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Trees with the Greatest Wiener and Edge−Wiener Index

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ABSTRACT

The Wiener index W and the edge-Wiener index W_e of G are defined as the sum of distances between all pairs of vertices in G and the sum of distances between all pairs of edges in G, respectively. In this paper, we identify the four trees, with the first through fourth greatest Wiener and edge−Wiener index among all trees of order $n \geq 10$.

1. INTRODUCTION

Throughout this paper we consider undirected graphs without loops and multiple edges. Let G be such a graph with vertex and edge sets $V(G)$ and $E(G)$, respectively. The distance between two vertices u and v in G, denoted by $d(u,v|G)$, is defined as the length of a shortest path between u and v. Let $f = xy$ and $g = uv$ be two edges of G. The distance between f and g is denoted by $d_e(f,g|G)$ and defined as the distance between the vertices of f and g in the line graph of G. The degree of a vertex v in G, $d_G(v)$, is the number of edges incident to v and $N[v,G]$ denotes the set of vertices adjacent to v. A pendent vertex is a vertex with degree one. We use the notations $\Delta = \Delta(G)$ and $n_i = n_i(G)$ to denote the maximum degree and the number of vertices of degree i in G, respectively. Obviously, $\sum_{i=1}^{\Delta(G)} n_i = |V(G)|$. Let $S \subseteq V(G)$ be any subset of vertices of G. Then the induced subgraph $G[S]$ is the graph whose vertex set is S and whose edge set consists of all of the

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edges in $E(G)$ that have both endpoints in S. If W is a subset of $V(G)$ then $G - W$ will be the subgraph of G obtained by deleting the vertices of W and similarly, for a subset F of $E(G)$, the subgraph obtained by deleting all edges in F is denoted by $G - F$. In the case that $W = \{v\}$ or $F = \{xy\}$, the subgraphs $G - W$ and $G - F$ will shortly be written as $G - v$ or $G - xy$, respectively. For any two nonadjacent vertices x and y in G, let $G + xy$ be the graph obtained from G by adding an edge xy.

If G is acyclic and connected graph, then G is a tree. Any tree with at least two vertices has at least two pendent vertices. The set of all n −vertex trees is denoted by $\tau(n)$. In chemical graph theory, a topological index is a number invariant under graph automorphisms. These numbers play a significant role in mathematical chemistry especially in the QSPR/QSAR investigations, see [7, 11].

Harold Wiener in [18], introduced **Wiener index** defined as

$$W(G) = \sum_{\{v,u\}\subseteq V(G)} d(u,v|G),$$

which is the sum of distances between all pairs of vertices of G. The **edge–Wiener** index of G, denoted by $W_e(G)$, is defined as

$$W_e(G) = \sum_{\{f,g\}\subseteq E(G)} d_e(f,g|G),$$

which is the sum of distances between all pairs of edges of G. This invariant was independently introduced in [10, 13]. Edge-Wiener index is one of the most interesting topological indices. Dankelmann et al. [5], recalled that, $W_e(G) \le \frac{2^5}{5^5}n^5 + O\left(n^{\frac{9}{2}}\right)$, for graphs of order n. Dou et al. [6], characterized the polyphenyl chains with minimum and maximum edge-Wiener indices among all the polyphenyl chains with h hexagons. They also characterized the explicit formulas for the edge-Wiener indices of extremal polyphenyl chains. Yousefi–Azari et al. [19], proved that for every tree T, $Sz_e(T) = W_e(T)$, $Sz_e(T)$ denotes the edge Szeged index of T. Nadjafi–Arani et al. [16], showed that for every connected graph G, $Sz_e(G) \ge W_e(G)$ with equality if and only if G is a tree. Alizadeh et al. [1], characterized the edge-Wiener index of suspensions, bottlenecks, and thorny graphs. Knor et al. [12], proved that $W_e(G) \ge \frac{\delta^2-1}{4}W(G)$ where δ denotes the minimum degree in G. Kelenc et al. [14], characterized an algorithm developed that, for a given benzenoid system G with m edges, computes the edge-Wiener index of G in $O(m)$ time. Chen et al. [4], studied explicit relation between the Wiener index and the edge-Wiener index of the catacondensed hexagonal systems. We refer the reader to [2, 9] for more information on the edge-Wiener index. Buckley in [3] and Tratnik et al. in [17], for a tree T with n vertices proved that:

