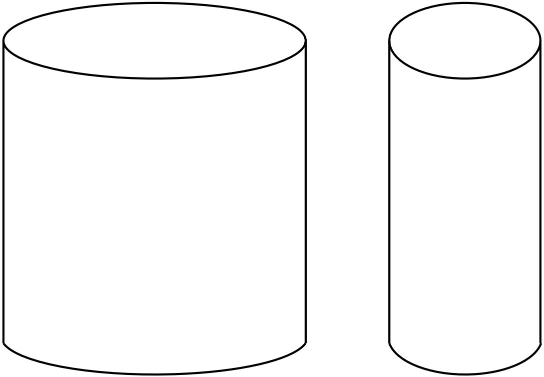
- 60 degrees around center of face
- 120 degrees around center of face
- 120 degrees around vertex
- 180 degrees around center of face
- 180 degrees around center of edge
- 240 degrees around center of face
- 240 degrees around vertex
- 300 degrees around center of face

# Existence of the 8 types



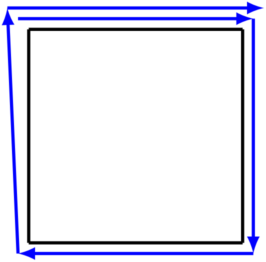
# Existence of the 8 types

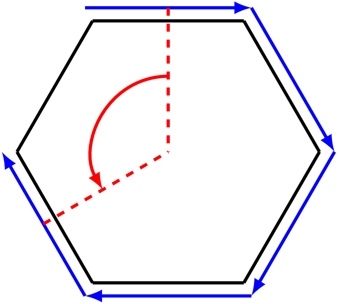




In nanotubes there is an infinite number of these equivalence classes.

# Quadrangle cones from hexagonal lattice





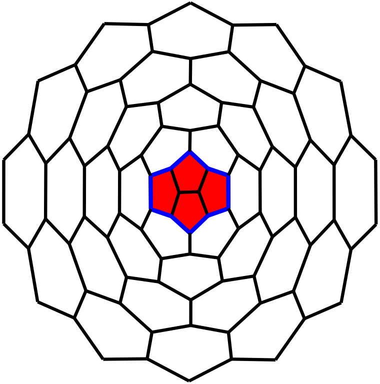
**One quadrangle (unique structure)**

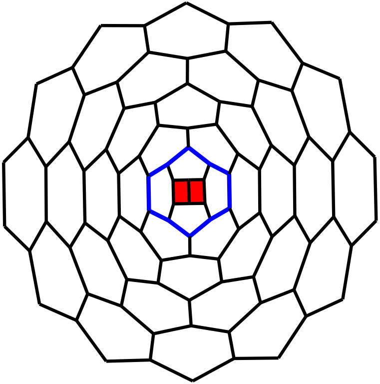
rotation of $120 = (6 - 4) \times 60$ degrees around center of face

Two quadrangles = rotation of 240 degrees

Two conjugacy classes:

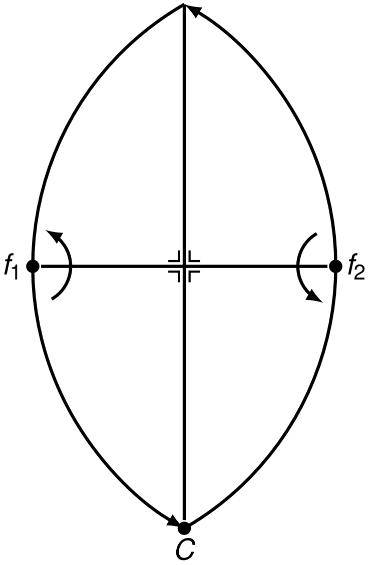
- around the center of a face
- around a vertex

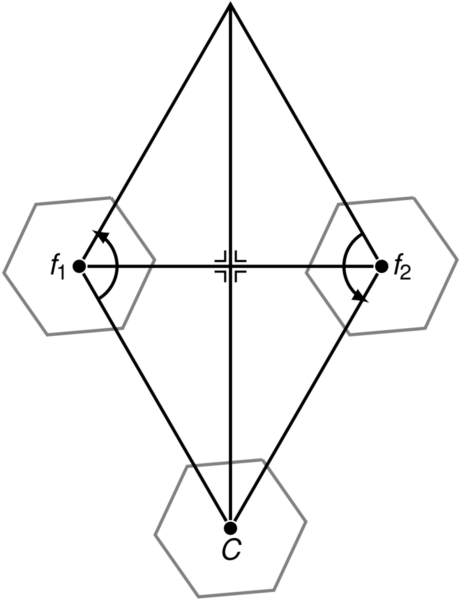




Does there exist a quadrangle cone corresponding to a rotation of 240 degrees around a vertex?


