MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **61** (2009) 487-494

ISSN 0340 - 6253

REMARKS ON MINIMAL ENERGIES OF UNICYCLIC BIPARTITE GRAPHS

Bing Zhang

Department of Computer Science, Guangdong Polytechnic Normal University, Guangzhou 510665, P. R. China

(Received June 4, 2008)

Abstract

If G is a graph and $\lambda_1, \lambda_2, \ldots, \lambda_n$ are its eigenvalues, then the energy of G is defined as $E(G) = |\lambda_1| + |\lambda_2| + \cdots + |\lambda_n|$. In this paper, we determine the graphs with minimal, second–minimal and third–minimal energies in the class of unicyclic bipartite graphs with n vertices.

1 Introduction

Let G be a simple graph with n vertices and $A(G)$ the adjacency matrix of G. The characteristic polynomial of G is $\phi(G, x) = \det(xI - A(G))$, where I stands for the unit matrix of order n. The roots $\lambda_1, \lambda_2, \ldots, \lambda_n$ of the equation $\phi(G, x) = 0$ are called the eigenvalues of the graph G. The energy of the graph G is then defined as

$$E(G) = \sum_{i=1}^{n} |\lambda_i|.$$

In chemistry the energy of a graph is extensively studied since it can be used to approximate the total π-electron energy of a molecule [1]. For a survey of the mathematical properties of $E(G)$ see the review [2].

If G is a bipartite graph with n vertices, then

$$\phi(G,x) = \sum_{k=0}^{\lfloor n/2 \rfloor} (-1)^k b(G,k) x^{n-2k} \tag{1}$$

and

$$E(G) = \frac{2}{\pi} \int_0^{+\infty} \frac{1}{x^2} \ln \left(\sum_{k=0}^{\lfloor n/2 \rfloor} b(G,k) x^{2k} \right) dx \,. \tag{2}$$

Let G and H be bipartite graphs with n vertices. If

$$b(G,k) \leq b(H,k) \text{ for all } k = 0,1,\ldots,\lfloor n/2 \rfloor \,, \tag{3}$$

then from (2) it follows that $E(G) \leq E(H)$. Further if there is a k_0 such that $b(G,k_0) < b(H,k_0)$, then (3) implies that $E(G) < E(H)$ (see [1, 3]).

Gutman [3] determined n-vertex trees with minimal, second-minimal, third-minimal and fourth-minimal energies. Zhang and Li [4] determined n-vertex trees of a perfect matching with minimal and second–minimal energies. Hou [5] and Chen et al. [6] determined the n-vertex unicyclic graphs with minimal, second–minimal and third–minimal energies, and Li et al. [7] determined the n-vertex unicyclic graphs for $n \geq 8$ with the fourth–, fifth– and sixth–minimal energies after deletion one, one and seven graphs respectively in the class of n-vertex unicyclic graphs. Other results on the energy of unicyclic graphs may be found in [8–16].

In this article, we determine the n-vertex unicyclic bipartite graphs for $n \geq 6$ with minimal, second–minimal and third–minimal energies.

2 Results

Let $\mathcal{U}(n)$ be the set of all unicyclic graphs with n vertices, and $\mathcal{U}(n,l)$ the set of all graphs in $\mathcal{U}(n)$ with a cycle C_l. Let $\mathcal{UB}(n)$ be the set of all bipartite graphs in $\mathcal{U}(n)$. Let S_n^l be the graph obtained by attaching $n-l$ pendent edges to a vertex of C_l. For graphs G and H, $G = H$ means that G and H are isomorphic.

