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MODIFIED WIENER INDICES OF TREES

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Abstract

For each tree T and each real number λ, $\lambda \neq 0$, the λ-modified Wiener index is defined as ${}^{m}W_{\lambda}(T) = \sum_{e \in E(T)} [n_{T,1}(e) \cdot n_{T,2}(e)]^{\lambda}$, where $n_{T,1}(e)$ and $n_{T,2}(e)$ denote the number of vertices of T lying on the two sides of the edge e. It provides a novel class of structure–descriptors which are suitable for modeling branching–dependent properties of organic compounds. Let $\mathcal{T}_{n,p}$ be the class of trees with n vertices, p of which are pendent vertices. In this paper, for each $\lambda \neq 0$ and each p with $3 \leq p \leq n-2$, we determine the trees in $\mathcal{T}_{n,p}$ with maximal and minimal λ-modified Wiener indices.

INTRODUCTION

The Wiener index (W) is one of the oldest and most useful molecular–graph–based structure–descriptors [1–3]. It is the sum of distances between all unordered pairs of vertices in the graph. Let T be a tree with vertex set $V(T)$ and edge set $E(T)$. For

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any $e \in E(T)$, $n_{T,1}(e)$ and $n_{T,2}(e)$ denote the number of vertices of T lying on the two sides of the edge e. For a long time it has been known [1, 3] that

$$W(T) = \sum_{e \in E(T)} n_{T,1}(e) \cdot n_{T,2}(e) \, .$$

For more mathematical properties of the Wiener index of trees, see the review [4].

Recently, Gutman et al. [5] put forward the λ-*modified Wiener index* ${}^{m}W_{\lambda}$, defined as

$$^{m}W_{\lambda}(T) = \sum_{e \in E(T)} \left[n_{T,1}(e) \cdot n_{T,2}(e)\right]^{\lambda} \tag{1}$$

where λ is a nonzero real number that may assume different values.

Obviously, for $\lambda = 1$ and $\lambda = -1$, the λ-modified Wiener index ${}^{m}W_{\lambda}$ reduces to the ordinary Wiener index W and the "modified Wiener index" ${}^{m}W$ studied in [6, 7], respectively.

The right–hand side of eq. (1) may be understood as a sum of increments, each associated with an edge. The contribution of the edge e, denoted by ${}^{m}W_{\lambda}(e,T)$, is clearly equal to $\left[n_{T,1}(e) \cdot n_{T,2}(e)\right]^{\lambda}$.

It is known [5] that for all nonzero real numbers λ, the λ-modified Wiener indices satisfy the basic requirement of being a branching index: For a tree T on n vertices, different from the n-vertex path P_n and the n-vertex star S_n,

$$^{m}W_{\lambda}(P_n) > {}^{m}W_{\lambda}(T) > {}^{m}W_{\lambda}(S_n) \quad \text{if} \quad \lambda > 0$$

$$^{m}W_{\lambda}(P_n) < {}^{m}W_{\lambda}(T) < {}^{m}W_{\lambda}(S_n) \quad \text{if} \quad \lambda < 0 \, .$$

Thus ${}^{m}W_{\lambda}$ provides a class of structure–descriptors which are suitable for modeling branching–dependent properties of organic compounds [5]. Vukičević [8] and Gorše and Žerovnik [9] showed that for arbitrary different λ_1, λ_2, there are trees (chemical trees if $\lambda_1, \lambda_2 > 0$) with the same number of vertices that are differently ordered by the indices ${}^{m}W_{\lambda_1}$ and ${}^{m}W_{\lambda_2}$. Vukičević and Gutman [10] deduced some conditions under which two trees are ordered the same by ${}^{m}W_{\lambda}$ for all positive or all negative values of λ. Some chemical properties of ${}^{m}W_{\lambda}$ were established by Gutman et al. [11] and Lučić et al. [12].

