Nanocones
A classification result in chemistry

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Carbon networks

- **Graphite**
- **Nanocone**
- **Nanotube**

All structures infinite

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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
unique structure – so 1 class only

Nanotubes (6 pentagons)
ininitely many structures and infinitely many equivalence classes
a finite number of tubes in each class
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Classification of cones

2 to 4 pentagons
infinitely many structures – 2 classes

5 pentagons
infinitely many structures – 1 class

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

<table>
<thead>
<tr>
<th>Number of Pentagons</th>
<th>Structures</th>
<th>Classes</th>
</tr>
</thead>
<tbody>
<tr>
<td>2 to 4</td>
<td>infinitely many</td>
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Each cone is equivalent to exactly one of the following cones (only caps shown)
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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Classification
Construction and results

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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 \( T \) 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 \( T \)
Take any closed path around the disorder.

Here: llrrrlrrlrrrr.

Follow the same path llrrrlrrlrrrr in the lattice.

A counterclockwise rotation by 60 degrees.
Take any closed path around the disorder.

Here: llrrlrrlrrrr.

Follow the same path lrrrlrrlrrrr in the lattice.

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.
This allows to determine possible equivalence classes.

Example: 3 pentagons

\[
\begin{align*}
60 \times 60 \times 60 &= 180
\end{align*}
\]

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.
Both classes exist for 3 pentagons

Balke: proof of existence for general disorders – not necessarily of the form needed here.
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Each cone is equivalent to exactly one of the following cones (only caps shown)
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.
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.
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 $m$).
Assume $2 \leq p \leq 5$ fixed.

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Definitions

"symmetric" conepath

\[(lr)^3 r^6 - p = (lr)^3 r^4\]

"nearsymmetric" conepath

\[(lr)^3 r^6 - p - 1 ((lr)^2 r) = (lr)^3 r^3 (lr)^2 r\]

Note: always \(6 - p\) edges with two times right

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Definitions

"symmetric" conepath

\[
((lr)^3 r)^6 - p = ((lr)^3 r)^4
\]

Note: always 6 - p edges with two times right

"nearsymmetric" conepath

\[
((lr)^3 r)^{6-p-1} ((lr)^2 r) = ((lr)^3 r)^3 ((lr)^2 r)
\]
A closed path in a cone is called a coneopath 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.
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.
Each cone is equivalent to exactly one of the following cones:

1. Hexagonal pyramid
2. Pentagonal pyramid
3. Hexagonal prism
4. Pentagonal prism
5. Hexagonal antiprism
6. Pentagonal antiprism
7. Hexagonal bipyramid
8. Pentagonal bipyramid
9. Hexagonal cupola
10. Pentagonal cupola
11. Hexagonal anticupola
12. Pentagonal anticupola
13. Hexagonal prismatohexagonal cupola
14. Pentagonal prismatopentagonal cupola
15. Hexagonal prismatohexagonal anticupola
16. Pentagonal prismatopentagonal anticupola
17. Hexagonal prismatohexagonal bipyramid
18. Pentagonal prismatopentagonal bipyramid
19. Hexagonal prismatohexagonal antiprism
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21. Hexagonal prismatohexagonal prism
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Sketch of the uniqueness proof

cone

\[ a_3 = 2 \quad a_0 = 2 \]

\[ a_2 = 4 \quad a_1 = 4 \]
Sketch of the uniqueness proof

cone

\[ a_0 = 2 \]
\[ a_1 = 4 \]
\[ a_3 = 2 \]

graphite lattice

\[ f(e, a_0, a_1, a_2, a_3) \]

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Sketch of the uniqueness proof

Method

- if two cone paths 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 \( a_i \)
Sketch of the uniqueness proof

Method

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- Solve the equations for the different possible variables \( a_i \).
Construction of cone caps

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

But: lots of optimizations to increase efficiency
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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

Numbers
# symmetric cones with two pentagons: \( \left\lfloor \frac{m+1}{2} \right\rfloor \)
# nearsymmetric cones with two pentagons: \( m + 1 \)
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Some results

Example: 3 pentagons, symmetric conepath

<table>
<thead>
<tr>
<th>sidelength</th>
<th>number cones</th>
<th>min atoms</th>
<th>max atoms</th>
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<td>50</td>
<td>13.955</td>
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<td>5.301</td>
</tr>
</tbody>
</table>
CaGe

The program can be used inside the environment CaGe:

http://caagt.ugent.be/CaGe