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MINIMAL ESTRADA INDICES OF THE TREES WITH A PERFECT MATCHING*

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Abstract. Let $\mathcal{H}_n$ be the set of the trees having a perfect matching with n vertices. The ordering of the trees in $\mathcal{H}_n$ according to their minimal Estrada indices is investigated. The trees with the smallest and the second smallest Estrada indices among $\mathcal{H}_n$, with $n \geq 6$, are obtained.

Key words. Estrada indices, Perfect matching, Trees.

AMS subject classifications. 05C05, 05C35.

1. Introduction. Let G be a simple graph with a vertex set $V(G)$, where $|V(G)| = n$. Let $\Phi(G, \lambda) = \det[\lambda I - A(G)]$ be the characteristic polynomial of G, where $A(G)$ is the adjacency matrix of G and I the unit matrix of order n [4]. Denote by $\lambda_1 \geq \cdots \geq \lambda_n$ the n roots of $\Phi(G, \lambda) = 0$. Obviously, $\lambda_1, \ldots, \lambda_n$ are all real numbers since $A(G)$ is a real symmetric matrix. The Estrada index (EI) of G, a newly proposed graph-spectrum-based invariant, is defined by [12]

$$EE(G) = \sum_{i=1}^{n} \mathrm{e}^{\lambda_i}. \tag{1.1}$$

Recall that a walk W of length k in G is any sequence of vertices and edges of G, namely $W = v_0, e_1, v_1, e_2, \ldots, v_{k-1}, e_k, v_k$ such that e_i is the edge joining vertices v_{i-1} and v_i for every $i = 1, 2, \ldots, k$. If $v_0 = v_k$, then the walk W is closed and is referred to as the (v_0, v_0)-walk of length k. For $u, v \in V(G)$, let $\mathcal{W}_k(G; u, v)$ be the set of the (u, v)-walks of length k in G, and $M_k(G; u, v)$ be the number of the elements in $\mathcal{W}_k(G; u, v)$. Similarly, let $\mathcal{W}_k(G; v)$ be the set of the (v, v)-walks of length k in G, and $M_k(G; v)$ be the number of the elements in $\mathcal{W}_k(G; v)$. Let $M_{2k}(G, u, [v])$ be the number of the close (u, u)-walks of length $2k$ starting at u and passing v in G. 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

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k in G [4]. From the Taylor expansion of e^{λ_i}, $EE(G)$ in (1.1) can be rewritten as

$$EE(G) = \sum_{k=0}^{\infty} \frac{M_k(G)}{k!}. \tag{1.2}$$

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

$$EE(G) = \sum_{k=0}^{\infty} \frac{M_{2k}(G)}{(2k)!}. \tag{1.3}$$

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 $EE(G_1) \geq EE(G_2)$ and we denote $G_1 \succeq G_2$. If $G_1 \succeq G_2$ and there is at least one positive integer k_0 such that $M_{2k_0}(G_1) > M_{2k_0}(G_2)$, then $EE(G_1) > EE(G_2)$ and we denote $G_1 \succ G_2$.

The EI has found numerical applications in biology, complex networks and chemistry. It was used to quantify the degree of folding of long-chain molecules, especially proteins [11, 12, 19]. It was also shown that the EI provides a measure of the centrality of complex network [13, 19]. In addition, a connection between the EI and the concept of extended atomic branching was pointed out by Estrada et al. [14]. For some mathematical properties of EI, including the lower and upper bounds for it, one can refer to [2, 15, 17].

In addition to the ordinary Estrada index, defined in terms of the eigenvalues of the adjacency matrix, Eq. (1.1), several analogous graph invariants have recently been considered. Of these worth mentioning are the Laplacian and signless Laplacian Estrada indices [1, 20], based on the eigenvalues of the Laplacian and signless Laplacian matrix, the resolvent Estrada index [3, 18], based on the resolvent of the adjacency matrix, and the skew Estrada index of oriented graphs [16].

The characterization of graphs having the extremal Estrada indices (EIs) is an interesting problem and has been obtained successfully. For the characterization of the unicyclic graphs, the bicyclic graphs and the tricyclic graphs, ect., one can refer to [8, 23, 24, 25, 27]. For the general trees and the trees with given parameters, such as the trees with a given matching number, the trees with a fixed diameter, and the trees with a given number of pendant vertices, etc., one can refer to [7, 5, 6, 10, 21, 26]. Recently, Wang [22] obtained the trees with the largest and the second largest Estrada indices among the set of trees with a perfect matching. From the references, one can find that many results are related to the graphs with the maximal EIs. However, until now, only a few results about the graphs having the minimal EIs have been obtained.

Recall that molecules with the Kekulé structures are molecular graphs with perfect matchings. Let $\mathcal{H}_n$ be the set of trees with a perfect matching having n vertices.

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Obviously, n is an even. In this paper, we will study the ordering of the trees in $\mathcal{H}_n$ in terms of their minimal EIs. Thus, we characterize the acyclic Kekuléan π-electron systems with the smallest and the second smallest EIs.

2. Transformations for studying the Estrada indices. To deduce the main results of this paper, Lemmas 2.1–2.4 are simply quoted here.

Let $v \in V(G)$, and $d_G(v)$ be the degree of v of G. A pendant path at v of G is a path in G connecting vertex v and a pendant vertex such that all internal vertices (if exist) in this path have degree two and $d_G(v) \geq 3$.

