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Wen-Huan Wang
Shanghai University,, whwang@shu.edu.cn

Chun-Xiang Zhai
Shanghai University

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MINIMAL ESTRADA INDEX OF THE TREES WITHOUT PERFECT MATCHINGS*

WEN-HUAN WANG† AND CHUN-XIANG ZHAI‡

Abstract. Trees possessing no Kekulé structures (i.e., perfect matching) with the minimal Estrada index are considered. Let $\overline{\mathcal{T}}_n$ be the set of the trees having no perfect matchings with n vertices. When n is odd and $n \geq 5$, the trees with the smallest and the second smallest Estrada indices among $\overline{\mathcal{T}}_n$ are obtained. When n is even and $n \geq 6$, the tree with the smallest Estrada index in $\overline{\mathcal{T}}_n$ is deduced.

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 $\boldsymbol{A}(G)$ be the adjacency matrix of G and $\boldsymbol{I}$ the identity matrix of order n. Let $\Phi(G, \lambda) = \det[\lambda \boldsymbol{I} - \boldsymbol{A}(G)]$ be the characteristic polynomial of G [3]. The n roots of $\Phi(G, \lambda) = 0$ are denoted by $\lambda_1 \geq \cdots \geq \lambda_n$. Since $\boldsymbol{A}(G)$ is a real symmetric matrix, $\lambda_1, \ldots, \lambda_n$ are all real numbers. The Estrada index (EI) of G, is defined by [9]

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

According to Estrada, the EI is useful to characterize the degree of folding of a protein chain, and to account for the contribution of amino acids to folding [9, 13, 14]. Later, the EI was extended to measure the centrality of complex network [10, 11], extended atomic branching [12], and the carbon-atom skeleton [18]. For a comprehensive survey of the index, one can refer to [16]. Since its inception in 2000, several analogous graph invariants, such as the Laplacian and signless Laplacian Estrada indices [1, 20] based respectively on the eigenvalues of Laplacian and signless Laplacian matrices, the resolvent Estrada indices [2, 17] based on the resolvent of the adjacency matrix, and the skew Estrada index of oriented graphs [15], have been considered.

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 $k \geq 0$, 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 [3]. From the Taylor expansion of e^{λ_i}, $EE(G)$ in (1.1) can be rewritten as

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

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†Department of Mathematics, Shanghai University, Shangda Road, Shanghai 200444, China (whwang@shu.edu.cn).
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‡Department of Mathematics, Shanghai University, Shangda Road, Shanghai 200444, China. Current address: Jiangqiao Experimental Middle School, Shanghai 201803, China.

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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 bipartite graphs of order n. If $M_{2k}(G_1) \geq M_{2k}(G_2)$ holds for each positive integer k, then $EE(G_1) \geq EE(G_2)$ and we write $G_1 \succeq G_2$. 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 write $G_1 \succ G_2$. If $G_1 \succeq G_2$ and $G_2 \succeq G_1$, then we write $G_1 \sim G_2$.

Within groups of isomers, it was found that the EI increases with the rising extend of branching of the carbon-atom skeleton [18, 21]. Therefore, the ordering of graphs with extremal Estrada indices (EIs) is of practical importance and theoretical interest in the subject of graph theory. In graph theory, a connected acyclic graph is called a tree. Therefore, the topological properties of acyclic molecules agree with those of trees. Based on the above relationship obtained from (1.3), a number of results have been reached for the graphs with the extremal EIs. 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, the trees with a given number of pendent vertices, and the trees with a given maximum degree, ect., one can refer to [4, 5, 6, 8, 21, 27]. For the characterization of the unicyclic graphs, the bicyclic graphs and the tricyclic graphs, ect., one can refer to [7, 22, 23, 25, 28].

Recall that conjugated molecules in chemistry may be classified into two groups: Kekuléan and non-Kekuléan molecules, depending on whether or not they possess the Kekulé structures, which are perfect matchings in the molecular graph corresponding to the carbon atom skeleton of a conjugated unsaturated hydrocarbon [19]. In the set of trees with perfect matchings, Wang [24] obtained the trees with the largest and the second largest EIs, Zhai and Wang [26] deduced the trees with the smallest and the second smallest EIs. However, the trees with the extremal EIs in the set of trees without perfect matchings remains unknown. For simplicity, $\mathcal{PM}$ stands for "perfect matching". Let $\overline{\mathcal{T}}_n$ be the set of the trees with n vertices having no $\mathcal{PM}$. In this paper, for completeness, in $\overline{\mathcal{T}}_n$, we will investigate the ordering of trees in terms of their minimal EIs. Thus, we characterize the acyclic non-Kekuléan π-electron systems with the minimal EIs.

2. Transformations for studying the Estrada indices. Let $v \in V(G)$, and $d_G(v)$ be the degree of v of G. A pendent path at v of G is a path in G connecting vertex v and a pendent vertex such that all internal vertices (if exist) in this path have degree two and $d_G(v) \geq 3$. Lemmas 2.1 and 2.2 are simply quoted.

Lemma 2.1. [21] *Let w be a vertex of the nontrivial connected graph G. For non-negative integers p and q, let $G(p,q)$ denote the graph obtained from G by attaching at w pendent paths $P \cong wv_1v_2\cdots v_p$ and $Q \cong wu_1u_2\cdots u_q$ 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. Let P_n be a path with n vertices.

