

On the Minimal Energy of Tetracyclic Graphs

Hongping Ma¹, Yongqiang Bai^{1,*}, Shengjin Ji²

¹*School of Mathematics and Statistics, Jiangsu Normal University,
Xuzhou 221116, China
hpma@163.com , bmbai@163.com*

²*School of Science, Shandong University of Technology,
Zibo, Shandong 255049, China
jishengjin2013@163.com*

(Received May 27, 2016)

Abstract

The energy of a graph is defined as the sum of the absolute values of the eigenvalues of its adjacency matrix. In this paper, we characterize the tetracyclic graph of order n with minimal energy. By this, the validity of a conjecture for the case $e = n + 3$ proposed by Caporossi et al. (1999) has been confirmed.

1 Introduction

Let G be a simple graph with n vertices and $A(G)$ the adjacency matrix of G . The eigenvalues $\lambda_1, \lambda_2, \dots, \lambda_n$ of $A(G)$ are said to be the eigenvalues of the graph G . The energy of G is defined as

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

The characteristic polynomial of $A(G)$ is also called the characteristic polynomial of G , denoted by $\phi(G, x) = \det(xI - A(G)) = \sum_{i=0}^k a_i(G)x^{n-i}$. Using these coefficients of $\phi(G, x)$, the energy of G can be expressed as the Coulson integral formula [14]:

$$E(G) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \frac{1}{x^2} \ln \left[\left(\sum_{i=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^i a_{2i}(G) x^{2i} \right)^2 + \left(\sum_{i=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^i a_{2i+1}(G) x^{2i+1} \right)^2 \right] dx. \quad (1)$$

*Corresponding author

For convenience, write $b_{2i}(G) = (-1)^i a_{2i}(G)$ and $b_{2i+1}(G) = (-1)^i a_{2i+1}(G)$ for $0 \leq i \leq \lfloor \frac{n}{2} \rfloor$.

Since the energy of a graph can be used to approximate the total π -electron energy of the molecular, it has been intensively studied. For details on graph energy, we refer the readers to the book [24], two reviews [11, 13] and some recent papers [5–10, 12, 15–23, 25–37].

A connected graph on n vertices with e edges is called an (n, e) -graph. We call an (n, e) -graph a unicyclic graph, a bicyclic graph, a tricyclic graph, and a tetracyclic graph if $e = n, n + 1, n + 2$ and $n + 3$, respectively. Follow [35], let $S_{n,e}$ be the graph obtained by the star S_n with $e - n + 1$ additional edges all connected to the same vertex, and $B_{n,e}$ be the bipartite (n, e) -graph with two vertices on one side, one of which is connected to all vertices on the other side.

In [1], Caporossi et al. gave the following conjecture:

Conjecture 1.1. [1] *Connected graphs G with $n \geq 6$ vertices, $n - 1 \leq e \leq 2(n - 2)$ edges and minimum energy are $S_{n,e}$ for $e \leq n + \lfloor (n - 7)/2 \rfloor$, and $B_{n,e}$ otherwise.*

This conjecture is true when $e = n - 1, 2(n - 2)$ [1], and when $e = n$ for $n \geq 6$ [15]. Li et al. [26] showed that $B_{n,e}$ is the unique bipartite graph of order n with minimal energy for $e \leq 2n - 4$. Hou [16] proved that for $n \geq 6$, $B_{n,n+1}$ has the minimal energy among all bicyclic graphs of order n with at most one odd cycle. Let $\mathcal{G}_{n,e}$ be the set of connected graphs with n vertices and e edges. Let $\mathcal{G}_{n,e}^1$ be the subset of $\mathcal{G}_{n,e}$ which contains no disjoint two odd cycles of length p and q with $p + q \equiv 2 \pmod{4}$, and $\mathcal{G}_{n,e}^2 = \mathcal{G}_{n,e} \setminus \mathcal{G}_{n,e}^1$. Zhang and Zhou [36] characterized the graphs with minimal, second-minimal and third-minimal energy in $\mathcal{G}_{n,n+1}^1$ for $n \geq 8$. Combining the results (Lemmas 5-9) in [36] with the fact that $E(B_{n,n+1}) < E(S_{n,n+1})$ for $5 \leq n \leq 7$, we can deduce the following theorem.

