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On the Anti–Kekulé and Anti–Forcing Number of Cata–condensed Phenylenes

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Abstract

The anti-forcing number is defined as the smallest number of edges that have to be removed in order that any graph remains with a single Kekulé structure. Similarly, the anti-Kekulé number is defined as the smallest number of edges that have to be removed in order that any graph remains connected but without any Kekulé structure. It is shown that the anti-Kekulé number of cata-condensed phenylenes is 3 and the anti-forcing number of a cata-condensed $[h]$-phenylene is h, where h is the number of the hexagons in the cata-condensed phenylene. Moreover, it is proved that for a Kekulé structure M of a cata-condensed $[h]$-phenylene, the forcing number $\varphi(M)$ is bounded by $\lceil \frac{h}{2} \rceil \leq \varphi(M) \leq h$.

1 Introduction

Let G be a graph and let M be a perfect matching(or Kekulé structure) of G. A subset S of M is said to force M if S is in no other perfect matching. The forcing number $\varphi(M)$ of M is the cardinality of a smallest subset S that forces M. The notion of forcing number of a perfect matching M is introduced by Harary et. al in [4], and it has arisen earlier in papers of Klein and Randić with the name “innate degree of freedom ”([5], [9]). Note that similar concept have been studied with different names in different fields

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(see [1]). While there are some study on forcing numbers (sets) of hexagonal systems in the context of chemistry, only few other classes of graphs have been considered, and there are also many interesting open problems on the forcing numbers (sets)(see, e.g. [1], [6], [8], [10], [15] and [16] and the references therein).

Very recently, two novel quantities that are opposite to the forcing number have been introduced by Vukičević and Trinajstić [13], i.e., the anti-forcing and anti-Kekulé number. Let $G = (V, E)$ be a graph that admits a perfect matching. A subset S of E is said to be an *anti-forcing set* of G if $G - S$ has only one perfect matching. The *anti-forcing number* $afn(G)$ of G is defined as the cardinality of a smallest anti-forcing set. A subset S of E is said to be an *anti-Kekulé set* of G if $G - S$ is connected, but has no perfect matching (Kekulé structure). The *anti-Kekulé number* $akn(G)$ of G is defined as the cardinality of a smallest anti-Kekulé set of G. In [13], the anti-Kekulé and anti-forcing number are determined for benzenoid parallelograms, and in [14] these two parameters are determined for cata-condensed benzenoids.

In this paper, we consider the anti-Kekulé and anti-forcing number of a special class of conjugated hydrocarbons-phenylenes [7]. These compounds are composed of six- and four-membered rings, where the six-membered rings (hexagons) are adjacent only to four-membered rings and every four-membered ring is adjacent to a pair of hexagons. A phenylene containing h hexagons is called an $[h]$-phenylne. It is assumed that the number of four-number rings of an $[h]$-phenylne amounts to $h - 1$, meaning that the structures in which alternating six-and four-membered rings are linked together in phenylenic super-rings are not considered in this paper. In Section 2, we determine the anti-Kekulé and anti-forcing number of cata-condensed phenylenes, and in Section 3, we present a lower and upper bounds for the forcing number of a given perfect matching of cata-condensed phenylenes.

2 Anti-Kekulé and anti-forcing number of cata-condensed phenylenes

The main results of this section are the following three theorems.

Theorem 2.1. *Let P be a cata-condensed phenylene. Then $akn(P) = 3$.*

Proof. We only prove the theorem for cata-condensed $[h]$-phenylenes without rings, the proof for ring cata-condensed phenylenes is similar.

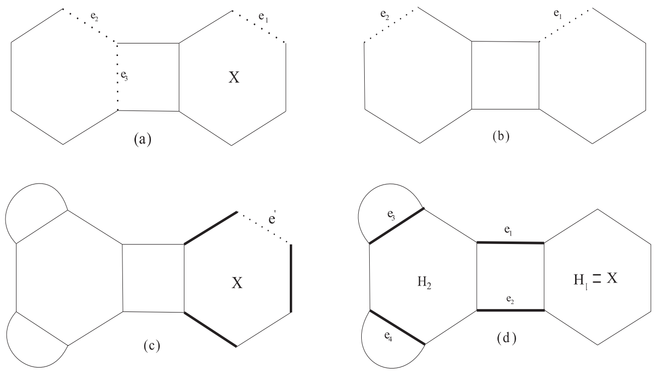

Figure 1:

First, we show that $akn(P) \leq 3$. Note that P has the segments presented below Figure 1:(a), where the hexagon denoted by X has no additional neighboring four-membered ring. It is easy to see that $P - \{e_1, e_2, e_3\}$ is a connected graph without Kekulé structure.