Let $\mathcal{T}_{n,p}$ be the class of trees with n vertices, p of which are pendent vertices, where

$2 \leq p \leq n-1$. Obviously, if $T \in \mathcal{T}_{n,2}$ then $T = P_n$, and if $T \in \mathcal{T}_{n,n-1}$ then $T = S_n$. So we can assume in the rest that $3 \leq p \leq n-2$.

In this paper, for each $\lambda \neq 0$ and each p with $3 \leq p \leq n-2$, we identify the trees in $\mathcal{T}_{n,p}$ with maximal and minimal λ-modified Wiener indices. It is also shown that these trees are unique and they depend only on the signs of λ and not on the actual values of λ. Our arguments also lead to a similar result for variable Wiener indices introduced in [13].

RESULTS

Let T be a tree. For $x \in V(T)$, $d_T(x)$ (or $d(x)$) denotes the degree of x. Let $V_1(T) = \{x \in V(T) | d(x) \geq 3\}$. There are $d(x)$ components in $T - x$, each containing a vertex that is adjacent to vertex x in T. These components are called the *branches* of T at x.

For $x, y \in V(T)$, $d_T(x,y)$ (or $d(x,y)$) denotes the distance between x and y in T, $P_T(x,y)$ (or $P(x,y)$) denotes the unique path in T joining x to y, $C_x(P,T)$ (or $C_x(P)$) denotes the component containing x in the forest formed by removing the edge incident with x in the path $P(x,y)$. For $P = P(x,y)$, let $n_x(P,T)$ (or $n_x(P)$) be the number of vertices $C_x(P,T)$.

It is easy to see that the function $f(t) = [t(n-t)]^\lambda$ is increasing if $\lambda > 0$ and decreasing if $\lambda < 0$ for $1 \leq t \leq \frac{n}{2}$. We will use this fact frequently in our proof.

For positive integers p and n with $3 \leq p \leq n-1$, let $k = \lfloor \frac{n-1}{p} \rfloor$ and $r = n-1-kp$. Let $F_{n,p}$ denote the tree formed by joining a vertex c to one end vertex of each of p paths, $p-r$ of which have k vertices and r of which have $k+1$ vertices. Clearly $F_{n,p} \in \mathcal{T}_{n,p}$.

Lemma 1. *Let $T \in \mathcal{T}_{n,p}$ with $|V_1(T)| \geq 2$. Then there is a tree $T^* \in \mathcal{T}_{n,p}$ with $|V_1(T^*)| = 1$ such that ${}^mW_\lambda(T^*) < {}^mW_\lambda(T)$ if $\lambda > 0$ and ${}^mW_\lambda(T^*) > {}^mW_\lambda(T)$ if $\lambda < 0$.*

Proof. Let $x, y \in V_1(T)$ so that $d(x,y)$ is as small as possible and $P = P(x,y)$. If $d(x,y) > 1$, then vertices on P except x and y all have degree two. Let $n_x = n_x(P)$ and $n_y = n_y(P)$. Assume that $n_y \leq n_x$. Then $n_y \leq \frac{n}{2}$.

Let z denote the vertex joined to y in the path P so that $z = x$ if $d(x, y) = 1$, and let w be one of the other vertices joined to y. Let n_w be the number of vertices separated from y by the edge yw. Let T' denote the tree formed from T by removing edge yw and replacing it with an edge zw joining vertices z and w. Note that $T' \in \mathcal{T}_{n,p}$. It is easy to see that

$$\begin{aligned} {}^{m}\!W_\lambda(T') - {}^{m}\!W_\lambda(T) &= {}^{m}\!W_\lambda(zy, T') - {}^{m}\!W_\lambda(zy, T) \\ &= [(n_y - n_w)(n - (n_y - n_w))]^\lambda - [n_y(n - n_y)]^\lambda . \end{aligned} \tag{2}$$

Suppose that $\lambda > 0$. Since $n_y - n_w < n_y \le \frac{n}{2}$ and $f(t) = [t(n-t)]^\lambda$ is an increasing function for $1 \le t \le \frac{n}{2}$, we have from (2) that ${}^{m}\!W_\lambda(T') < {}^{m}\!W_\lambda(T)$.