Lemma 2.1. [21] *Let w be a vertex of the nontrivial connected graph G. For nonnegative integers p and q, let $G(p,q)$ denote the graph obtained from G by attaching at w pendant paths $P = wv_1v_2 \cdots v_p$ and $Q = wu_1u_2 \cdots u_q$ of lengths p and q, respectively. If $p \geq q \geq 1$, then $EE(G(p,q)) > EE(G(p+1, q-1))$.*

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.

Lemma 2.2. [9] *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 2.3. [8, 22] *Let A, B and C be three connected graphs, and 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.*

Lemma 2.4. [7] *Let u be a non-isolated vertex of a simple graph H. If H_1 and H_2 are the graphs obtained from H by identifying an end vertex v_1 and an internal vertex v_t of the path P_{a+b+1} with u, respectively (see Figs. 2.1(a) and 2.1(b)), then $M_{2k}(H_2) > M_{2k}(H_1)$ for $n \geq 3$ and $k \geq 2$.*

3. The smallest and the second smallest trees with the minimal Estrada indices in $\mathcal{H}_n$. In this section, we study the ordering of the trees in $\mathcal{H}_n$ according to their minimal EIs. Some definitions are introduced first.

We classify $\mathcal{H}_n$ into three subsets $\mathcal{H}_n^1$, $\mathcal{H}_n^2$ and $\mathcal{H}_n^3$, where $\mathcal{H}_n^1$ is the subset of

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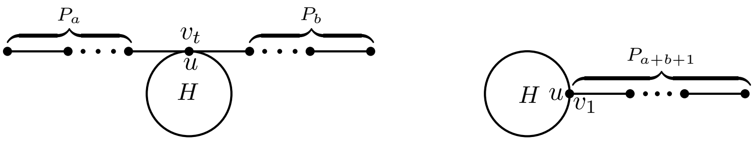

(a) H_2. (b) H_1.

FIG. 2.1. *The transformation in Lemma 2.4.*

$\mathcal{H}_n$ in which there exists at most one vertex having degree 3 and all other vertices having degrees 2 or 1; $\mathcal{H}_n^2$ is the subset of $\mathcal{H}_n$ in which there exists at least one vertex having degree greater than 3; and $\mathcal{H}_n^3$ is the subset of $\mathcal{H}_n$ in which there exist at least two vertices having degrees 3 and all other vertices having degrees 2 or 1. Obviously, $\mathcal{H}_n = \mathcal{H}_n^1 \cup \mathcal{H}_n^2 \cup \mathcal{H}_n^3$.

Let ${}^l\mathrm{T}_b^r$ be the tree obtained by attaching three pendant paths of length l, r and b at a common vertex u, where $l + r + b + 1 = n$, l and r are even with $l, r \geq 0$ and b is odd with $b \geq 1$. Specially, if at least one of l and r is 0, then ${}^l\mathrm{T}_b^r$ is the path P_n. Obviously, ${}^l\mathrm{T}_b^r$ has a perfect matching. By the definition of $\mathcal{H}_n^1$, if $T \in \mathcal{H}_n^1$, then T is ${}^l\mathrm{T}_b^r$. For example, ${}^l\mathrm{T}_b^r$ is shown in Fig. 3.1.

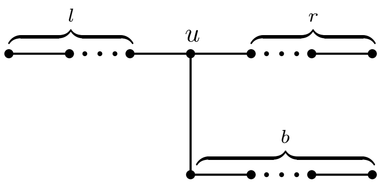

FIG. 3.1. ${}^lT_b^r$ *with* $l + r + b + 1 = n$.

Let G in Lemma 2.1 be P_{b+1}. Repeatedly using Lemma 2.1, we can obtain Corollary 3.1.

COROLLARY 3.1. ${}^l\mathrm{T}_b^r \succ^{l-2} \mathrm{T}_b^{r+2} \succ \cdots \succ^4 \mathrm{T}_b^{n-b-5} \succ^2 \mathrm{T}_b^{n-b-3} \succ^0 \mathrm{T}_b^{n-b-1} \cong P_n$, *where* $r \geq l \geq 2$ *and* $b \geq 1$.

Let G in Lemma 2.1 be P_{l+1}. Repeatedly using Lemma 2.1, we get Corollaries 3.2 and 3.3.

COROLLARY 3.2. ${}^l\mathrm{T}_b^r \succ^l \mathrm{T}_{r-1}^{b+1} \succ \cdots \succ^l \mathrm{T}_3^{n-l-4} \succ^l \mathrm{T}_{n-l-3}^2 \succ^l \mathrm{T}_1^{n-l-2} \succ^l \mathrm{T}_{n-l-1}^0 \cong P_n$, *where* $b > r \geq 2$.

COROLLARY 3.3. ${}^l\mathrm{T}_b^r \succ^l \mathrm{T}_{r+1}^{b-1} \succ \cdots \succ^l \mathrm{T}_3^{n-l-4} \succ^l \mathrm{T}_{n-l-3}^2 \succ^l \mathrm{T}_1^{n-l-2} \succ^l \mathrm{T}_{n-l-1}^0 \cong P_n$, *where* $r > b \geq 1$.

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By Corollaries 3.2 and 3.3, we get Corollary 3.4.

Corollary 3.4. *As* $r \geq 4$ *and* $b \geq 3$, ${}^l\mathrm{T}_b^r \succeq^l \mathrm{T}_3^{n-l-4} \succ^l \mathrm{T}_{n-l-3}^2 \succ^l \mathrm{T}_1^{n-l-2} \succ^l \mathrm{T}_{n-l-1}^0 \cong P_n$, *with* $EE({}^l\mathrm{T}_b^r) = EE({}^l\mathrm{T}_3^{n-l-4})$ *if and only if* $b = 3$.