$$W_e(T) = W(T) - \frac{n(n-1)}{2}. \quad (1)$$

Deng [8], the trees with the greatest Wiener index were investigated, where the trees on n vertices ($n \geq 9$) with the first to seventeenth greatest Wiener index were found. However, it turned out that the results in [8] were not correct and therefore, paper [15] was published. In that paper, the trees on n vertices ($n \geq 28$) with the first to fifteenth greatest Wiener index were found. Hence by Equation (1), the trees on n vertices ($n \geq 28$) with the first to fifteenth greatest Wiener index in [15] are the trees on n vertices ($n \geq 28$) with the first to fifteenth greatest edge-Wiener index. In this paper, we identify the four trees, with the first through fourth greatest Wiener and edge-Wiener index among all trees of order $n \geq 10$.

2. Main Results

In this section, some graph transformations are presented by which we can increase the edge-Wiener index of trees. By applying these graph operations, we identify the four trees, with the first through fourth greatest edge-Wiener index among all trees of order $n \geq 10$.

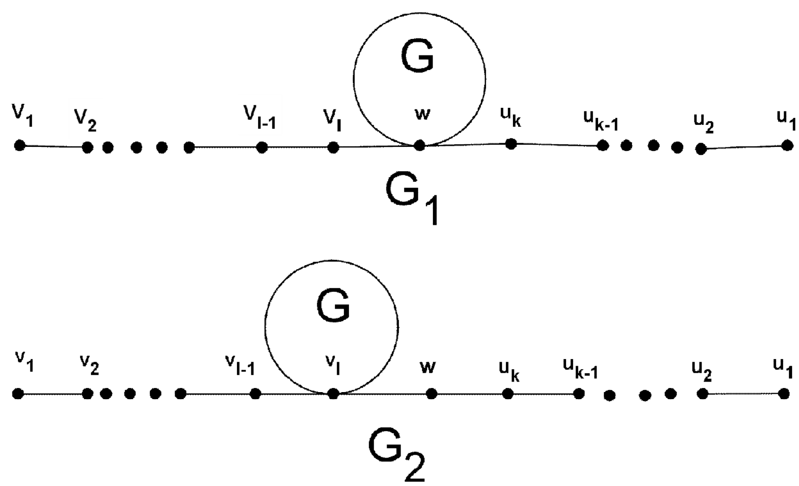

Figure 1. The graphs P, Q, G, G_1 and G_2 in Transformation A.

Transformation A**.** Suppose w is a vertex in a connected graph G with at least two vertices and $N[w,G] = \{x_1, x_2, \dots, x_{d_G(w)}\}$. In addition, we assume that $P : u_k u_{k-1} \dots u_2 u_1$ and $Q : v_l v_{l-1} \dots v_2 v_1$, are two new paths of lengths k, l ($k \geq l \geq 1$), respectively. Let G_1 be the graph obtained from G, P and Q by attaching edges $v_l w$, $w u_k$, and $G_2 = G_1 - \{w x_i : x_i \in N[w,G]\} + \{v_l x_i : x_i \in N[w,G]\}$. Such graphs have been illustrated in Figure 1.