Lemma 1. [5] *Let G be a bipartite graph and uv be an edge of G with the pendent vertex v. Then $b(G,k) = b(G-v,k) + b(G-v-u,k-1)$.*

Lemma 2. [5] *Let $G \in \mathcal{U}(n,l) \setminus \{S_n^l\}$. Then $E(G) > E(S_n^l)$.*

Lemma 3. [5, 6] *If $n \geq l > 4$, then $E(S_n^l) > E(S_n^4)$, and if $n \geq l > 6$, then $E(S_n^l) > E(S_n^6)$.*

Denote by T_n^4 the graph obtained by attaching $n-5$ pendent edges and a pendent edge to two non-adjacency vertices of a C_4, respectively.

Lemma 4. [6] *Let $G \in \mathcal{U}(n,4) \setminus \{S_n^4\}$ with $n \geq 6$. Then $E(G) \geq E(T_n^4)$ with equality if and only if $G = T_n^4$.*

Theorem 5. *If $G \in \mathcal{UB}(n)$, then $E(G) \geq E(S_n^4)$ with equality if and only if $G = S_n^4$. Moreover, if $G \in \mathcal{UB}(n) \setminus \{S_n^4\}$ with $n \geq 6$, then $E(G) \geq E(T_n^4)$ with equality if and only if $G = T_n^4$.*

Proof. The first part of the theorem follows immediately from Lemmas 2 and 3. We need only to prove the second part.

Suppose G contains a cycle C_l. If $l \geq 6$, then by Lemmas 2 and 3 again, we have $E(G) \geq E(S_n^l) \geq E(S_n^6)$. It is easy to see that

$$\begin{aligned} \phi(S_n^6, x) &= x^n - nx^{n-2} + (4n-15)x^{n-4} - (3n-14)x^{n-6}\,, \\ \phi(T_n^4, x) &= x^n - nx^{n-2} + (3n-13)x^{n-4}\,. \end{aligned}$$

Obviously, $b(S_n^6, k) \geq b(T_n^4, k)$, for $k = 0, 1, 2, \ldots, \lfloor n/2 \rfloor$ and $b(S_n^6, 2) > b(T_n^4, 2)$. Thus we have $E(S_n^6) > E(T_n^4)$. So if $l \geq 6$ then $E(G) \geq E(S_n^6) > E(T_n^4)$. By Lemma 4, the result follows. $\square$

Remark. We note that Theorem 5 follows also from the results in [5, 6]. However, our proof is different.

Let $\mathcal{S}(n,4)$ be the class of graphs G in $\mathcal{U}_n$ such that $G - C_4$ consists of $n-4$ isolated vertices. A graph in $\mathcal{S}(n,4)$ obtained by attaching l, m, p and q pendent edges to four vertices of C_4, respectively, where $l, m, p, q \geq 0$ and $l + m + p + q = n - 4$, is denoted by $S_{l,m,p,q}$. Let $T_n'^4 = S_{n-5,1,0,0}$, $H_n = S_{n-6,0,2,0}$. Let $\mathcal{S}_1(n,4) = \{S_{l,0,p,0} : l + p = n - 4, l, p > 0\}$.

Lemma 6. *If $G \in \mathcal{S}(n,4) \setminus (\mathcal{S}_1(n,4) \cup \{S_n^4\})$, then $b(G,2) \geq b(T_n'^4, 2)$ and $b(G,3) \geq b(T_n'^4, 3)$ with equality if and only if $G = T_n'^4$.*

Proof. By direct calculations,

$$\begin{aligned} b(S_{l,m,p,q}, 2) &= lm + lp + lq + mp + mq + pq + 2(n-4) \\ &\geq l(n-4-l) + 2(n-4) \geq 3n - 13\,. \end{aligned}$$

So $b(G,2) \geq 3n-13$ with equality if and only if $G = T_n'^4$.