Similarly, if $\lambda < 0$, then ${}^{m}\!W_\lambda(T') > {}^{m}\!W_\lambda(T)$.

Iterating the transformation from T to T' yields the tree T^* as required. $\square$

Lemma 2. *Let $T \in \mathcal{T}_{n,p}$ with $V_1(T) = \{c\}$ and $T \neq F_{n,p}$. Then ${}^{m}\!W_\lambda(T) > {}^{m}\!W_\lambda(F_{n,p})$ if $\lambda > 0$ and ${}^{m}\!W_\lambda(T) < {}^{m}\!W_\lambda(F_{n,p})$ if $\lambda < 0$.*

Proof. Since T has p pendent vertices, the degree of c is p and the remaining $n-1-p$ vertices all have degree two. Since $T \neq F_{n,p}$, there are two branches, say B_1 and B_2 of T at c with $B_1 = P_a$, $B_2 = P_b$ such that $b \ge a + 2$ and $a \ge 1$. Let u (resp. v) be the pendent vertices of T in the branches B_1 (resp. B_2). Let u_1 (resp. v_1) be the neighbors of c in B_1 (resp. B_2). Let T' denote the tree formed from T by removing the edge incident with v and adding an edge uv joining v to u. Since $d(c, v) = b \ge 3 > 1$, we have $T' \in \mathcal{T}_{n,p}$. Clearly, $a + b + 1 < n$ and

$$\begin{aligned} {}^{m}\!W_\lambda(T') - {}^{m}\!W_\lambda(T) &= {}^{m}\!W_\lambda(cu_1, T') - {}^{m}\!W_\lambda(cv_1, T) \\ &= [(a+1)(n-a-1)]^\lambda - [b(n-b)]^\lambda . \end{aligned}$$

Since $a+1 < \min\{b, n-b\} \le \frac{n}{2}$, we have ${}^{m}\!W_\lambda(T') < {}^{m}\!W_\lambda(T)$ if $\lambda > 0$ and ${}^{m}\!W_\lambda(T') > {}^{m}\!W_\lambda(T)$ if $\lambda < 0$.

Iterating the transformation from T to T' yields the tree T^* as required. $\square$

Theorem 3. *Let $T \in \mathcal{T}_{n,p}$ and $T \neq F_{n,p}$, where $3 \leq p \leq n-2$. Then*

$$^{m}W_{\lambda}(T) > {^{m}W_{\lambda}}(F_{n,p}) \quad \textit{if} \quad \lambda > 0$$

$$^{m}W_{\lambda}(T) < {^{m}W_{\lambda}}(F_{n,p}) \quad \textit{if} \quad \lambda < 0\,.$$

Proof. Since $p \geq 3$, we have $|V_1(T)| \geq 1$. If $|V_1(T)| \geq 2$, we have by Lemmas 1 and 2 that there is a tree $T^* \in \mathcal{T}_{n,p}$ with $|V_1(T^*)| = 1$ such that ${^{m}W_{\lambda}}(F_{n,p}) \leq {^{m}W_{\lambda}}(T^*) < {^{m}W_{\lambda}}(T)$ if $\lambda > 0$ and ${^{m}W_{\lambda}}(F_{n,p}) \geq {^{m}W_{\lambda}}(T^*) > {^{m}W_{\lambda}}(T)$ if $\lambda < 0$. So suppose that $|V_1(T)| = 1$. Since $T \neq F_{n,p}$, the result follows from Lemma 2. $\square$

In the proof of Theorem 3, we use the techniques from [14], where the total distance was studied.

For integer r with $1 \leq r \leq \lfloor \frac{p}{2} \rfloor$, let $D_{n,p,r}$ be the tree formed by attaching r and $p-r$ pendent edges to the two end vertices of a path P_{n-p}. Clearly, $D_{n,p,r} \in \mathcal{T}_{n,p}$. We call $D_{n,p,r}$ a *generalized double star*. Let $S_{n,p} = D_{n,p,\lfloor \frac{p}{2} \rfloor}$.

