MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **75** (2016) 373-383

ISSN 0340 - 6253

Estrada Indices of the Trees with a Perfect Matching

Wen–Huan Wang*

Department of Mathematics, Shanghai University, Shanghai 200444, China

(Received October 17, 2015)

Abstract

Let $\mathcal{H}_{2n}$ be the set of the trees having a perfect matching with $2n$ vertices. In $\mathcal{H}_{2n}$, ordering the trees in terms of their maximal Estrada indices is considered. A new transformation is introduced. As an application of the new transformation, we give a simpler proof for the result in Deng's paper [H. Deng, MATCH Commun. Math. Comput. Chem. 62 (2009) 607–610]. Then, we obtain the trees with the largest and the second largest Estrada indices among $\mathcal{H}_{2n}$ with $n \geq 5$.

1 Introduction

Let G be a simple graph with n vertices and $A(G)$ its adjacency matrix. The characteristic polynomial of G is $\Phi(G, \lambda) = \det[\lambda I - A(G)]$, where I is the unit matrix of order n [1]. The n roots of $\Phi(G, \lambda) = 0$ are denoted by $\lambda_1 \geq \cdots \geq \lambda_n$. Since $A(G)$ is a real symmetric matrix, $\lambda_1, \cdots, \lambda_n$ are all real numbers. The Estrada index (EI), put forward by Estrada [2] is defined as

$$EE(G) = \sum_{i=1}^{n} \mathrm{e}^{\lambda_i} \ . \tag{1}$$

In the last decade the EI had numerous applications and attracted much attention of mathematicians. For example, it can measure the degree of protein folding [2] and the centrality of complex (communication, social, metabolic, ect.) networks [3]. It is shown that there is a connection between the EI and the concept of extended atomic branching [4]. Some mathematical properties of the EI and the lower and upper bounds for EI may

*Corresponding author, email: whwang@shu.edu.cn

be found in Refs. [5–7]. For the characterization of graphs with the extremal EI and some other results on the EI, one can refer to Refs. [8–13].

A walk W of length k in G is any sequence of vertices and edges of G, namely $W = v_0, e_1, v_1, e_2, \cdots, v_{k-1}, e_k, v_k$ such that e_i is the edge joining vertices v_{i-1} and v_i for every $i = 1, 2, \cdots, k$. If $v_0 = v_k$, the walk is closed and is referred to as the (v_0, v_0)-walk of length k. For $k \geq 0$, we denote $M_k(G) = \sum_{i=1}^{n} \lambda_i^k$ and refer to $M_k(G)$ as the k-th spectral moment of G. It is well known that $M_k(G)$ is equal to the number of the closed walks of length k in G [1]. From the Taylor expansion of e^{λ_i}, $EE(G)$ in (1) can be rewritten as

$$EE(G) = \sum_{k=0}^{\infty} \frac{M_k(G)}{k!} \ . \tag{2}$$

In particular, if G is a bipartite graph, then $M_{2k+1}(G) = 0$ for $k \geq 0$. Hence, we have

$$EE(G) = \sum_{k=0}^{\infty} \frac{M_{2k}(G)}{(2k)!} \ . \tag{3}$$

Let G_1 and G_2 be two bipartite graphs of order n. If $M_{2k}(G_1) \geq M_{2k}(G_2)$ holds for any positive integer k, then $EE(G_1) \geq EE(G_2)$. Moreover, if the strict inequality $M_{2k}(G_1) > M_{2k}(G_2)$ holds for at least one integer k, then $EE(G_1) > EE(G_2)$.

The characterization of graphs with the extremal Estrada indices (EIs) is an interesting problem. Recently, the trees and cyclic graphs with the extremal Estrada indices have successfully been characterized [8–13]. For the general trees [14–17], the trees with a fixed maximal degree [18], the trees with a perfect matching and a maximal degree [18], the trees with a given matching number [8], the trees with a fixed diameter [8], the trees with a given number of pendant vertices [9], and the trees with an independence number [9], etc., some results were recently reported.

Let $\mathcal{H}_{2n}$ be the set of trees with a perfect matching having $2n$ vertices. In this paper, we will study the trees with the largest and the second largest EIs in $\mathcal{H}_{2n}$. Recall that molecular graphs with perfect matchings correspond to molecules with the Kekulé structures. This, in particular, means that the trees with a perfect matching in which the maximum vertex degree is 3, are the molecular graphs of acyclic polyenes. Thus we will characterize the acyclic Kekuléan π-electron systems with the largest Estrada indices.

