MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **67** (2012) 281-288

ISSN 0340 - 6253

On the Anti-Kekulé Number of Fullerenes[1]

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(Received September 24, 2010)

Abstract

The anti-Kekulé number of a connected graph G is the smallest number of edges whose removal from G results in a connected subgraph without Kekulé structures (perfect matchings). K. Kutnar et al. showed that the anti-Kekulé number of leapfrog fullerene graphs is either 3 or 4 [On the anti-Kekulé number of leapfrog fullerenes, J. Math. Chem. 45 (2009) 431-441]. In this paper, we show that the anti-Kekulé number is always equal to 4 for all fullerene graphs.

1 Introduction

A *fullerene* is a spherically shaped molecule consisting of only carbon atoms such that every carbon atom has bonds to three other atoms, and the length of each carbon ring is either 5 or 6. Ever since the first fullerene, the famous football structure C_{60}, was

[1]This work was supported by NSFC grant no. 10831001.
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discovered by Kroto et al. in 1985 [6], fullerenes have been applied extensively in many fields, such as physics, biology, chemistry, material science, etc. [9, 12]. As a molecular graph of a fullerene, a *fullerene graph* is a 3-connected planar cubic graph with only pentagonal and hexagonal faces. By Euler's polyhedron formula, every fullerene graph with n vertices has exactly 12 pentagonal faces and $(n/2 - 10)$ hexagonal faces.

An edge set M of a graph G is called a *matching* if no two edges in M have a common endvertex. A matching M of G is *perfect* if every vertex of G is incident with an edge in M. In organic molecule graphs, perfect matchings correspond to Kekulé structures, playing an important role in analysis of the resonance energy and stability of hydrocarbon compounds. Cyvin and Gutman systematically gave [1] detailed enumeration formulas for Kekulé structures of various types of benzenoids. Kardoš et al. showed [5] that fullerene graphs have exponentially many Kekulé structures.

The *anti-Kekulé number* of a connected graph G is the smallest number of edges such that the remaining graph obtained from G by deleting these edges is still connected but has no Kekulé structures. For benzenoids, Vukičević and Trinajstić showed [16] that the anti-Kekulé number of parallelograms with at least three rows and at least three columns is equal to 2, and they also showed [15] that cata-condensed benzenoids have anti-Kekulé number either 2 or 3 and both classes are characterized. Afterwards, Veljan and Vukičević [14] demonstrated that the anti-Kekulé numbers of the infinite triangular, rectangular and hexagonal grids are 9, 6 and 4, respectively.

For fullerene graphs, D. Vukičević showed that the anti-Kekulé number of the icosahedron C_{60} (buckminsterfullerene) is 4. The leapfrog transformation of fullerenes is defined in [3], and the icosahedron C_{60} is the smallest leapfrog fullerene graph. In general, Kutnar et al. [8] proved that the anti-Kekulé number of all leapfrog fullerene graphs is either 3 or 4, and for each leapfrog fullerene graph the anti-Kekulé number can be established by observing finite number of cases not depending on the size of the fullerene graph.

By taking into account some structural properties of fullerene graphs and applying Tutte's theorem on perfect matching of graphs, in this paper we show that the anti-Kekulé number of all fullerene graphs is always equal to 4.

2 Preliminary

Let $G = (V(G), E(G))$ be a connected graph with at least one perfect matching (i.e. Kekulé structure). For $S \subseteq E(G)$, let $G - S$ denote the graph obtained from G by deleting all the edges in S. We call S an *anti-Kekulé set* if $G - S$ is connected but has no perfect matchings. The smallest cardinality of anti-Kekulé sets of G is called the *anti-Kekulé number*, and denoted by $ak(G)$.

A connected graph G with at least $2k + 2$ vertices is called to be *k-extendable* if any matching of G with size k is contained in some perfect matching of G.

Theorem 2.1 ([18]). *Every fullerene graph is 2-extendable.*

For a proper subset $X \neq \emptyset$ of $V(G)$, let $\bar{X} = V(G) \backslash X$ and $G[X]$ denote the subgraph of G induced by the vertices of X. Then $[X, \bar{X}]$, the set of k edges with one endvertex in X and the other one in $\bar{X}$, is a k-edge-cut of G. Further it is a minimal edge-cut if each proper subset cannot be an edge-cut of G. It is known that an edge-cut $[X, \bar{X}]$ is minimal if and only if both $G[X]$ and $G[\bar{X}]$ are connected.