Theorem 1.2. [36] *The graph with minimal energy in $\mathcal{G}_{n,n+1}^1$ is $S_{n,n+1}$ for $n = 4$ or $n \geq 8$, and $B_{n,n+1}$ for $5 \leq n \leq 7$, respectively.*

Li et al. [22] proved that $B_{n,n+2}$ has minimal energy in $\mathcal{G}_{n,n+2}^1$ for $7 \leq n \leq 9$, and for $n \geq 10$, they wanted to characterize the graphs with minimal and second-minimal energy in $\mathcal{G}_{n,n+2}^1$, but left four special graphs without determining their ordering. Huo et al. solved this problem in [18], and the results on minimal energy can be restated as follows.

Theorem 1.3. *The graph with minimal energy in $\mathcal{G}_{n,n+2}^1$ is $B_{n,n+2}$ for $7 \leq n \leq 9$ [22], and $S_{n,n+2}$ for $n \geq 10$ [18], respectively.*

In [35], the authors claimed that they gave a complete solution to conjecture 1.1 for $e = n + 1$ and $e = n + 2$ by showing the following two results.

Theorem 1.4. (Theorem 1 of [35]) *Let G be a connected graph with n vertices and $n + 1$ edges. Then*

$$E(G) \geq E(S_{n,n+1})$$

with equality if and only if $G \cong S_{n,n+1}$.

Theorem 1.5. (Theorem 2 of [35]) *Let G be a connected graph with n vertices and $n + 2$ edges. Then*

$$E(G) \geq E(S_{n,n+2})$$

with equality if and only if $G \cong S_{n,n+2}$.

Note that $E(B_{n,n+1}) < E(S_{n,n+1})$ for $5 \leq n \leq 7$, and $E(B_{n,n+2}) < E(S_{n,n+2})$ for $6 \leq n \leq 9$. Hence Theorems 1.4 and 1.5 do not hold for smaller n , respectively. Moreover, even for large n , there is a little gap in the original proofs of Theorems 1.4 and 1.5 in [35], respectively. For completeness, we will prove the following two results in Section 2.

Theorem 1.6. *$S_{n,n+1}$ if $n = 4$ or $n \geq 8$, $B_{n,n+1}$ if $5 \leq n \leq 7$ has minimal energy in $\mathcal{G}_{n,n+1}$.*

Theorem 1.7. *The complete graph K_4 if $n = 4$, $S_{n,n+2}$ if $n = 5$ or $n \geq 10$, $B_{n,n+2}$ if $6 \leq n \leq 9$ has minimal energy in $\mathcal{G}_{n,n+2}$. Furthermore, $S_{6,8}$ has second-minimal energy in $\mathcal{G}_{6,8}$.*

Li and Li [21] discussed the graph with minimal energy in $\mathcal{G}_{n,n+3}^1$, and claimed that the graph with minimal energy in $\mathcal{G}_{n,n+3}^1$ is $B_{n,n+3}$ for $9 \leq n \leq 17$, and $S_{n,n+3}$ for $n \geq 18$, respectively. Note that $E(S_{n,n+3}) < E(B_{n,n+3})$ for $n \geq 12$. In Section 3, we will first illustrate the correct version of this result, and then we will show the following theorem.

Theorem 1.8. *The wheel graph W_5 if $n = 5$, the complete bipartite graph $K_{3,3}$ if $n = 6$, $B_{n,n+3}$ if $7 \leq n \leq 11$, $S_{n,n+3}$ if $n \geq 12$ has minimal energy in $\mathcal{G}_{n,n+3}$. Furthermore, $S_{n,n+3}$ has second-minimal energy in $\mathcal{G}_{n,n+3}$ for $6 \leq n \leq 7$.*

Lemma 1.9. [35] *$E(S_{n,e}) < E(B_{n,e})$ if $n - 1 \leq e \leq \frac{3}{2}n - 3$; $E(B_{n,e}) < E(S_{n,e})$ if $\frac{3}{2}n - \frac{5}{2} \leq e \leq 2n - 4$.*

From Lemma 1.9, we know that the bound $e \leq n + [(n - 7)/2]$ in Conjecture 1.1 should be understood that $e \leq n + [(n - 7)/2]$. With Theorems 1.6, 1.7 and 1.8, we give a complete solution to Conjecture 1.1 for $e = n + 1, n + 2$ and $n + 3$.