The rest of this paper is organized as follows. In Section 2, a new transformation is introduced (see Lemma 7) for studying the EI. As an application of the new transformation, we give a simpler proof for the result which has been obtained by Deng [17]. In

Section 3, with the aid of the new transformation, we deduce the trees with the largest and the second largest EIs in $\mathcal{H}_{2n}$ as $n \geq 5$.

2 Transformations for Studying the Estrada Indices

To deduce the main results of this paper, Lemmas 1–6 are simply quoted here.

Let the coalescence $G(u) \cdot H(v)$ be the graph obtained from G and H by identifying u of G with v of H. Let $M_k(G, u)$ be the number of closed walks of length k starting at u in G.

Lemma 1 ([8]) *If G_1 and G_2 are two bipartite graphs satisfying $M_{2k}(G_1) \geq M_{2k}(G_2)$ and $M_{2k}(G_1, w) \geq M_{2k}(G_2, u)$ for any positive integer k, then $M_{2k}(G) \geq M_{2k}(G')$ for any positive integer k, where $G \cong G_1(w) \cdot G_3(a)$ and $G' \cong G_2(u) \cdot G_3(a)$. Furthermore, if $M_{2k}(G_1, w) > M_{2k}(G_2, u)$ for some positive integer k, then there must exist a positive integer l such that $M_{2l}(G) > M_{2l}(G')$.*

Lemma 2 ([19]) *Let G and H be two vertex-disjoint graphs with $u, v \in V(G)$ and $z \in V(H)$, where $|V(H)| \geq 2$. For each positive integer k, if $M_k(G; u) \geq M_k(G; v)$ and there exists at least one k such that $M_k(G; u) > M_k(G; v)$ holds, then $EE(G(u) \cdot H(z)) > EE(G(v) \cdot H(z))$.*

Lemma 3 ([20]) *Let A, B, and C be three connected graphs, each of which has at least two vertices. Let u and v be two different vertices of C, $u' \in V(A)$ and $v' \in V(B)$. Let $H = A(u') \cdot C(u)$, $G = H(v) \cdot B(v')$ and $G' = H(u) \cdot B(v')$. Suppose that there exists an automorphism θ of C such that $\theta(u) = v$, then*

(i) $M_k(H, u) \geq M_k(H, v)$ for all positive integer k and it is strict for some positive integer k_0;

(ii) $M_k(G') \geq M_k(G)$ for all positive integer k and it is strict for some positive integer k_0.

Proof. Lemma 3(i) is Lemma 2.4(i) in Ref. [20]. Lemma 3(ii) follows from Lemma 3(i) and Lemma 2. ∎

Remark: It should be noted that Deng and Chen [20] deduced Lemma 3(ii) by Lemma 3(i) and Lemma 1. Bearing the condition of Lemma 1 in mind, we point out that H in Lemma 2.4 in Ref. [20] must be a bipartite graph.

Lemma 4 ([10]) *Let A be the adjacency matrix of a connected graph G with n vertices. For two vertices v_i and v_j in G, the number of the walks of length k from v_i to v_j is $A^k_{i,j} = \sum_{v_h \in N_G(v_j)} A^{k-1}_{ih}$, where $N_G(v_j)$ is the set of the vertices which are adjacent to the vertex v_j in G and A^k_{ij} is the element of A^k which lies in the i-th row and the j-th column with $1 \leq i, j \leq n$. Furthermore, $A^k_{i,j} = A^k_{j,i}$.*

Lemma 5 has been obtained by Zhang et al. [8]. For completeness, we give another proof for Lemma 5. For $v \in V(G)$, let $d_G(v)$ be the degree of v.

Lemma 5 ([8]) *Let G and H be two vertex-disjoint connected graphs with $|V(G)| \geq 3$ and $|V(H)| \geq 2$. Let $z \in V(H)$ and $v_s, v_{s-1} \in V(G)$, where v_s and v_{s-1} are adjacent, $d_G(v_s) = 1$, and $d_G(v_{s-1}) \geq 2$. We have $M_k(G; v_{s-1}) \geq M_k(G; v_s)$ and there exists at least one k such that the inequality holds. Furthermore, $EE(G(v_{s-1}) \cdot H(z)) > EE(G(v_s) \cdot H(z))$.*

Proof. Let A be the adjacency matrix of G. Obviously, $M_k(G; v_i) = A^k_{i,i}$.

