MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **55** (2006) 95-102

ISSN 0340 - 6253

Energy Ordering of Unicycle graphs

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(Received April 26, 2005)

Abstract

If G is a graph with n vertices and $\lambda_1, \lambda_2, \ldots, \lambda_n$ are its eigenvalues, then the energy of G is defined as $E(G) = |\lambda_1| + |\lambda_2| + \cdots + |\lambda_n|$. Let $\mathcal{G}(n)$ be the set of all unicyclic graphs with n vertices. Y. Hou obtained the minimum value on the energies of the graphs in $\mathcal{G}(n)$ and determined the corresponding graph in [10]. In this paper we give the second and third minimum values of the energies of graphs in $\mathcal{G}(n)$ and determine their corresponding graphs, respectively.

1. Introduction

Let G be a graph of order n with vertex set $\{v_1, v_2, \ldots, v_n\}$. Its adjacency matrix $A(G) = (a_{ij})$ is defined to be the $n \times n$ matrix (a_{ij}), where $a_{ij} = 1$ if v_i is adjacent to v_j, and $a_{ij} = 0$ otherwise. The characteristic polynomial of $A(G)$ is defined by

$$P(G, x) = \det(xI - A(G)) = \sum_{i=0}^{n} a_i x^{n-i}, \tag{1}$$

where I stands for the identity matrix of order n, is called the *characteristic polynomial* of the graph G. The n roots of the equation $P(G, x) = 0$, denoted by $\lambda_1, \lambda_2, \ldots, \lambda_n$, are called the *eigenvalues of the graph* G. Since $A(G)$ is a real symmetric matrix, all of its eigenvalues are real.

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* The work was supported by the National Natural Science Foundation of China (No.10371019), SDFFZU(No.2003-XQ-22)); and Faculty Research Grant, Hong Kong Baptist University

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In chemistry the experimental heats from the formation of conjugated hydrocarbons are closely related to the total electron energy. And the calculation of the total energy of all electrons in conjugated hydrocarbons can be reduced to (within the framework of HMO approximation) (see [1])

$$E(G) = \sum_{i=1}^{n} |\lambda_i|, \tag{2}$$

where $\lambda_1, \lambda_2, \ldots, \lambda_n$ are all eigenvalues of the corresponding molecular graph G. $E(G)$ can be expressed as the coulson integral formula (see[1])

$$E(G) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{1}{x^2} \ln[(\sum_{j=0}^{[n/2]} (-1)^j a_{2j} x^{2j})^2 + (\sum_{j=0}^{[n/2]} (-1)^j a_{2j+1} x^{2j+1})^2] dx, \tag{3}$$

where $a_1, a_2, \ldots, a_n$ are the coefficients of the characteristic polynomial of G.

The right-hand side of equation (2) is defined for all graphs (no matter whether they are molecular graphs or not). In view of this, if G is a graph, then by means of equation (2), one can defines and calls it the *energy of the graph* G. For a survey of the mathematical properties of $E(G)$, see [1, Chapter 12] and [2].

There are a lot of results on the bounds for which pertains to special types of graphs: bipartite, benzenoid and trees. However, up to now, very little is known for graphs with extremal energy. Graphs with extremal energy have been determined only for trees and trees with perfect matching (see [7]). Let $\mathcal{G}(n)$ denote the set of all unicyclic graphs with n vertices. Let S_n^3 be the graph obtained from the star graph with n vertices by adding an edge. Recently, Y. Hou [10] proved that among all graphs in $\mathcal{G}(n)$ the graph S_n^3 is the unique graph with minimum energy. In this paper we will give the second and third minimal values for the graphs in $\mathcal{G}(n)$ and give their corresponding graphs.

2. Results

In this paper, we consider only connected simple graph, and denote by $K_{1,n-1}$, C_n and P_n the star graph, the cycle graph, and the path graph with *n* vertices, respectively. Let $\mathcal{G}(n)$ denote the set of all unicyclic graphs with n vertices, and $\mathcal{G}(n,l)$ the set of all unicyclic graphs with n vertices which contains the cycle C_l. Set $b_i(G) = |a_i|$, $i = 0,1,\ldots,n$, where a_i are defined in (1). Notice that $b_0(G) = 1$, and $b_2(G)$ is the number of edges of G. Denote the number of *k*-matchings of a graph G by $m(G,k)$. If G is acyclic, then $b_{2k} = m(G,k)$ and $b_{2k+1}(G) = 0$ for $k \geq 0$.