$f_1$
$f_2$


$f_1$
$f_2$
$c$

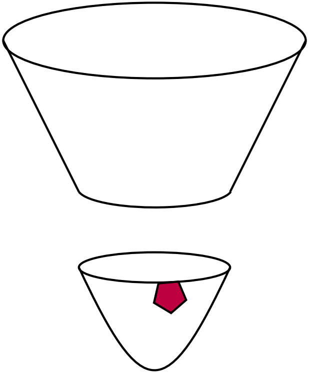

$f_1$
$f_2$
$c$

# 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* (cap)!

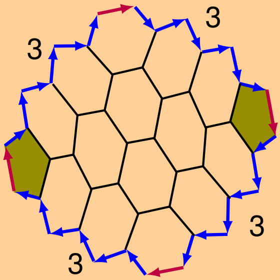
## Aim

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



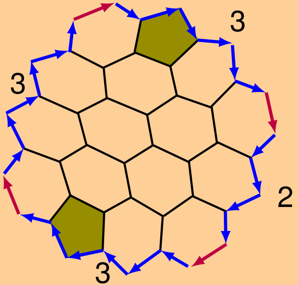
# Definitions

*"symmetric"* conepath




$$((lr)^m r)^{6-p} = ((lr)^3 r)^4$$

*"nearsymmetric"* conepath




$$((lr)^m r)^{6-p-1}((lr)^{m-1} r) = ((lr)^3 r)^3((lr)^2 r$$

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

# 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 $m$).

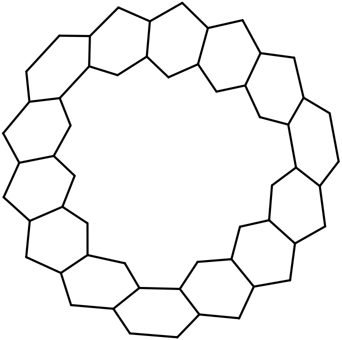
## Definition

A closed path of the form $((lr)^m r)^{6-p-1}((lr)^{m-1} r)$ (for some $m$) is called a nearsymmetric path (for $p$ and $m$).

## Definition

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

# Adding a layer of hexagons



$$((lr)^4 r)^2((lr)^3 r) \rightarrow ((lr)^5 r)^2((lr)^4 r)$$

# Finer classification of cones

**Theorem**

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

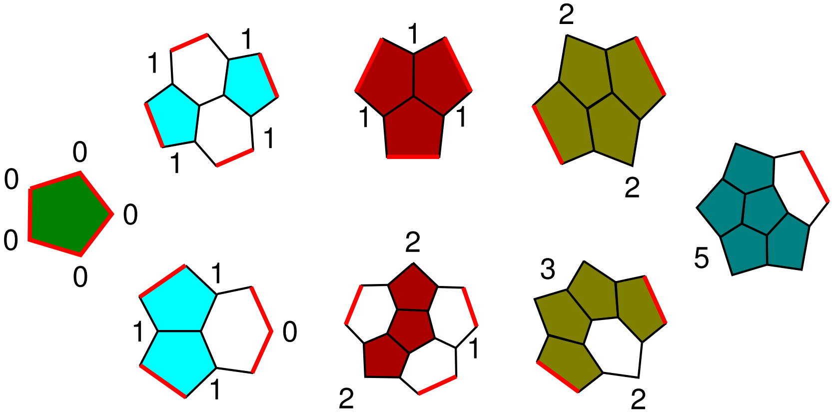
  **unless** *$p = 2$ and there is a nearsymmetric conepath. In this case there are exactly two isomorphic conepaths with isomorphic interior.*

# Finer classification of cones

**Theorem**

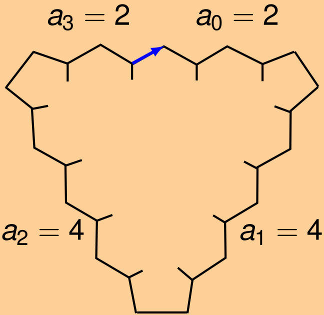
*So there is a 1-1 correspondence between caps (interiors of cone paths) and cones.*