As $k = 1$, $A^k_{s-1,s-1} = A^k_{s,s} = 0$. As $k = 2$, since $d_G(v_s) = 1$ and $d_G(v_{s-1}) \geq 2$, we have $A^k_{s-1,s-1} \geq 2 > 1 = A^k_{s,s}$. Let $k \geq 3$. Since v_s and v_{s-1} are adjacent, $d_G(v_s) = 1$, and $d_G(v_{s-1}) \geq 2$, by Lemma 4, we get

$$A^k_{s-1,s-1} = A^{k-1}_{s-1,s} + \sum_{v_h \in N_G(v_{s-1}) \setminus \{v_s\}} A^{k-1}_{s-1,h} \geq A^{k-1}_{s-1,s} = A^{k-1}_{s,s-1} = A^k_{s,s}. \quad (4)$$

Thus, we get $M_k(G; v_{s-1}) \geq M_k(G; v_s)$ and there exists at least one $k = 2$ such that $M_k(G; v_{s-1}) > M_k(G; v_s)$ holds. Furthermore, by Lemma 2, we get Lemma 5. ■

By Lemma 5, we have another proof for Lemma 6 which has been obtained by Du and Zhou [19].

Lemma 6 ([19]) *Let G_1 and G_2 be two connected graphs, $u \in V(G_1)$, and $v \in V(G_2)$. Let G be the graph obtained from G_1 and G_2 by joining u and v with an edge. Let G' be the graph obtained from G_1 and G_2 by identifying u with v, and attaching a pendant vertex to the common vertex $u(v)$. If $d_G(u) \geq 2$ and $d_G(v) \geq 2$, then $EE(G') > EE(G)$.*

Proof. Let A be $G_2(v) \cdot P_2(v_1)$, where $P_2 = v_0v_1$. Obviously, v_0 and v_1 of A are adjacent, $d_A(v_0) = 1$, $d_A(v_1) \geq 2$, $A(v_1) \cdot G_1(u) = G'$, and $A(v_0) \cdot G_1(u) = G$. By Lemma 5, we have $EE(G') > EE(G)$. ■

To get our main results of this paper, Lemma 7 is introduced as follows.

Lemma 7 *Let G and H be two vertex-disjoint connected graphs with $|V(G)| \geq 4$ and $|V(H)| \geq 2$. Let $z \in V(H)$ and $v_s, v_{s-1}, v_{s-2} \in V(G)$, where $d_G(v_s) = 1$, $d_G(v_{s-1}) = 2$, $d_G(v_{s-2}) \geq 2$, and v_{s-1} is adjacent to v_s and v_{s-2}. We have $M_k(G; v_{s-2}) \geq M_k(G; v_{s-1})$ for all positive k. Furthermore, if there exists at least one k such that $M_k(G; v_{s-2}) > M_k(G; v_{s-1})$, then $EE(G(v_{s-2}) \cdot H(z)) > EE(G(v_{s-1}) \cdot H(z))$.*

Proof. Let A be the adjacency matrix of G. Obviously, $M_k(G; v_i) = A^k_{i,i}$. We prove $M_k(G; v_{s-2}) \geq M_k(G; v_{s-1})$ by induction on k.

As $k = 1$, $A^k_{s-2,s-2} = A^k_{s-1,s-1} = 0$. As $k = 2$, since $d_G(v_{s-1}) = 2$ and $d_G(v_{s-2}) \geq 2$, we have $A^k_{s-2,s-2} \geq 2 = A^k_{s-1,s-1}$. As a fixed k with $k \geq 3$, we suppose $M_k(G; v_{s-2}) \geq M_k(G; v_{s-1})$. Next, we prove $M_{k+1}(G; v_{s-2}) \geq M_{k+1}(G; v_{s-1})$.