2 The graphs with minimal energy in $\mathcal{G}_{n,n+1}$ and $\mathcal{G}_{n,n+2}$

The following three lemmas are needed in the sequel.

Lemma 2.1. [9] *If F is an edge cut of a simple graph G , then $E(G - F) \leq E(G)$, where $G - F$ is the subgraph obtained from G by deleting the edges in F .*

Lemma 2.2. [35] (1) *Suppose that $n_1, n_2 \geq 3$ and $n = n_1 + n_2$. Then*

$$E(S_{n_1, n_1} \cup S_{n_2, n_2}) \geq E(S_{n-3, n-3} \cup C_3)$$

with equality if and only if $\{n_1, n_2\} = \{3, n - 3\}$.

(2) $E(S_{n-3, n-3} \cup C_3) > E(S_{n, n+1})$ for $n \geq 6$.

(3) $E(S_{n, n+1}) > E(S_{n, n})$ for $n \geq 4$.

(4) $E(S_{n-3, n-3} \cup C_3) > E(S_{n, n+2})$ for $n \geq 6$.

Lemma 2.3. (1) [15] $S_{n, n}$ has minimal energy in $\mathcal{G}_{n, n}$ for $n = 3$ or $n \geq 6$.

(2) $B_{n, n}$ and $S_{n, n}$ have, respectively, minimal and second-minimal energy in $\mathcal{G}_{n, n}$ for $4 \leq n \leq 5$. In particular, $S_{n, n}$ is the unique non-bipartite graph in $\mathcal{G}_{n, n}$ with minimal energy for $4 \leq n \leq 5$.

Proof. By Table 1 of [3], there are two (4, 4)-graphs and five (5, 5)-graphs. By simple computation, we can obtain the result (2). ■

Proof of Theorem 1.6: By Theorem 1.2, it suffices to prove that $E(G) > E(S_{n, n+1})$ when $n = 4$ or $n \geq 8$, and $E(G) > E(B_{n, n+1})$ when $5 \leq n \leq 7$ for $G \in \mathcal{G}_{n, n+1}^2$.

Suppose that $G \in \mathcal{G}_{n, n+1}^2$. As there is nothing to prove for the case $n \leq 5$, we suppose that $n \geq 6$. Then G has a cut edge f such that $G - f$ contains exactly two components, say G_1 and G_2 , which are non-bipartite unicyclic graphs. Let $|V(G_1)| = n_1$, $|V(G_2)| = n_2$, and $n_1 + n_2 = n$. By Lemmas 2.1, 2.2 and 2.3, we have

$$E(G) \geq E(G_1 \cup G_2) \tag{2}$$

$$\geq E(S_{n_1, n_1} \cup S_{n_2, n_2}) \tag{3}$$

$$\geq E(S_{n-3, n-3} \cup C_3) \tag{4}$$

$$> E(S_{n, n+1}). \tag{5}$$

In particular, $E(G) > E(S_{n, n+1}) > E(B_{n, n+1})$ for $6 \leq n \leq 7$. The proof is thus complete. ■

Remark 2.4. The proof of Theorem 1.6 (for large n) is similar to that of Theorem 1.4 except that in [35], the authors did not point out that G_1 and G_2 are non-bipartite unicyclic graphs. Without this assumption, we know that the inequality (3) does not hold when n_1 or n_2 equals to 4 or 5 by Lemma 2.3 (2). Moreover, the inequality $E(G_1 \cup G_2) \geq E(S_{n-3, n-3} \cup C_3)$ does not hold. For example: $E(C_4 \cup S_{n-4, n-4}) < E(S_{n-3, n-3} \cup C_3)$ for $n \geq 7$, since $E(C_4) = E(C_3) = 4$ and $E(S_{n-4, n-4}) < E(S_{n-3, n-3})$ by Lemma 2.1.

Lemma 2.5. $S_{n, n+1}$ is the unique non-bipartite graph in $\mathcal{G}_{n, n+1}$ with minimal energy for $5 \leq n \leq 7$. Furthermore, $S_{n, n+1}$ has second-minimal energy in $\mathcal{G}_{n, n+1}$ for $n = 5$ or 7 , and $S_{6, 7}$ has third-minimal energy in $\mathcal{G}_{6, 7}$.