Since $G \in \mathcal{S}(n,4) \setminus (\mathcal{S}_1(n,4) \cup \{S_n^4\})$, we may assume that $G = S_{l,m,p,q}$ with $l = \max\{l,m,p,q\}$. Then one of m and q is nonzero and so $b(G,3) = lmp + lmq + lpq + mpq + lm + mp + pq + ql \geq l(n-4-l) \geq n-5$. It follows that $b(G,3) \geq n-5$ with equality if and only if $G = T_n'^4$. □

Let R_n^4 denote the graph obtained by attaching $n-6$ pendent edges and a path of length two to a vertex of C_4. Let W_n denote the graph obtained by attaching $n-5$ pendent edges to the unique pendent vertex of S_5^4. Let v be the vertex of C_4 satisfying $d(v) = 3$ in W_{n-1}. Let M_1, M_2, M_3, M_4 be the n-vertex graph obtained from W_{n-1} by attaching a pendent vertex to v, the vertex non-adjacency to v in C_4, the vertex adjacency to v in C_4, a pendent vertex, respectively.

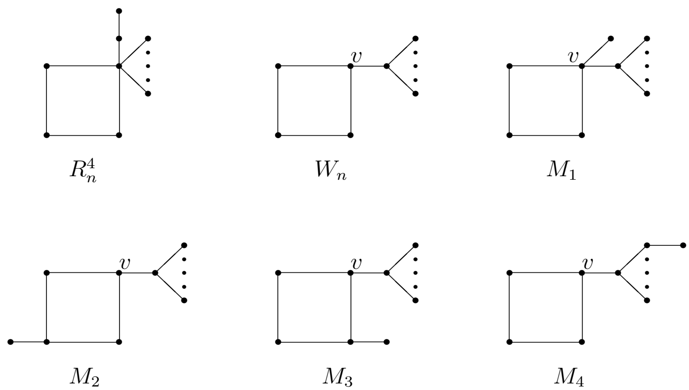

Figure 1. Graphs $R_n^4, W_n, M_1, M_2, M_3, M_4$.

Lemma 7. *Let $G \in \mathcal{U}(n,4) \setminus (\mathcal{S}_1(n,4) \cup \{S_n^4, W_n\})$ with $n \geq 6$. Then $E(G) \geq E(T_n'^4)$ with equality if and only if $G = T_n'^4$.*

Proof. It is easy to see that $\phi(T_n'^4, x) = x^n - nx^{n-2} + (3n-13)x^{n-4} - (n-5)x^{n-6}$ and $b(T_n'^4, 2) = b(T_{n-1}'^4, 2) + b(P_4, 1) = b(T_{n-1}'^4, 2) + 3$.

Firstly, we prove $b(G,2) \geq b(T_n'^4, 2)$ by induction on n. If $n = 6$, then the inequality clearly follows. Suppose that $n \geq 7$ and that the inequality holds for graphs with $n-1$ vertices. Let $G \in \mathcal{U}(n,4) \setminus (\mathcal{S}_1(n,4) \cup \{S_n^4, W_n\})$. If $G \in \mathcal{S}(n,4)$, then from Lemma 6, we have $b(G,2) \geq b(T_n'^4, 2)$ with equality if and only if $G = T_n'^4$. Otherwise, there is a pendent vertex v, being adjacent to vertex u, such that $G-v \in \mathcal{U}(n-1,4)$ and $G-v-u$ contains a cycle C_4. There are three cases:

Case 1. $G-v = S_{n-1}^4, W_{n-1}$. Then $G \in \{R_n^4, M_1, M_2, M_3, M_4\}$. It is not difficult to check that

$$b(R_n^4,2) = 3n-12\,,\quad b(M_1,2) = 5n-26\,,\quad b(M_2,2) = 5n-25\,,$$
$$b(M_3,2) = 5n-25\,,\quad b(M_4,2) = 5n-24\,.$$

So $b(G,2) > b(T_n'^4,2)$.

Case 2. $G-v \in \mathcal{S}_1(n-1,4)$. Then G is obtained by attaching one pendent edge to a pendent vertex of a $S_{l,0,n-5-l,0}$ for some l with $1 \le l \le n-6$. So $b(G,2) = l(n-5-l) + 3(n-4) \ge 1 \times (n-6) + 3(n-4) = 4n-18 > b(T_n'^4,2)$.