Since $d_G(v_{s-2}) \geq 2$, we can choose a vertex v_y which is adjacent to v_{s-2} and $v_y \neq v_{s-1}$. By using Lemma 4 twice, we get

$$\begin{aligned} A^{k+1}_{s-2,s-2} &= A^k_{s-2,s-1} + \sum_{v_h \in N_G(v_{s-2}) \setminus \{v_{s-1}\}} A^k_{s-2,h} \\ &\geq A^k_{s-2,s-1} + A^k_{s-2,y} \\ &= A^k_{s-2,s-1} + \sum_{v_h \in N_G(v_y)} A^{k-1}_{s-2,h} \\ &\geq A^k_{s-2,s-1} + A^{k-1}_{s-2,s-2}. \end{aligned} \tag{5}$$

Since $d_G(v_s) = 1$, $d_G(v_{s-1}) = 2$, and v_{s-1} is adjacent to v_s and v_{s-2}, by using Lemma 4 twice, we get

$$A^{k+1}_{s-1,s-1} = A^k_{s-1,s-2} + A^k_{s-1,s} = A^k_{s-2,s-1} + A^{k-1}_{s-1,s-1}. \tag{6}$$

By the induction assumption, we have $A^{k-1}_{s-2,s-2} \geq A^{k-1}_{s-1,s-1}$ for a fixed k with $k \geq 3$. Therefore, by (5) and (6), we get $A^{k+1}_{s-2,s-2} \geq A^{k+1}_{s-1,s-1}$. Namely, we obtain $M_k(G; v_{s-2}) \geq M_k(G; v_{s-1})$ for all positive k. Furthermore, if there exists at least one k such that $M_k(G; v_{s-2}) > M_k(G; v_{s-1})$ holds, then by Lemma 2, we get Lemma 7. ■

Lemma 7 will provide us with a useful and direct method to compare EIs for two graphs. For example, we show some applications of Lemma 7 as follows.

(i) By Lemma 7, we have a simpler proof for Theorem 1 which has been obtained by Deng [17].

(ii) By Lemmas 5 and 7, we get Lemma 8 in Section 3. By Lemma 7, we get Lemma 9 in Section 3.

For $n \geq 2$, let P_n and X_n be a path and a star graph, respectively, where n is the number of vertices. Let $S_n^4 = P_5(v_2) \cdot X_{n-4}(v)$ and $S_n^5 = P_5(v_1) \cdot X_{n-4}(v)$, where $P_5 = v_0 \cdots v_4$, v is the center vertex of X_{n-4}, and $n \geq 6$.

Theorem 1 *[17] $EE(S_n^4) > EE(S_n^5)$ for $n \geq 6$.*

Proof. Since $P_5 = v_0 \cdots v_4$, we have $d_{P_5}(v_0) = 1$, $d_{P_5}(v_1) = 2$, $d_{P_5}(v_2) = 2$, and v_1 is adjacent to v_0 and v_2. By Lemma 7, we get $M_k(P_5; v_2) \geq M_k(P_5; v_1)$. Furthermore, by Lemma 3.1 in Ref. [18], for sufficiently large k, $M_k(P_5; v_2) > M_k(P_5; v_1)$ holds. Since $S_n^4 = P_5(v_2) \cdot X_{n-4}(v)$ and $S_n^5 = P_5(v_1) \cdot X_{n-4}(v)$, by Lemma 7 again, we obtain Theorem 1. ■

3 The Largest and the Second Largest Trees with the Maximal Estrada Indices in $\mathcal{H}_{2n}$

In this section, we study the trees with the largest and the second largest EIs in $\mathcal{H}_{2n}$. Some definitions are introduced first.

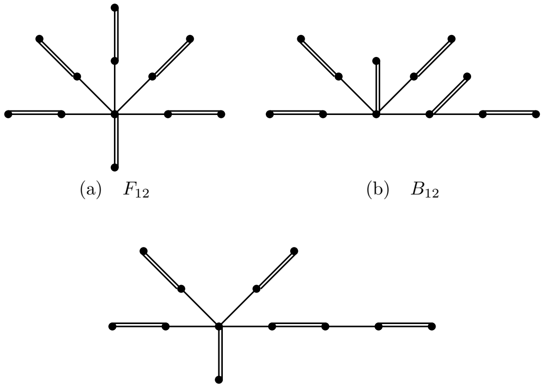
For $T \in \mathcal{H}_{2n}$, let $Q(T) = L(T) - M(T)$, where $L(T)$ is the edge set of T and $M(T)$ the perfect matching of T. It is clear that $|M(T)| = n$ and $|Q(T)| = n - 1$, where $|M(T)|$ and $|Q(T)|$ are the numbers of edges in $M(T)$ and $Q(T)$, respectively. Let $\widehat{T}$ be the graph induced by $Q(T)$, namely $\widehat{T} = T - M(T) - S_0$, where S_0 is the set of singletons in $T - M(T)$. We call $\widehat{T}$ the capped graph of T and T the original graph of $\widehat{T}$.