Lemma 2.1. *Let G_1 and G_2 be two graphs as shown in Figure 1. Then we have*

$$W_e(G_1) < W_e(G_2).$$

Proof. Let $E^*(G) = E(G) \backslash \{xw | x \in N[w,G]\}$ and $\bar{E}(G) = E^*(G) \cup \{x v_l | x \in N[w,G]\}$. From definition,

$$
\begin{aligned}
W_e(G_1) - W_e(G_2) &= \sum_{i=1}^{l-1} \sum_{f \in E(G)} d_e(f, v_i v_{i+1} | G_1) + \sum_{i=1}^{k-1} \sum_{f \in E(G)} d_e(f, u_i u_{i+1} | G_1) \\
&+ \sum_{f \in E(G)} d_e(f, w u_k | G_1) \\
&- \left[\sum_{i=1}^{l-1} \sum_{f \in \bar{E}(G)} d_e(f, v_i v_{i+1} | G_2) + \sum_{i=1}^{k-1} \sum_{f \in \bar{E}(G)} d_e(f, u_i u_{i+1} | G_2) \right. \\
&\left. + \sum_{f \in \bar{E}(G)} d_e(f, w u_k | G_2) \right] \\
&= \sum_{i=1}^{l-1} \sum_{f \in E(G)} d_e(f, v_i v_{i+1} | G_1) + \sum_{i=1}^{k-1} \sum_{f \in E(G)} d_e(f, u_i u_{i+1} | G_1) \\
&+ \sum_{f \in E(G)} d_e(f, w u_k | G_1) \\
&- \left[\sum_{i=1}^{l-1} \sum_{f \in E(G)} (d_e(f, v_i v_{i+1} | G_1) - 1) \right. \\
&+ \sum_{i=1}^{k-1} \sum_{f \in E(G)} (d_e(f, u_i u_{i+1} | G_1) + 1) \\
&\left. + \sum_{f \in E(G)} (d_e(f, w u_k | G_1) + 1) \right] \\
&= \sum_{i=1}^{l-1} \sum_{f \in E(G)} 1 - \sum_{i=1}^{k-1} \sum_{f \in E(G)} 1 - \sum_{f \in E(G)} 1 < 0 \ as\ k \geq l \geq 1.
\end{aligned}
$$

which completes the proof. □

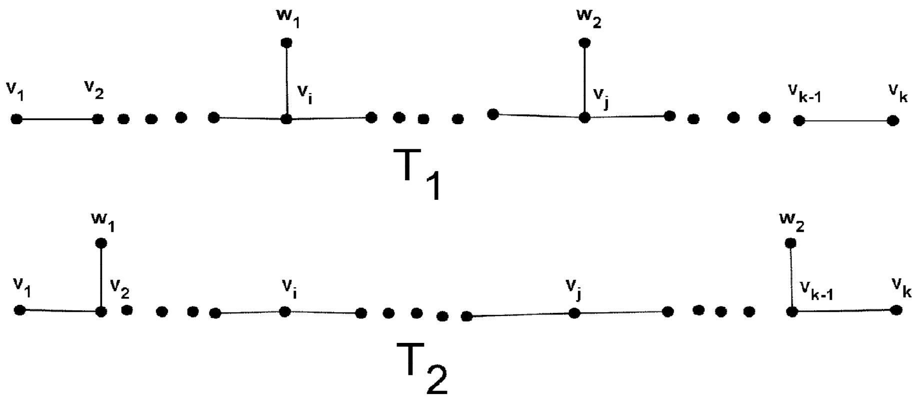

Figure 2. The graphs G_1, G_2, P , T_1 and T_2 in Transformation B

Transformation B**.** Suppose G_1 and G_2 are two trivial graphs with vertices w_1 and w_2, respectively. In addition, we assume that $P : v_1v_2 \dots v_{k-1}v_k$ is a path of length k $(k \geq 5)$. Let T_1 be the graph obtained from G_1, G_2 and P by attaching edges w_1v_i, w_2v_j, and $T_2 = T_1 - \{w_1v_i, w_2v_j\} + \{w_1v_2, w_2v_{k-1}\}$, such that at least one of the two $i \neq 2, j \neq k-1$ is true and $1 < i < j < k$. Such graphs have been illustrated in Figure 2.