Case 3. $G-v \notin \mathcal{S}_1(n-1,4) \cup \{S_{n-1}^4, W_{n-1}\}$. By the induction assumption, we have $b(G-v,2) \ge b(T_{n-1}'^4,2)$. By Lemma 1,

$$b(G,2) = b(G-v,2) + b(G-v-u,1) \ge b(G-v,2) + 4 > b(T_n'^4,2).$$

It follows that if $G \in \mathcal{U}(n,4) \setminus (S_1(n,4) \cup \{S_n^4, W_n\})$. Then $b(G,2) \ge b(T_n'^4,2)$, and the equality holds if and only if $G = T_n'^4$.

Next, we prove $b(G,3) \ge b(T_n'^4,3)$ by induction on n. If $n=6$, then the inequality clearly follows. Suppose that $n \ge 7$ and that the inequality holds for graphs with $n-1$ vertices. Let $G \in \mathcal{U}(n,4) \setminus (\mathcal{S}_1(n,4) \cup \{S_n^4, W_n\})$. If $G \in \mathcal{S}(n,4)$, then from Lemma 6, we have $b(G,3) \ge b(T_n'^4,3)$ with equality if and only if $G = T_n'^4$. Otherwise, there is a pendent vertex v, being adjacent to vertex u, such that $G-v \in \mathcal{U}(n-1,4)$ and $G-v-u$ contains a cycle C_4. There are three cases:

Case i. $G-v = S_{n-1}^4, W_{n-1}$. Then $G \in \{R_n^4, M_1, M_2, M_3, M_4\}$. It is not difficult to check that

$$b(R_n^4,3) = 2n-12\,,\quad b(M_1,3) = 2n-12\,,\quad b(M_2,3) = 2n-12\,,$$
$$b(M_3,3) = 2n-11\,,\quad b(M_4,3) = 4n-26\,.$$

So $b(G,3) > b(T_n'^4,3)$.

Case ii. $G-v \in \mathcal{S}_1(n-1,4)$. Then G is obtained by attaching one pendent edge to a pendent vertex of a $S_{l,0,n-5-l,0}$ for some l with $1 \le l \le n-6$. So $b(G,3) = l(n-l-4) + (n-7) \ge 1 \times (n-5) + n-7 = 2n-12 \ge b(T_n'^4,3); b(G,3) = l(n-l-6) + 2(n-6) \ge n-7 + 2(n-6) = 3n-19 \ge b(T_n'^4,3)$.

Case iii. $G-v \notin \mathcal{S}_1(n-1,4) \cup \{S_{n-1}^4, W_{n-1}\}$. By the induction assumption, we have $b(G-v,3) \ge b(T_{n-1}'^4,3)$. By Lemma 1,

$$b(G,3) = b(G-v,3) + b(G-v-u,2) \ge b(G-v,3) + 2 \ge b(T_n'^4,3).$$

It follows that if $G \in \mathcal{U}(n,4) \setminus (S_1(n,4) \cup \{S_n^4, W_n\}$. Then $b(G,3) \geq b(T_n^{'4}, 3)$ with equality if and only if $G = T_n^{'4}$.

This proves the lemma. $\square$

Lemma 8. *Let $G \in \mathcal{UB}(n) \setminus (\mathcal{S}_1(n,4) \cup \{S_n^4, W_n\})$ with $n \geq 6$. Then $E(G) \geq E(T_n^{'4})$ with equality if and only if $G = T_n^{'4}$.*

Proof. If length of the unique cycle of G is at least 6, then by Lemma 3, $E(G) \geq E(S_n^6)$. It is easy to see that

$$\begin{aligned} \phi(S_n^6, x) &= x^n - nx^{n-2} + (4n-15)x^{n-4} - (3n-14)x^{n-6}\,, \\ \phi(T_n^{'4}, x) &= x^n - nx^{n-2} + (3n-13)x^{n-4} - (n-5)x^{n-6}\,. \end{aligned}$$