For $n \geq 4$, let Y_n be the graph obtained from $P_4 = v_0v_1v_2v_3$ by attaching $n-4$ pendant edges to v_2.

Let F_{2n} (for $n \geq 3$) and B_{2n} (for $n \geq 4$) be respectively the trees obtained from the star graph X_n and Y_n by attaching a pendant edge to every vertex. As $n \geq 3$, let the center vertex of F_{2n} be the vertex of $\widehat{F}_{2n} = X_n$ with degree $n-1$. For $n = 2$, let F_{2n} be P_4 and the center vertex of F_4 be the second vertex of P_4. For $n = 1$, let F_{2n} be P_2 and the center vertex of F_2 be the pendant vertex of P_2. For $n \geq 4$, let M_{2n} be the tree obtained from P_7 by attaching $n - 4$ paths of length 2 and a pendant edge to the third vertex of P_7. Obviously, $\widehat{F}_{2n} = X_n$, $\widehat{B}_{2n} = Y_n$, and $\widehat{M}_{2n} = X_{n-1} \cup P_2$. For example, F_{12}, B_{12}, and M_{12} are shown in Fig. 1.

By Lemmas 5 and 7, we get Lemma 8.

Lemma 8 *$EE(F_{2n}) > EE(B_{2n}) > EE(M_{2n})$ for $n \geq 4$.*



(a) F_{12} (b) B_{12}

(c) M_{12}

Figure 1: F_{12}, B_{12}, and M_{12}

Proof. Let G in Lemmas 5 and 7 be F_{2n-2} with $n \geq 4$. Let $v_s, v_{s-1}, v_{s-2} \in V(F_{2n-2})$ be the three vertices as follows. (i) v_{s-2} is the center vertex of F_{2n-2}. (ii) v_{s-1} is a vertex adjacent to v_{s-2} with $d_{F_{2n-2}}(v_{s-1}) = 2$. (iii) v_s is the pendant vertex adjacent to v_{s-1}. Obviously, $d_{F_{2n-2}}(v_s) = 1$ and $d_{F_{2n-2}}(v_{s-2}) \geq 3$ since $n \geq 4$. Note that $F_{2n} = F_{2n-2}(v_{s-2}) \cdot P_3(v_0)$, $B_{2n} = F_{2n-2}(v_{s-1}) \cdot P_3(v_0)$, and $M_{2n} = F_{2n-2}(v_s) \cdot P_3(v_0)$, where $P_3 = v_0v_1v_2$. Obviously, $M_2(F_{2n-2}; v_{s-2}) \geq 3 > 2 = M_2(F_{2n-2}; v_{s-1})$. By Lemma 7, we obtain $EE(F_{2n}) > EE(B_{2n})$ as $n \geq 4$. By Lemma 5, we have $EE(B_{2n}) > EE(M_{2n})$ as $n \geq 4$. ∎

Let $c(\widehat{T})$ be the component numbers of $\widehat{T}$ hereinafter. Let $d(G)$ be a diameter of G.

Lemma 9 *For $T_1 \in \mathcal{H}_{2n}$ with $n \geq 5$, if $c(\widehat{T_1}) = 1$ and $d(\widehat{T_1}) \geq 4$, then there exists a tree $T_2 \in \mathcal{H}_{2n}$ with $c(\widehat{T_2}) = 1$ and $d(\widehat{T_2}) = d(\widehat{T_1}) - 1$, satisfying $EE(T_2) > EE(T_1)$.*

Proof. Let $T_1 \in \mathcal{H}_{2n}$ with $n \geq 5$, $c(\widehat{T_1}) = 1$, and $d(\widehat{T_1}) \geq 4$. As $c(\widehat{T_1}) = 1$, we get that T_1 is the tree obtained from $\widehat{T_1}$ by attaching a pendant edge to each vertex of $\widehat{T_1}$. As $d(\widehat{T_1}) \geq 4$, we have $d(T_1) \geq 6$. Let $P_{d+1} = v_0v_1v_2 \cdots v_d$ be a diameter of T_1, where $d \geq 6$. Since T_1 has a perfect matching, P_{d+1} is a diameter of T_1, and $c(\widehat{T_1}) = 1$, we get that T_1 is the tree obtained from P_{d+1} with the following three properties:

(i) v_0, v_1, v_{d-1}, v_d of P_{d+1} of T are attached by no trees, namely, $v_0v_1, v_{d-1}v_d \in M(T)$;

(ii) v_2 (resp., v_{d-2}) of P_{d+1} of T is identified with the center vertex of F_{n_2} (resp., $F_{n_{d-2}}$), where $n_2, n_{d-2} \geq 2$;

(iii) v_i $(3 \leq i \leq d-3)$ of P_{d+1} of T is attached by a tree (denoted by $T^i_{n_i}$), where n_i is the number of the vertices of $T^i_{n_i}$ (including the vertex v_i). Obviously, n_i is an even and $n_i \geq 2$.