Next we show $akn(P) \geq 3$.

Obviously, $P - e$ has a Kekulé structure for any $e \in E(P)$.

Now let e', e'' be any two edges of P, we distinguish the following cases.

Case 1. e', e'' belong to the same hexagon. Then either $P - \{e', e''\}$ is disconnected or has a Kekulé structure.

Case 2. e', e'' belong to the two distinct hexagons.

Obviously $P - \{e', e''\}$ has a Kekulé structure.

Case 3. e' belongs to some six-membered ring and e'' belongs to some four-membered ring.

Then again $P - \{e', e''\}$ has a Kekulé structure.

Case 4. Both e', e'' belong to the four-membered ring(s).

Then either $P - \{e', e''\}$ is disconnected or has a Kekulé structure.

Hence $akn(P) \geq 3$ and the claim follows. □

Theorem 2.2. *Let P be a cata-condensed $[h]$-phenylene without rings. Then $afn(P) = h$.*

Proof. First, we show $afn(P) \leq h$ by induction on h. Consider the case when $h = 2$ exemplified in Figure 1:(b). If $S = \{e_1, e_2\}$, then obviously $P - S$ possess only one Kekulé structure. Now suppose that the claim holds for all cata-condensed $[k]$-phenylenes with $1 \leq k \leq h-1$ and let P be a cata-condensed $[h]$-phenylenes. Let us present this case by Figure 1:(c). Note that edge e' fixes double bonds of X as depicted in the figure. Eliminating the vertices covered by these double bonds, we get phenylene P' with $h-1$ hexagons. Hence there is, by induction hypothesis, a set S' with $h-1$ elements that fixes all double bonds on P'. And then the set $S' \cup \{e'\}$ with h elements fixes all double bonds on P.

Next, we show $afn(P) \geq h$ by induction on h. If $h = 1, 2$, the claim is obvious. Hence, suppose that the claim holds for all cata-condensed $[k]$-phenylenes with $1 \leq k \leq h-1$ and let P be a cata-condensed $[h]$-phenylenes with $h \geq 3$. Again we denote by X a hexagon that has only one neighboring four-membered ring. Set $P' = P - V(X)$, then P' is a cata-condensed $[h-1]$-phenylene.

Case 1. The restriction of the only Kekulé structure κ (of P) to P' is a Kekulé structure of P'.

In this case, obviously, the restriction of the only Kekulé structure κ to $P - P'$ is a Kekulé structure of $P - P'$. Therefore $afn(P) \geq afn(P') + afn(P - P') \geq$\{by induction hypothesis\}$\geq h - 1 + 1 = h$.

Case 2. The restriction of the only Kekulé structure κ (of P) to P' is not a Kekulé structure of P' as depicted in Figure1:(d).

In this case, $e_1, e_2 \in \kappa$. If $e_3, e_4 \in \kappa$, from the uniqueness of κ, it follows that there are at least two edges of H_1, H_2 in S. Also note that the restriction of κ to $P - V(H_1 \cup H_2)$ is the Kekulé structure of $P - V(H_1 \cup H_2)$ and then it follows that $afn(P) \geq 2 + afn(P - V(H_1 \cup H_2)) \geq$\{by induction hypothesis\}$\geq 2 + h - 2 = h$. Suppose that e_3 does not belong to κ or e_4 does not belong to κ, as shown in Figure 2:(a). Because of the uniqueness of κ, there are at least i edges of $H_1 \cup H_2 \cup \cdots \cup H_i$ in S. (As each four-membered ring is an alternating cycle, there is at least an edge of a four-membered ring in S. Also note that the border is an alternating cycle. So there are at least i edges of $H_1 \cup H_2 \cup \cdots \cup H_i$ in S.) Similarly, $afn(P) \geq i + afn(P - V(H_1 \cup H_2 \cup \cdots \cup H_i)) \geq i + h - i = h$.