Lemma 2.2. [6] *Let u be a non-isolated vertex of a simple graph H. Let $H_1 \cong H(u) \cdot P_n(v_1)$ (as shown in Figure 1(a)) and $H_2 \cong H(u) \cdot P_n(v_t)$ (as shown in Figure 1(b)), where $P_n \cong v_1v_2\cdots v_n$. As $n \geq 3$ and $k \geq 2$, we have $M_{2k}(H_2) > M_{2k}(H_1)$.*

To obtain our results, Lemma 2.3 is introduced as follows.

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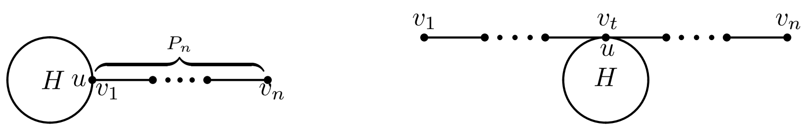

(a) H_1 (b) H_2

FIGURE 1. *The transformation in Lemma 2.2.*

(a) G (b) G'

FIGURE 2. *The transformation in Lemma 2.3.*

LEMMA 2.3. *Let G_1 be a connected graph, $u \in V(G_1)$ and $|V(G_1)| \geq 2$. Let G_2 be a tree with $n \geq 3$ vertices, $G_2 \ncong P_n$ and $v \in V(G_2)$. Let $G \cong G_1(u) \cdot G_2(v)$ (as shown in Figure 2(a)) and $G' \cong G_1(u) \cdot P_n(v)$ (as shown in Figure 2(b)), where $P_n \cong vv_2 \cdots v_n$. We have $EE(G) > EE(G')$.*

Proof. Let G be the graph as shown in Figure 2(a). Two cases are considered as follows.

Case (i). $d_{G_2}(v) = 1$.

In G, since $G_2 \ncong P_n$, we can choose one vertex (denoted by w) of G_2 such that $d_{G_2}(w) \geq 3$ and there are $(d_{G_2}(w) - 1)$ pendent paths attached at w. By using Lemma 2.2 $(d_{G_2}(w) - 2)$ times on w in G, we get a new graph H satisfying $d_H(w) = 2$ and $G \succ H$. By using the same procedure on all the vertices in G_2 which have degrees three or more, we can obtain a graph G' such that $H \succeq G'$, where G' is the graph as shown in Figure 2(b). Thus, we get $G \succ G'$.

Case (ii). $d_{G_2}(v) \geq 2$.

Subcase (ii.i). $d_{G_2}(v) \geq 2$ and all the vertices in $V(G_2) \setminus \{v\}$ have degrees 2 or 1.

Obviously, G is the graph obtained from G_1 by attaching $d_{G_2}(v)$ pendent paths at u of G_1. By using Lemma 2.2 $(d_{G_2}(v) - 1)$ times on v in G, we have $G \succ G'$.

Subcase (ii.ii). $d_{G_2}(v) \geq 2$ and there exist $k \geq 1$ vertices in $V(G_2) \setminus \{v\}$ having degrees three or more.

In G, we can choose one vertex (denoted by s) of $V(G_2) \setminus \{v\}$ such that $d_{G_2}(s) \geq 3$ and there are $(d_{G_2}(s) - 1)$ pendent paths attached at s. By using Lemma 2.2 $(d_{G_2}(s) - 2)$ times on s of G, we get a new graph H satisfying $d_H(s) = 2$ and $G \succ H$. In G, by using the same procedure on all the vertices in G_2 which have degrees three or more (except for v), we can obtain a graph H' such that $H \succeq H'$, where H' is the graph obtained from G_1 by attaching $d_{G_2}(v)$ pendent paths at u in G_1. By using Lemma 2.2 $(d_{G_2}(v) - 1)$ times on v in H', we get $H' \succ G'$. Thus, $G \succ G'$. ∎

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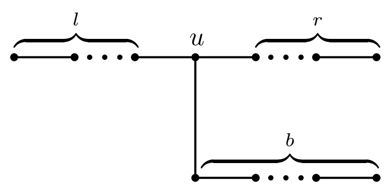

FIGURE 3. ${}^{l}T_{b}^{r}$ *with* $l+r+b+1=n$.

3. Ordering of the trees in $\overline{\mathcal{T}}_n$ according to their minimal Estrada indices for odd n. Let ${}^{l}\mathrm{T}_{b}^{r}$ be the tree obtained by attaching three pendent paths of length l, r and b at a common vertex u, where $l+r+b+1=n$. For example, ${}^{l}\mathrm{T}_{b}^{r}$ is shown in Figure 3.

For a tree T with n vertices, if n is odd, then T has no $\mathcal{PM}$, namely $T \in \overline{\mathcal{T}}_n$. We have $\overline{\mathcal{T}}_2 = \emptyset$, $\overline{\mathcal{T}}_3 = \{P_3\}$, and $\overline{\mathcal{T}}_4 = \{{}^{1}\mathrm{T}_{1}^{1}\}$. Next, in $\overline{\mathcal{T}}_n$, when n is odd and $n \geq 5$, we obtain the trees with the smallest and the second smallest EIs in Theorem 3.1.

