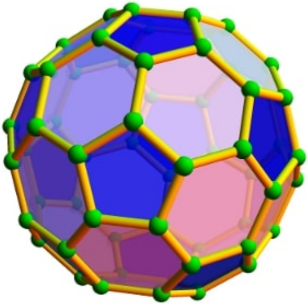


Spectral classification of fullerenes

Joint work with Artur Bille (Skoltech/UUlm) and
Victor Buchstaber (Steklov Math. Inst./Skoltech)

Evgeny Spodarev | Ulm University | 3.12.2018

Spectral classification of fullerenes

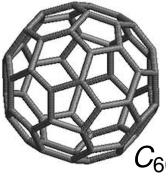
Outline of the talk

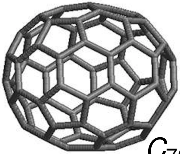
- What is a fullerene?
- Why do we care?
- Isomers of fullerenes
- Spectral clustering of isomers
- Example of C_{60}
  - Dimension reduction
  - 5 interesting isomers
- Outlook
- References

What is a fullerene?

Chemical point of view:

- Molecule C_n with n carbon atoms
- Closed cage-like hollow sphere
- Any atom belongs to exactly three carbon rings
- Carbon rings can be pentagons or hexagons only


C_{60}


C_{70}

Nobel Prize in Chemistry 1996 (R. Curl, H. Kroto, R. Smalley)

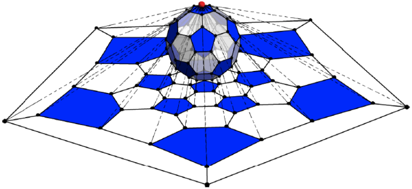
What is a fullerene?

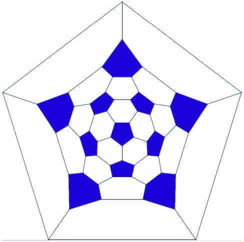
Mathematical point of view:

A fullerene C_n is a simple 3–convex polytope with all facets being regular pentagons or hexagons.

Numer of vertices: $n \geq 20$, even.

Schlegel diagram:



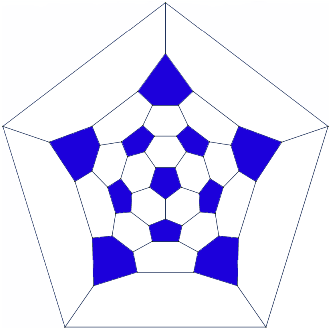


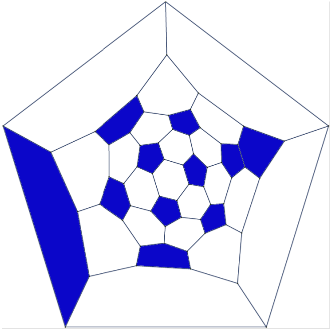
Why do we study fullerenes?

- Wide variety of applications: artificial photosynthesis, nonlinear optics, nanostructures etc.
- Young research area:
  What fullerenes can be synthesized?
  Are there any particularly stable fullerenes? $\rightarrow$ IPR–Isomers
  (IPR- isolated penagon rule. All pentagon facets are isolated)
- How can fullerenes be simulated?
- How can one cluster fullerene isomers?

What are isomers and how many do exist?

Two combinatorially nonequivalent fullerenes with the same number of hexagons are called combinatorial isomers.





Number of C_n–Isomers

n	# C_n–Isomers	# IPR–Isomers
20	1	0
22	0	0
24	1	0
60	1812	1
68	6332	0
70	8149	1
80	31 92	7
100	285 914	450

$$\Rightarrow \#C_n\text{–Isomers} = \mathcal{O}\left(n^9\right)$$

How to cluster these Isomers?

Our approach:

1. Construct an adjacency matrix A of all hexagons .
2. Calculate the k–th power of A and trace $t_k := tr\left(A^k\right)$, $2 \leq k \leq N$.
3. For every k check how many different values one gets.
4. Cluster all C_n–isomers based on these values.

Remark:

It holds $tr\,(A) = 0$ for all C_n–Isomers by definition of A, $t_k \in \mathbb{N}$ for all k.

Question: What is minimal N needed?