All the cases are exhausted and the theorem is proved. □

Theorem 2.3. *Let P be a ring $[h]$-phenylene. Then $afn(P) = h$.*

Proof. By Theorem 2.2, it is easy to see that $afn(P) \geq h$.

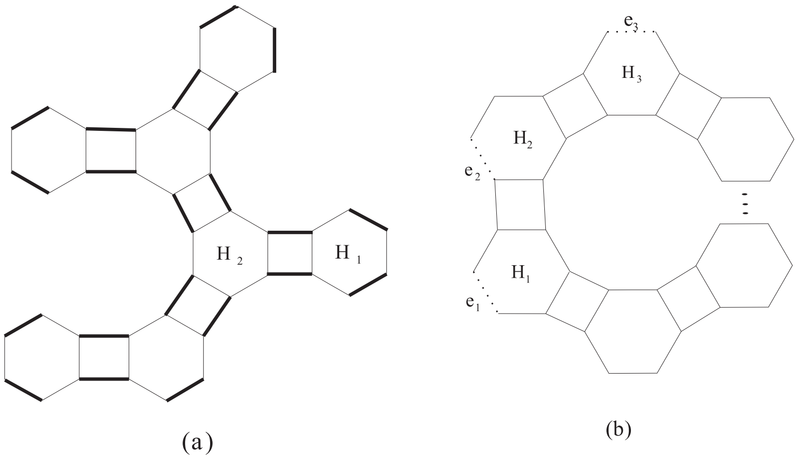

Figure 2:

Next we prove $afn(P) \leq h$. We choose three hexagons H_1, H_2, H_3 and take an edge e_i on $H_i (i = 1, 2, 3)$, see Figure 2:(b).

Again by Theorem 2.2, there is a set S' with $h-3$ elements that fixes all double bonds on $P - V(H_1 \cup H_2 \cup H_3)$. But then the set $S' \cup \{e_1, e_2, e_3\}$ with h elements fixes all double bonds on P. Hence $afn(P) = h$. □

3 Forcing number of cata-condensed phenylenes

We first define some terms which will be used in the proof of the main result of this section.

Let G be a graph and let M be a perfect matching of G. Recall that the forcing number $\varphi(M)$ of M is defined as the smallest number of double edges that completely determine M.

Definition 3.1. *An alternating path in a matching M is a sequence $v_1, e_1, v_2,$ $e_2, v_3, e_3, \cdots, v_{n-1}, e_{n-1}, v_n$ satisfying*

(i) v_i and v_{i+1} belong to the edge e_i.

(ii) $e_i \in M$ when i is odd and $e_i \notin M$ when i is even.

Alternating cycles are alternating paths where the final vertex is the same as the initial vertex.

Edges in an alternating path which are not in the matching will be called *alternate edges*. If all the edges in an alternating path(resp. cycle) are distinct, the alternating path(resp. cycle) will be called *simple*.

Definition 3.2. *We shall denote by $c(M)$ the maximum number of disjoint, simple, alternating cycles in a matching M of a graph G.*

Definition 3.3. *Let G be a finite directed graph. A feedback set is a set of edges in G that contains at least one edge of each directed cycle of G.*

Using the terminology of Alon et al.[2], we shall say that a directed graph G has the *cycle-packing property* if the maximum size of a collection of edge disjoint cycles equals the minimum size of a feedback set. An undirected graph will be said to have the cycle-packing property if every orientation of the edges results in a directed graph with the cycle-packing property.

Theorem 3.4 ([8]). *Let M be a perfect matching M of a bipartite graph G with the cycle-packing property. Then $\varphi(M) = c(M)$.*

Theorem 3.5. *Let P be a cata-condensed $[h]$-phenylene and let M be a perfect matching of P. The forcing number of M is bounded by $\lceil \frac{h}{2} \rceil \leq \varphi(M) \leq h$.*

Proof. Obviously, P is a bipartite graph. Next, we prove that P satisfy the cycle-packing property by induction on h. We only prove that cata-condensed phenylenes without rings satisfy the cycle-packing property, the proof for ring cata-condensed phenylenes is similar.