# Existence of cone paths

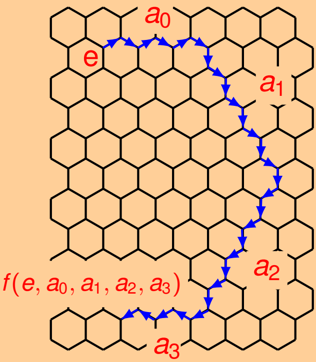


# Sketch of the uniqueness proof

## cone




## hexagonal lattice



# Sketch of the uniqueness proof

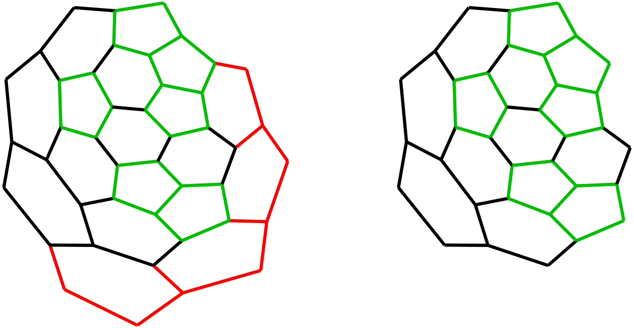
## Method

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

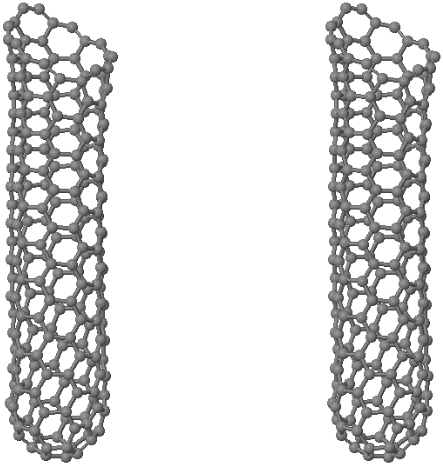
# Finer classification of cones

**Note**

The corresponding result does not hold for nanotubes.



$$rlrlrlrlrlrllrlrlrlr = (rl)^5(lr)^4$$



# Outline

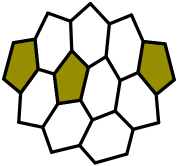
# Patch

## Definition

A patch is a finite, bridgeless, plane graph with three kinds of faces:

- 1 outer face with unrestricted size,
- 1 to 5 pentagons, and
- an unrestricted number of hexagons.

Furthermore, all internal vertices have degree 3 and all other vertices have degree 2 or 3.



# Pseudo-convex patch

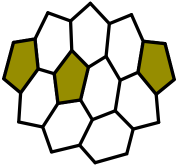
**Definition**

A pseudo-convex patch is a patch such that the cyclic sequence of degrees on the boundary does not contain two consecutive 3's.

**Definition**

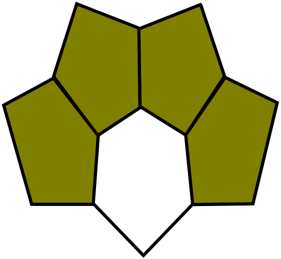
A break-edge is a boundary edge which is incident with two vertices of degree 2.

A patch with $p$ pentagons contains $6 - p$ break-edges.



# Pseudo-convex patch

Interior of a cone path is a pseudo-convex patch.