Remark. By the definition of ${}^l\mathrm{T}_b^r$, all the graphs in Corollaries 3.1–3.4 have a perfect matching.

Let $\mathcal{H}_n^{1,1} = \{{}^l\mathrm{T}_b^r | b = 1, l, r \geq 0\}$ and $\mathcal{H}_n^{1,2} = \{{}^l\mathrm{T}_b^r | b \geq 3, l, r \geq 0\}$. Obviously, $\mathcal{H}_n^1 = \mathcal{H}_n^{1,1} \cup \mathcal{H}_n^{1,2}$. From Corollaries 3.1 and 3.3, we obtain, in Theorem 3.5, the complete ordering of the trees in $\mathcal{H}_n^{1,1}$ in terms of their minimal EIs.

Theorem 3.5. *For* ${}^l\mathrm{T}_1^r \in \mathcal{H}_n^{1,1}$ *with* $n \geq 8$, *we have the ordering as follows.*

(i) *As* $n = 4h$ *with* $h \geq 2$, ${}^{\frac{n}{2}-2}\mathrm{T}_1^{\frac{n}{2}} \succ^{\frac{n}{2}-4} \mathrm{T}_1^{\frac{n}{2}+2} \succ \cdots \succ^2 \mathrm{T}_1^{n-4} \succ^2 \mathrm{T}_{n-3}^0 \cong P_n$.

(ii) *As* $n = 4h+2$ *with* $h \geq 2$, ${}^{\frac{n}{2}-1}\mathrm{T}_1^{\frac{n}{2}-1} \succ^{\frac{n}{2}-3} \mathrm{T}_1^{\frac{n}{2}+1} \succ \cdots \succ^2 \mathrm{T}_1^{n-4} \succ^2 \mathrm{T}_{n-3}^0 \cong P_n$.

Proof. As $n \geq 8$, by Corollary 3.3, we get ${}^2\mathrm{T}_1^{n-4} \succ^2 \mathrm{T}_{n-3}^0 \cong P_n$. In Corollary 3.1, let $b = 1$. Using Corollary 3.1 repeatedly, we obtain Theorem 3.5. ☐

From Corollaries 3.3 and 3.4, we obtain the first four trees in $\mathcal{H}_n^{1,2}$ with the minimal EIs in Theorem 3.6.

Theorem 3.6. *Let* $T \in \mathcal{H}_n^{1,2} \backslash \{P_n, {}^2\mathrm{T}_{n-5}^2, {}^2\mathrm{T}_3^{n-6}\}$ *and* $n \geq 8$. *We have*

$$T \succ^2 \mathrm{T}_3^{n-6} \succeq^2 \mathrm{T}_{n-5}^2 \succ^2 \mathrm{T}_1^{n-4} \succ^2 \mathrm{T}_{n-3}^0 \cong P_n,$$

where $EE({}^2\mathrm{T}_3^{n-6}) = EE({}^2\mathrm{T}_{n-5}^2)$ *if and only if* $n = 8$.

Proof. As $n \geq 8$, it follows directly from Corollary 3.3 (let $l = 2$) that ${}^2\mathrm{T}_3^{n-6} \succeq^2 \mathrm{T}_{n-5}^2 \succ^2 \mathrm{T}_1^{n-4} \succ^2 \mathrm{T}_{n-3}^0 \cong P_n$, where $EE({}^2\mathrm{T}_3^{n-6}) = EE({}^2\mathrm{T}_{n-5}^2)$ if and only if $n = 8$.

Next, let ${}^l\mathrm{T}_b^r \in \mathcal{H}_n^{1,2} \backslash \{P_n, {}^2\mathrm{T}_{n-5}^2, {}^2\mathrm{T}_3^{n-6}\}$. As $b \geq 3$ and $n \geq 8$, we will prove

$$ {}^l\mathrm{T}_b^r \succ^2 \mathrm{T}_3^{n-6}. \tag{3.1}$$

In ${}^l\mathrm{T}_b^r$, we have $l, r \geq 2$ since ${}^l\mathrm{T}_b^r \ncong P_n$. We assume $r \geq l \geq 2$. As $l = 2$, we have $r \geq 4$ since ${}^l\mathrm{T}_b^r \ncong^2 \mathrm{T}_{n-5}^2$. Thus, as $r \geq 4$ and $b \geq 3$, (3.1) follows from Corollary 3.4 directly. As $l \geq 4$, we have $r \geq l \geq 4$. It follows from Corollary 3.1 that ${}^l\mathrm{T}_b^r \succ^2 \mathrm{T}_b^{l+r-2}$. Since $l + r - 2 \geq 6$ and $b \geq 3$, by Corollary 3.4, we get ${}^2\mathrm{T}_b^{l+r-2} \succeq^2 \mathrm{T}_3^{n-6}$. Therefore, we have ${}^l\mathrm{T}_b^r \succ^2 \mathrm{T}_3^{n-6}$. Namely, (3.1) holds. Theorem 3.6 is thus proved. ☐

Lemma 3.7. *If* H_2 *(see Fig. 2.1(a)) in Lemma 2.4 has a perfect matching, then* H_1 *(see Fig. 2.1(b)) has a perfect matching too.*

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Proof. If H_2 has a perfect matching, then the vertex u of H_2 (as shown in Fig. 2.1(a)) must be matched with another vertex (denoted by w) of H_2. If $w \in V(H)\backslash\{u\}$, then a and b are even. If $w \notin V(H)$, then one of a and b is odd and the another is even. We can easily check that H_1 has a perfect matching too. $\square$

By Lemmas 2.4 and 3.7, we obtain Corollary 3.8 as follows.