THEOREM 3.1. *Let $T \in \overline{\mathcal{T}}_n \setminus \{P_n, {}^{1}\mathrm{T}_{n-3}^{1}\}$ and n be odd, where $n \geq 5$. We have $EE(T) > EE({}^{1}\mathrm{T}_{n-3}^{1}) > EE(P_n)$.*

Proof. Let n be odd and $n \geq 5$. By Lemma 2.1, we obtain ${}^{1}\mathrm{T}_{n-3}^{1} \succ P_n$. Let $T \in \overline{\mathcal{T}}_n \setminus \{P_n, {}^{1}\mathrm{T}_{n-3}^{1}\}$. Next, we prove

$$T \succ {}^{1}\mathrm{T}_{n-3}^{1}. \tag{3.4}$$

Since $T \ncong P_n$, T has at least one vertex having a degree three or more. We consider two cases as follows.

Case (i). Only one vertex of T (denoted by u) has a degree three or more.

In this case, all the degrees of the vertices in $V(T) \setminus \{u\}$ are 2 or 1. Namely, T is the tree obtained by attaching $d_T(u)$ pendent paths at a common vertex u. By using Lemma 2.2 $(d_T(u)-3)$ times on u in T, we get $T \succeq {}^{l}\mathrm{T}_{b}^{r}$, where $T \sim {}^{l}\mathrm{T}_{b}^{r}$ holds if and only if $T \cong {}^{l}\mathrm{T}_{b}^{r}$. Since ${}^{l}\mathrm{T}_{b}^{r}$ has $n \geq 5$ vertices, where n is odd, ${}^{l}\mathrm{T}_{b}^{r} \in \overline{\mathcal{T}}_n$.

Suppose $r \geq l \geq 1$. By applying Lemma 2.1 $(l-1)$ times, we obtain ${}^{l}\mathrm{T}_{b}^{r} \succ {}^{l-1}\mathrm{T}_{b}^{r+1} \succ \cdots \succ {}^{1}\mathrm{T}_{b}^{l+r-1}$. Without loss of generality, let $b \geq l+r-1$. By using Lemma 2.1 $(n-b-3)$ times again, we have ${}^{1}\mathrm{T}_{b}^{l+r-1} \succ {}^{1}\mathrm{T}_{b+1}^{l+r-2} \succ \cdots \succ {}^{1}\mathrm{T}_{n-3}^{1}$. Therefore, we get ${}^{l}\mathrm{T}_{b}^{r} \succ {}^{1}\mathrm{T}_{n-3}^{1}$.

Case (ii). There exist $k \geq 2$ vertices in T having degrees three or more.

In this case, we can choose one vertex (denoted by w) in T such that $d_T(w) \geq 3$ and there are $(d_T(w)-1)$ pendent paths attached at w. By using Lemma 2.2 $(d_T(w)-2)$ times on w in T, we obtain a new tree $T' \in \overline{\mathcal{T}}_n$ (since n is odd) satisfying $d_{T'}(w) = 2$ and $T \succ T'$. By using the same procedure, we can obtain a tree $T'' \in \overline{\mathcal{T}}_n$ (since n is odd) such that $T' \succeq T''$, where T'' has only one vertex having a degree three or more and all the other vertices in T'' having degrees 2 or 1. Furthermore, by the proof of case (i), we have $T'' \succeq {}^{1}\mathrm{T}_{n-3}^{1}$. Therefore, we obtain $T \succ {}^{1}\mathrm{T}_{n-3}^{1}$.

By the combination of the proofs of cases (i) and (ii), we get (3.4). ∎

Next, in Section 4, among $\overline{\mathcal{T}}_n$, when n is even, we will deduce the tree with the minimal EI by using a different method. The reason is given in the following remark.

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REMARK 3.2. In Lemma 2.2, if H_2 (as shown in Figure 1(b)) has even number of vertices and has no $\mathcal{PM}$, then H_1 (as shown in Figure 1(a)) may have a $\mathcal{PM}$. Therefore, in $\overline{\mathcal{T}}_n$, if n is even, then Lemma 2.2 can not be used to obtain the ordering of the trees according to their minimal EIs.

4. Trees with the minimal Estrada index in $\overline{\mathcal{T}}_n$ for even n. In this section, among $\overline{\mathcal{T}}_n$, when n is even, we will investigate the tree with the minimal EI in $\overline{\mathcal{T}}_n$. Since the trees in $\overline{\mathcal{T}}_n$ have no $\mathcal{PM}$, we get $P_n \notin \overline{\mathcal{T}}_n$. Let $\overline{\mathcal{T}}_n = \overline{\mathcal{T}}_n^1 \bigcup \overline{\mathcal{T}}_n^2$, where $\overline{\mathcal{T}}_n^1$ is the subset of $\overline{\mathcal{T}}_n$, in which each tree has only one vertex having degree 3 and all the other vertices having degrees 2 or 1, and $\overline{\mathcal{T}}_n^2$ is the subset of $\overline{\mathcal{T}}_n$, in which each tree has at least two vertices having degrees three or more or only one vertex having a degree four or more.

In ${}^l\mathrm{T}_b^r$, we have $l + r + b + 1 = n$. If n is even, then only one of l, r and b is odd or all of l, r and b are odd. Therefore, if ${}^l\mathrm{T}_b^r \in \overline{\mathcal{T}}_n$ and n is even, then l, r and b must be all odd. Otherwise, if only one of l, r and b is odd, then ${}^l\mathrm{T}_b^r$ has a $\mathcal{PM}$. By the definition of $\overline{\mathcal{T}}_n^1$, we get that $\overline{\mathcal{T}}_n^1 = \{{}^l\mathrm{T}_b^r |\ l, r \text{ and } b \text{ are all positive odd numbers}\}$.

Let G in Lemma 2.1 be P_{b+1}. By using Lemma 2.1, we can obtain Corollary 4.1.