Let T'_1 be the tree obtained from T_1 by replacing $T^i_{n_i}$ with F_{n_i} for each $3 \leq i \leq d-3$. Namely, in T'_1, each v_i of P_{d+1} of T'_1 with $3 \leq i \leq d-3$ is identified with the center vertex of F_{n_i}. Obviously, $c(\widehat{T'_1}) = 1$ and $d(\widehat{T'_1}) = d(\widehat{T_1})$. We prove Claims 1 and 2 as follows.

Claim 1 *$EE(T'_1) \geq EE(T_1)$, with the equality if and only if $T'_1 = T_1$.*

For each i with $3 \leq i \leq d-3$, if $n_i = 2$ or $n_i = 4$, then each v_i of P_{d+1} of T_1 is identified with the center vertex of F_{n_i}. Namely, $T'_1 = T_1$. Obviously, Claim 1 holds since $EE(T'_1) = EE(T_1)$.

Next, we suppose that there exists one tree $T^j_{n_j}$ of T_1 (attached at v_j) with $T^j_{n_j} \neq F_{n_j}$ and $n_j \geq 6$, where $3 \leq j \leq d-3$. Since $T^j_{n_j} \neq F_{n_j}$ and T_1 has a perfect matching, in $T^j_{n_j}$, there exists one vertex (denoted by u) with a degree not less than 3 in such a way: (i) u is adjacent to v_j and a pendant vertex (denoted by s); and (ii) u is identified with a vertex z of a tree H of order at least 3 (including z), where $uv_j, us \notin E(H)$ and $us \in M(T)$. Let G in Lemma 7 be the graph obtained from T_1 by deleting all the vertices in $V(H)$ (except for z, namely u). Obviously, $G(u) \cdot H(z) = T_1$, $d_G(s) = 1$, $d_G(u) = 2$, $d_G(v_j) \geq 3$, and $M_2(G; v_j) \geq 3 > 2 = M_2(G; u)$. By Lemma 7, we have $EE(G(v_j) \cdot H(z)) > EE(G(u) \cdot H(z)) = EE(T_1)$. Repeatedly using the same procedure, we get Claim 1.

Claim 2 *There exists a tree $T_2 \in \mathcal{H}_{2n}$ with $c(\widehat{T_2}) = 1$ and $d(\widehat{T_2}) = d(\widehat{T_1}) - 1$, satisfying $EE(T_2) > EE(T'_1)$.*

Let the two components of $T'_1 - v_{d-2}v_{d-3}$ be A and B, where A and B contain v_{d-3} and v_{d-2}, respectively. Obviously, $B = F_{n_{d-2}+2}$. In B, we denote the pendant vertex adjacent to v_{d-2} by v'_{d-2}. Let G in Lemma 7 be $A(v_{d-3}) \cdot P_3(v_{d-3})$, where $P_3 = v_{d-3}v_{d-2}v'_{d-2}$. Let H in Lemma 7 be $B - v'_{d-2}$. Obviously, $d_G(v'_{d-2}) = 1$, $d_G(v_{d-2}) = 2$, and $d_G(v_{d-3}) \geq 3$. Since v_{d-3} of P_{d+1} of T'_1 is attached by at least a pendant edge, we have $M_2(G; v_{d-3}) \geq 3 > 2 = M_2(G; v_{d-2})$. By Lemma 7, we have $EE(G(v_{d-3}) \cdot H(v_{d-2})) > EE(G(v_{d-2}) \cdot H(v_{d-2}))$, where $G(v_{d-2}) \cdot H(v_{d-2})$ is T'_1. Let $T_2 = G(v_{d-3}) \cdot H(v_{d-2})$. Obviously, $T_2 \in \mathcal{H}_{2n}$, $c(\widehat{T_2}) = 1$, and $d(\widehat{T_2}) = d(\widehat{T_1}) - 1$. Thus, we get Claim 2.

