Digest Journal of Nanomaterials and Biostructures Vol. 6, No 2, April - June 2011, p. 439-443

ON THE ANTI-KEKULE NUMBER OF THREE FENCE GRAPHS

SIPING TANG, HANYUAN DENG*
School of Mathematics and Computing Science, Hunan University of Science and Technology, Xiangtan, Hunan 411201, P. R. China
School of Mathematics and Computing Science, Hunan Normal University, Changsha, Hunan 410081, P. R. China

The anti-Kekule number is the smallest number of edges that must be removed from a connected graph with a perfect matching so that the graph remains connected, but has no perfect matchings. The calculation of this invariant is demonstrated on ladders, cyclic ladders and Mobius ladders in this paper by analyzing the structures of their graphs, and it is shown that the anti-Kekule numbers of these models are 3 or 4.

(Received December 20, 2010; accepted February 22. 2011)

Keywords: anti-Kekule number, Kekule structure, ladder, Mobius ladder.

1. Introduction

Graph theory models have been extensively used as predictors of the properties of chemical compounds (see [1] and references within). The concept of perfect matchings corresponds to the notion of Kekule structure in chemistry and plays a very important role [2]. For example, it is well known that carbon compounds without Kekule structures are unstable. The study of Kekule structures of chemical compounds is very important, because they have many “hidden treasures” [3] that may explain their physical and chemical properties. Kekule, anti-Kekule and related structures are also discussed in terms of the current aromaticity and reactivity indices. Kekule is predicted to be aromatic and stable. This prediction is in agreement with experimental findings. Anti-Kekule is predicted to be nonaromatic and reactive. The synthesis of anti-Kekule has not yet been accomplished, but it seems that its preparation is imminent and difficult [4].

The anti-Kekule number [5] of a graph is the smallest number of edges that have to be removed from a graph in order that it remains connected, but without any Kekule structure (perfect matching). Vukicevic and Trinajstic [5] showed that all cata-benzenoids have anti-Kekule number either 2 or 3 and both classes are characterized. It was found that the anti-Kekule number of the smallest leapfrog fullerenes C_{60} is equal to 4. Further, Kutnar, Sedlar and Vukicevic [6] proved that the anti-Kekule number of all fullerenes is either 3 or 4 and that for each leapfrog fullerene the anti-Kekule number can be established by observing finite number of cases not depending on the size of the fullerene. Both of them attracted considerable interest in graph theory and chemistry.

*Corresponding author: hydeng@hunnu.edu.cn

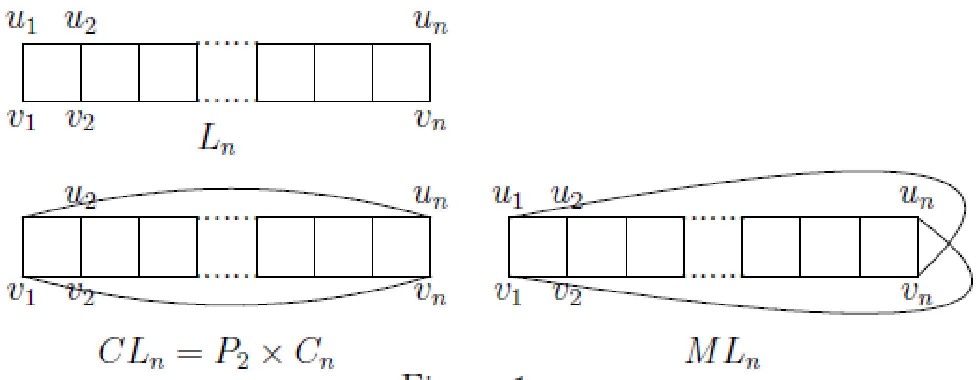


Figure 1.

It is well known [7,8] that ladder graphs are defined as $P_2 \times P_n$ and cyclic ladder graphs (prisms) as $P_2 \times C_n$, where P_n and C_n are the path and the cycle of order n, respectively. For another chemical reason, the prism or cyclic ladder graph has been called the Huckel ladder graph. A Mobius ladder graph as in Figure 1 just by a physical twist of a cyclic ladder graph. Accordingly, several interesting mathematical features including the Kekule number, characteristic polynomial and basis number have been discussed [8,9,10].