COROLLARY 4.1. *${}^l\mathrm{T}_b^r \succ {}^{l-2}\,\mathrm{T}_b^{r+2} \succ \cdots \succ {}^5\,\mathrm{T}_b^{n-b-6} \succ {}^3\,\mathrm{T}_b^{n-b-4} \succ {}^1\,\mathrm{T}_b^{n-b-2}$, where $r \geq l$ and $l,\ r,\ b$ are all positive odd numbers.*

Let G in Lemma 2.1 be P_{l+1}. By using Lemma 2.1, we get Corollaries 4.2 and 4.3.

COROLLARY 4.2. *${}^l\mathrm{T}_b^r \succ {}^l\,\mathrm{T}_{b+2}^{r-2} \succ \cdots \succ {}^l\,\mathrm{T}_{n-l-6}^5 \succ {}^l\,\mathrm{T}_{n-l-4}^3 \succ {}^l\,\mathrm{T}_{n-l-2}^1$, where $b \geq r$ and $l,\ r,\ b$ are all positive odd numbers.*

COROLLARY 4.3. *${}^l\mathrm{T}_b^r \succ {}^l\,\mathrm{T}_{b-2}^{r+2} \succ \cdots \succ {}^l\,\mathrm{T}_5^{n-l-6} \succ {}^l\,\mathrm{T}_3^{n-l-4} \succ {}^l\,\mathrm{T}_1^{n-l-2}$, where $r \geq b$ and $l,\ r,\ b$ are all positive odd numbers.*

By Corollaries 4.2 and 4.3, we get Corollary 4.4.

COROLLARY 4.4. *${}^l\mathrm{T}_b^r \succeq {}^l\,\mathrm{T}_{n-l-4}^3 \succ {}^l\,\mathrm{T}_{n-l-2}^1$, with ${}^l\mathrm{T}_b^r \sim {}^l\,\mathrm{T}_{n-l-4}^3$ if and only if $r = 3$ or $b = 3$, where $r,\ b \geq 3$ and $l,\ r,\ b$ are all positive odd numbers.*

REMARK 4.5. By the definition of ${}^l\mathrm{T}_b^r$, if $l,\ r,\ b$ are all positive odd numbers, then all the graphs in Corollaries 4.1–4.4 have no $\mathcal{PM}$.

For n is even, let $\overline{\mathcal{T}}_n^1 = \overline{\mathcal{T}}_n^{1,1} \bigcup \overline{\mathcal{T}}_n^{1,2}$, where $\overline{\mathcal{T}}_n^{1,1} = \{{}^l\mathrm{T}_b^r \mid r \geq 1,\ b \geq l = 1\}$ and $\overline{\mathcal{T}}_n^{1,2} = \{{}^l\mathrm{T}_b^r \mid b \geq 3,\ r \geq l \geq 3\}$. Since $l + r + b + 1 = n$, we get $n \geq 4$ in $\overline{\mathcal{T}}_n^{1,1}$ and $n \geq 10$ in $\overline{\mathcal{T}}_n^{1,2}$.

From Corollary 4.2 (let $l = 1$), we obtain, in Theorem 4.6, the complete ordering of the trees in $\overline{\mathcal{T}}_n^{1,1}$ in terms of their minimal EIs.

THEOREM 4.6. *For ${}^1\mathrm{T}_b^r \in \overline{\mathcal{T}}_n^{1,1}$, we have the ordering as follows.*

(i) For $n = 4t$ with $t \geq 1$, ${}^1\mathrm{T}_{\frac{n}{2}-1}^{\frac{n}{2}-1} \succ {}^1\,\mathrm{T}_{\frac{n}{2}+1}^{\frac{n}{2}-3} \succ \cdots \succ {}^1\,\mathrm{T}_{n-5}^3 \succ {}^1\,\mathrm{T}_{n-3}^1$.

(ii) For $n = 4t + 2$ with $t \geq 1$, ${}^1\mathrm{T}_{\frac{n}{2}}^{\frac{n}{2}-2} \succ {}^1\,\mathrm{T}_{\frac{n}{2}+2}^{\frac{n}{2}-4} \succ \cdots \succ {}^1\,\mathrm{T}_{n-5}^3 \succ {}^1\,\mathrm{T}_{n-3}^1$.

From Corollaries 4.1 and 4.4, we get Theorem 4.7 as follows.

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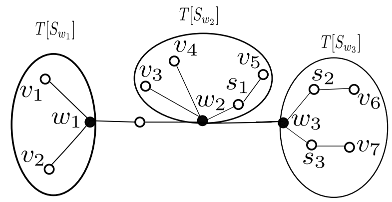

FIGURE 4. T.

THEOREM 4.7. *Let* ${}^l\mathrm{T}_b^r \in \overline{\mathcal{T}}_n^{1,2} \backslash \{{}^3\mathrm{T}_{n-7}^3\}$, *$n$ be even and* $n \geq 10$. *We have*

$$ {}^l\mathrm{T}_b^r \succ^3 \mathrm{T}_{n-7}^3 \succ^1 \mathrm{T}_{n-7}^5 \succeq^1 \mathrm{T}_{n-5}^3 \succ^1 \mathrm{T}_{n-3}^1, $$

with ${}^1\mathrm{T}_{n-7}^5 \sim^1 \mathrm{T}_{n-5}^3$ *if and only if* $n = 10$.