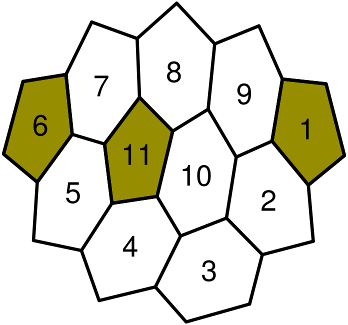


$l \to 3 \quad r \to 2$

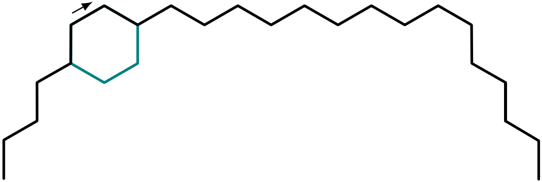
# Outer spiral

**Brinkmann-Dress, 1997**

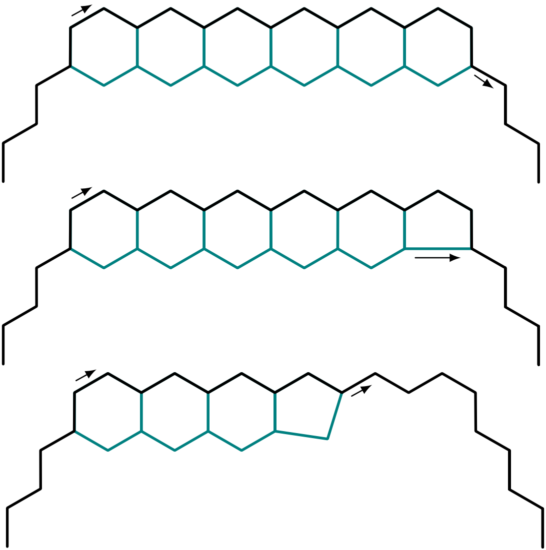
Pseudo-convex patches have an outer spiral.



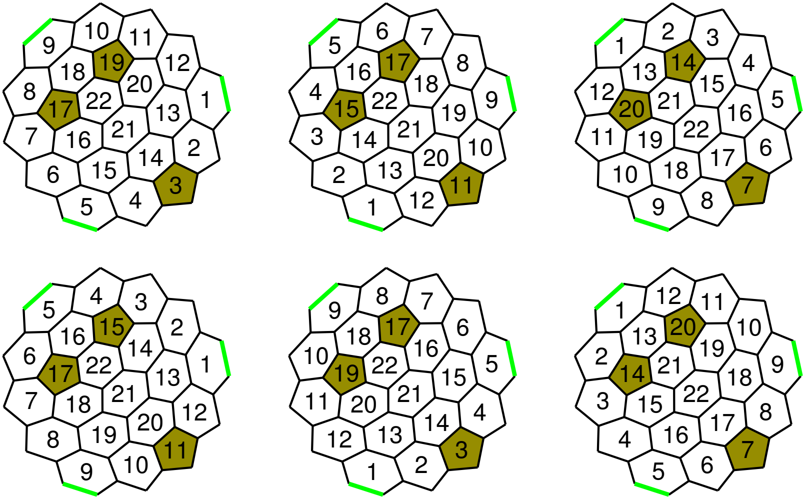
# Filling the boundary



# Next pseudo-convex boundary



# Multiple outer spirals



# Starting points

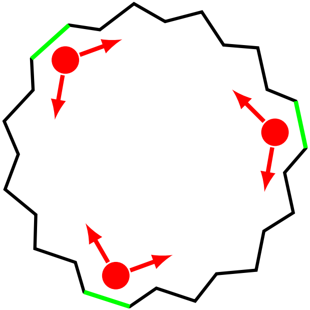
Fix the starting point and starting direction

Consider all equivalent starting points!

# Starting points

## Symmetric cone path

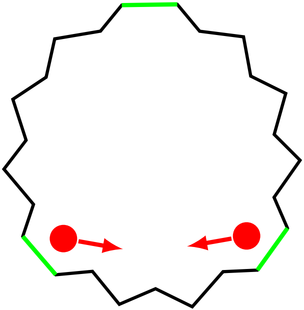
Each break-edge and each direction



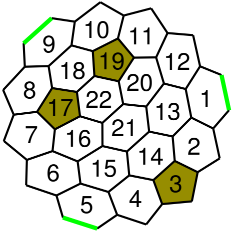
# Starting points

## Nearsymmetric cone path

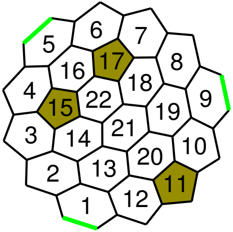
Break-edge next to shortest side and only in the direction of the shortest side



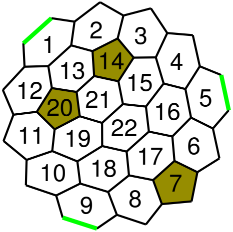
# Minimal spiral code



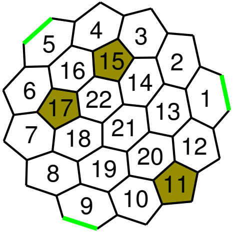

[3,17,19]



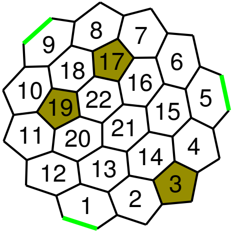

[11,15,17]