When $h = 1, 2$, it is easy to check that every orientation of the edges results in a directed graph with the cycle-packing property.

Now, suppose that the claim holds for all cata-condensed $[k]$-phenylenes with $1 \leq k \leq h-1$ and let P be a cata-condensed $[h]$-phenylene with $h \geq 3$. Recall that the graph P' is obtained from P by deleting the vertices of a hexagon X that has only one neighboring four-membered ring. It is easy to see that the maximum size of a collection of edge disjoint cycles of P is either the maximum size or the maximum size + 1 of a collection of edge disjoint cycles of P'. By induction hypothesis, the maximum size of collection of edge disjoint cycles equals the minimum size of a feedback set of every orientation of P.

Also, it is obvious $\lceil \frac{h}{2} \rceil \leq c(M) \leq h$, and then the claims follows from Theorem 3.4, $\lceil \frac{h}{2} \rceil \leq \varphi(M) \leq h$. □

Note that for linear phenylenes these bounds are sharp.

4 Conclusion

The analysis of cata-condensed phenylenes shows that these phenylenes possess only one value of the anti-Kekulé number: 3. The anti-forcing number of cata-condensed phenylenes is h, where h is the number of hexagons in a cata-condensed phenylene. It is also shown that for a Kekulé strcture M of an $[h]$-phenylene, the forcing number $\varphi(M)$ of M is bounded by $\lceil \frac{h}{2} \rceil \leq \varphi(M) \leq h$.

References

[1] P. Adams, M. Mahdian, E. S. Mahmoodian, On the forcing matching numbers of bipartite graphs, *Discr. Math.* **281** (2004) 1–12.

[2] N. Alon, C. McDiarmid, M. Molloy, Edge–disjoint cycles in regular directed graphs, *J. Graph Theory* **22** (1996) 231–237.

[3] I. Gutman, S. J. Cyvin, *Introduction to Theory of Benzenoid Hydrocarbons*, Springer–Verlag, Berlin, 1989.

[4] F. Harary, D. J. Klein, T. P. Živković, Graphical properties of polyhexes: perfect matching vector and forcing, *J. Math. Chem.* **6** (1991) 295–306.

[5] D. J. Klein, M. Randić, Innate degree of freedom of a graph, *J. Comput. Chem.* **8** (1987) 516–521.

[6] F. Lam, L. Pachter, Forcing number of stop signs, *Theor. Comput. Sci.* **303** (2003) 409–416.

[7] S. Marković, Tenth spectral moment for molecular graphs of phenylenes, *J. Chem. Inf. Comput. Sci.* **39** (1999) 654–658.

[8] L. Pachter, P. Kim, Forcing number on square grids, *Discr. Math.* **190** (1998) 287–294.

[9] M. Randić, D. J. Klein, Kekulé valence structures revisited, in: N. Trinajstić (Ed.), *Mathematical and Computational Concepts in Chemistry*, Wiley, New York, 1985.

[10] M. Riddle, The minimum forcing number for the torus and hypercube, *Discr. Math.* **245** (2002) 283–292.

[11] J. Schulman, R. Disch, H. Jiao, P. Schleyer, Chemical shifts of the [N]phenylenes and related compunds, *J. Phys. Chem. A* **102** (1998) 8051–8055.

[12] N. Trinajstić, *Chemical Graph Theory*, CRC Press, Boca Raton, 1992.

[13] D. Vukičević, N. Trinajstić, On the forcing number of benzenoids, *J. Math. Chem.* **42** (2007) 575–583.

[14] D. Vukičević, N. Trinajstić, On the anti–Kekulé number and anti–forcing number of cata–condensed benzenoids, *J. Math. Chem.* **43** (2008) 719–726.

[15] D. Vukičević, J. Sedlar, Total forcing number of the trianglar grid, *Math. Commun.* **9** (2004) 169–179.

[16] F. Zhang, X. Li, Hexagonal systems with forcing edges, *Discr. Math.* **140** (1995) 253–263.