Lemma 1[10]**.** *Let* $G \in \mathcal{G}(n)$. *Then* $E(G)$ *can be expressed as the following integral formula:*

$$E(G)=\frac{1}{\pi}\int_{0}^{+\infty}\frac{1}{x^2}\ln[(\sum_{j=0}^{[n/2]}b_{2j}(G)x^{2j})^2+(\sum_{j=0}^{[n/2]}b_{2j+1}(G)x^{2j+1})^2]dx. \quad (4)$$

Moreover, $E(G)$ *is a monotonically increasing function of* $b_i(G)$, $i=0,1,\ldots,n$.

Thus, suppose G_1 and G_2 are two graphs in $\mathcal{G}(n)$. By Lemma 1 if

$$b_i(G_1)\geq b_i(G_2) \quad (5)$$

for all $i\geq 0$, then

$$E(G_1)\geq E(G_2) \quad (6)$$

and the equality in (6) holds only if (5) is an equality for all $i\geq 0$. This is the main idea which we used in the following to deal with the ordering graphs in $\mathcal{G}(n)$ by their energies.

Lemma 2[10]**.** *Let* $G\in\mathcal{G}(n)$*, and edge* uv *be an edge of* G *with the pendant vertex* v*. Then* $b_i(G)=b_i(G-v)+b_{i-2}(G-v-u)$.

Let S_n^l denote the graph obtained from the cycle C_l by adding $n-l$ pendant edges to a vertex of C_l (See Fig. 1).

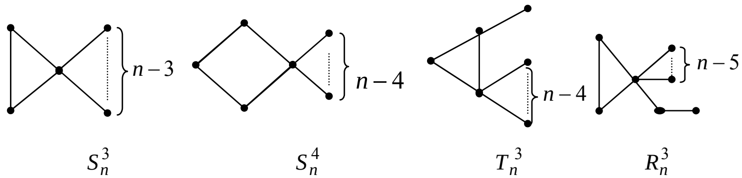


Fig. 1 S_n^3, S_n^4, T_n^3 and R_n^3

Lemma 3[10]**.** *Let* $G\in\mathcal{G}(n,l)\setminus\{S_n^l\}$. *Then* $E(G_l)>E(S_n^l)$.

Lemma 4[10]**.** *Let* $n\geq l\geq 5$, *Then* $E(S_n^l)>E(S_n^4)$.

Let T_n^3 be the graph obtained from the cycle C_3 by attaching $n-4$ pendant edges and a pendant edge to two vertices of C_3, respectively, and R_n^3 the graph obtained from the cycle C_3 by attaching $n-5$ edges and a path of length two to a vertex of C_3 (see Figure 1).

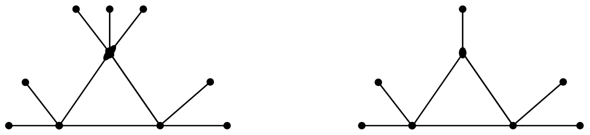
Lemma 5. *Let* $n\geq 5$, *then* $E(R_n^3)>E(T_n^3)$.

Proof. It is not difficult to get that the characteristic polynomials of T_n^3 and R_n^3 are

$$P(T_n^3,\chi)=\chi^n-n\chi^{n-2}-2\chi^{n-3}+(2n-7)\chi^{n-4} \text{ and}$$

$$P(R_n^3,\chi)=\chi^n-n\chi^{n-2}-2\chi^{n-3}+(2n-6)\chi^{n-4}+(n-5)\chi^{n-6},$$

respectively. Obviously, $b_i(R_n^3)\ge b_i(T_n^3)$ ($i=1,2,\ldots,n$) and $b_4(R_n^3)>b_4(T_n^3)$. Thus, we have $E(R_n^3)>E(T_n^3)$. □



$S_{3,2,2}$ $S_{2,2,1}$

Fig. 2. $S_{3,2,2}$ and $S_{2,2,1}$

Let $S_{l,m,n}$ denote the graph obtained from the cycle C_3 by attaching l, m and n pendant edges to three vertices of C_3, respectively (see Figure 2). Similar to the proof of Lemma 5, we can get the following result.