A k-edge-cut E of a connected graph G is *cyclic* if $G - E$ has at least two components, each containing a cycle. The minimum value of k such that G has a cyclic k-edge-cut is called the *cyclic edge-connectivity* of G, dented by $c\lambda(G)$. For a positive integer k, G is *cyclically k-edge-connected* if $k \leq c\lambda(G)$. The following basic result has been obtained in several different ways.

Theorem 2.2 ([2, 4, 11]). *Every fullerene graph has the cyclic edge-connectivity 5.*

An edge cut is called *trivial* if all of its edges are incident with the same vertex. The following results are related to edge-cuts of fullerene graphs, or generally cyclically 5-edge-connected cubic graphs.

Lemma 2.3. *Let $E = [X, \bar{X}]$ be a minimal edge-cut of a cyclically 5-edge-connected cubic graph G with $|X| \leq |\bar{X}|$. We have the following statements:*
(i) If $|E| = 3$, then E is trivial and $|X| = 1$,
(ii) If $|E| = 4$, then $|X| = 2$, and
(iii) If $|E| = 5$, then either E is a cyclic 5-edge-cut or $|X| = 3$.

Proof. Suppose that E is not a cyclic edge-cut of G. Without loss of generality, suppose that $G[X]$ is a tree with n vertices and m edges. By degree-sum formula of graph $G[X]$

and tree property, we have that

$$2m = 3n - |E| = 2(n-1),$$

which implies that $n = |E| - 2$. Hence the lemma follows. $\square$

The following result was previously proved to be true for leapfrog fullerene graphs [8], and now we extend this result to all fullerene graphs.

Lemma 2.4. *Let G be a fullerene graph. Then $3 \leq ak(G) \leq 4$.*

Proof. To prove this upper bound on $ak(G)$, it suffices to find an anti-Kekulé set of G with the size 4. Let $v_1v_2v_3$ be a path of length 2 of G. Let e_1, e_2 be the incident edges with v_1 other than v_1v_3, and e_3, e_4 the incident edges with v_2 other than v_2v_3 (see Fig. 1). We can show that $S := \{e_1, e_2, e_3, e_4\}$ is an anti-Kekulé set of G. Let $G' := G - S$. Then G' has no perfect matchings since G' has two 1-degree vertices v_1 and v_2 adjacent to the same vertex v_3. Next, we will show that G' is connected. If G' is not connected, then S is a minimal edge-cut of G by Lemma 2.3 (i) and 3-connectivity of G. Since G' has one component containing vertices v_1, v_2 and v_3, and only v_1 and v_2 are adjacent to vertices of the other component of G' in G. Hence v_1v_3 and v_2v_3 also form an edge cut of G, contradicting that G is 3-edge-connected. Consequently, S is an anti-Kekulé set of G.

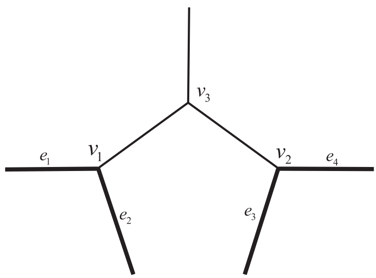

Figure 1: An anti-Kekulé set $\{e_1, e_2, e_3, e_4\}$ (bold edges) of a fullerene graph.

To prove that lower bound on $ak(G)$, choose any pair of edges e_1, e_2 of G. It suffices to show that G has a perfect matching M such that $M \cap \{e_1, e_2\} = \emptyset$. Since G is 2-connected, we can choose a cycle C of G containing e_1 and e_2. Since G is cyclically 5-edge-connected (Theorem 2.2), C has length at least 5 [7, Proposition 2.1]. So there exist two edges e_a and e_b of C such that e_a and e_b are disjoint, and adjacent to e_1 and e_2 respectively. Since

G is 2-extendable (Theorem 2.1), G has a perfect matching M containing e_a and e_b. So $M \cap \{e_1, e_2\} = \emptyset$. That is, $\{e_1, e_2\}$ is not anti-Kekulé set of G. □

3 Main results

The following well-known 1-factor theorem due to Tutte plays a crucial role in proving our main result.