COROLLARY 3.8. *Let $T \in \mathcal{H}_n$ with $n \geq 6$. In T, if there exists an vertex (denoted by u) satisfying that $d_T(u) \geq 3$ and there are two pendant paths attaching at u of T, then we have another tree $T' \in \mathcal{H}_n$ satisfying $d_{T'}(u) = d_T(u) - 1$ and $EE(T) > EE(T')$.*

From Corollary 3.8, we deduce Lemmas 3.9 and 3.10 as follows.

LEMMA 3.9. *If $T \in \mathcal{H}_n^2$, then there exists a tree $T_1 \in \mathcal{H}_n^2$ (see Fig. 3.2(a)) such that $EE(T) \geq EE(T_1)$, with the equality if and only if $T \cong T_1$.*

Proof. Let $T \in \mathcal{H}_n^2$. By the definition of $\mathcal{H}_n^2$, we get that T has at least one vertex having degree greater than 3.

Case (i): Only one vertex of T (denoted by u) has degree greater than 3.

Subcase (i.i): All the degrees of the vertices in $V(T) \setminus \{u\}$ are 2 or 1.

Obviously, u of T is attached by $d_T(u)$ pendant paths of T. Using Corollary 3.8 $(d_T(u) - 4)$ times on u of T, we get Lemma 3.9.

Subcase (i.ii): There exist $k \geq 1$ vertices in $V(T) \setminus \{u\}$ having degree 3.

We can choose one vertex (denoted by s) of T such that $d_T(s) = 3$ and s is attached by two pendant paths of T. By Corollary 3.8, we get $EE(T) > EE(T')$, where $T' \in \mathcal{H}_n^2$, $d_{T'}(s) = 2$, and T' has $k-1$ vertices having degree 3. Repeatedly using the same procedure, we obtain $EE(T') \geq EE(T'')$, where $T'' \in \mathcal{H}_n^2$, T'' has only one vertex u having degree greater than 3 and all other vertices of T'' having degrees 2 or 1. Furthermore, by the proof of Subcase (i.i), we can get that there exists a tree $T_1 \in \mathcal{H}_n^2$ with $EE(T'') \geq EE(T_1)$. Thus, we obtain $EE(T) > EE(T_1)$.

Case (ii): There exist $k \geq 2$ vertices of T having degrees greater than 3.

In this case, we can choose one vertex (denoted by w) of T such that $d_T(w) \geq 3$ and w is attached by $(d_T(w) - 1)$ pendant paths. Repeatedly using Corollary 3.8 $(d_T(w) - 2)$ times on w of T, we get a new tree $T' \in \mathcal{H}_n^2$ satisfying $d_{T'}(w) = 2$ and $EE(T) > EE(T')$. Repeatedly using the same procedure, we can obtain a tree $T'' \in \mathcal{H}_n^2$ such that $EE(T') \geq EE(T'')$, where T'' has only one vertex having degree greater than 3 and all other vertices of T'' having degrees 2 or 1. Furthermore, by the proof of Subcase (i.i), we can get that there exists a tree $T_1 \in \mathcal{H}_n^2$ with

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$EE(T'') \geq EE(T_1)$. Thus, we obtain $EE(T) > EE(T_1)$. □

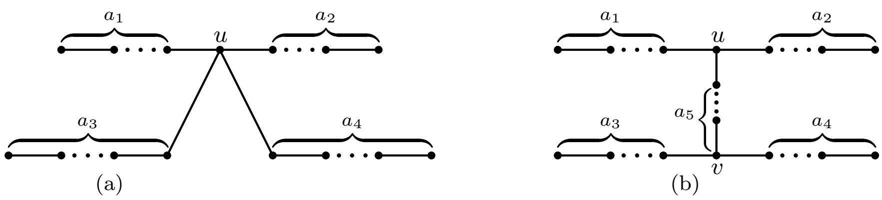

FIG. 3.2. *(a)* $T_1 : \sum_{i=1}^{4} a_i = n-1$ *with* $a_i \geq 1$. *(b)* $T_2 : \sum_{i=1}^{5} a_i = n-1$ *with* $a_i \geq 1$.

LEMMA 3.10. *If* $T \in \mathcal{H}_n^3$*, then there exists a tree* $T_2 \in \mathcal{H}_n^3$ *(see Fig. 3.2(b)) such that* $EE(T) \geq EE(T_2)$*, with the equality if and only if* $T \cong T_2$.

Proof. Let $T \in \mathcal{H}_n^3$. We get that T has at least two vertices having degree 3 and all other vertices of T having degrees 2 or 1. If T has two vertices (denoted by u and v) having degree 3, then $T \cong T_2$. If T has at least three vertices having degree 3, then by the methods similar to those for Subcase (i.ii) in Lemma 3.9, we get Lemma 3.10. □

In T_2, if $a_1 = a_2 = a_3 = a_4 = 2$, then we denote T_2 by I_n.

THEOREM 3.11. *Let* $T \in \mathcal{H}_n^2$ *and* $n \geq 10$*, we have* $T \succ^2 \mathrm{T}_3^{n-6}$ *or* $T \succ I_n$.