By the proofs of Claims 1 and 2, we obtain Lemma 9. ■

Lemma 10 *For $T \in \mathcal{H}_{2n}$ with $n \geq 5$, if $c(\widehat{T}) = 1$ and $d(\widehat{T}) = 3$, we have $EE(B_{2n}) \geq EE(T)$, where the equality holds if and only if $T = B_{2n}$.*

Proof. Let Q be the tree obtained from $P_6 = v_0v_1 \cdots v_5$ by attaching a pendant edge to v_2 and v_3. For $T \in \mathcal{H}_{2n}$, if $c(\widehat{T}) = 1$ and $d(\widehat{T}) = 3$, then T must be the tree obtained from Q by attaching pathes of length two to v_2 and v_3. In Lemma 3, let C be Q, A be the graph attached at v_2 of Q of T, and B be the graph attached at v_3 of Q of T. Obviously, there exists an automorphism θ of C such that $\theta(v_2) = v_3$. Thus, by Lemma 3, we get Lemma 10. ■

Lemma 11 *For $T \in \mathcal{H}_{2n}$ with $n \geq 5$, if $c(\widehat{T}) \geq 2$, then $EE(B_{2n}) > EE(T)$.*

Proof. Let $T \in \mathcal{H}_{2n}$ and $c(\widehat{T}) \geq 2$. Let $\widetilde{T}$ be the tree obtained from $\widehat{T}$ by coalescing the two vertices in T which are incident with a common edge in $M(T)$. Obviously, $\widetilde{T}$ is a tree with n vertex and the edges of $\widetilde{T}$ are those of $\widehat{T}$. Two cases are considered as follows.

Case (i) $\widetilde{T} = X_n$.

As $\widetilde{T} = X_n$, we have $\widehat{T} = X_{a+1} \cup X_{b+1}$, where $a, b \geq 1$ and $a + b = n - 1$.

If $a = 1$ or $b = 1$, then $T = M_{2n}$. By Lemma 8, we have $EE(B_{2n}) > EE(M_{2n})$ as $n \geq 5$.

Next, let $a, b \geq 2$. Hence $n \geq 5$ and T is the tree obtained from $P_6 = v_0v_1v_2v_3v_4v_5$ by attaching $a - 1$ paths of length two to v_2 and $b - 1$ paths of length two to v_3. In Lemma 3, let C be P_6, A and B be the graphs attached at v_2 and v_3 of P_6 of T, respectively. Obviously, there exists an automorphism θ of C such that $\theta(v_2) = v_3$. Thus, by Lemma 3, we get $EE(M_{2n}) \geq EE(T)$. Furthermore, by Lemma 8, we obtain $EE(B_{2n}) > EE(T)$ as $n \geq 5$.

Case (ii) $\widetilde{T} \neq X_n$.

For $T \in \mathcal{H}_{2n}$, if $c(\widehat{T}) \geq 2$, then there exists a cut edge $e = uv \in M(T)$ which is not a pendant edge, where $d_T(u), d_T(v) \geq 2$. Let T_1 be the tree obtained from T by identifying u with v, and attaching a pendant vertex to the common vertex u (namely v) of T. Obviously, $T_1 \in \mathcal{H}_{2n}$ and $c(\widehat{T_1}) = c(\widehat{T}) - 1$. By Lemma 6, we have $EE(T_1) > EE(T)$. Repeatedly using the same procedure until all the edges in $M(T_1)$ are pendant edges, we can get a tree $T_2 \in \mathcal{H}_{2n}$ with $c(\widehat{T_2}) = 1$ such that $EE(T_2) \geq EE(T_1)$. Bearing the definition of $\widetilde{T}$ in mind, we have $\widehat{T_2} = \widetilde{T}$. As $\widetilde{T} \neq X_n$, we get $\widehat{T_2} \neq X_n$. Namely, $d(\widehat{T_2}) \geq 3$. By Lemmas 9 and 10, we obtain $EE(B_{2n}) \geq EE(T_2)$. Therefore, $EE(B_{2n}) > EE(T)$.

By the proofs of Cases (i) and (ii), we get Lemma 11. ■

By Lemmas 8–11, we obtain the trees with the largest and the second largest EIs in $\mathcal{H}_{2n}$ with $n \geq 5$.