It follows that $b(S_n^6, k) \geq b(T_n^{'4}, k)$, $b(S_n^6, k) \geq b(H_n, k)$, $k = 1, \ldots, \lfloor n/2 \rfloor$ and $b(S_n^6, 2) > b(T_n^{'4}, 2), b(S_n^6, 2) > b(H_n, 2)$, and so $E(S_n^6) > E(T_n^{'4})$. By Lemma 7, the result follows. $\square$

Theorem 9. *Let $G \in \mathcal{UB}(n) \setminus (S_n^4 \cup T_n^4\})$ with $n \geq 6$.*
(i) If $n = 6, 7$, then $E(G) \geq E(W_n)$ with equality if and only if $G = W_n$;
(ii) If $n \geq 8$, then $E(G) \geq E(H_n)$ with equality if and only if $G = H_n$.

Proof. Note that

$$\begin{aligned} \phi(H_n, x) &= x^n - nx^{n-2} + (4n-20)x^{n-4}\,, \\ \phi(W_n, x) &= x^n - nx^{n-2} + (4n-18)x^{n-4}\,. \end{aligned}$$

and then $E(W_n) > E(H_n)$ and that if $G \in \mathcal{S}_1(n,4) \setminus \{T_n^4, H_n\}$, then $E(G) > E(H_n)$. By Lemma 8, if $G \in \mathcal{UB}(n) \setminus \{S_n^4, T_n^4\}$. Then $E(G) \geq \min\{E(T_n^{'4}), E(H_n)\}$ for $n \geq 8$ and $E(G) \geq \min\{E(T_n^{'4}), E(W_n)\}$ for $n = 6, 7$. Note that

$$\begin{aligned} E(T_6^{'4}) &= 7.202\,, \quad E(W_6) = 6.602\,, \\ E(T_7^{'4}) &= 7.9925\,, \quad E(W_7) = 7.3006\,. \end{aligned}$$

Then (i) follows. Supposed $n \geq 8$. To prove (ii), we need only to compare the energies of $T_n^{'4}$ and H_n. Note that

$$\begin{aligned} \phi(T_n^{'4}, x) &= x^n - nx^{n-2} + (3n-13)x^{n-4} - (n-5)x^{n-6}\,, \\ &= x^{n-6}\left[x^6 - nx^4 + (3n-13)x^2 - (n-5)\right]\,. \end{aligned}$$

Suppose that

$$\begin{aligned} & x^6 - nx^4 + (3n-13)x^2 - (n-5) \\ = \; & (x-\sqrt{a})(x-\sqrt{b})(x-\sqrt{c})(x+\sqrt{a})(x+\sqrt{b})(x+\sqrt{c}). \end{aligned}$$

Then $a+b+c = n, ab+bc+ca = 3n-13$ and $abc = n-5$.

$$\begin{aligned} \left[\frac{E(T_n'^4)}{2}\right]^2 &= \left[\sqrt{a}+\sqrt{b}+\sqrt{c}\right]^2 \\ &= a+b+c+2\left(\sqrt{ab}+\sqrt{ba}+\sqrt{ca}\right) \\ &= n+2\left(\sqrt{ab}+\sqrt{ba}+\sqrt{ca}\right) . \end{aligned}$$

Similarly, we have

$$\begin{aligned} \left[\frac{E(H_n)}{2}\right]^2 &= \left[\sqrt{d}+\sqrt{e}\right]^2 \\ &= n+2\sqrt{de}\,. \end{aligned}$$