Lemma 6. *Suppose* $l\ge m\ge n$. *Then*

$$E(S_{l+1,m-1,n})>E(S_{l,m,n}) \text{ and } E(S_{l,m+1,n-1})>E(S_{l,m,n}).$$

Theorem 1. *Let* $n\ge 5$ *and* $G\in\mathcal{G}(n,3)\setminus\{S_n^3\}$. *Then* $E(G)\ge E(T_n^3)$, *and the equality holds if and only if* $G\cong T_n^3$.

Proof. Let $G\in\mathcal{G}(n,3)\setminus\{S_n^3\}$. Obviously, $b_i(G)=b_i(T_n^3)$ for all $0\le i\le 3$, and $b_i(T_n^3)=0$ for all $5\le i\le n$.

Now we prove $b_4(G)\ge b_4(T_n^3)$ by induction on n. If $n=5$, then the inequality clearly follows. Let $p\ge 6$ and suppose the inequality holds for $n<p$. Now we consider $n=p$. By Lemma 2, we have $b_4(T_n^3)=b_4(T_{n-1}^3)+b_2(K_{1,2})=b_4(T_{n-1}^3)+2$. We distinguish the following three cases.

Case 1. $G\cong R_n^3$. By the proof of Lemma 5, we have $b_4(G)>b_4(T_n^3)$.

Case 2. $G\ncong R_n^3$, and $G\ncong S_{l,m,n}$. Then G must have a pendant vertex v, such that the distance between v and a vertex on C is at least 2. Suppose that v is adjacent to vertex u, then $G-v\in\mathcal{G}(n-1,3)\setminus\{S_{n-1}^3\}$ (otherwise $G\cong R_n^3$), and $G-v-u$ contains the cycle C_3 as its subgraph. Thus by induction assumption, we have

$$b_4(G)=b_4(G-v)+b_2(G-v-u)\ge b_4(G-v)+3\ge b_4(T_{n-1}^3)+3.$$

Since $b_4(T_n^3)=b_4(T_{n-1}^3)+2$, we have $b_4(G)>b_4(T_n^3)$.

Case 3. $G\cong S_{l,m,n}$. By the proof of Lemma 6, we have $b_4(G)\ge b_4(T_n^3)$.

Therefore, if $G\in\mathcal{G}(n,3)\setminus\{S_n^3\}$, then we have $b_i(G)\ge b_i(T_n^3)$ for all $i=0,1,\ldots,n$.

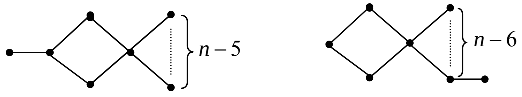
Thus $E(G) \ge E(T_n^3)$. The equality holds if and only if G is in Case 3, $b_2(G-v-u)=2$ and $b_4(G-v)=b_4(T_{n-1}^3)$. Hence $G-v \cong T_{n-1}^3$. This implies that $G \cong T_n^3$. □

Similar to the proof of Lemma 5, we can get the following result.

Lemma 7. *Suppose* $n \ge 5$. *We have* $E(S_n^4) < E(T_n^3)$.

Theorem 2. *Let* $G \in \mathcal{G}(n)$ *with* $n \ge 5$. *Then* $E(G) \ge E(S_n^4)$ *and the equality holds if and only if* $G \cong S_n^4$.

Denote by T_n^4 the graph obtained from C_4 by attaching $n-5$ pendant edges and a pendant edge to two vertices of C_4, respectively. Let R_n^4 denote the graph obtained by the cycle C_4 by attaching $n-6$ edges and a path of length two to a vertex of C_3 (see Figure 3).