Theorem 2 *Let $T \in \mathcal{H}_{2n}$ with $n \geq 5$. We have $EE(F_{2n}) > EE(B_{2n}) > EE(T)$, where $T \neq F_{2n}, B_{2n}$.*

Proof. By Lemma 8, we get $EE(F_{2n}) > EE(B_{2n})$ as $n \geq 5$. Let $T \in \mathcal{H}_{2n} \setminus \{F_{2n}, B_{2n}\}$ and $n \geq 5$.

Let $|c(\widehat{T})| = 1$. As $d(\widehat{T}) = 2$, $\mathcal{H}_{2n}$ has only one tree F_{2n}. As $d(\widehat{T}) = 3$, by Lemma 10, we have $EE(B_{2n}) > EE(T)$. As $d(\widehat{T}) \geq 4$, by Lemmas 9 and 10, we obtain $EE(B_{2n}) > EE(T)$.

Let $|c(\widehat{T})| \geq 2$. By Lemma 11, we get $EE(B_{2n}) > EE(T)$. ■

Acknowledgment: The work was supported by the National Natural Science Foundation of China under Grant No. 11001166 and the Shanghai Leading Academic Discipline Project under Project No. S30104. The author thanks the anonymous reviewer for his/her useful suggestion which leads to an improvement of the introduction.

References

[1] D. M. Cvetković, M. Doob, S. Hachs, *Spectra of Graphs Theory and Application*, Academic Press, New York, 1980.

[2] E. Estrada, Characterization of 3D molecular structure, *Chem. Phys. Lett.* **319** (2000) 713–718.

[3] E. Estrada, Topological structural classes of complex networks, *Phys. Rev. E* **75** (2007) 016103.

[4] E. Estrada, J. A. Rodriguez–Velazquez, M. Randić, Atomic branching in molecules, *Int. J. Quantum Chem.* **106** (2006) 823–832.

[5] B. Zhou, On Estrada index, *MATCH. Commun. Math. Comput. Chem.* **60** (2008) 485–492.

[6] G. H. Fath-Tabar, A. R. Ashrafi, New upper bounds for Estrada index of bipartite graphs, *Lin. Algebra Appl.* **435** (2011) 2607–2611.

[7] A. R. Ashrafi, G. H. Fath-Tabar, Bounds on the Estrada index of isr (4,6)-fullerenes, *Appl. Math. Lett.* **24** (2011) 337–339.

[8] J. Zhang, B. Zhou, J. Li, On Estrada index of trees, *Lin. Algebra Appl.* **434** (2011) 215–223.

[9] Z. Du, B. Zhou, The Estrada index of trees, *Lin. Algebra Appl.* **435** (2011) 2462–2467.

[10] W. H. Wang, W. W. Xu, Graphs with the maximal Estrada indices, *Lin. Algebra Appl.* **446** (2014) 314–328.

[11] Z. X. Zhu, L. S. Tan, Z. Y. Qiu, Tricyclic graph with maximal Estrada index, *Discr. Appl. Math.* **162** (2014) 364–372.

[12] F. Huang, X. Li, S. Wang, On maximum Estrada indices of bipartite graphs with some given parameters, *Lin. Algebra Appl.* **465** (2015) 283–295.

[13] L. Wang, Y. Z. Fan, Y. Wang, Maximum Estrada index of bicyclic graphs, *Discr. Appl. Math.* **180** (2015) 194–199.

[14] H. Deng, A proof of a conjecture on the Estrada index, *MATCH. Commun. Math. Comput. Chem.* **62** (2009) 599–606.

[15] K. C. Das, S. G. Lee, On the Estrada index conjecture, *Lin. Algebra Appl.* **431** (2009) 1351–1359.

[16] H. Zhao, Y. Jia, On the Estrada index of bipartite graph, *MATCH. Commun. Math. Comput. Chem.* **61** (2009) 495–501.

[17] H. Deng, A note on the Estrada index of trees, *MATCH. Commun. Math. Comput. Chem.* **62** (2009) 607–610.

[18] A. Ilić, D. Stevanović, The Estrada index of chemical trees, *J. Math. Chem.* **47** (2010) 305–314.

[19] Z. Du, B. Zhou, On the Estrada index of graphs with given number of cut edges, *El. J. Lin. Algebra* **22** (2011) 586–592.

[20] Q. Y. Deng, H. Y. Chen, On extremal bipartite unicyclic graphs, *Lin. Algebra Appl.* **444** (2014) 89–99.