Proof. Let $T \in \mathcal{H}_n^2$ and $n \geq 10$. By Lemma 3.9, there exists a tree T_1 such that $T_1 \in \mathcal{H}_n^2$ and $T \succeq T_1$. Since T_1 has a perfect matching, in T_1, only one of a_i $(1 \leq i \leq 4)$ is odd. We assume that a_1 is odd. Therefore, a_2, a_3, and a_4 are even. We let $a_4 \geq a_3 \geq a_2 \geq 2$. Two cases are considered as follows.

Case (i): At least one of a_2, a_3 and a_4 is not less than 4.

Without loss of generality, we let $a_4 \geq 4$. Since $a_4 \geq a_3 \geq 2$, by Corollaries 3.8 and 3.1, $T_1 \succ^{a_3} \mathrm{T}_{a_1+a_2}^{a_4} \succeq^2 \mathrm{T}_{a_1+a_2}^{a_3+a_4-2}$. Since $a_1 + a_2 \geq 3$ and $a_3 + a_4 - 2 \geq 4$, ${}^2\mathrm{T}_{a_1+a_2}^{a_3+a_4-2} \succeq^2 \mathrm{T}_3^{n-6}$ follows from Corollary 3.4. In conclusion, we get $T \succeq T_1 \succ^2 \mathrm{T}_3^{n-6}$.

Case (ii): $a_2 = a_3 = a_4 = 2$.

Let C in Lemma 2.3 be $P_{n-4} = v_1 v_2 \cdots v_{n-5} v_{n-4}$, u in Lemma 2.3 be v_3 of P_{n-4}, and v in Lemma 2.3 be v_{n-6} of P_{n-4}. In C, we can check that there exists an automorphism θ such that $\theta(u) = v$. Let $H = P_{n-4}(v_3) \cdot P_3(v_0)$, where $P_3 = v_0 v_1 v_2$. Since $T_1 \cong H(u) \cdot P_3(v_0)$ and $I_n \cong H(v) \cdot P_3(v_0)$, by Lemma 2.3, we obtain $T_1 \succ I_n$ as $n \geq 10$. Therefore, $T \succeq T_1 \succ I_n$ as $n \geq 10$. □

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To obtain the tree with the minimal EI in $\mathcal{H}_n^3$, we introduce Lemmas 3.12 and 3.13 first. Two trees J_n and K_n are introduced. In T_2, if $a_1 = a_2 = a_3 = 2$ and $a_4 = 4$, then we denote T_2 by J_n. In T_2, if $a_2 = a_3 = 2$ and $a_1 = a_4 = 4$, then we denote T_2 by K_n.

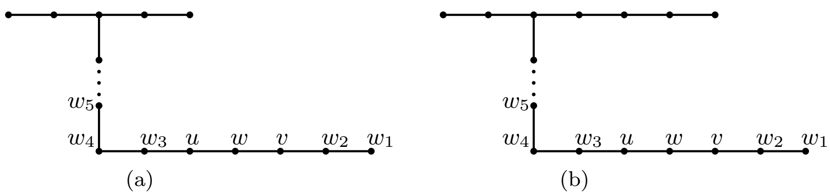

FIG. 3.3. *(a)* ${}^2T_{n-7}^2$. *(b)* ${}^2T_{n-9}^4$.

LEMMA 3.12. *As $n \geq 12$, we have $J_n \succ I_n$.*

Proof. For simplicity, let H be ${}^2T_{n-7}^2$ (see Fig. 3.3(a)), where $n \geq 12$. In ${}^2T_{n-7}^2$, let u, v, w, and w_i with $1 \leq i \leq 5$ be the eight vertices, as shown in Fig. 3.3(a). Next, we prove

$$M_k(H; u) \geq M_k(H; v) \tag{3.2}$$

holds for all $k \geq 0$ and there exists a $k_0 \geq 0$ such that $M_{k_0}(H; u) > M_{k_0}(H; v)$.

Let H_1 be one of the two components of $H - \{uw\}$ which contains the vertex v of H, namely, H_1 is the path $P_4 = wvw_2w_1$. Similarly, let H_2 be one of the two components of $H - \{vw\}$ which contains the vertex u of H. We can easily check that H_1 is isomorphic to a subgraph (denoted by H_2') of H_2, where H_2' is the path $P_4 = w_4w_3uw$. Obviously, for all $k \geq 0$, $M_k(H_2'; u) = M_k(H_1; v)$. Thus, for all $k \geq 0$, we have

$$\begin{aligned} M_k(H_2; u) &= M_k(H_2'; u) + M_k(H_2; u, [w_5]) \\ &= M_k(H_1; v) + M_k(H_2; u, [w_5]) \\ &\geq M_k(H_1; v) \end{aligned} \tag{3.3}$$

since $M_k(H_2; u, [w_5]) \geq 0$. As $k = 6$, we can check that $M_k(H_2; u, [w_5]) = 1 > 0$. Therefore, $M_6(H_2; u) > M_6(H_1; v)$. Namely, there exist a k_0 such $M_{k_0}(H_2; u) > M_{k_0}(H_1; v)$. By the methods similar to those for (3.3), we can prove $M_k(H_2; u, w) \geq M_k(H_1; v, w)$ for all $k \geq 0$.

As $k \geq 0$, we obtain

$$M_k(H; v) = M_k(H; v, [u]) + M_k(H_1; v), \tag{3.4}$$

$$M_k(H; u) = M_k(H; u, [v]) + M_k(H_2; u). \tag{3.5}$$

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From (3.4) and (3.5), to obtain (3.2), we only need to prove

$$M_k(H; u, [v]) \geq M_k(H; v, [u])$$

since (3.3) holds.