T_n^4 R_n^4

Fig.3. T_n^4 and R_n^4

Theorem 3. *Let* $n \ge 6$ *and let* $G \in \mathcal{G}(n,4) \setminus \{S_n^4\}$. *Then* $E(G) \ge E(T_n^4)$ *and the equality holds if and only if* $G \cong T_n^4$.

Proof. Firstly, we prove $b_4(G) \ge b_4(T_n^4)$ by induction on n. If $n=5$, then the inequality clearly follows. Let $p \ge 7$ and suppose that the inequality holds for $n<p$. Now we consider $n=p$. Obviously, $b_4(T_n^4)=b_4(T_{n-1}^4)+b_2(K_{1,3})=b_4(T_{n-1}^4)+3$. We distinguish three cases.

Case 1. $G \cong R_n^4$. It is not difficult to check that $b_4(G) > b_4(T_n^4)$.

Case 2. $G \not\cong R_n^4$. Then G must have a pendant vertex v such that the distance between v and a vertex on G is at least 2. Suppose that v is adjacent to vertex u, then $G-v \in \mathcal{G}(n-1,4) \setminus \{S_{n-1}^4\}$ (otherwise $G \cong R_n^4$), and $G-v-u$ contains C_4 as its subgraph. Thus

$$b_4(G)=b_4(G-v)+b_2(G-v-u) \ge b_4(G-v)+4.$$

Recall that $b_4(T_n^4)=b_4(T_{n-1}^4)+3$ and by the induction assumption, we have $b_4(G) > b_4(T_n^4)$.

Case 3. The distance between each pendant vertex and a vertex C_4 is 1. Since $n \ge 6$, G has a pendant vertex v, which is adjacent to a vertex u. Then $G-v \in \mathcal{G}(n-1,4) \setminus \{S_{n-1}^4\}$, and $G-v-u$ contains the star graph $K_{1,3}$ as its subgraph. Thus

$$b_4(G)=b_4(G-v)+b_2(G-v-u)\geq b_4(G-v)+3\geq b_4(T_{n-1}^3)+3=b_4(T_n^4).$$

From the above, we get that if $G\in\mathcal{G}(n,4)\setminus\{S_n^4\}$, then $b_4(G)\geq b_4(T_n^4)$, and the equality holds if and only if G is in Case 3, $b_2(G-v-u)=3$ and $b_4(G-v)=b_4(T_{n-1}^3)$. By induction assumption, we have $G-v\cong T_{n-1}^4$ and hence $G\cong T_n^4$. Moreover, $b_i(G)\geq b_i(T_n^4)$ holds for all $0\leq i\leq 3$ and $b_i(T_n^4)=0$ for all $5\leq i\leq n$. Thus $E(G)\geq E(T_n^4)$, with the equality holds if and only if $G\cong T_n^4$. □

Lemma 8. *Suppose* $n\geq 7$. *We have* $E(T_n^4)>E(T_n^3)$.

Proof. The characteristic polynomials of T_n^3 and T_n^4 are

$$P(T_n^3,\chi)=\chi^n-n\chi^{n-2}-2\chi^{n-3}+(2n-7)\chi^{n-4} \text{ and}$$

$$P(T_n^4,\chi)=\chi^n-n\chi^{n-2}+(3n-13)\chi^{n-4},$$

respectively. By Lemma 1, we have

$$E(T_n^4)-E(T_n^3)=\frac{1}{\pi}\int_0^{+\infty}\frac{1}{\chi^2}ln\frac{\left[1+n\chi^2+(3n-13)\chi^4\right]^2}{\left[1+n\chi^2+(2n-7)\chi^4\right]^2+4\chi^6}d\chi .$$

Let

$$\begin{aligned}F(\chi)&=[1+n\chi^2+(3n-13)\chi^4]^2-[1+n\chi^2+(2n-7)\chi^4]^2-4\chi^6\\&=2(n-6)\chi^4+2(n^2-6n-4)\chi^6+5(n^2-10n+2)\chi^8.\end{aligned}$$

It is not difficult to check that $F(\chi)>0$ ($\chi\neq 0$) for $n\geq 7$. Thus, we have $E(T_n^4)>E(T_n^3)$ when $n\geq 7$. □

Theorem 4. *Suppose* $l_0\geq 6$ *is an even integer. If* $l>l_0$,*then* $E(S_n^l)>E(S_n^{l_0})$.