Example: Hierarchical clustering of C_{60}

Vector	# Cluster	# Cluster with one element
(t_2)	18	5
(t_2, t_3)	42	7
(t_2, t_3, t_4)	372	130
(t_2, t_3, t_4, t_5)	1068	670
$(t_2, t_3, t_4, t_5, t_6)$	1747	1686
$(t_2, t_3, t_4, t_5, t_6, t_7)$	1808	1804
$(t_2, t_3, t_4, t_5, t_6, t_7, t_8)$	1812	1812
(t_6, t_7, t_8)	1812	1812

N=8

Single-step clustering of C_{60}

t_k	# Cluster	# Cluster with one element
$k = 2$	18	5
$k = 3$	23	5
$k = 4$	218	47
$k = 5$	219	36
$k = 6$	1233	845
$k = 7$	1241	825
$k = 8$	1784	1757
$k = 9$	1781	1750
$k = 10$	1807	1802
$k = 11$	1810	1808
$k = 12$	1812	1812

N=12

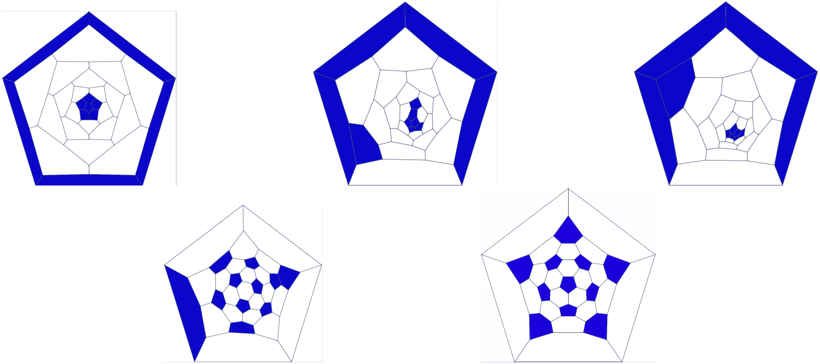
Five special C_{60}–Isomers

For $k = 2$ one gets 18 different values (= 18 clusters).
Five of these clusters consist of one C_{60}–Isomer only.

$tr\left(A^2\right)$	# C_{60}–Isomers
60	1
64	1
66	3
68	17
70	86
72	254
74	262
76	413
78	297

$tr\left(A^2\right)$	# C_{60}–Isomers
80	197
82	96
84	50
86	19
88	10
90	2
92	1
96	1
100	1

Five special C_{60}–Isomers: physical interpretation



Three least stable and two most stable isomers

Relative Energy

Top: Highest relative energy and less spherical structure
$\Rightarrow$ least stable isomers

Bottom: Smallest relative energy and more spherical structure
$\Rightarrow$ most stable isomers

Compare the paper

R. Sure, A. Hansen, et al. *Phys. Chem. Chem. Phys.* (2017)

Outlook

- Classification of isomers of C_n for $n = 70, 80, 82, \ldots$
- Search for potentially interesting isomers for large n
- Dimension reduction: a formula for the least possible N

References

V. Andova, F. Kardoš, and R. Škrekovski, *Mathematical aspects of fullerenes*, Ars Mathematica Contemporanea 11, 2016, 252-279

A. Bille, V. Buchstaber, M. Schandar, E. Spodarev, *Spectral clustering of combinatorial fullerene isomers based on their facet eigenstructure*, Preprint, 2018

V. Buchstaber, N. Erokhovets, *Fullerenes, polytopes and toric topology*, 67-178, Lect. Notes Ser. Inst. Math. Sci. Natl. Univ. Singap., 35, World Sci. Publ., 2018

F. Cataldo, A. Graovac, O. Ori, *The Mathematics and Topology of Fullerenes*, Springer, 2011

P. W. Fowler, D. E. Manolopoulos, *An Atlas of Fullerenes*, Dover Publ., NY, 2006

I. Gutman, D. Vidović, and L. Popović, *Graph representation of organic molecules*, J. Chem. Soc., Faraday Trans., 1998, 94(7), 857–860

R. Sure, A. Hansen, P. Schwerdtfeger, S. Grimme, *Comprehensive theoretical study of all 1812 C_{60} isomers*, Phys. Chem. Chem. Phys., The Royal Society of Chemistry, 2017, 19, 14296