Lemma 4. *Let $T \in \mathcal{T}_{n,p}$ with $|V_1(T)| \geq 3$. Then there is a tree $T^* \in \mathcal{T}_{n,p}$ with $|V_1(T^*)| = 2$ such that ${^{m}W_{\lambda}}(T^*) > {^{m}W_{\lambda}}(T)$ if $\lambda > 0$ and ${^{m}W_{\lambda}}(T^*) < {^{m}W_{\lambda}}(T)$ if $\lambda < 0$.*

Proof. Let $x, y \in V_1(T)$ such that $d(x,y)$ is as large as possible. Let $P = P(x,y)$ with $n_x = n_x(P)$ and $n_y = n_y(P)$.

Choose $w, z \in V_1(T)$ in the path P such that both $d(x,w)$ and $d(z,y)$ are as small as possible.

Obviously, $\min\{n_x + d(x,w), n_y + d(z,y)\} \leq \frac{n}{2}$. Assume that $n_y + d(z,y) \leq n_x + d(x,w)$ and then $n_y + d(z,y) \leq \frac{n}{2}$.

Let $d(z,y) = r$ and let $z = z_0, z_1, \ldots, z_r = y$ be the path from z to y. Let n'_z be the total number of vertices of the branches at z except the two branches containing a vertex in the path P.

Let $u_1, u_2, \ldots, u_{d_T(z)-2}$ be the neighbors of z outside P in T. Let T' be the tree obtained from T by removing edge zu_i and replacing it with an edge yu_i for all $i = 1, 2, \ldots, d_T(z)-2$.

It is easy to see that

$$ {}^{m}W_\lambda(T') - {}^{m}W_\lambda(T) = \sum_{i=1}^{r} [{}^{m}W_\lambda(z_{i-1}z_i, T') - {}^{m}W_\lambda(z_{i-1}z_i, T)] $$

with

$$ {}^{m}W_\lambda(z_{i-1}z_i, T') = [(r-i+n_y+n'_z)\,(n-(r-i+n_y+n'_z))]^\lambda $$

$$ {}^{m}W_\lambda(z_{i-1}z_i, T) = [(r-i+n_y)\,(n-(r-i+n_y))]^\lambda . $$

For $i = 1, 2, \dots, r$, since

$$ \begin{aligned} & n-(r-i+n_y+n'_z)-(r-i+n_y) \\ = \; & n-2r-2n_y-n'_z+2i \\ = \; & (n-r-n_y)-(r+n_y+n'_z)+2i \\ \geq \; & d(x,w)+n_x+n'_z-(r+n_y+n'_z)+2i \\ = \; & d(x,w)+n_x-(r+n_y)+2i > 0 \,, \end{aligned} $$

we have $r-i+n_y < n-(r-i+n_y+n'_z)$. So for $i = 1, 2, \dots, r$, we have $r-i+n_y < \min\{r-i+n_y+n'_z, n-(r-i+n_y+n'_z)\} \leq \frac{n}{2}$, which implies that ${}^{m}W_\lambda(z_{i-1}z_i, T') > {}^{m}W_\lambda(z_{i-1}z_i, T)$ if $\lambda > 0$ and ${}^{m}W_\lambda(z_{i-1}z_i, T') < {}^{m}W_\lambda(z_{i-1}z_i, T)$ if $\lambda < 0$. Hence we have ${}^{m}W_\lambda(T') > {}^{m}W_\lambda(T)$ if $\lambda > 0$ and ${}^{m}W_\lambda(T') < {}^{m}W_\lambda(T)$ if $\lambda < 0$. $\square$