The aim of this paper is to analyze the anti-Kekule number of these three models.

Main results

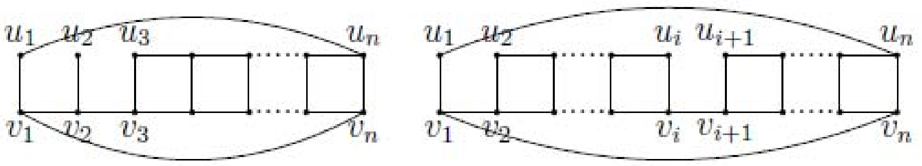
All graphs in this paper are simple and connected with a perfect matching, if not explicitly stated otherwise. A perfect matching (or Kekule structure) in a graph G is a set M of edges of G such that every vertex of G is incident with exactly one edge from M.

An anti-Kekule set of G with Kekule structures is the set S such that G-S is a connected graph and it has no Kekule structures. An anti-Kekule set of the smallest cardinality is called a minimal anti-Kekule set, and its cardinality is the anti-Kekule number of G and it is denoted by ak(G).

Theorem 1. $ak(CL_n) = \begin{cases} 3, & \text{if } n \geq 3 \text{ is odd;} \\ 4, & \text{if } n \geq 4 \text{ is even.} \end{cases}$

Proof. Let $C_1=u_1u_2...u_nu_1$ and $C_2=v_1v_2...v_nv_1$ be two cycles of length n in CL_n, see Figure 1.
It is easy to see that the graph obtained from CL_n by deleting any two edges has a Kekule structure, and $ak(CL_n)>2$.
If $n \geq 3$ is odd, then CL_n-$\{u_1u_2, u_2u_3, v_2v_3\}$ is connected and bipartite with vertex classes V_1 and V_2, where $V_1=\{u_1, u_2, u_4, u_6, ..., u_{n-1}\} \cup \{v_2, v_4, ..., v_n\}$ and $V_2=\{u_3, u_5, ..., u_n\} \cup \{v_1, v_3, ..., v_{n-1}\}$. So, CL_n-$\{u_1u_2, u_1v_1, u_nv_1\}$ has no Kekule structures and $ak(CL_n)=3$ for odd n.
If $n \geq 4$ is even, let e_1, e_2, e_3 be any three edges of CL_n such that $G=CL_n$-$\{e_1, e_2, e_3\}$ is connected, we will prove that G has a Kekule structure and $ak(CL_n)>3$.

Case I. $e_1, e_2, e_3 \in E(C_1) \cup E(C_2)$. Then $u_1v_1, u_2v_2, ..., u_nv_n$ is a Kekule structure of G.



(1) (2)

Figure 2.

Case II. Exactly two of e_1, e_2, e_3 belong to $E(C_1) \cup E(C_2)$. Without loss of generality, we assume that $e_3 \notin E(C_1) \cup E(C_2)$.

(i) $e_1, e_2 \in E(C_1)$. We may assume that $e_1=u_1u_2$ and $e_2=u_iu_{i+1}$ ($2 \le i \le n$, $u_{n+1}=u_1$).

When i=2, $e_3 \ne u_2v_2$ since G is connected. If $e_3 \ne u_1v_1$, then $u_2v_2v_3 \ldots v_nv_1u_1u_nu_{n-1} \ldots u_3$ is a Hamilton path of G, see Figure 2(1); Otherwise, $e_3 \ne u_3v_3$, then $u_2v_2v_1v_nv_{n-1} \ldots v_3u_3u_4 \ldots u_nu_1$ is a Hamilton path of G. So, G has a Kekule structure.

When i=n, the result holds similarly.

Now, we consider 2<i<n. Then at most one of u_1v_1, u_2v_2, u_iv_i, $u_{i+1}v_{i+1}$ is e_3. Without loss of generality, we assume that $e_3 \ne u_1v_1, u_2v_2$, then $u_iu_{i-1} \ldots u_2v_2v_3 \ldots v_nv_1u_1u_nu_{n-1} \ldots u_{i+1}$ is a Hamilton path of G, see Figure 2(2), and G has a Kekule structure.

(ii) $e_1, e_2 \in E(C_2)$. Similarly to (i).

(iii) $e_1 \in E(C_1)$, $e_2 \in E(C_2)$. We may assume that $e_1=u_1u_2$ and $e_2=v_iv_{i+1}$.