Proof. By Table 1 of [3], there are five (5, 6)-graphs. By simple calculation, we can prove the theorem for $n = 5$. By Table 1 of [4], there are 19 (6, 7)-graphs. By direct computation, we can prove the theorem for $n = 6$. By the results (Lemmas 5-9) in [36], we can obtain that $S_{7, 8}$ has second-minimal energy in $\mathcal{G}_{7, 8}^1$. On the other hand, from the proof of Theorem 1.6, $E(G) > E(S_{7, 8})$ for $G \in \mathcal{G}_{7, 8}^2$. Therefore $S_{7, 8}$ has second-minimal energy in $\mathcal{G}_{7, 8}$, and so the theorem is true for $n = 7$. ■

Proof of Theorem 1.7: Since K_4 is the unique graph in $\mathcal{G}_{4, 6}$, the theorem holds for $n = 4$. By Table 1 of [3], there are four (5, 7)-graphs. By simple calculation, we can prove the theorem for $n = 5$. By Table 1 of [4], there are 22 (6, 8)-graphs. By direct computation, we can prove the theorem for $n = 6$. Now suppose that $n \geq 7$. By Theorem 1.3, it suffices to prove that $E(G) > E(S_{n, n+2})$ when $n \geq 10$, and $E(G) > E(B_{n, n+2})$ when $7 \leq n \leq 9$ for $G \in \mathcal{G}_{n, n+2}^2$.

Suppose that $G \in \mathcal{G}_{n, n+2}^2$ and C_p, C_q are two disjoint odd cycles with $p + q \equiv 2 \pmod{4}$. Then there are at most two edge disjoint paths in G connecting C_p and C_q .

Case 1. There exists exactly an edge disjoint path P connecting C_p and C_q . Then there exists an edge e of P such that $G - e = G_1 \cup G_2$, where G_1 is a non-bipartite bicyclic graph with $n_1 \geq 4$ vertices and G_2 is a non-bipartite unicyclic graph with $n_2 \geq 3$ vertices. By Lemmas 2.1, 2.2, 2.3, 2.5 and Theorem 1.6, we have

$$\begin{aligned} E(G) &\geq E(G_1 \cup G_2) \geq E(S_{n_1, n_1+1} \cup S_{n_2, n_2}) > E(S_{n_1, n_1} \cup S_{n_2, n_2}) \\ &\geq E(S_{n-3, n-3} \cup C_3) > E(S_{n, n+2}). \end{aligned}$$

In particular, $E(G) > E(S_{n, n+2}) > E(B_{n, n+2})$ for $7 \leq n \leq 9$.

Case 2. There exist exactly two edge disjoint paths P^1 and P^2 connecting C_p and C_q . Then there exist two edges e_1 and e_2 such that e_i is an edge of P^i for $i = 1, 2$,

and $G - \{e_1, e_2\} = G_3 \cup G_4$, where G_3 and G_4 are non-bipartite unicyclic graphs. Let $|V(G_3)| = n_1$ and $|V(G_4)| = n_2$. Then by Lemmas 2.1, 2.2 and 2.3, we have

$$E(G) \geq E(G_3 \cup G_4) \geq E(S_{n_1, n_1} \cup S_{n_2, n_2}) \geq E(S_{n-3, n-3} \cup C_3) > E(S_{n, n+2}).$$

In particular, $E(G) > E(S_{n, n+2}) > E(B_{n, n+2})$ for $7 \leq n \leq 9$. The proof is thus complete. ■

Remark 2.6. *The proof of Theorem 1.7 (for large n) is similar to that of Theorem 1.5 except that in [35], the authors did not point out that G_1 and G_2 are non-bipartite graphs.*

3 The graph with minimal energy in $\mathcal{G}_{n, n+3}$

Li and Li [21] discussed the graph with minimal energy in $\mathcal{G}_{n, n+3}^1$, and we first restate their results.

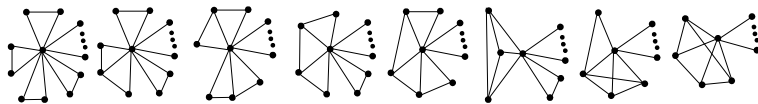


Figure 1. Graphs $G_1, G_2, G_3, G_4, G_5, G_6, G_7$ and G_8 .