Lemma 2.2. *Let T_1 and T_2 be two graphs as shown in Figure 2. Then we have*

$$W_e(T_1) < W_e(T_2).$$

Proof. Let $S = \{v_1, v_2, \dots, v_i, v_{i+1}, w_1\}$ and $R = \{v_{j-1}, v_j, \dots, v_{k-1}, v_k, w_2\}$. Then from definition $T_1[S] \cong T_2[S]$ and $T_1[R] \cong T_2[R]$. Therefore, we have,

$$\begin{aligned} W_e(T_1) - W_e(T_2) = & \sum_{h=i+1}^{k-1} d_e(w_1v_i, v_hv_{h+1}|T_1) + \sum_{h=1}^{j-2} d_e(w_2v_j, v_hv_{h+1}|T_1) \\ & + d_e(w_1v_i, w_2v_j|T_1) \\ & - \left[\sum_{h=i+1}^{k-1} d_e(w_1v_2, v_hv_{h+1}|T_2) + \sum_{h=1}^{j-2} d_e(w_2v_{k-1}, v_hv_{h+1}|T_2) \right. \\ & + d_e(w_1v_2, w_2v_{k-1}|T_2)] \\ = & \sum_{h=i+1}^{k-1} d_e(w_1v_i, v_hv_{h+1}|T_1) + \sum_{h=1}^{j-2} d_e(w_2v_j, v_hv_{h+1}|T_1) \\ & + d_e(w_1v_i, w_2v_j|T_1) \\ & - \left[\sum_{h=i+1}^{k-1} (d_e(w_1v_i, v_hv_{h+1}|T_1) + i - 2) \right. \\ & + \sum_{h=1}^{j-2} (d_e(w_2v_j, v_hv_{h+1}|T_1) + k - j - 1) \end{aligned}$$

$$+ \left(d_e\left(w_1v_i, w_2v_j\middle|T_1\right) + k + i - j - 3\right)\Big]$$
$$= -\left[\sum_{h=i+1}^{\mathrm{k}-1}(i-2) + \sum_{h=1}^{j-2}(k-j-1) + (k+i-j-3)\right].$$

Now, suppose that $i \neq 2$. So,

$$W_e(T_1) - W_e(T_2) = -\left[\sum_{h=i+1}^{k-1}(i-2) + \sum_{h=1}^{j-2}(k-j-1) + (k+i-j-3)\right]$$
$$\leq -\left[\sum_{h=i+1}^{k-1}(3-2) + \sum_{h=1}^{j-2}[(k-(k-1)-1) + 1\right] < 0.$$

If $j \neq k - 1$, then we have,

$$W_e(T_1) - W_e(T_2) = -\left[\sum_{h=i+1}^{k-1}(i-2) + \sum_{h=1}^{j-2}[(k-j-1) + (k+i-j-3)]\right]$$
$$\leq -\left[\sum_{=i+1}^{k-1}(2-2) + \sum_{=1}^{j-2}[(k-(k-2)-1) + (\mathrm{k}+2-(\mathrm{k}-2)-3)\right] < 0,$$

which completes the proof. □

Let the vertices of the path P_{n-1} be numbered consecutively by $1, 2, \ldots, n-1$. Construct the graph $P_{n-1}(j)$ by attaching a pendent vertex at position j of the $(n-1)-$vertex path. For positive integers $x_1, \ldots, x_m$, and $y_1, \ldots, y_m$, let $T({y_1}^{x_1}, \ldots, {y_m}^{x_m})$ be the class of trees with x_i vertices of degree y_i, $i = 1, \ldots, m$. For some values of $x_1, \ldots, x_m$, and $y_1, \ldots, y_m$, the class $T({y_1}^{x_1}, \ldots, {y_m}^{x_m})$ may be empty.

Lemma 2.3. *Let $P_{n-1}(2)$, $P_{n-1}(3)$, $P_{n-1}(4)$, T_1, T_2 and T_3 be six trees with $n(\geq 10)$ vertices as shown in Figure 3. Then we have*
$W_e(P_n) > W_e\left(P_{n-1}(2)\right) > W_e\left(P_{n-1}(3)\right) > W_e(T_1) > \max\left\{W_e\left(P_{n-1}(4)\right), W_e(T_2), W_e(T_3)\right\}$.