Lemma 5. *Let $T \in \mathcal{T}_{n,p}$ with $V_1(T) = \{x, y\}$. Let $P = P_T(x, y)$ with $n_y = n_y(P) \leq \frac{n}{2}$. If $C_y(P)$ is not a star, then there is a tree $T^* \in \mathcal{T}_{n,p}$ with $V(T^*) = V(T)$, $|V_1(T^*)| = \{x, y^*\}$ and $P^* = P_{T^*}(x, y^*)$ such that $n_x(P^*, T^*) = n_x(P, T)$, $C_{y^*}(P^*, T^*)$ is a star, ${}^{m}W_\lambda(T^*) > {}^{m}W_\lambda(T)$ if $\lambda > 0$ and ${}^{m}W_\lambda(T^*) < {}^{m}W_\lambda(T)$ if $\lambda < 0$.*

Proof. Since $C_y(P)$ is not a star, it has a branch B at y, which is a path P_s with $s \geq 2$. Let v be the vertex in B that is adjacent to y in T. Denote by $u_1, u_2, \dots, u_{d_T(y)-2}$ all other neighbors of y outside P. Let T' be the tree obtained from T by removing edge yu_i and replacing it with an edge vu_i for all $i = 1, 2, \dots, d_T(y)-2$. It is easy to see that

$$ \begin{aligned} {}^{m}W_\lambda(T') - {}^{m}W_\lambda(T) &= {}^{m}W_\lambda(yv, T') - {}^{m}W_\lambda(yv, T) \\ &= [(n_y-1)(n-n_y+1)]^\lambda - [s(n-s)]^\lambda . \end{aligned} $$

Since $s < n_y - 1 < \frac{n}{2}$, we have ${}^{m}W_\lambda(T') > {}^{m}W_\lambda(T) > 0$ if $\lambda > 0$ and ${}^{m}W_\lambda(T') < {}^{m}W_\lambda(T) > 0$ if $\lambda < 0$. $\square$

Lemma 6. *Let $T \in \mathcal{T}_{n,p}$ with $V_1(T) = \{x, y\}$. Let $P = P_T(x, y)$ with $n_x = n_x(P) > \frac{n}{2}$. If $C_x(P, T)$ is not a star and $C_y(P, T)$ is a star, then either there is a tree $T^* \in \mathcal{T}_{n,p}$ with $V(T^*) = V(T)$, $V_1(T^*) = V_1(T)$ and $P_{T^*}(x, y) = P$ such that $n_x(P, T^*) \leq \frac{n}{2}$, $C_x(P, T^*)$ has exactly one branch with at least two vertices and $C_y(P, T^*)$ is a star, or $T^* = D_{n,p,1}$. In either case, ${}^{m}W_\lambda(T^*) \geq {}^{m}W_\lambda(T)$ if $\lambda > 0$ and ${}^{m}W_\lambda(T^*) \leq {}^{m}W_\lambda(T)$ if $\lambda < 0$.*

Proof. There are two cases.

Case 1. There are two branches, say B_1 and B_2 of $C_x(P, T)$ at x with $B_1 = P_{s_1}$, $B_2 = P_{s_2}$, and $s_2 \geq s_1 \geq 2$. Let u (resp. v) be the pendent vertex of T in B_1 (resp. B_2). Let T' be the tree obtained from T by removing the edge incident with u and adding an edge vu. By similar argument as in Lemma 2, we have ${}^{m}W_\lambda(T') > {}^{m}W_\lambda(T)$ if $\lambda > 0$ and ${}^{m}W_\lambda(T') < {}^{m}W_\lambda(T)$ if $\lambda < 0$.

Case 2. There is exactly one branch, say P_s of $C_x(P, T)$ at x with $s \geq 2$. Label the vertices of P as $x = z_0, z_1, \ldots, z_r = y$. For a pendent edge xu of T, let T' be the tree obtained from T by removing edge xu and replacing it with an edge yu. It is easy to see that

$$\begin{aligned} {}^{m}W_\lambda(T') - {}^{m}W_\lambda(T) &= {}^{m}W_\lambda(z_0z_1, T') - {}^{m}W_\lambda(z_{r-1}z_r, T) \\ &= [(n_x - 1)(n - n_x + 1)]^\lambda \\ &\quad - [(n_x + r - 1)(n - n_x - r + 1)]^\lambda . \end{aligned}$$

Subcase 2.1. $n_x > \frac{n+1}{2}$. We have $n_x \geq \frac{n}{2} + 1$ and then $n - n_x - r + 1 < n - n_x + 1 \leq \frac{n}{2}$. Thus we have ${}^{m}W_\lambda(T') > {}^{m}W_\lambda(T)$ if $\lambda > 0$ and ${}^{m}W_\lambda(T') < {}^{m}W_\lambda(T)$ if $\lambda < 0$.