Follow [21], let G_1, G_2, \dots, G_8 be eight special graphs in $\mathcal{G}_{n, n+3}$ as shown in Figure 1.

Let $\mathcal{I}_n = \{S_{n, n+3}, B_{n, n+3}, G_1, G_2, G_3, G_4, G_5, G_6, G_7, G_8\}$.

Lemma 3.1. [21] *If $G \in \mathcal{G}_{n, n+3}^1$ and $G \notin \mathcal{I}_n$, then $E(G) > E(B_{n, n+3})$ for $n \geq 9$.*

In fact, Lemma 3.1 is also true for $n = 8$.

Lemma 3.2. *If $G \in \mathcal{G}_{8, 11}^1$ and $G \notin \mathcal{I}_8 \setminus \{G_1\}$, then $E(G) > E(B_{8, 11})$.*

Proof. By the results (see the proofs of Lemma 2.2 and Proposition 2.3) of [21], all we need is to show that $b_4(G) - b_4(B_{8, 11}) > 0$ when G contains exactly i ($i = 10, 12, 13, 14, 15$) cycles (see Case 7 of Lemma 2.2). From [21], we have

$$b_4(G) - b_4(B_{8, 11}) \geq \frac{1}{2}n^2 + \frac{3}{2}n - 12 - 2s - (5n - 35),$$

where s is the number of quadrangles in G . It is easy to check that in this case, G has at most 13 quadrangles. Therefore

$$b_4(G) - b_4(B_{8, 11}) \geq \frac{1}{2}n^2 + \frac{3}{2}n - 12 - 26 - (5n - 35) = \frac{1}{2}n(n - 7) - 3 = 1 > 0.$$

The proof is thus complete. ■

Lemma 3.3. [21] For each $G_j \in \mathcal{S}_n$ ($j = 1, \dots, 8$), $E(S_{n,n+3}) < E(G_j)$ for $n \geq 9$ and $E(B_{n,n+3}) < E(G_j)$ for $9 \leq n \leq 17$.

By the proof of Lemma 2.4 of [21], we can get the following result for $n = 8$.

Lemma 3.4. For each $G_j \in \mathcal{S}_n \setminus \{G_1\}$ ($j = 2, \dots, 8$), $E(B_{n,n+3}) < E(G_j)$ for $n = 8$.

Li and Li [21] claimed that the graph with minimal energy in $\mathcal{G}_{n,n+3}^1$ is $B_{n,n+3}$ for $9 \leq n \leq 17$, and $S_{n,n+3}$ for $n \geq 18$, respectively. However, from Lemma 1.9, we can obtain the following result.

Corollary 3.5. $E(S_{n,n+3}) < E(B_{n,n+3})$ for $n \geq 12$, and $E(B_{n,n+3}) < E(S_{n,n+3})$ for $7 \leq n \leq 11$.

The authors of [21] failed to get the above result in that (in the proof of Proposition 2.5 of [21]) they used the wrong formula $b_4(S_{n,n+3}) = 4n - 18$ instead of the correct one $b_4(S_{n,n+3}) = 4n - 24$. In fact, by Lemmas 3.1, 3.2, 3.3,3.4 and Corollary 3.5, we can characterize the graph with minimal energy in $\mathcal{G}_{n,n+3}^1$ as follows.

Theorem 3.6. The graph with minimal energy in $\mathcal{G}_{n,n+3}^1$ is $B_{n,n+3}$ for $8 \leq n \leq 11$, and $S_{n,n+3}$ for $n \geq 12$, respectively.

To prove Theorem 1.8, we need the following two lemmas.

Lemma 3.7. (1) $E(K_4) > E(S_{4,4})$, and $E(B_{n,n+2}) > E(S_{n,n})$ for $7 \leq n \leq 9$.

(2) $E(S_{n,n+2}) > E(S_{n,n})$ for $n \geq 5$.

Proof. (1) It is easy to obtain that $E(K_4) = 6$, $E(S_{4,4}) \doteq 4.96239$, $E(B_{7,9}) \doteq 7.21110$, $E(S_{7,7}) \doteq 6.64681$, $E(B_{8,10}) \doteq 7.91375$, $E(S_{8,8}) \doteq 7.07326$, $E(B_{9,11}) \doteq 8.46834$ and $E(S_{9,9}) \doteq 7.46410$. Hence the result (1) follows.