Proof. Firstly, we prove by induction on $n-l_0$ that if $l_0\geq 6$ is an even integer and $l>l_0$, then we have $b_i(S_n^l)\geq b_i(S_n^{l_0})$ for all $i=0,1,2,\ldots,n$, and $b_{n-1}(S_n^l)>b_{n-1}(S_n^{l_0})$.

If $n-l_0=1$, then $b_n(S_n^{l_0})=0$; and if $0\leq i\leq 3$, then $b_i(S_n^l)=b_i(S_n^{l_0})$ and; if $4\leq i\leq n-2$, then

$$b_i(S_n^{l_0})=b_i(C_{n-1})+b_{i-2}(P_{n-1})=b_i(P_{n-1})+b_{i-2}(P_{n-2})+b_{i-2}(P_{n-3})$$

and $$b_i(S_n^l)=b_i(P_n)+b_{i-2}(P_{n-2})=b_i(P_{n-1})+b_{i-2}(P_{n-2})+b_{i-2}(P_{n-2}).$$

Obviously, $b_i(S_n^l)=b_i(S_n^{l_0})$ is true for all $4\leq i\leq n-2$. Since

$$\begin{aligned}b_{n-1}(S_n^l)&=b_{n-1}(C_n)=b_{n-1}(P_{n-1})+2b_{n-3}(P_{n-2})\\&=b_{n-1}(P_{n-1})+b_{n-3}(P_{n-2})+b_{n-3}(P_{n-3})+b_{n-5}(P_{n-4}).\end{aligned}$$

Moreover, if $l_0 \equiv 2 \pmod 4$, then $b_{n-1}(S_n^{l_0}) = b_{n-1}(P_{n-1}) + b_{n-3}(P_{n-2}) + b_{n-3}(P_{n-3}) - 2$; and if $l_0 \equiv 0 \pmod 4$, then $b_{n-1}(S_n^{l_0}) = b_{n-1}(P_{n-1}) + b_{n-3}(P_{n-2}) + b_{n-3}(P_{n-3}) + 2$. Thus, we get $b_{n-1}(S_n^{l}) > b_{n-1}(S_n^{l_0})$.

Let $p \geq 2$ and suppose that the inequalities hold for $n < p$. Now we consider $n = p$. Obviously, $b_i(S_n^{l_0}) = b_i(S_{n-1}^{l_0}) + b_{i-2}(P_{l_0-1})$ and $b_i(S_n^{l}) = b_i(S_{n-1}^{l}) + b_{i-2}(P_{l-1})$.

By the induction assumption, we have $b_i(S_n^{l}) \geq b_i(S_n^{l_0})$, $i = 0,1,2,\ldots,n$ and $b_{n-1}(S_n^{l}) > b_{n-1}(S_n^{l_0})$.

Hence, by Lemma 1, we get that the result. □

Corollary 2. *Suppose* $l > 6$. *Then* $E(S_n^{l}) > E(S_n^{6})$.

Similar to the proof of Lemma 8, we can get following Lemmas 9 and 10.

Lemma 9. *Suppose* $l > 6$. *Then* $E(S_n^{6}) > E(S_n^{5})$.

Lemma 10. *Suppose* $n \geq 7$. *Then* $E(S_n^{5}) > E(T_n^{4})$.

The next result follows immediately by above discussions.

Theorem 5. *Suppose* $n \geq 7$ *and* $G \in \mathcal{G}(n) \setminus \{S_n^3, S_n^4\}$. *Then* $E(G) \geq E(T_n^3)$ *and the equality holds if and only if* $G \cong T_n^3$.

Combining with Theorems 2 and 5, we restate our main results as the following: Graphs S_n^4 and T_n^3 are the graphs with second and third minimum values of energies among all graphs in $\mathcal{G}(n)$, respectively.

Acknowledgements

The authors thanks the referee for his/her a lot of valuable comments which make a number of improvements on this paper.

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