Proof. By Lemma 2.1, we have $W_e(P_n) > W_e\left(P_{n-1}(2)\right) > W_e\left(P_{n-1}(3)\right)$. Now, it is easy to see, $P_{n-1}(3)[\{1,2, \ldots, n-2\}] \cong P_{n-1}(4)[\{1,2, \ldots, n-2\}] \cong T_1[\{\mathrm{v}_1, \mathrm{v}_2, \ldots, \mathrm{v}_{n-2}\}]$, and $\sum_{i=2}^{n-3} d_e\left((n-1)(n-2), (i)(i+1)\middle|P_{n-1}(3)\right) = \sum_{\mathrm{i}=2}^{\mathrm{n}-3} d_e((\mathrm{n}-1)(\mathrm{n}-2), (\mathrm{i})(\mathrm{i}+1)|$
$P_{n-1}(4)) = \sum_{i=1}^{n-4} d_e(\mathrm{v}_{\mathrm{n}-1}\mathrm{v}_{\mathrm{n}-3}, \mathrm{v}_\mathrm{i}\mathrm{v}_{\mathrm{i}+1}|T_1)$. Then for $n \geq 10$, we have

$$W_e\left(P_{n-1}(3)\right) - W_e(T_1) = 1 + 2 + n - 3 + \sum_{i=1}^{n-4} i - [1 + 1 + n - 4 + \sum_{i=1}^{n-4} i] > 0$$

and

$$W_e(T_1) - W_e\left(P_{n-1}(4)\right) = 1 + 1 + n - 4 + \sum_{i=1}^{n-4} i + -\left[1 + 2 + n - 3 + \sum_{i=1}^{n-5} i\right].$$

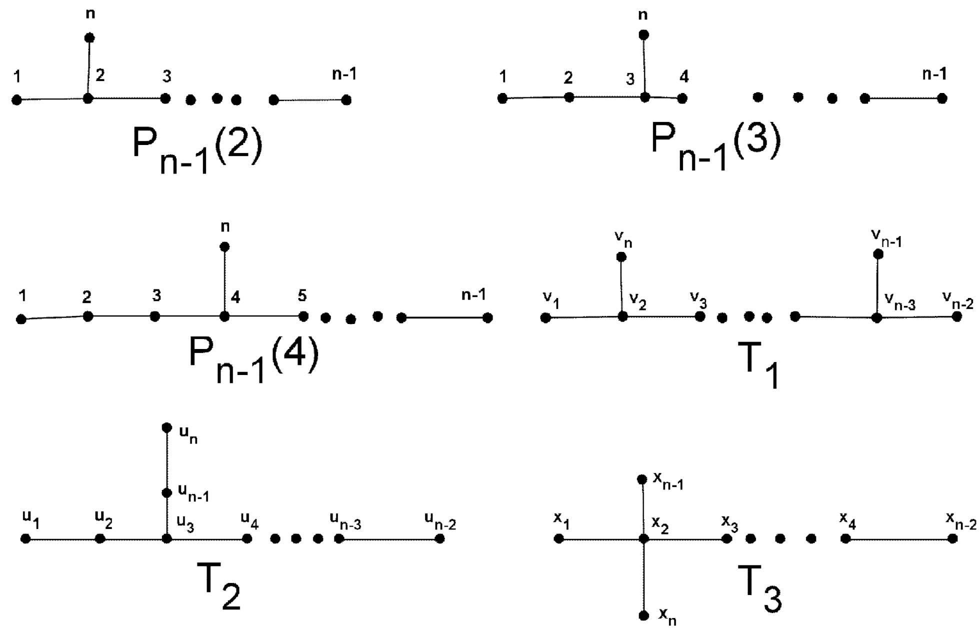

Figure 3. The trees in Lemma 2.3 ($T_1 \in T(3^2, 2^{n-6}, 1^4)$, $T_2 \in T(3^1, 2^{n-4}, 1^3)$, $T_3 \in T(4^1, 2^{n-5}, 1^4)$).