So

$$\begin{aligned} & E(T_n'^4) > E(H_n) \\ \Leftrightarrow \; & \sqrt{ab}+\sqrt{bc}+\sqrt{ca} > \sqrt{de} \\ \Leftrightarrow \; & ab+bc+ca+2\sqrt{abc}(\sqrt{a}+\sqrt{b}+\sqrt{c}) > de \\ \Leftrightarrow \; & 3n-13+2\sqrt{n-5}(\sqrt{a}+\sqrt{b}+\sqrt{c}) > 4n-20 \\ \Leftrightarrow \; & E(T_n'^4) > \tfrac{n-7}{\sqrt{n-5}} \end{aligned}$$

From [2], we have $E(T_n'^4) > E(S_n) = 2\sqrt{n-1} > \frac{n-7}{\sqrt{n-5}}$, and then $E(T_n'^4) > E(H_n)$. Now (ii) follows. □

By Theorems 5 and 9, the graphs S_n^4 and T_n^4 are respectively the unique graphs with minimal, second–minimal energies in $\mathcal{UB}(n)$ for $n \geq 6$, while W_n for $n = 6, 7$, and H_n for $n \geq 8$ is the unique graph with third–minimal energies in $\mathcal{UB}(n)$.

References

[1] I. Gutman, O. E. Polansky, *Mathematical Concepts in Organic Chemistry*, Springer–Verlag, Berlin, 1986.

[2] I. Gutman, The energy of a graph: old and new results, in: A. Betten, A. Kohnert, R. Laue, A. Wassermann (Eds.), *Algebraic Combinatorics and Applications*, Springer–Verlag, Berlin, 2001, pp. 196–211.

[3] I. Gutman, Acyclic systems with extremal Hücklel π-electron energy, *Theor. Chim. Acta* **45** (1977) 79–87.

[4] F. Zhang, H. Li, On acyclic conjugated molecules with minimal energies, *Discr. Appl. Math.* **92** (1999) 71–84.

[5] Y. Hou, Unicyclic graphs with minimal energy, *J. Math. Chem.* **28** (2001) 163–168.

[6] A. Chen, A. Chang, W. Shiu, Energy ordering of unicyclic graph, *MATCH Commun. Math. Comput. Chem.* **55** (2006) 95–102.

[7] S. Li, X. Li, Z. Zhu, On minimal energy and Hosoya index of unicyclic graphs, *MATCH Commun. Math. Comput. Chem.* **61** (2009) 325–339.

[8] F. Li, B. Zhou, Minimal energy of bipartite unicyclic graphs of a given bipartition, *MATCH Commun. Math. Comput. Chem.* **54** (2005) 379–388.

[9] W. Wang, A. Chang, L. Zhang, D. Lu, Unicyclic Hücklel molecular graphs with minimal energy, *J. Math. Chem.* **39** (2006) 231–241.

[10] H. Hua, On minimal energy of unicyclic graphs with prescribed grith and pendent vertices, *MATCH Commun. Math. Comput. Chem.* **57** (2007) 351–361.

[11] I. Gutman, B. Furtula, H. Hua, Bipartite unicyclic graphs with maximal, second–maximal, and third–maximal energy, *MATCH Commun. Math. Comput. Chem.* **58** (2007) 85–92.

[12] H. Hua, M. Wang, Unicyclic graphs with given number of pendent vertices and minimal energy, *Lin. Algebra Appl.* **426** (2007) 478–489.

[13] W. Wang, A. Chang, D. Lu, Unicyclic graphs possessing Kekulé structures with minimal energy, *J. Math. Chem.* **42** (2007) 311–320.

[14] X. Li, J. Zhang, B. Zhou, On unicyclic conjugated molecules with minimal energies, *J. Math. Chem.* **42** (2007) 729–740.

[15] F. Li, B. Zhou, Minimal energy of unicyclic graphs of a given diameter, *J. Math. Chem.* **43** (2008) 476–484.

[16] Y. Yang, B. Zhou, Remarks on minimal energies of bipartite unicyclic graphs of a given bipartition, to appear.