For an arbitrary $W \in \mathcal{W}_k(H; v, [u])$, we decompose W into $W_1 W_2$, where W_1 is the shortest (v, u)-section of W (consisting of a (v, w)-walk in H_1 and a single edge wu), and W_2 is the remaining (u, v)-section of W. Thus, we get

$$M_k(H; v, [u]) = \sum_{\substack{k_1 + k_2 = k \\ k_1, k_2 \geq 2 \\ k_1, k_2 \text{ are all even}}} M_{k_1 - 1}(H_1; v, w) M_{k_2}(H; u, v). \tag{3.6}$$

Similarly,

$$M_k(H; u, [v]) = \sum_{\substack{k_1 + k_2 = k \\ k_1, k_2 \geq 2 \\ k_1, k_2 \text{ are all even}}} M_{k_1 - 1}(H_2; u, w) M_{k_2}(H; v, u). \tag{3.7}$$

For all even $k_2 \geq 0$, obviously $M_{k_2}(H; u, v) = M_{k_2}(H; v, u)$. Since for all $k_1 \geq 0$, $M_{k_1 - 1}(H_2; u, w) \geq M_{k_1 - 1}(H_1; v, w)$, it follows from (3.6) and (3.7) that

$$M_k(H; u, [v]) \geq M_k(H; v, [u]).$$

Furthermore, by (3.3), (3.4), and (3.5), we get (3.2).

Obviously, $J_n \cong H(u) \cdot P_3(v_0)$ and $I_n \cong H(v) \cdot P_3(v_0)$, where $P_3 = v_0 v_1 v_2$. Thus, by Lemma 2.2, we obtain Lemma 3.13. $\square$

Lemma 3.13. *As $n \geq 14$, we have $K_n \succ J_n \succ I_n$.*

Proof. For simplicity, let Q be ${}^2T^4_{n-9}$ (see Fig. 3.3(b)), where $n \geq 14$. In ${}^2T^4_{n-9}$, let u, v, w, and w_i with $1 \leq i \leq 5$ be the eight vertices, as shown in Fig. 3.3(b). By the methods similar to those for (3.3) in Lemma 3.12, we can prove $M_k(Q; u) \geq M_k(Q; v)$ for all $k \geq 0$ and there exists a $k_0 = 6$ such that $M_{k_0}(Q; u) > M_{k_0}(Q; v)$.

Obviously, $K_n \cong Q(u) \cdot P_3(v_0)$ and $J_n \cong Q(v) \cdot P_3(v_0)$, where $P_3 = v_0 v_1 v_2$. By Lemma 2.2, we get $K_n \succ J_n$ as $n \geq 14$. Furthermore, by Lemma 3.12, we obtain Lemma 3.13. $\square$

Let $\mathcal{H}^{3,1}_n = \{T \in H^3_n \,|\, \exists T_2$ such that $T \succeq T_2$ and T_2 has $a_1 = a_3 = 1$ and $a_2, a_4 \geq 2\}$ and $\mathcal{H}^{3,2}_n = \mathcal{H}^3_n \backslash \mathcal{H}^{3,1}_n$. By Lemmas 3.10–3.13, we get Theorem 3.14 as follows.

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THEOREM 3.14. *Let* $T \in \mathcal{H}_n^3$ *and* $n \geq 14$.

(i) *If* $T \in \mathcal{H}_n^{3,1}$, *then* $T \succ^2 \mathrm{T}_1^{n-4}$.

(ii) *If* $T \in \mathcal{H}_n^{3,2}$, *then* $T \succ^2 \mathrm{T}_{n-5}^2$ *or* $T \succeq I_n$.

Proof. (i) $T \in \mathcal{H}_n^{3,1}$ with $n \geq 14$.

If $T \in \mathcal{H}_n^{3,1}$, then by Lemma 3.10, there exists a tree T_2 such that $T_2 \in \mathcal{H}_n^3$ and $T \succeq T_2$. Furthermore, by the definition of $\mathcal{H}_n^{3,1}$, T_2 (see Fig. 3.2(b)) has $a_1 = a_3 = 1$. Since T_2 has a perfect matching, a_2 and a_4 of T_2 must be even with $a_2, a_4 \geq 2$. As $a_3 + a_4 + a_5 \geq 4$, by Corollaries 3.8 and 3.1, we obtain $T_2 \succ^{a_2} \mathrm{T}_1^{a_3+a_4+a_5} \succeq^2 \mathrm{T}_1^{n-4}$. Thus, Theorem 3.14(i) holds.

(ii) $T \in \mathcal{H}_n^{3,2}$ with $n \geq 14$.

If $T \in \mathcal{H}_n^{3,2}$, then by Lemma 3.10, there exists a tree T_2 such that $T_2 \in \mathcal{H}_n^3$ and $T \succeq T_2$. Since T_2 has a perfect matching, all a_i $(1 \leq i \leq 4)$ of T_2 are even or at most two of a_i $(1 \leq i \leq 4)$ are odd. Two cases are considered as follows.

Case (i): All a_i of T_2 are even with $a_i \geq 2$, where $1 \leq i \leq 4$.

Subcase (i.i): At least one of $a_1 + a_2$ and $a_3 + a_4$ is not less than 8.

