Resonance Polynomials of Cata-condensed Hexagonal Systems

Xi Chen

Joint work with Dong Ye & Xiaoya Zha

Middle Tennessee State University

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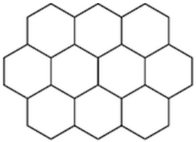
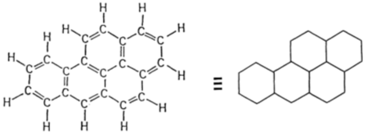
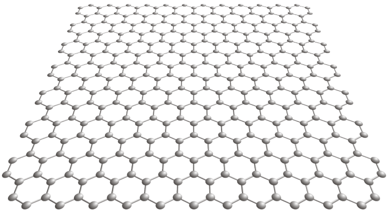
A *hexagonal system* is a finite 2-connected plane bipartite graph in which each interior face is bounded by a regular hexagon of side length one.



Benzenoid hydrocarbon:



Graphene:



Question: Is there some connections between structures of these molecules and their chemical stability?

- Homo-Lumo Gap ($\triangle = \lambda_H - \lambda_L$, difference between two middle eigenvalues)
- Kekulé count (# of perfect matchings)
- Clar number (the maximum # of disjoint hexagons)

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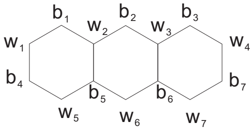
F. J. Rispoli gave a method to compute Kekulé count (# of perfect matchings) in hexagonal systems.

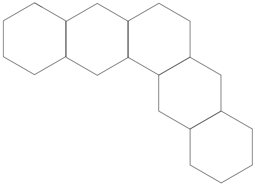
- Let $A(a_{ij})$ be the biadjacency matrix of a hexagonal system G.
- $$\Phi(G) = |det(A)|.$$

  Note: $\Phi(G)$ is the number of perfect matchings of G.

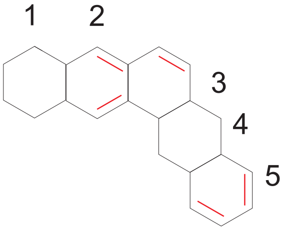


G

A hexagonal system is *cata-condensed* if all vertices appear on its boundary.



- A set of disjoint hexagons $\mathcal{H}$ of a hexagonal system G is a *resonant set* if a subgraph G' consisting of deleting all vertices covered by $\mathcal{H}$ from G has a perfect matching.
- A resonant set is a *forcing resonant set* if G' has a unique perfect matching.



Disjoint hexagonal set: $\{1,4\}$

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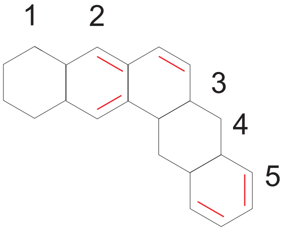

Disjoint hexagonal set: $\{1,4\}$

- (Zheng & Hanse, 1993)
  The Clar number problem of hexagonal system can be solved by an integer program.
- (Abeledo & Atkinson, 2006)
  The Clar number problem of hexagonal system can be solved by an linear programming which was conjectured by Zheng & Hanse.

- (Zheng & Chen, 1985)
  A maximum resonant set of a hexagonal system is a forcing resonant set.
- The *spectrum* of forcing resonant set can be defined as:
  $spec_{FRS}(G) = \{|\mathcal{H}| : \mathcal{H}$ is a forcing resonant set of $G\}$.

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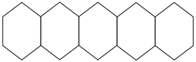
Definition 1

Let G be a cata-condensed hexagonal system. The forcing resonant polynomial $P_G(x)$ can be defined as

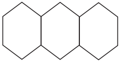
$$P_G(x) = \sum_{i=0}^{cl(G)} a_i x^i \quad (1)$$

where a_i is the number of forcing resonant sets of size i.

- (Zhang, Chen, Guo & Gutman, 1991)
  A hexagonal system H has $cl(H) = 1$ if and only if H is a linear chain.
- $spec_{FRS}(L_k) = \{1\}$



G_1



G_2

The coefficient vector of G:

$$a = \begin{bmatrix} a_{cl(G)} \\ a_{cl(G)-1} \\ \vdots \\ a_1 \end{bmatrix}$$

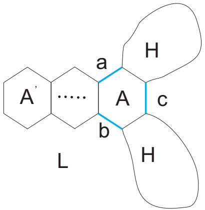
where a_i is the coefficient of x^i in $P_G(x)$, then a is called the the *coefficient vector* of G.