Theorem 3.1 (Tutte's Theorem, [10, 13]). *A graph G has a perfect matching if and only if for any $X \subseteq V(G)$, $o(G - X) \leq |X|$, where $o(G - X)$ denotes the number of odd components of $G - X$.*

We now describe our main result on the anti-Kekulé number of fullerene graphs as follows, and prove it by applying the similar technique used in the proof of Theorem 2.2 in [17], together with 2-extendability and cyclic edge-connectivity 5 of fullerene graphs, and Lemmas 2.3 and 2.4.

Theorem 3.2. *Let G be a fullerene graph. Then $ak(G) = 4$.*

Proof. By Lemma 2.4, we have that $ak(G)$ is either 3 or 4. Suppose to the contrary that $ak(G) = 3$. Then there exists an anti-Kekulé set $S = \{e_1, e_2, e_3\}$ of G. That is, $G' := G - S$ is connected but has no perfect matchings.

Claim 1. Any two edges in S do not have a common adjacent edge.

Suppose there exist two edges in S, say e_1 and e_2, having a common adjacent edge e_a. Then, either both e_1 and e_2 are incident to the same end-vertex of e_a or to different endvertices of e_a. For the former, $e_a \neq e_3$; for the latter, $e_a = e_3$ may be allowed. If $e_a = e_3$, choose edges e'_1 and e'_2 such that e'_1 is adjacent to both e_1 and e_a, and e'_2 adjacent to both e_2 and e_a. Then e'_1 and e'_2 are disjoint. By the 2-extendability of a fullerene graph (Theorem 2.1), $\{e'_1, e'_2\}$ is contained in a perfect matching of G avoiding e_1, e_2 and e_3. That is, G' has a perfect matching, a contradiction.

So suppose $e_a \neq e_3$. Then G has a cycle C that contains both e_a and e_3 since G is 2-connected. We have that C has length at least 5 by Theorem 2.2; see the proof of Lemma 2.4. Note that $E(C) \cap \{e_a, e_1, e_2\}$ induces a path on C. So C contains an edge e_b different from e_1, e_2 and e_a such that e_b is adjacent to e_3 but not to e_a. So e_a and e_b are two disjoint edges of G. By the similar reason as above, $\{e_a, e_b\}$ can be extended to a perfect matching of G avoiding e_1, e_2 and e_3. That is, G' has a perfect matching, a contradiction.

Claim 2. G' is 2-edge-connected.

If not, there exists a cut edge, say e, of G'. If $S' = S \cup \{e\}$, then $G - S'$ is not connected. By Claim 1 and Lemma 2.3 (i), S' is a minimal 4-edge-cut of G. Hence $S' = [X, \overline{X}]$ for some $\emptyset \neq X \subset V(G)$. Using Lemma 2.3 (ii), one of the $|X|$ and $|\overline{X}|$ is 2. Since $|S| = 3$, there must exist two edges in S that have a common adjacent edge, contradicting Claim 1.

Claim 3. G' is a bipartite graph.

Since G' has no perfect matchings, Tutte's theorem ensures the existence of a subset $X \subseteq V(G')$ such that $o(G' - X) > |X|$. Since $|V(G')|$ is even, $o(G' - X)$ and $|X|$ have the same parity. Consequently,

$$o(G' - X) \geq |X| + 2. \tag{1}$$

For the sake of convenience, let $\alpha := o(G' - X)$, and let $G_1, G_2, \cdots, G_\alpha$ denote the odd components of $G' - X$. By Claim 1, the endvertices of edges e_1, e_2 and e_3 are pairwise different.

Since $ak(G) = 3$, adding any edge in S to G' results in a spanning subgraph of G with at least one perfect matching. Hence by Tutte's theorem we can see that every edge of S must join two different odd components in $G' - X$. That is, adding an edge in S to G' will decrease the number of odd components of $G' - X$ by 2. Then $\alpha - 2 \leq |X|$ by Tutte's theorem. Taking (1) into account, we know that

$$\alpha = |X| + 2. \tag{2}$$

Let T be the set of odd components of $G' - X$ which contain at least one vertex incident with one of edges e_1, e_2 and e_3. It is easy to see that $|T| \leq 6$.