We assume $a_1 + a_2 \geq 8$. Since $a_1 + a_2 - 2 \geq 6$ and $a_3 + a_4 + a_5 \geq 5$, by Corollaries 3.8, 3.1 and 3.4, $T_2 \succ^{a_1} \mathrm{T}_{a_3+a_4+a_5}^{a_2} \succeq^2 \mathrm{T}_{a_3+a_4+a_5}^{a_1+a_2-2} \succ^2 \mathrm{T}_3^{n-6}$. Thus, we have $T \succeq T_2 \succ^2 \mathrm{T}_3^{n-6} \succ^2 \mathrm{T}_{n-5}^2$ (by Corollary 3.3).

Subcase (i.ii): $a_1 + a_2$ and $a_3 + a_4$ are less than 8.

If $a_1 + a_2 = 4$ and $a_3 + a_4 = 4$, then $T_2 \cong I_n$, namely $T \succeq T_2 \cong I_n$. If $a_1 + a_2 = 4$ and $a_3 + a_4 = 6$ or $a_1 + a_2 = 6$ and $a_3 + a_4 = 4$, then $T_2 \cong J_n$. By Lemma 3.12, we have $J_n \succ I_n$. Thus, $T \succeq T_2 \cong J_n \succ I_n$. If $a_1 + a_2 = a_3 + a_4 = 6$, then $T_2 \cong K_n$. From Lemma 3.13, we get $T \succeq T_2 \cong K_n \succ I_n$.

Case (ii): At most two of a_i $(1 \leq i \leq 4)$ of T_2 are odd.

Subcase (ii.i): One of a_i $(1 \leq i \leq 4)$ of T_2 is odd.

We assume that a_1 is odd. Obviously, a_2, a_3, a_4 are all even and not less than 2. As $a_1 \geq 1$, from Corollary 3.8, Corollary 3.1 and Theorem 3.5, we obtain $T_2 \succ^{a_3} \mathrm{T}_{a_1+a_2+a_5}^{a_4} \succeq^2 \mathrm{T}_{a_1+a_2+a_5}^{a_3+a_4-2} \succeq^2 \mathrm{T}_{n-5}^2$ since $a_3 \geq 2$ and $a_1 + a_2 + a_5 \geq 4$. Thus, $T \succeq T_2 \succ^2 \mathrm{T}_{n-5}^2$.

Subcase (ii.ii): Two of a_i $(1 \leq i \leq 4)$ of T_2 are odd.

Let a_1 and a_3 be odd. Obviously, a_2 and a_4 are even and not less than 2. Since $T \notin \mathcal{H}_n^{3,1}$, one of a_1 and a_3 is not less than 3. Let $a_3 \geq 3$. From Corollaries 3.8,

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3.1 and 3.4, we get $T_2 \succ^{a_4} \mathrm{T}_{a_3}^{a_1+a_2+a_5} \succeq^2 \mathrm{T}_{a_3}^{a_1+a_2+a_5+a_4-2} \succeq^2 \mathrm{T}_{n-6}^{3}$ since $a_3 \geq 3$ and $a_1+a_2+a_5+a_4-2 \geq 4$. Therefore, $T \succeq T_2 \succ^2 \mathrm{T}_3^{n-6} \succ^2 \mathrm{T}_{n-5}^2$ (by Corollary 3.3). ◻

From Theorems 3.5–3.14, we obtain the ordering of the trees in $\mathcal{H}_n$ according to their minimal EIs, as shown in Theorem 3.15.

THEOREM 3.15. *Let $T \in \mathcal{H}_n$ and $n \geq 14$.*

(i) *If $T \in \mathcal{H}_n^{1,1} \cup \mathcal{H}_n^{3,1}$, then $EE(T) > EE(^2T_1^{n-4}) > EE(P_n)$, where $T \ncong P_n,\ ^2T_1^{n-4}$.*

(ii) *If $T \in \mathcal{H}_n^{1,2} \cup \mathcal{H}_n^{2} \cup \mathcal{H}_n^{3,2}$, then $EE(T) > EE(^2T_{n-5}^2) > EE(^2T_1^{n-4}) > EE(P_n)$, where $T \ncong P_n,\ ^2T_1^{n-4}, ^2T_2^{n-5}$.*

Proof. Let $T \in \mathcal{H}_n$ with $n \geq 14$ and $T \ncong P_n,\ ^2T_1^{n-4}$. From Theorems 3.5 and 3.14(i), we get Theorem 3.15(i). As $n \geq 14$, $^2T_3^{n-6} \succ^2 T_{n-5}^2$ follows from Corollary 3.3 and $I_n \succ^2 T_{n-5}^2$ follows from Corollary 3.8. By Theorems 3.6, 3.11, and 3.14(ii), we get Theorem 3.15(ii). ◻

Let $T \in \mathcal{H}_n$. We can check that $T \cong P_2$ as $n = 2$, $T \cong P_4$ as $n = 4$, and $T \cong P_6, ^2T_1^2$ as $n = 6$. By Lemma 2.4, we have $EE(^2T_1^{n-4}) > EE(P_n)$ as $n = 6$. Next, for $n = 8, 10, 12$, we have Theorem 3.16 as follows.

THEOREM 3.16. *Let $T \in \mathcal{H}_n$ and $n = 8, 10, 12$. We have*

$$EE(T) > EE(^2T_1^{n-4}) > EE(P_n),$$

where $T \ncong P_n,\ ^2T_1^{n-4}$.