Proof. Let n be even and $n \geq 10$. It follows from Corollary 4.1 that ${}^3\mathrm{T}_{n-7}^3 \succ^1 \mathrm{T}_{n-7}^5$. Since $n-7 \geq 3$, by Corollary 4.4 (let $l=1$), we obtain ${}^1\mathrm{T}_{n-7}^5 \succeq^1 \mathrm{T}_{n-5}^3$ with ${}^1\mathrm{T}_{n-7}^5 \sim^1 \mathrm{T}_{n-5}^3$ if and only if $n = 10$. Since $n-5 \geq 5$, by Corollary 4.4 (let $l=1$) again, we get ${}^1\mathrm{T}_{n-5}^3 \succ^1 \mathrm{T}_{n-3}^1$. Namely, we have ${}^3\mathrm{T}_{n-7}^3 \succ^1 \mathrm{T}_{n-7}^5 \succeq^1 \mathrm{T}_{n-5}^3 \succ^1 \mathrm{T}_{n-3}^1$.

Next, let ${}^l\mathrm{T}_b^r \in \overline{\mathcal{T}}_n^{1,2} \backslash \{{}^3\mathrm{T}_{n-7}^3\}$. We will prove

$$ {}^l\mathrm{T}_b^r \succ^3 \mathrm{T}_{n-7}^3. \tag{4.5} $$

By the definition of $\overline{\mathcal{T}}_n^{1,2}$, in ${}^l\mathrm{T}_b^r$, we have $b \geq 3$ and $r \geq l \geq 3$. By Corollary 4.1, we obtain ${}^l\mathrm{T}_b^r \succ^{l-2} \mathrm{T}_b^{r+2} \succ \cdots \succ^3 \mathrm{T}_b^{l+r-3}$. Since $l+r-3 \geq 3$ and $b \geq 3$, by Corollary 4.4 (let $l=3$), we get ${}^3\mathrm{T}_b^{l+r-3} \succeq^3 \mathrm{T}_{n-7}^3$ with ${}^3\mathrm{T}_b^{l+r-3} \sim^3 \mathrm{T}_{n-7}^3$ if and only if ${}^3\mathrm{T}_b^{l+r-3} \cong^3 \mathrm{T}_{n-7}^3$. Therefore, if ${}^l\mathrm{T}_b^r \ncong^3 \mathrm{T}_{n-7}^3$, then we have ${}^l\mathrm{T}_b^r \succ^3 \mathrm{T}_{n-7}^3$. Namely, (4.5) holds. Theorem 4.7 is thus proved. $\square$

Next, we consider the tree with the minimal EI in $\overline{\mathcal{T}}_n^2$. By the definition of $\overline{\mathcal{T}}_n^2$, we have $\overline{\mathcal{T}}_n^2 = \emptyset$ when $n = 4$. In $\overline{\mathcal{T}}_n^2$, we assume that n is even and $n \geq 6$. To obtain the tree with the minimal EI in $\overline{\mathcal{T}}_n^2$, we first give some definitions and proposition and then introduce Lemma 4.9.

Let $T \in \overline{\mathcal{T}}_n$. For two vertices $u, v \in V(T)$, let $d(u,v)$ be the distance between u and v. Let $V_p(T) = \{v \in V(T) \mid d_T(v) = 1\}$ and $\mathcal{A}(T) = \{w \in V(T) \mid d_T(w) \geq 3\}$. For a given vertex $w \in \mathcal{A}(T)$, let

$$ P_w(T) = \{v \in V_p(T) \mid d(v,w) < d(v,x), \text{ for any } x \in \mathcal{A}(T) \setminus \{w\}\}. $$

For example, let T be the tree as shown in Figure 4. We have $\mathcal{A}(T) = \{w_1, w_2, w_3\}$, $P_{w_1}(T) = \{v_1, v_2\}$, $P_{w_2}(T) = \{v_3, v_4, v_5\}$, and $P_{w_3}(T) = \{v_6, v_7\}$. For any $v \in V_p(T)$, there exists a vertex $w \in \mathcal{A}(T)$ such that $v \in P_w(T)$. For any $w \in \mathcal{A}(T)$, there exists at least one vertex $v \in P_w(T)$, namely $|P_w(T)| \geq 1$.

For $w \in \mathcal{A}(T)$, let $S_w = \{w\} \cup P_w(T) \cup Q_w(T)$, where $Q_w(T)$ is the set of vertices lying on the pendent paths between v of $P_w(T)$ and w (other than v and w) for all $v \in P_w(T)$. For example, for T in Figure 4, $S_{w_1} = \{w_1, v_1, v_2\}$, $S_{w_2} = \{w_2, s_1, v_3, v_4, v_5\}$, and $S_{w_3} = \{w_3, s_2, s_3, v_6, v_7\}$. We denote by $T[S_w]$ the induced subtree of T, where the vertex set of $T[S_w]$ is S_w, and the edge set of $T[S_w]$ is the set of those edges of T that have both ends in S_w. We say that the induced subtree $T[S_w]$ is the pendent subtree attached at w. For example, for T in Figure 4, $T[S_{w_1}]$, $T[S_{w_2}]$ and $T[S_{w_3}]$ are the three pendent subtrees attached at w_1, w_2 and w_3, respectively. By the definition of $T[S_w]$, we get that $d_{T[S_w]}(w) \geq 3$ and all the degrees of the vertices in $V(T[S_w]) \setminus \{w\}$ are 2 or 1.