Subcase 2.2. $n_x = \frac{n+1}{2}$ and $r > 1$. Then we have $n - n_x - r + 1 = \frac{n+1}{2} - r < \frac{n-1}{2} = n_x - 1$ and so ${}^{m}W_\lambda(T') > {}^{m}W_\lambda(T)$ if $\lambda > 0$ and ${}^{m}W_\lambda(T') < {}^{m}W_\lambda(T)$ if $\lambda < 0$.

Subcase 2.3. $n_x = \frac{n+1}{2}$ and $r = 1$. Then we have $n - n_x - r + 1 = \frac{n-1}{2} = n_x - 1$ and so ${}^{m}W_\lambda(T') = {}^{m}W_\lambda(T)$.

Iterating the transformations from T to T' in Cases 1 and 2 yields the tree T^* as required. $\square$

Lemma 7. *Let $T = D_{n,p,r}$ with $r < \lfloor \frac{p}{2} \rfloor$. Then ${}^{m}W_{\lambda}(S_{n,p}) > {}^{m}W_{\lambda}(T)$ if $\lambda > 0$ and ${}^{m}W_{\lambda}(S_{n,p}) < {}^{m}W_{\lambda}(T)$ if $\lambda < 0$.*

Proof. Since $r < \lfloor \frac{p}{2} \rfloor$, it is easy to see that

$${}^{m}W_{\lambda}(D_{n,p,r+1}) - {}^{m}W_{\lambda}(D_{n,p,r}) = [(n-p+r)(p-r)]^{\lambda} - [(r+1)(n-r-1)]^{\lambda}.$$

Since $r+1 < \min\{n-p+r, p-r\} \le \frac{n}{2}$, we have ${}^{m}W_{\lambda}(D_{n,p,r+1}) > {}^{m}W_{\lambda}(D_{n,p,r})$ if $\lambda > 0$ and ${}^{m}W_{\lambda}(D_{n,p,r+1}) < {}^{m}W_{\lambda}(D_{n,p,r})$ if $\lambda < 0$. Iterating the procedure, we prove the lemma. $\square$

Theorem 8. *Let $T \in \mathcal{T}_{n,p}$ and $T \neq S_{n,p}$, where $3 \le p \le n-2$. Then*

$${}^{m}W_{\lambda}(T) < {}^{m}W_{\lambda}(S_{n,p}) \quad \textit{if} \quad \lambda > 0$$

$${}^{m}W_{\lambda}(T) > {}^{m}W_{\lambda}(S_{n,p}) \quad \textit{if} \quad \lambda < 0.$$

Proof. If $|V_1(T)| = 1$ and $T \neq D_{n,p,1}$, then from the proof of Lemma 2 we have ${}^{m}W_{\lambda}(D_{n,p,1}) > {}^{m}W_{\lambda}(T)$ for $\lambda > 0$ and ${}^{m}W_{\lambda}(D_{n,p,1}) < {}^{m}W_{\lambda}(T)$ for $\lambda < 0$.

If $|V_1(T)| \ge 3$, then by Lemma 4, there is a tree $T^* \in \mathcal{T}_{n,p}$ with $|V_1(T^*)| = 2$ such that ${}^{m}W_{\lambda}(T^*) > {}^{m}W_{\lambda}(T)$ for $\lambda > 0$ and ${}^{m}W_{\lambda}(T^*) < {}^{m}W_{\lambda}(T)$ for $\lambda < 0$. So suppose that $|V_1(T)| = 2$. Let $V_1(T) = \{x, y\}$ and $P = P_T(x,y)$, $n_x = n_x(P,T)$ and $n_y = n_y(P,T)$.