In addition, $T_1[\{v_1, v_2, \dots, v_{n-2}\}] \cong T_2[\{u_1, u_2, \dots, u_{n-2}\}]$, $\sum_{i=2}^{n-3} d_e(v_n v_2, v_i v_{i+1} | T_1) = \sum_{i=3}^{n-3} d_e(u_n u_{n-1}, u_i u_{i+1} | T_2) + d_e(u_n u_{n-1}, u_{n-1} u_3 | T_2)$ and $\sum_{i=2}^{n-4} d_e(v_{n-1} v_{n-3}, v_i v_{i+1} | T_1) = \sum_{i=3}^{n-3} d_e(u_{n-1} u_3, u_i u_{i+1} | T_2)$. Then we have

$$W_e(T_1) - W_e(T_2) = 1 + 1 + n - 4 + n - 4 - (2 + 3 + 1 + 2) > 0 \ as \ n \geq 10.$$

Finally,

$$T_1[\{v_1, v_2, \dots, v_{n-2}\}] \cong T_3[\{x_1, x_2, \dots, x_{n-2}\}],$$
$$\sum_{i=2}^{n-3} d_e(v_n v_2, v_i v_{i+1} | T_1) = \sum_{i=2}^{n-3} d_e(x_{n-1} x_2, x_i x_{i+1} | T_3),$$
$$\sum_{i=1}^{n-4} d_e(v_{n-1} v_{n-3}, v_i v_{i+1} | T_1) = \sum_{i=2}^{n-3} d_e(x_n x_2, x_i x_{i+1} | T_3).$$

Then we have,

$$W_e(T_1) - W_e(T_3) = n - 4 - (1 + 1 + 1) > 0 \ as \ n \geq 10.$$

which completes the proof. □

Theorem 2.4. *Let $P_{n-1}(2)$, $P_{n-1}(3)$ and T_1 be trees with n vertices as shown in Figure 3. If $n \geq 10$ and $T \in \tau(n) \backslash \{P_n, P_{n-1}(2), P_{n-1}(3), T_1\}$, then*

$$W_e(P_n) > W_e(P_{n-1}(2)) > W_e(P_{n-1}(3)) > W_e(T_1) > W_e(\mathrm{T}).$$

Proof. From Lemma 2.3, $W_e(P_n) > W_e(P_{n-1}(2)) > W_e(P_{n-1}(3)) > W_e(T_1)$. Now, suppose that $\Delta(T) = 3$ and $n_3(T) = 1$. In this case, if $T \in \left\{P_{n-1}(i): i = 4,5, \ldots, \left\lceil\frac{n}{2}\right\rceil\right\}$ then by Lemma 2.1 and Lemma 2.3, $W_e(T_1) > W_e(P_{n-1}(4)) \geq W_e(\mathrm{T})$. Otherwise, by Lemma 2.1 and Lemma 2.3, $W_e(T_1) > W_e(T_2) \geq W_e(\mathrm{T})$. For the case of $\Delta(T) = 3$ and $n_3(T) \geq 2$, by Lemma 2.1 and Lemma 2.2, $W_e(T_1) > W_e(\mathrm{T})$. If $\Delta(T) \geq 4$, then by Lemma 2.1 and Lemma 2.3, $W_e(T_1) > W_e(T_3) \geq W_e(\mathrm{T})$. Otherwise, $T \in \{P_n, P_{n-1}(2), P_{n-1}(3), T_1\}$. This proves our theorem. □

Corollary 2.5. *Among all trees with $n(\geq 10)$ vertices, P_n, $P_{n-1}(2)$, $P_{n-1}(3)$ and T_1 have the maximum values of first through fourth Wiener index, respectively.*

Proof. Equation (1) and Theorem 2.4 give us the result. □

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