(2) Since $6 = E(S_{5,7}) > E(S_{5,5}) \doteq 5.62721$, we now suppose $n \geq 6$. By direct computation, we have that $\phi(S_{n,n+2}, x) = x^n - (n+2)x^{n-2} - 6x^{n-3} + (3n-15)x^{n-4}$ and $\phi(S_{n,n}, x) = x^n - nx^{n-2} - 2x^{n-3} + (n-3)x^{n-4}$. By Eq. (1), we obtain that

$$\begin{aligned} E(S_{n,n+2}) &= \frac{1}{2\pi} \int_{-\infty}^{+\infty} \frac{1}{x^2} \ln((1 + (n+2)x^2 + (3n-15)x^4)^2 + (6x^3)^2) dx \\ &> \frac{1}{2\pi} \int_{-\infty}^{+\infty} \frac{1}{x^2} \ln((1 + nx^2 + (n-3)x^4)^2 + (2x^3)^2) dx = E(S_{n,n}). \end{aligned}$$

■

Lemma 3.8. $E(S_{n-3,n-3} \cup C_3) > E(S_{n,n+3})$ for $n \geq 6$.

Proof. For $6 \leq n \leq 14$, the result follows by direct computation. Suppose that $n \geq 15$. By direct calculation, we have that $\phi(S_{n,n+3}, x) = x^n - (n+3)x^{n-2} - 8x^{n-3} + (4n-24)x^{n-4}$. Let $f(x) = x^4 - (n+3)x^2 - 8x + 4n - 24$. Then we have that $f(-\sqrt{n-1}) > 0$, $f(-2) < 0$, $f(0) > 0$, $f(2) < 0$ and $f(\sqrt{n+3}) > 0$. Hence

$$E(S_{n,n+3}) < 4 + \sqrt{n-1} + \sqrt{n+3}.$$

On the other hand, we have $E(S_{n-3,n-3} \cup C_3) > 4 + \sqrt{2} + 2\sqrt{n-4}$ [35], and so $E(S_{n-3,n-3} \cup C_3) > E(S_{n,n+3})$. ■

Proof of Theorem 1.8: By Table 1 of [3], there are two (5, 8)-graphs. By simple calculation, we can prove the theorem for $n = 5$. By Table 1 of [4], there are 20 (6, 9)-graphs. By direct computation, we can prove the theorem for $n = 6$. By [2], there are 132 (7, 10)-graphs. By direct computing, we can prove the theorem for $n = 7$. Now suppose that $n \geq 8$. By Theorem 3.6 and Corollary 3.5, it suffices to prove that $E(G) > E(S_{n,n+3})$ for $G \in \mathcal{G}_{n,n+3}^2$.

Suppose that $G \in \mathcal{G}_{n,n+3}^2$ and C_p, C_q are two disjoint odd cycles with $p + q \equiv 2 \pmod{4}$. Then there are at most three edge disjoint paths in G connecting C_p and C_q .

Case 1. There exists exactly an edge disjoint path P^1 connecting C_p and C_q . Then there exists an edge e_1 of P^1 such that $G - e_1 = G_1 \cup G_2$, where either both G_1 and G_2 are non-bipartite bicyclic graphs, or G_1 is an non-bipartite tricyclic graph and G_2 is an non-bipartite unicyclic graph. Let $|V(G_1)| = n_1$ and $|V(G_2)| = n_2$.

Subcase 1.1. Both G_1 and G_2 are non-bipartite bicyclic graphs. Then by Lemmas 2.1, 2.2, 2.5, 3.8 and Theorem 1.6, we have

$$\begin{aligned} E(G) &\geq E(G_1 \cup G_2) \geq E(S_{n_1, n_1+1} \cup S_{n_2, n_2+1}) > E(S_{n_1, n_1} \cup S_{n_2, n_2}) \\ &\geq E(S_{n-3, n-3} \cup C_3) > E(S_{n, n+3}). \end{aligned}$$

Subcase 1.2. G_1 is an non-bipartite tricyclic graph and G_2 is an non-bipartite unicyclic graph. It follows from Theorem 1.7 and Lemma 3.7 that $E(G_1) > E(S_{n_1, n_1})$. Therefore by Lemmas 2.1, 2.2, 2.3 and 3.8, we have

$$E(G) \geq E(G_1 \cup G_2) > E(S_{n_1, n_1} \cup S_{n_2, n_2}) \geq E(S_{n-3, n-3} \cup C_3) > E(S_{n, n+3}).$$