Now we consider the number of edges from X to G_i. For $i = 1, 2, \cdots, \alpha$, let n_i denote the number of edges of G' from X to G_i. Since G is 3-edge-connected and G' is 2-edge-connected, we have

$$n_i \geq 3 \quad \text{for each } G_i \notin T; \quad n_i \geq 2 \quad \text{for each } G_i \in T. \tag{3}$$

Then

$$3|X| \geq \sum_{i=1}^{\alpha} n_i \geq 3(\alpha - |T|) + 2|T| = 3|X| + (6 - |T|) \geq 3|X|. \tag{4}$$

In the above expression, the first inequality holds because the edges between X and the odd components of $G' - X$ are partial edges from X towards outside; Inequality (3) implies the second inequality; Take into account of (2) and $|T| \leq 6$, the rest of the relationship holds.

We can see that all equalities in (4) hold. Hence X is an independent set of G', $G' - X$ has no even components, $n_i = 3$ for each $G_i \notin T$, and $|T| = 6$ and $n_i = 2$ for each $G_i \in T$. Further, each odd component G_i in T is joined by exactly one edge in S to the other in T, and there are exactly three edges of G from each G_i going outward. Lemma 2.3 (i) implies that each such three edges form a trivial edge-cut of G and hence every odd component of $G' - X$ is a singleton. Then G' is a bipartite graph and Claim 3 follows. That is, G' has no cycles of odd length.

Since G is a fullerene graph, there are 12 pentagons in G. After deleting three edges from G, there are at least six pentagons in the remaining graph. So G' contains pentagons, contradicting Claim 3. Therefore, $ak(G) = 4$. $\square$

References

[1] S. J. Cyvin, I. Gutman, *Kekulé Structures in Benzenoid Hydrocarbons*, Springer–Verlag, Berlin, 1988.

[2] T. Došlić, Cyclical edge–connectivity of fullerene graphs and (k,6)-cages, *J. Math. Chem.* **33** (2003) 103–111.

[3] P. Fowler, T. Pisanski, Leapfrog transformation and polyhedra of Clar type, *J. Chem. Soc. Faraday Trans.* **90** (1994) 2865–2871.

[4] F. Kardoš, R. Škrekovski, Cyclic edge-cuts in fullerene graphs, *J. Math. Chem.* **44** (2008) 121–132.

[5] F. Kardoš, D. Král, J. Miškuf, J. Sereni, Fullerene graphs have exponentially many perfect matchings, *J. Math. Chem.* **46** (2009) 443–447.

[6] H. W. Kroto, J. R. Heath, S. C. O Brian, R. F. Curl, R. Smalley, C_{60}: Buckminsterfullerene, *Nature* **318** (1985) 162–163.

[7] K. Kutnar, D. Marušič, On cyclic edge-connectivity of fullerenes, *Discr. Appl. Math.* **156** (2008) 1661–1669.

[8] K. Kutnar, J. Sedlar, D. Vukičević, On the anti-Kekulé number of leapfrog fullerenes, *J. Math. Chem.* **45** (2009) 431–441.

[9] F. Langa, J. F. Nierengarten, *Fullerenes: Principles and Applications*, RSC, Cambridge, 2007.

[10] L. Lovász, M. D. Plummer, *Matching Theory*, North–Holland, Amsterdam, 1986.

[11] Z. Qi, H. Zhang, A note on the cyclical edge-connectivity of fullerene graphs, *J. Math. Chem.* **43** (2008) 134–140.

[12] T. D. Ros, G. Spalluto, M. Prato, Biological applications of fullerene derivatives: A brief overview, *Croat. Chem. Acta* **74** (2001) 743–755.

[13] W. T. Tutte, The factorization of linear graphs, *J. London Math. Soc.* **22** (1947) 107–111.

[14] D. Veljan, D. Vukičević, The anti-Kekulé number of the infinte triangular, rectangular and hexagonal grids, *Glas Mat.* **43** (2008) 243–252.

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

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

[17] D. Ye, Z. Qi, H. Zhang, On k-resonant fullerene graphs, *SIAM J. Discr. Math.* **23** (2009) 1023–1044.

[18] H. Zhang, F. Zhang, New lower bound on the number of perfect matchings in fullerene graphs, *J. Math. Chem.* **30** (2001) 343–347.