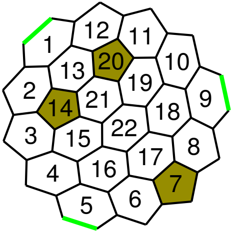

[7,14,20]




[11,15,17]

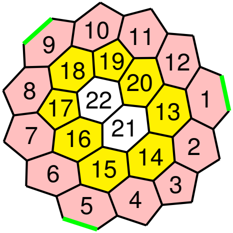


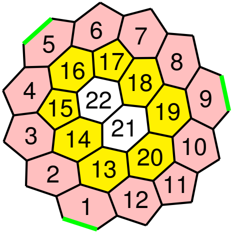

[3,17,19]




[7,14,20]

# Layers


9
10
11
12
1
8
18
19
20
22
13
17
21
2
7
16
14
6
15
3
4
5


5
6
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3
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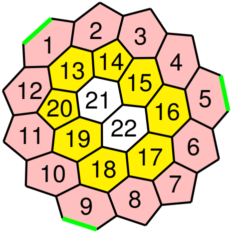
11
12
1


1
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12
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16
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22
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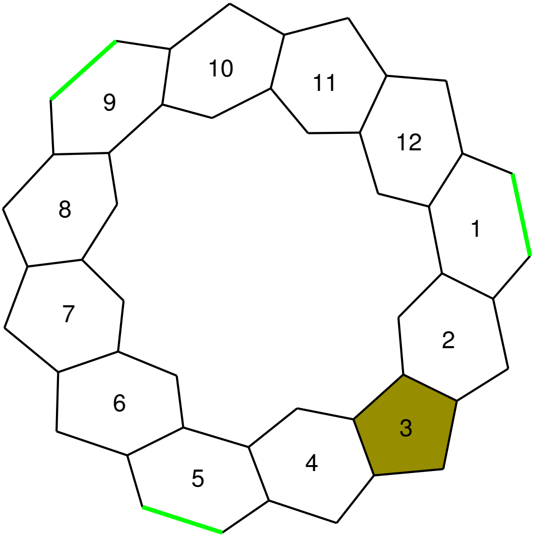
17
10
18
7
8
9

# Layer by layer



# Isolated pentagons

While constructing the pseudo-convex patch, a pentagon neighbouring a new face can only appear at two positions:

- at a break-edge in the previous layer, and
- as the last added face.

# Number of cones per length of short side

| | 3<br>s | 3<br>n | 4<br>s | 4<br>n | 5 |
|---|---|---|---|---|---|
| 1 | 1 | 2 | 0 | 0 | 0 |
| 2 | 3 | 8 | 1 | 2 | 0 |
| 3 | 5 | 18 | 4 | 9 | 0 |
| 4 | 12 | 37 | 16 | 32 | 0 |
| 5 | 18 | 63 | 37 | 89 | 1 |
| 10 | 124 | 413 | 975 | 2 272 | 212 |
| 15 | 387 | 1 288 | 7 040 | 16 032 | 3 941 |
| 20 | 915 | 2 960 | 29 342 | 65 056 | 31 025 |
| 25 | 1 757 | 5 646 | 88 918 | 194 044 | 150 732 |
| 30 | 3 039 | 9 640 | 220 741 | 475 422 | 547 166 |
| 35 | 4 793 | 15 138 | 476 101 | 1 016 193 | 1 620 501 |
| 35 | 0.1s | 0.4s | 4.4s | 9.8s | 4.1s |

Timings for Intel I5 processor (1.7 GHz)

# 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

# Two pentagons

## Symmetric cone patches with two pentagons

There are $\lceil \frac{n+1}{2} \rceil$ pairwise non-isomorphic cone patches with boundary $(2(23)^n)^4$ and they have spiral code $[i, 2n+i]$ with $i \in \{0, \ldots, \lceil \frac{n+1}{2} \rceil - 1\}$.

## Nearsymmetric cone patches with two pentagons

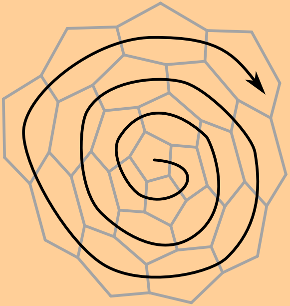
There are $n+1$ pairwise non-isomorphic cone patches with boundary $2(23)^n(2(23)^{n+1})^3$ and they have spiral code $[i, 2n+1+i]$ with $i \in \{n+1, \ldots, n+2+\lfloor \frac{n+1}{2} \rfloor, 2n+2, \ldots, 3n+1-\lfloor \frac{n}{2} \rfloor\}$.