Case 2. There exist exactly two edge disjoint paths P^2 and P^3 connecting C_p and C_q . Then there exist two edges e_2 and e_3 such that e_i is an edge of P^i for $i = 2, 3$, and $G - \{e_2, e_3\} = G_3 \cup G_4$, where G_3 is an non-bipartite bicyclic graph with n_1 vertices and

G_4 is an non-bipartite unicyclic graph with n_2 vertices. By Lemmas 2.1, 2.2, 2.3, 2.5, 3.8 and Theorem 1.6, we have

$$\begin{aligned} E(G) &\geq E(G_3 \cup G_4) \geq E(S_{n_1, n_1+1} \cup S_{n_2, n_2}) > E(S_{n_1, n_1} \cup S_{n_2, n_2}) \\ &\geq E(S_{n-3, n-3} \cup C_3) > E(S_{n, n+3}). \end{aligned}$$

Case 3. There exist exactly three edge disjoint paths P^4 , P^5 and P^6 connecting C_p and C_q . Then there exist three edges e_4 , e_5 and e_6 such that e_i is an edge of P^i for $i = 4, 5, 6$, and $G - \{e_4, e_5, e_6\} = G_5 \cup G_6$, where G_5 and G_6 are non-bipartite unicyclic graphs. Let $|V(G_5)| = n_1$ and $|V(G_6)| = n_2$. Then by Lemmas 2.1, 2.2, 2.3 and 3.8, we have

$$E(G) \geq E(G_5 \cup G_6) \geq E(S_{n_1, n_1} \cup S_{n_2, n_2}) \geq E(S_{n-3, n-3} \cup C_3) > E(S_{n, n+3}).$$

The proof is thus complete. ■

Acknowledgment: This work was supported by NNSFC (Nos. 11101351, 11401348 and 11561032), Jiangsu Government Scholarship for Overseas Studies and NSF of the Jiangsu Higher Education Institutions (No. 11KJB110014).

References

- [1] G. Caporossi, D. Cvetković, I. Gutman, P. Hansen, Variable neighborhood search for extremal graphs. 2. Finding graphs with extremal energy, *J. Chem. Inf. Comput. Sci.* **39** (1999) 984–996.
- [2] D. Cvetković, M. Doob, I. Gutman, A. Torgašev, *Recent Results in the Theory of Graph Spectra*, North-Holland, Amsterdam, 1988.
- [3] D. Cvetković, M. Doob, H. Sachs, *Spectra of Graphs – Theory and Application*, Academic Press, New York, 1980.
- [4] D. Cvetković, M. Petrić, A table of connected graphs on six vertices, *Discr. Math.* **50** (1984) 37–49.
- [5] K. C. Das, S. A. Mojallal, Relation between energy and (signless) Laplacian energy of graphs, *MATCH Commun. Math. Comput. Chem.* **74** (2015) 359–366.
- [6] K. C. Das, S. A. Mojallal, Relation between signless Laplacian energy, energy of graph and its line graph, *Lin. Algebra Appl.* **493** (2016) 91–107.
- [7] K. C. Das, S. A. Mojallal, I. Gutman, On energy of line graphs, *Lin. Algebra Appl.* **499** (2016) 79–89.