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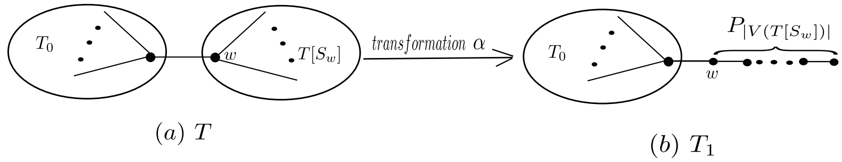

Figure 5. *Transformation α: $T \succ T_1$.*

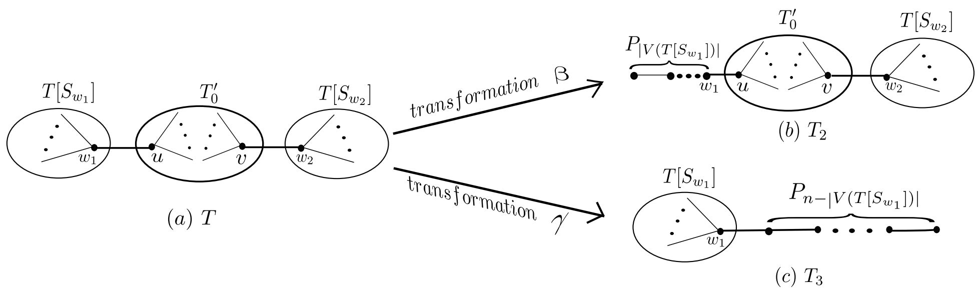

Figure 6. *Transformation β: $T \succ T_2$.* *Transformation γ: $T \succ T_3$.*

Let $|\mathcal{A}(T)|$ be the number of vertices in $\mathcal{A}(T)$. When $|\mathcal{A}(T)| \geq 2$, let $\mathcal{A}(T) = \{w_1, w_2, \ldots, w_t\}$, where $t \geq 2$. In $\mathcal{A}(T)$, when $t \geq 2$, we can choose two vertices (denoted by w_1 and w_2) such that

$$d(w_1, w_2) = \max\ \{d(w_i, w_j)|w_i, w_j \in \mathcal{A}(T), 1 \leq i < j \leq t\}. \tag{4.6}$$

Proposition 4.8. *Let $T \in \overline{\mathcal{T}}_n^2$. For $|\mathcal{A}(T)| \geq 2$, let w_1 and w_2 be the two vertices as defined in (4.6).*

(i) There exist two pendent subtrees $T[S_{w_1}]$ and $T[S_{w_2}]$ attached at w_1 and w_2, respectively.

(ii) $|P_{w_1}(T)| \geq 2$ and $|P_{w_2}(T)| \geq 2$.

Proof. (i) Let $T \in \overline{\mathcal{T}}_n^2$ and w_1 and w_2 be the two vertices as defined in (4.6). We can choose one vertex $u \in V(T)$ (u can be w_2) such that u is adjacent to w_1 and $T - w_1u = T_1' \cup T_2'$, where T_1' and T_2' are the two components of $T - w_1u$ which contain w_1 and w_2, respectively. Suppose that there exists a vertex (let it be x, $x \neq w_1$) in T_1' which has a degree three or more. Then $d(x, w_2) = d(x, w_1) + d(w_1, w_2) > d(w_1, w_2)$, which contradicts the definition of w_1 and w_2. Thus, all the vertices of T_1' (except for w_1) have degrees 2 or 1. Namely, T_1' is the pendent subtree attached at w_1. Similarly, we can get that there exists a pendent subtree attached at w_2. Thus, we get Proposition 4.8(i).

(ii) Since $d_T(w_1) \geq 3$, we get $d_{T_1'}(w_1) \geq 2$. Furthermore, since T_1' is the pendent subtree attached at w_1, we get $|P_{w_1}(T)| \geq 2$. Similarly, we can get $|P_{w_2}(T)| \geq 2$. Thus, we get Proposition 4.8(ii). ◻

Lemma 4.9. *Let $T \in \overline{\mathcal{T}}_n^2$, n be even, and $n \geq 6$. We get that there exists a tree ${}^l\mathrm{T}_b^r \in \overline{\mathcal{T}}_n^1$ such that $EE(T) > EE({}^l\mathrm{T}_b^r)$.*

Proof. Let $T \in \overline{\mathcal{T}}_n^2$, n be even, and $n \geq 6$. By the definition of $\overline{\mathcal{T}}_n^2$, we have $|\mathcal{A}(T)| \geq 1$. We prove Lemma 4.9 by induction on $|\mathcal{A}(T)|$.

(I). $|\mathcal{A}(T)| = 1$.

Since $T \in \overline{\mathcal{T}}_n^2$ and $|\mathcal{A}(T)| = 1$, by the definition of $\overline{\mathcal{T}}_n^2$, in T, there is only one vertex (let it be w) having a degree four or more and all the other vertices of T have degrees 2 or 1. Namely, T is a starlike

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tree obtained from w by attaching $d_T(w) \geq 4$ pendent paths at w. Let the lengths of the $d_T(w)$ pendent paths be $r_1, r_2, \ldots, r_{d_T(w)}$, where $\sum_{i=1}^{d_T(w)} r_i = n-1$. Let $\mathcal{R} = \{r_i |\ r_i \text{ is odd}, 1 \leq i \leq d_T(w)\}$. Since n is even, $|\mathcal{R}|$ must be odd number. Furthermore, since T has no $\mathcal{PM}$, $|\mathcal{R}| \geq 3$. Otherwise, if $|\mathcal{R}| = 1$, then T has a $\mathcal{PM}$. Therefore, we can choose $r_s,\ r_t \in \mathcal{R}$, where $1 \leq s,\ t \leq d_T(w)$. By employing Lemma 2.2 on w in T $(d_T(w) - 3)$ times, we get $T \succ^{r_s} \mathrm{T}^{r_t}_{n-r_s-r_t-1}$ since $d_T(w) \geq 4$. Since r_s and r_t are odd numbers and n is even, $n - r_s - r_t - 1$ is odd number. Therefore, ${}^{r_s}\mathrm{T}^{r_t}_{n-r_s-r_t-1} \in \overline{\mathcal{T}}^1_n$. Thus, we get Lemma 4.9 when $|\mathcal{A}(T)| = 1$.