Proposition 1

Let G be a graph of disjoint union of cata-condensed hexagonal systems $G_1, G_2, ...G_k$. Then

$$P_G(x) = \prod_{i=1}^{k} P_{G_i}(x). \tag{2}$$

A pendant chain L:



Lemma 2

Let G be a cata-condensed hexagonal system. Every forcing resonant set of G contains exactly one hexagon of L if L is not a non-pendant chain with two hexagons.

Corollary 3

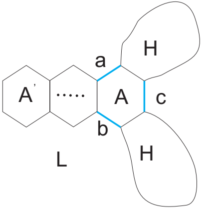
Every forcing resonant set $\mathcal{H}$ hits every maximal linear hexagonal chain.

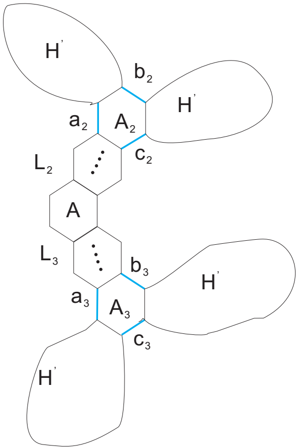
Lemma 4

Let G be a cata-condensed hexagonal system. Let A be a hexagon of G. Then,

$$P_G(x) = P_G(x, A^C) + P_G(x, A)$$

Theoretical part



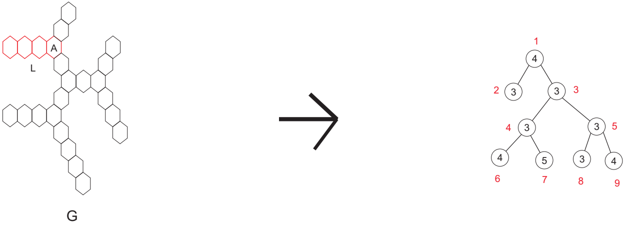


Theorem 5

Let G be a cata-condensed hexagonal system and L be a pendant chain with r hexagons. Let H be the subgraph consisting of all hexagons of G except these in L, and H' be the subgraph of H consisting of all hexagons except these contained in the maximal linear chains of G with a common hexagon with L. Then,

$$P_G(x) = (r-1)xP_H(x) + xP_{H'}(x) \tag{3}$$

How to construct the weighted tree:



Steps:

- Start with a pendant chain L. L corresponds with the fist vertex in (T, w).
- The children of a vertex v in (T, w) are defined to be the maximal linear hexagonal chains which share a common hexagon with the corresponding chain of the vertex v.
- Continue to do step 2 until the number of vertices equals the number of maximal linear hexagon chains.

Note that the vertex which corresponds with the initial pendant hexagonal chain L is the root of (T, w).

function cal_poly

if *Tree is empty* **then**

   $P_{tree}(x) = 1$;

else

   Find left subtree and right subtree of the tree T;
   Find left subtree and right subtree of the left subtree;
   Find left subtree and right subtree of the right subtree;
   Recursive formula;