If i=1, then at most one of u_1v_1, u_2v_2 is e_3, and $u_1u_nu_{n-1} \ldots u_2v_2v_3v_nv_1$ or $u_2u_3 \ldots u_nu_1v_1v_nv_{n-1} \ldots v_2$ is a Hamilton path of G. So, G has a Kekule structure.

If i=2, note that n is even, u_2u_3, u_4u_5, ..., u_nu_1, v_1v_2, v_3v_4, ..., $v_{n-1}v_n$ is a Kekule structure of G.

If i=n, i.e., $e_2=v_nv_1$, then G has a Kekule structure similarly to i=2.

If 2<i<n, then at most one of u_1v_1, u_2v_2, u_iv_i, $u_{i+1}v_{i+1}$ is e_3. Without loss of generality, we assume that $e_3 \ne u_1v_1, u_2v_2$, then $v_iv_{i-1} \ldots v_2u_2u_3 \ldots u_nu_1v_1v_nv_{n-1} \ldots v_{i+1}$ is a Hamilton path of G, and G has a Kekule structure.

(iv) $e_1 \in E(C_2)$, $e_2 \in E(C_1$. Similarly to (iii).

Case III. Exactly one of e_1, e_2, e_3 belong to $E(C_1) \cup E(C_2)$. Without loss of generality, we assume that $e_1=u_1u_2 \in E(C_1) \cup E(C_2)$.

If $\{e_2, e_3\}=\{u_1v_1, u_2v_2\}$, then $u_2u_3v_3v_2v_1v_nv_{n-1} \ldots v_4u_4u_5 \ldots u_nu_1$ is a Hamilton path of G; Otherwise, we may assume that $u_1v_1 \ne e_2, e_3$. Then $u_2u_3 \ldots u_nu_1v_1v_2 \ldots v_n$ is a Hamilton path of G. So, G has a Kekule structure.

Case IV. $e_1, e_2, e_3 \notin E(C_1) \cup E(C_2)$. Then there is $1 \le i \le n$ such that $u_iv_i \ne e_1, e_2, e_3$ since

G is connected, and $u_{i+1}u_{i+2}...u_nu_1...u_iv_iv_{i+1}...v_nv_1v_2...v_{i-1}$ is a Hamilton path of G. So, G has a Kekule structure.

Finally, we can see that CL_n-{u_1v_1, u_1u_n, u_3v_3, u_3u_4} is connected and has no Kekule structures, and

$\mathrm{ak}(CL_n) \leq 4$.

Hence, $\mathrm{ak}(CL_n)=4$.

Theorem 2. $$\mathrm{ak}(ML_n) = \begin{cases} 3, & \text{if } n \geq 2 \text{ is even;} \\ 4, & \text{if } n \geq 3 \text{ is odd.} \end{cases}$$

Proof. Let $E_0=\{u_iv_i|i=1, 2, ..., n\}$ be an edge-subset of ML_n, see Figure 1.

It is easy to see that the graph obtained from ML_n by deleting any two edges has a Kekule structure, and $\mathrm{ak}(ML_n)>2$.

If $n \geq 2$ is even, then ML_n-{u_1u_2, u_1v_1, u_nv_1} is connected and bipartite with vertex classes V_1 and V_2, where $V_1=\{u_1, u_2, u_4, u_6, ..., u_n\} \cup \{v_1, v_3, ..., v_{n-1}\}$ and $V_2=\{u_3, u_5, ..., u_{n-1}\} \cup \{v_2, v_4, ..., v_n\}$. So, ML_n-{u_1u_2, u_1v_1, u_nv_1} has no Kekule structures and $\mathrm{ak}(ML_n)=3$ for even n.

If $n \geq 3$ is odd, let e_1, e_2, e_3 be three edges of ML_n such that $G=ML_n$-{e_1, e_2, e_3} is connected, we will prove that G has a Kekule structure and $\mathrm{ak}(ML_n)>3$.

Case I. $e_1, e_2, e_3 \in E_0$. Then $C_0=u_1u_2...u_nv_1v_2...v_nu_1$ is a Hamilton cycle in G, and G has a Kekule structure.

Case II. Exactly two of e_1, e_2, e_3 belong to E_0. Without loss of generality, we assume $e_3 \notin E_0$. Then C_0-{e_3} is a Hamilton path of G, and G has a Kekule structure.