# Number of hexagons

## General pseudoconvex patches

Bornhöft, Brinkmann, Greinus (2003)

Extremal case is spiral that starts with all pentagons and then hexagons



# Number of hexagons

## General pseudoconvex patches

Upperbounds by Bornhöft, Brinkmann, Greinus (2003)

$$p = 1 \Rightarrow h \leq \frac{b^2 - 25}{40}$$

$$p = 2 \Rightarrow h \leq \frac{b^2 - 64}{32}$$

$$p = 3 \Rightarrow h \leq \frac{b^2 - 81}{24}$$

$$p = 4 \Rightarrow h \leq \frac{b^2 - 100}{16}$$

$$p = 5 \Rightarrow h \leq \frac{b^2 - 113}{8}$$

# Number of hexagons in cone patches

Pentagon in boundary! ⇒ maximal spiral not possible

## Idea

- insert vertex into boundary edge of a pentagon
- boundary length increases by one
- number of faces equal
- upperbound on number of hexagons is one more than upperbound of original patch

# Number of hexagons in cone patches

## symmetric

$$p = 2 \Rightarrow h \leq \frac{8m^2 + 10m - 5}{5}$$

$$p = 3 \Rightarrow h \leq \frac{9m^2 + 12m - 44}{16}$$

$$p = 4 \Rightarrow h \leq \frac{2m^2 + 3m - 12}{3}$$

$$p = 5 \Rightarrow h \leq \frac{m^2 + 2m - 28}{4}$$

## nearsymmetric

$$p = 2 \Rightarrow h \leq \frac{8m^2 + 22m + 7}{5}$$

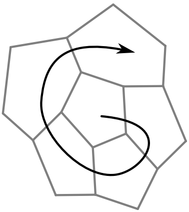
$$p = 3 \Rightarrow h \leq \frac{9m^2 + 24m - 32}{16}$$

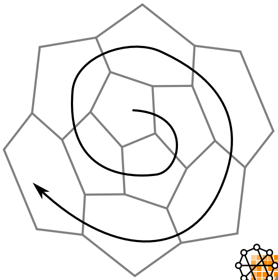
$$p = 4 \Rightarrow h \leq \frac{2m^2 + 5m - 10}{3}$$

# Number of hexagons in cone patches

## 5 pentagons

$h \leq \left\lfloor \frac{m^2 + 2m - 28}{4} \right\rfloor$ is sharp



# Number of hexagons in cone patches

## 2 pentagons

$h \leq \left\lfloor \frac{8m^2+10m-5}{5} \right\rfloor$ (symmetric case) and

$h \leq \left\lfloor \frac{8m^2+22m+7}{5} \right\rfloor$ (nearsymmetric case) are *not* sharp

$h \leq \left\lfloor \frac{5m^2+8m-4}{4} \right\rfloor$ (symmetric case) and

$h \leq \left\lfloor \frac{5m^2+16m+4}{4} \right\rfloor$ (nearsymmetric case) are sharp

# Outline

# CaGe

The program can be used inside the environment CaGe:

http://caagt.ugent.be/CaGe
https://www.math.uni-bielefeld.de/~CaGe/

https://github.com/CaGe-graph/CaGe

# What is CaGe?

**C**hemical and **a**bstract **G**raph **e**nvironment

a graphical user interface for a set of commandline generators and embedders

**user interface**

written in Java

**generators and embedders**

written in C and Java (any language will do)

# User interface

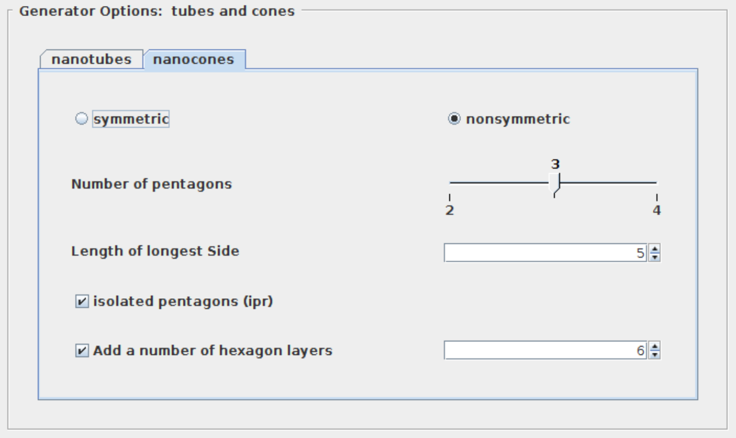
Having a user interface
$\neq$
Being a user friendly program

# Example

```
cone -i -e p 3 4 n 6
```

generates all nanocones with exactly 3 isolated pentagons that have a cone path of the form $2(23)^4(2(23)^5)^2$ and adds six layers of hexagons to the patch.