end

end

G. Brinkmann, G. Caporppssi and P. Hansen proposed a method to construct enumerate fusenes and bezenoids in 2002.

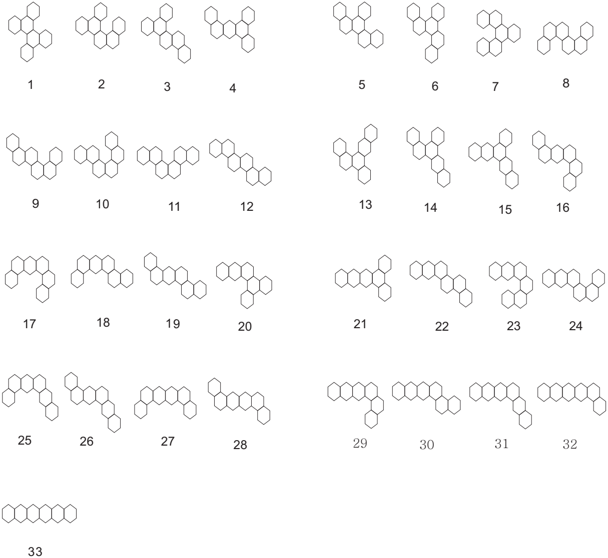


Table III
CATA-CONDENSED BENZENOID SYSTEM WITH 6 HEXAGONS

Graph number	Polynomial	Clar number	Coefficient vector	x coordinate	HOMO-LUMO gap	$\Phi(G)$
1	x^4+2x^3	4	[1 2 0 0]	15	1.0229	24
2	$x^4+x^3+2x^2$	4	[1 1 2 0]	14	1.0901	23
3	$x^4+x^3+2x^2$	4	[1 1 2 0]	14	1.0727	23
4	$x^4+x^3+x^2$	4	[1 1 1 0]	13	1.0449	22
5	$5x^3$	3	[0 5 0 0]	12	1.0929	22
6	$5x^3$	3	[0 5 0 0]	12	1.0083	22
7	$5x^3$	3	[0 5 0 0]	12	0.9411	22
8	$4x^3+x^2$	3	[0 4 1 0]	11	1.0785	21
9	$4x^3+x^2$	3	[0 4 1 0]	11	1.0133	21
10	$4x^3+x^2$	3	[0 4 1 0]	11	1.0044	21
11	$4x^3+x^2$	3	[0 4 1 0]	11	0.9969	21
12	$4x^3+x^2$	3	[0 4 1 0]	11	0.9428	21
13	$4x^3+x^2$	3	[0 4 1 0]	11	0.8933	20
14	$4x^3+x^2$	3	[0 4 1 0]	11	0.8902	20
15	$4x^3+x$	3	[0 4 0 1]	10	1.0115	19
16	$3x^3+2x^2$	3	[0 3 2 0]	9	0.9013	19
17	$3x^3+2x^2$	3	[0 3 2 0]	9	0.9011	19
18	$3x^3+2x^2$	3	[0 3 2 0]	9	0.8755	19
19	$3x^3+2x^2$	3	[0 3 2 0]	9	0.8571	19
20	$3x^3+2x^2$	3	[0 3 2 0]	9	0.7910	19
21	$3x^3+x$	3	[0 3 0 1]	8	0.7114	17
22	$2x^3+4x^2$	3	[0 2 4 0]	7	0.8528	18
23	$2x^3+4x^2$	3	[0 2 4 0]	7	0.8400	18
24	$2x^3+4x^2$	3	[0 2 4 0]	7	0.8387	18
25	$2x^3+3x^2$	3	[0 2 3 0]	6	0.8969	17
26	$2x^3+3x^2$	3	[0 2 3 0]	6	0.8575	17
27	$2x^3+2x^2$	3	[0 2 2 0]	5	0.7213	16
28	$2x^3+2x^2$	3	[0 2 2 0]	5	0.7168	16
29	$7x^2$	2	[0 0 7 0]	4	0.6142	14
30	$7x^2$	2	[0 0 7 0]	4	0.6066	14
31	$6x^2+x$	2	[0 0 6 1]	3	0.6715	13
32	$4x^2+x$	2	[0 0 4 1]	2	0.4872	11
33	$6x$	1	[0 0 0 6]	1	0.3387	7

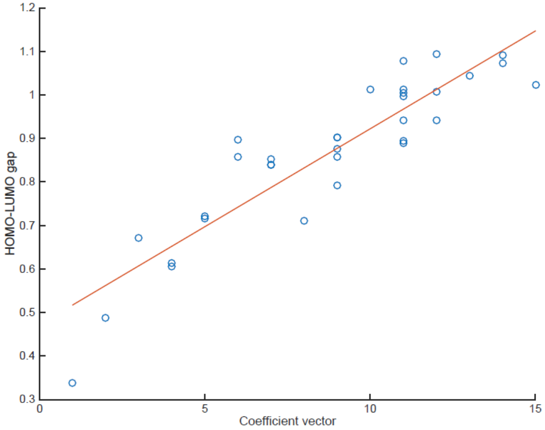


Figure 2: Using least square method to fit the data points from tab 3

We obtain the following conclusions by comparing the experiment results:

- The coefficient vector we proposed increases as the HOMO-LUOM gap increases.
- The stability of G is relative with the coefficient vector. The one that has larger coefficient vector has better stability.
- The coefficient vector we proposed is a refined indicator than the existing method, Clar number, to predict the stability of G.

Thanks!