Case III. Exactly one of e_1, e_2, e_3 belongs to E_0. Without loss of generality, we assume $e_2, e_3 \notin E_0$ and $e_2=u_1u_2$.

(i) If $e_3=u_2u_3$, then $e_1 \neq u_2v_2$ since G is connected. Note that $G_1=ML_n$-{u_2, v_2} is a ladder and $e_2, e_3 \notin G_1$, G_1-{e_1} has a perfect matching M. So, $M \cup \{u_2v_2\}$ is a Kekule structure of G.

(ii) If $e_3=v_2v_3$, then $C_1=u_1v_1v_2u_2u_3v_3v_4u_4u_5...v_{n-2}v_{n-1}u_{n-1}u_nv_nu_1$ is a Hamilton cycle of ML_n-{e_2, e_3} since $n \geq 3$ is odd, see Figure 3. So, $G=ML_n$-{e_1, e_2, e_3} has a Kekule structure.

(iii) If $e_3=u_1v_n$ or $e_3=u_nv_1$, then, similarly to (i)-(ii), we can prove that G also has a Kekule structure.

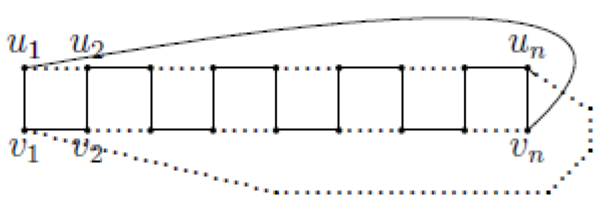


Figure 3.

(iv) If $e_3=u_iu_{i+1}$ or $e_3=v_iv_{i+1}$, $3 \leq i \leq n-1$, let $f_1=v_1v_2$ and

$$f_2 = \begin{cases} v_i v_{i+1}, \text{ if } e_3 = u_i u_{i+1}; \\ u_i u_{i+1}, \text{ if } e_3 = v_i v_{i+1}. \end{cases}$$

then ML_n-{e_2, e_3, f_1, f_2} is the disjoint union of two ladders L_r and L_s, where $r \geq 2$, $s \geq 2$ and r+s=n. So, $L_r \cup L_s$-{e_1} has a perfect matching, and G also has a Kekule structure.

Case IV. None of e_1, e_2, e_3 belong to E_0. Then E_0 is a Kekule structure of G.

From Cases I-IV, we know $ak(ML_n)>3$ for odd n.

Finally, we can see that ML_n-{u_1v_1, u_1v_n, u_3v_3, u_3u_4} is connected and has no Kekule structures, and $ak(ML_n) \leq 4$.

Hence, ak(ML_n)=4.

Similarly to Theorems 1 and 2, we can obtain the anti-Kekule number of ladders, its proof is omitted here.

Theorem 3. $ak(L_n) = \begin{cases} 2, \text{ if } n = 3; \\ 3, \text{ if } n \geq 4. \end{cases}$

Acknowledgements

Project supported by Hunan Provincial Natural Science Foundation of China (09JJ6009).

References

[1] R. Todescini, V. Consonni, Handbook of Molecular Descriptors, Wiley-VCH, Weinheim, (2000).
[2] I. Gutman, O. Polansky, Mathematical Concepts in Organic Chemistry, Springer-Verlag, Berlin, (1986).
[3] M. Randic, Chem. Rev. **103**, 3449 (2003).
[4] D. Babic, N. Trinajstic, J. Molecular Structure: THEOCHEM, 314, 321 (1994).
[5] D. Vukicevic, N. Trinajstic, J. Math. Chem. **43**(2), 719(2008) .
[6] K. Kutnar, J. Sedlar, D. Vukicevic, J. Math. Chem. **45**, 431 (2009).
[7] F. Harary, Graph Theory, Addison-Wesley, Reading, (1969).
[8] N. Biggs, Algebraic Graph Theory, 2nd Ed., Cambridge University Press, Cambridge (1993).
[9] H. Hosoya, F. Harary, J. Math. Chem. **12**, 211 (1993) .
[10] M. Y. Alzoubi, M. M. M. Jaradat, International J. Mathematics and Mathematical Sciences, **12**, 1861 (2005).