- [8] K. C. Das , S. A. Mojallal, I. Gutman, On energy and Laplacian energy of bipartite graphs, *Appl. Math. Comput.* **273** (2016) 759–766.
- [9] J. Day, W. So, Graph energy change due to edge deletion, *Lin. Algebra Appl.* **428** (2008) 2070–2078.
- [10] M. A. A. de Freitas, M. Robbiano, A. S. Bonifácio, An improved upper bound of the energy of some graphs and matrices, *MATCH Commun. Math. Comput. Chem.* **74** (2015) 307–320.
- [11] 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.
- [12] I. Gutman, Kragujevac trees and their energy, *Sci. Publ. State Univ. Novi Pazar A* **6** (2014) 71–79.
- [13] I. Gutman, X. Li, J. Zhang, Graph energy, in: M. Dehmer, F. Emmert–Streib (Eds.), *Analysis of Complex Networks: From Biology to Linguistics*, Wiley–VCH, Weinheim, 2009, 145–174.
- [14] I. Gutman, O. E. Polansky, *Mathematical Concepts in Organic Chemistry*, Springer–Verlag, Berlin, 1986.
- [15] Y. Hou, Unicyclic graphs with minimal energy, *J. Math. Chem.* **29** (2001) 163–168.
- [16] Y. Hou, Bicyclic graphs with minimum energy, *Lin. Multilin. Algebra* **49** (2001) 347–354.
- [17] M. Hu, W. Yan, W. Qiu, Maximal energy of subdivisions of graphs with a fixed chromatic number, *Bull. Malays. Math. Sci. Soc.* **38** (2015) 1349–1359.
- [18] B. Huo, S. Ji, X. Li, Solutions to unsolved problems on the minimal energies of two classes of graphs, *MATCH Commun. Math. Comput. Chem.* **66** (2011) 943–958.
- [19] B. Huo, X. Li, Y. Shi, Complete solution to a conjecture on the maximal energy of unicyclic graphs, *Eur. J. Comb.* **32** (2011) 662–673.
- [20] D. P. Jacobs, V. Trevisan, F. Tura, Eigenvalues and energy in threshold graphs, *Lin. Algebra Appl.* **465** (2015) 412–425.
- [21] S. Li, X. Li, On tetracyclic graphs with minimal energy, *MATCH Commun. Math. Comput. Chem.* **60** (2008) 395–414.
- [22] S. Li, X. Li, Z. Zhu, On tricyclic graphs with minimal energy, *MATCH Commun. Math. Comput. Chem.* **59** (2008) 397–419.

- [23] X. Li, Y. Mao, M. Wei, More on a conjecture about tricyclic graphs with maximal energy, *MATCH Commun. Math. Comput. Chem.* **73** (2015) 11–26.
- [24] X. Li, Y. Shi, I. Gutman, *Graph Energy*, Springer, New York, 2012.
- [25] X. Li, Y. Shi, M. Wei, J. Li, On a conjecture about tricyclic graphs with maximal energy, *MATCH Commun. Math. Comput. Chem.* **72** (2014) 183–214.
- [26] X. Li, J. Zhang, L. Wang, On bipartite graphs with minimal energy, *Discr. Appl. Math.* **157** (2009) 869–873.
- [27] H. Ma, Some relations on the ordering of trees by minimal energies between subclasses of trees, *J. Appl. Math. Comput.* **45** (2014) 111–135.
- [28] H. Ma, Y. Bai, S. Ji, On the minimal energy of conjugated unicyclic graphs with maximum degree at most 3, *Discr. Appl. Math.* **186** (2015) 186–198.
- [29] C. A. Marín, J. Monsalve, J. Rada, Maximum and minimum energy trees with two and three branched vertices, *MATCH Commun. Math. Comput. Chem.* **74** (2015) 285–306.
- [30] S. Renqian, Y. Ge, B. Huo, S. Ji, Q. Diao, On the tree with diameter 4 and maximal energy, *Appl. Math. Comput.* **268** (2015) 364–374.
- [31] O. Rojo, Effects on the energy and Estrada indices by adding edges among pendent vertices, *MATCH Commun. Math. Comput. Chem.* **74** (2015) 343–358.
- [32] T. Tian, W. Yan, S. Li, On the minimal energy of trees with a given number of vertices of odd degree, *MATCH Commun. Math. Comput. Chem.* **73** (2015) 3–10.
- [33] W. H. Wang, L. Y. Kang, Ordering of unicyclic graphs by minimal energies and Hosoya indices, *Util. Math.* **97** (2015) 137–160.
- [34] W. H. Wang, W. So, Graph energy change due to any single edge deletion, *El. J. Lin. Algebra* **29** (2015) 59–73.
- [35] J. Zhang, H. Kan, On the minimal energy of graphs, *Lin. Algebra Appl.* **453** (2014) 141–153.
- [36] J. Zhang, B. Zhou, On bicyclic graphs with minimal energies, *J. Math. Chem.* **37** (4) (2005) 423–431.
- [37] J. Zhu, J. Yang, Bipartite unicyclic graphs with large energies, *J. Appl. Math. Comput.* **48** (2015), 533–552.