(II). When $|\mathcal{A}(T)| = k$ and $k \geq 1$, we suppose there exists a tree ${}^l\mathrm{T}^r_b \in \overline{\mathcal{T}}^1_n$ such that $T \succ^l \mathrm{T}^r_b$.

(III). When $|\mathcal{A}(T)| = k+1$ and $k \geq 1$, next, we will prove that Lemma 4.9 holds.

Let $\mathcal{A}'(T) = \{w_i \in \mathcal{A}(T) | |P_{w_i}(T)| \geq 2, 1 \leq i \leq t\}$. Obviously, $\mathcal{A}'(T) \subseteq \mathcal{A}(T)$. Let $\mathcal{A}'(T) = \{w_1, w_2, \ldots, w_h\}$. By Proposition 4.8(ii), in $\mathcal{A}'(T)$, $h \geq 2$. For w_i $(1 \leq i \leq h)$ in $\mathcal{A}'(T)$, let $\mathcal{T_S} = \{T[S_{w_1}], T[S_{w_2}], \ldots, T[S_{w_h}]\}$.

Next, when $|\mathcal{A}(T)| = k+1$ with $k \geq 1$, we consider two cases according to the trees in $\mathcal{T_S}$ having $\mathcal{PM}$ or not.

Case (i). There exists at least one pendent subtree in $\mathcal{T_S}$ having $\mathcal{PM}$.

Let T be the graph as shown in Figure 5(a). Let $T[S_w]$ be the pendent subtree in $\mathcal{T_S}$ having a $\mathcal{PM}$. Since T has no $\mathcal{PM}$, we get that T_0 has no $\mathcal{PM}$. By employing Lemma 2.3 on T (namely, transformation α in Figure 5), we can get a new tree T_1 (as shown in Figure 5(b)) such that $T \succ T_1$. Obviously, $|\mathcal{A}(T_1)| = |\mathcal{A}(T)| - 1 = k$ and T_1 has no $\mathcal{PM}$ since T_0 has no $\mathcal{PM}$. By the induction, we can get that there exists a tree ${}^l\mathrm{T}^r_b \in \overline{\mathcal{T}}^1_n$ such that $T_1 \succeq^l \mathrm{T}^r_b$. Therefore, we obtain $T \succ^l \mathrm{T}^r_b$.

Case (ii). All the pendent subtrees in $\mathcal{T_S}$ do not have $\mathcal{PM}$.

Let T be the tree as shown in Figure 6(a). Let w_1 and w_2 be the two vertices as defined in (4.6). By Proposition 4.8, we get that there exist two pendent subtrees $T[S_{w_1}]$ and $T[S_{w_2}]$ attached at w_1 and w_2, respectively, and $|P_{w_1}(T)|, |P_{w_2}(T)| \geq 2$.

Subcase (ii.i). $|V(T[S_{w_1}])| \equiv 1 \pmod 2$ or $|V(T[S_{w_2}])| \equiv 1 \pmod 2$.

Without loss of generality, we assume $|V(T[S_{w_1}])| \equiv 1 \pmod 2$.

In T, if the induced graph $T[V(T_0{}') \bigcup V(T[S_{w_2}]) \bigcup \{w_1\}]$ has no $\mathcal{PM}$, then by employing Lemma 2.3 on T (namely, transformation β in Figure 6), we can get a new tree T_2 (as shown in Figure 6(b)) having no $\mathcal{PM}$ such that $T \succ T_2$. Since $|\mathcal{A}(T_2)| = |\mathcal{A}(T)| - 1 = k$, by the induction, we get $T_2 \succeq^l \mathrm{T}^r_b$. Therefore, $T \succ^l \mathrm{T}^r_b$, where ${}^l\mathrm{T}^r_b \in \overline{\mathcal{T}}^1_n$.

In T, if the induced graph $T[V(T_0{}') \bigcup V(T[S_{w_2}]) \bigcup \{w_1\}]$ has $\mathcal{PM}$, then w_1 (as shown in Figure 6(a)) is saturated with another vertex in $T[V(T_0{}') \bigcup V(T[S_{w_2}]) \bigcup \{w_1\}]$. Since T has no $\mathcal{PM}$, we can deduce that, in $T[S_{w_1}]$, there exist at least one vertex (except for w_1) which is unsaturated. By employing Lemma 2.3 on T (namely, transformation γ in Figure 6), we can get a new tree T_3 (as shown in Figure 6(c)) such that $T \succ T_3$, where T_3 has no $\mathcal{PM}$. Since $|\mathcal{A}(T_3)| = 1$, by the proof for (I) with $|\mathcal{A}(T)| = 1$, we get $T_3 \succeq^l \mathrm{T}^r_b$. Thus, $T \succ^l \mathrm{T}^r_b$, where ${}^l\mathrm{T}^r_b \in \overline{\mathcal{T}}^1_n$.