Proof. Let $T \in \mathcal{H}_n$ with $n = 8, 10, 12$ and $T \ncong P_n,\ ^2T_1^{n-4}$. If $T \in \mathcal{H}_n^1$, then by Theorems 3.5 and 3.6, we get Theorem 3.16. If $T \in \mathcal{H}_n^2 \cup \mathcal{H}_n^3$, then by Lemma 3.9, Lemma 3.10 and Corollary 3.8, there exits a tree $^lT_b^r \in \mathcal{H}_n^1$ such that $EE(T) > EE(^lT_b^r)$, where $^lT_b^r \ncong P_n$. Furthermore, by Theorems 3.5 and 3.6, we have $EE(^lT_b^r) \geq EE(^2T_1^{n-4})$, where $^lT_b^r \ncong P_n$. Thus, we get Theorem 3.16 as $T \in \mathcal{H}_n^2 \cup \mathcal{H}_n^3$. ◻

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REFERENCES

[1] S. Azami. On Laplacian and signless Laplacian Estrada indices of graphs. *MATCH–Communications in Mathematical and in Computer Chemistry*, 74:411–418, 2015.

[2] H. Bamdad, F. Ashraf, and I. Gutman. Lower bounds for Estrada index and Laplacian Estrada index. *Applied Mathematics Letters*, 23:739–742, 2010.

[3] X.D. Chen and J.G. Qian. On resolvent Estrada index. *MATCH–Communications in Mathematical and in Computer Chemistry*, 73:163–174, 2015.

[4] D.M. Cvetković, M. Doob, and H. Sachs. *Spectra of Graphs Theory and Application*. Academic Press, New York, 1980.

[5] K.C. Das and S.G. Lee. On the Estrada index conjecture. *Linear Algebra and its Applications*, 431:1351–1359, 2009.

[6] H.Y. Deng. A note on the Estrada index of trees. *MATCH–Communications in Mathematical and in Computer Chemistry*, 62:607–610, 2009.

[7] H.Y. Deng. A proof of a conjecture on the Estrada index. *MATCH–Communications in Mathematical and in Computer Chemistry*, 62:599–606, 2009.

[8] Q.Y. Deng and H.Y. Chen. On extremal bipartite unicyclic graphs. *Linear Algebra and its Applications*, 444:89–99, 2014.

[9] Z.B. Du and B. Zhou. On the Estrada index of graphs with given number of cut edges. *Electronic Journal of Linear Algebra*, 22:586–592, 2011.

[10] Z.B. Du and B. Zhou. The Estrada index of trees. *Linear Algebra and its Applications*, 435:2462–2467, 2011.

[11] E. Estrada. Characterization of the amino acid contribution to the folding degree of proteins. *Proteins: Structure, Function, and Bioinformatics*, 54:727–737, 2004.

[12] E. Estrada. Characterization of 3D molecular structure. *Chemical Physics Letters*, 319:713–718, 2000.

[13] E. Estrada and J.A. Rodriguez-Velazquez. Subgraph centrality in complex networks. *Physical Review E*, 71:056103, 2005.

[14] E. Estrada, J.A. Rodriguez-Velazquez, and M. Randić. Atomic branching in molecules. *International Journal of Quantum Chemistry*, 106:823–832, 2006.

[15] G.H. Fath-Tabar and A.R. Ashrafi. New upper bounds for Estrada index of bipartite graphs. *Linear Algebra and its Applications*, 435:2607–2611, 2011.

[16] N. Gao, L. Qiao, B. Ning, and S.G. Zhang. Coulson-type integral formulas for the Estrada index of graphs and the skew Estrada index of oriented graphs. *MATCH–Communications in Mathematical and in Computer Chemistry*, 73:133–148, 2015.

[17] I. Gutman. Lower bounds for Estrada index. *Publications de lInstitut Mathematique*, 83:1–7, 2008.

[18] I. Gutman, B. Furtula, X. Chen, and J. Qian. Resolvent Estrada index – Computational and mathematical studies. *MATCH–Communications in Mathematical and in Computer Chemistry*, 74:431–440, 2015.

[19] I. Gutman and A. Graovac. Estrada index of cycles and paths. *Chemical Physics Letters*, 436:294–296, 2007.

[20] F. Huang, X.L. Li, and S.J. Wang. On maximum Laplacian Estrada indices of trees with some given parameters. *MATCH–Communications in Mathematical and in Computer Chemistry*, 74:419–429, 2015.

[21] A. Ilić and D. Stevanović. The Estrada index of chemical trees. *Journal of Mathematical Chemistry*, 47:305–314, 2010.

[22] W.H. Wang. Estrada indices of the trees with a perfect matching. *MATCH–Communications in Mathematical and in Computer Chemistry*, 75:373–383, 2016.

[23] L. Wang, Y.Z. Fan, and Y. Wang. Maximum Estrada index of bicyclic graphs. *Discrete Applied Mathematics*, 180:194–199, 2015.

Electronic Journal of Linear Algebra ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 31, pp. 134-146, March 2016

ELA
http:/repository.uwyo.edu/ela

[24] H.Z. Wang, L.Y. Kang, and E.F. Shan. On the Estrada index of cacti. *Electronic Journal of Linear Algebra*, 27:798–808, 2014.

[25] W.H. Wang and W.W. Xu. Graphs with the maximal Estrada indices. *Linear Algebra and its Applications*, 446:314–328, 2014.

[26] J.B. Zhang, B. Zhou, and J.P. Li. On Estrada index of trees. *Linear Algebra and its Applications*, 434:215–223, 2011.

[27] Z.X. Zhu, L.S. Tan, and Z.Y. Qiu. Tricyclic graph with maximal Estrada index. *Discrete Applied Mathematics*, 162:364–372, 2014.