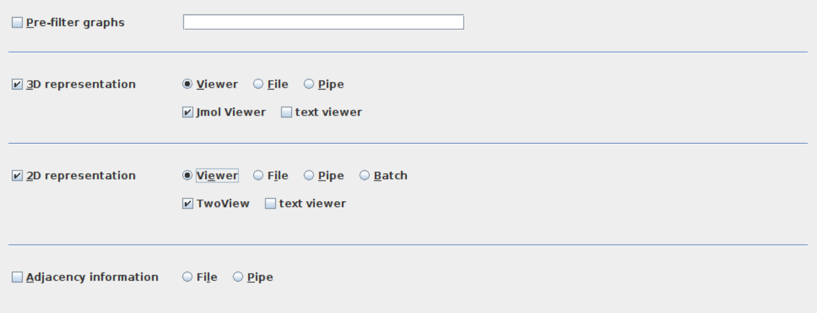
# And now with CaGe



```
3e 3e 70 6c 61 6e 61 72 5f 63 6f 64 65 3c 3c 00 6a 01 02 00 36
00 00 00 03 00 01 00 00 00 04 00 37 00 02 00 00 00 05 00 03 00
00 00 06 00 39 00 04 00 00 00 07 00 05 00 00 00 08 00 3b 00 06
00 00 00 09 00 07 00 00 00 0a 00 3d 00 08 00 00 00 0b 00 09 00
00 00 0c 00 3f 00 0a 00 00 00 0d 00 0b 00 00 00 0e 00 41 00 0c
00 00 00 0f 00 0d 00 00 00 10 00 43 00 0e 00 00 00 11 00 0f 00
00 00 12 00 45 00 10 00 00 00 13 00 11 00 00 00 14 00 47 00 12
00 00 00 15 00 13 00 00 00 16 00 49 00 14 00 00 00 17 00 15 00
00 00 18 00 4b 00 16 00 00 00 19 00 17 00 00 00 1a 00 4d 00 18
00 00 00 1b 00 19 00 00 00 1c 00 4f 00 1a 00 00 00 1d 00 1b 00
00 00 1e 00 1c 00 00 00 1f 00 51 00 1d 00 00 00 20 00 1e 00 00
00 21 00 52 00 1f 00 00 00 22 00 20 00 00 00 23 00 54 00 21 00
00 00 24 00 22 00 00 00 25 00 56 00 23 00 00 00 26 00 24 00 00
00 27 00 58 00 25 00 00 00 28 00 26 00 00 00 29 00 5a 00 27 00
00 00 2a 00 28 00 00 00 2b 00 5c 00 29 00 00 00 2c 00 2a 00 00
00 2d 00 5e 00 2b 00 00 00 2e 00 2c 00 00 00 2f 00 60 00 2d 00
00 00 30 00 2e 00 00 00 31 00 62 00 2f 00 00 00 32 00 30 00 00
00 33 00 64 00 31 00 00 00 34 00 32 00 00 00 35 00 66 00 33 00
```

# Output

`cone` and the other generators in CaGe output a binary format, e.g., planar code.



# Recent additions

- Rotation and stepless scaling of vertices in 2D viewer
- Batch export of 2D images
- `buckygen` as generator for fullerenes
- Upgraded `plantri` to version 4.5
- New embedder for benzenoids
- New generator for 5-regular plane graphs
- New generator for generalised fusenes
- Made default embedder more customisable
- Export for 3D printing

# CaGe

The program can be used inside the environment CaGe:

http://caagt.ugent.be/CaGe
https://www.math.uni-bielefeld.de/~CaGe/

https://github.com/CaGe-graph/CaGe

# Nanocones

## A classification and generation result in chemistry

Gunnar Brinkmann Nico Van Cleemput

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Department of Applied Mathematics, Computer Science and Statistics
Ghent University