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Subcase (ii.ii). $|V(T[S_{w_1}])| \equiv 0 \pmod 2$ and $|V(T[S_{w_2}])| \equiv 0 \pmod 2$.

By employing Lemma 2.3 on T (namely, transformation γ in Figure 6), we get a new tree T_3 (as shown in Figure 6(c)) such that $T \succ T_3$, where T_3 has no $\mathcal{PM}$ since $T[S_{w_1}]$ has no $\mathcal{PM}$. Obviously, $|\mathcal{A}(T_3)| = 1$. By the proof for (I) with $|\mathcal{A}(T)| = 1$, we have $T_3 \succeq^l \mathrm{T}_b^r$. Therefore, we get $T \succ^l \mathrm{T}_b^r$, where ${}^l\mathrm{T}_b^r \in \overline{\mathcal{T}}_n^1$.

By the combination of the proofs of cases (i) and (ii), we get that Lemma 4.9 holds when $|\mathcal{A}(T)| = k+1$. Therefore, by the proofs of (I)–(III) and the induction on $|\mathcal{A}(T)|$, we obtain Lemma 4.9. ∎

Remark 4.10. In the proof for case (ii) of Lemma 4.9, if $u = w_2$ or $u = v$ (u, w_2 and v are shown in Figure 6(a), then we can check that the technique used in case (ii) of Lemma 4.9 remains valid.

By Theorem 4.6, Theorem 4.7 and Lemma 4.9, we obtain the tree with the minimal EI in $\overline{\mathcal{T}}_n$ when n is even.

Theorem 4.11. *Let $T \in \overline{\mathcal{T}}_n$, n be even and $n \geq 4$. We have $EE(T) \geq EE({}^1\mathrm{T}_{n-3}^1)$, with the equality if and only if $T \cong^1 \mathrm{T}_{n-3}^1$.*

Proof. Let $T \in \overline{\mathcal{T}}_n$, n be even and $n \geq 4$. For $n = 4$, $T \cong^1 T_1^1$. Let $n \geq 6$. For $T \in \overline{\mathcal{T}}_n^1$, obviously, $T \cong^l \mathrm{T}_b^r$. For $T \in \overline{\mathcal{T}}_n^2$, by Lemma 4.9, there exists a tree ${}^l\mathrm{T}_b^r \in \overline{\mathcal{T}}_n^1$ such that $T \succ^l \mathrm{T}_b^r$. Furthermore, by Theorems 4.6 and 4.7, we obtain Theorem 4.11. ∎

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

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

[4] K.C. Das and S.G. Lee. On the Estrada index conjecture. *Linear Algebra and its Applications*, 431(8):1351–1359, 2009.

[5] H.Y. Deng. A note on the Estrada index of trees. *MATCH – Communications in Mathematical and in Computer Chemistry*, 62(3):607–610, 2009.

[6] H.Y. Deng. A proof of a conjecture on the Estrada index. *MATCH – Communications in Mathematical and in Computer Chemistry*, 62(3):599–606, 2009.

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

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

[9] E. Estrada. Characterization of 3D molecular structure. *Chemical Physics Letters*, 319(5-6):713–718, 2000.

[10] E. Estrada and J.A. Rodriguez-Velázquez. Spectral measures of bipartivity in complex networks. *Physical Review E*, 72(4):046105, 2005.

[11] E. Estrada and J.A. Rodriguez-Velázquez. Subgraph centrality in complex networks. *Physical Review E*, 71(5):056103, 2005.

[12] E. Estrada, J.A. Rodriguez-Velázquez, and M. Randić. Atomic branching in molecules. *International Journal of Quantum Chemistry*, 106(4):823–832, 2006.

[13] E. Estrada. Characterization of the folding degree of proteins. *Bioinformatics*, 18(5):697–704, 2002.

[14] E. Estrada. Characterization of the amino acid contribution to the folding degree of proteins. *Proteins: Structure, Function, and Bioinformatics*, 54(4):727–737, 2004.

[15] 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.

[16] I. Gutman, H. Deng, and S. Radenković. The Estrada index: an updated survey. In: D. Cvetković and I. Gutman (editors), *Selected Topics on Applications of Graph Spectra*, Math. Inst., Beograd, 155–174, 2011.

Electronic Journal of Linear Algebra, ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 35, pp. 408-417, September 2019.
http://repository.uwyo.edu/ela

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

[18] I. Gutman, B. Furtula, V. Marković, and B. Glisić. Alkanes with greatest Estrada index. *Zeitschrift Fur Naturforschung*, 62(9):495–498, 2007.

[19] H. Hosoya. Introduction to graph theory. In: D.D Bonchev and O.G. Mekenyan (editors), *Graph Theoretical Approaches to Chemical Reactivity*, Kluwer Academic Publishers, Dordrecht, 1–36, 1994.

[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(1):305–314, 2010.

[22] 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.

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

[24] W.H. Wang. Estrada indices of the trees with a perfect matching. *MATCH – Communications in Mathematical and in Computer Chemistry*, 75(3):373–383, 2016.

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

[26] C.X. Zhai and W.H. Wang. Minimal Estrada indices of the trees with a perfect matching. *Electronic Journal of Linear Algebra*, 31:134–146, 2016.

[27] J.B. Zhang, B. Zhou, and J.P. Li. On Estrada index of trees. *Linear Algebra and its Applications*, 434(1):215–223, 2011.

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