Suppose that T is not a generalized double star. There are two cases.

Case 1. $n_x, n_y \le \frac{n}{2}$. By Lemma 5, there is a generalized double star $D \in \mathcal{T}_{n,p}$ satisfying ${}^{m}W_{\lambda}(D) > {}^{m}W_{\lambda}(T)$ if $\lambda > 0$ and ${}^{m}W_{\lambda}(D) < {}^{m}W_{\lambda}(T)$ if $\lambda < 0$.

Case 2. $\max\{n_x, n_y\} > \frac{n}{2}$, say, $n_x > \frac{n}{2}$. Then $n_y < \frac{n}{2}$. If $C_y(P,T)$ is not a star, we have by Lemma 5 that there is a tree $T' \in \mathcal{T}_{n,p}$ with $V(T') = V(T)$, $|V_1(T')| = \{x, y'\}$ and $P' = P_{T'}(x,y')$ such that $n_x(P',T') = n_x$, $C_{y'}(P',T')$ is a star, ${}^{m}W_{\lambda}(T') > {}^{m}W_{\lambda}(T)$ if $\lambda > 0$ and ${}^{m}W_{\lambda}(T') < {}^{m}W_{\lambda}(T)$ if $\lambda < 0$. If $C_x(P',T')$ is not a star, we have by Lemma 6 that either there is a tree $T'' \in \mathcal{T}_{n,p}$ with $V(T'') = V(T')$, $V_1(T'') = V_1(T')$, $P_{T''}(x,y') = P'$ such that $n_x(P',T'') \le \frac{n}{2}$, $C_x(P',T'')$ has exactly one branch with at least two vertices and $C_{y'}(P',T'')$ is a star, or T'' is the generalized double star $D_{n,p,1}$, satisfying ${}^{m}W_{\lambda}(T'') \ge {}^{m}W_{\lambda}(T')$ if $\lambda > 0$ and ${}^{m}W_{\lambda}(T'') \le {}^{m}W_{\lambda}(T')$

if $\lambda < 0$ in either case. Now using Lemma 5 again if $T'' \neq D_{n,p,1}$, there is a generalized double star $D' \in \mathcal{T}_{n,p}$ satisfying ${}^{m}W_{\lambda}(D') > {}^{m}W_{\lambda}(T'') > {}^{m}W_{\lambda}(T)$ if $\lambda > 0$ and ${}^{m}W_{\lambda}(D') < {}^{m}W_{\lambda}(T'') < {}^{m}W_{\lambda}(T)$ if $\lambda < 0$. Thus for $D = D'$ or $D_{n,p,1}$, we have ${}^{m}W_{\lambda}(D) > {}^{m}W_{\lambda}(T)$ if $\lambda > 0$ and ${}^{m}W_{\lambda}(D) < {}^{m}W_{\lambda}(T)$ if $\lambda < 0$.

Combining Cases 1 and 2 and using Lemma 7, the result follows. $\square$

By Theorems 3 and 8, we obtain the main result of this paper:

Theorem 9. *Let $T \in \mathcal{T}_{n,p}$ and $T \neq F_{n,p}, S_{n,p}$, where $3 \leq p \leq n-2$. Then*

$$ {}^{m}W_{\lambda}(F_{n,p}) < {}^{m}W_{\lambda}(T) < {}^{m}W_{\lambda}(S_{n,p}) \quad \textit{if} \quad \lambda > 0 $$

$$ {}^{m}W_{\lambda}(S_{n,p}) < {}^{m}W_{\lambda}(T) < {}^{m}W_{\lambda}(F_{n,p}) \quad \textit{if} \quad \lambda < 0\,. $$

By Theorem 9, the trees in $\mathcal{T}_{n,p}$ with the smallest and the largest λ-modified Wiener indices are determined for any nonzero real λ. The λ-modified Wiener indices of the extremal trees are given by

$$ {}^{m}W_{\lambda}(F_{n,p}) = p \sum_{i=1}^{k} [i(n-i)]^{\lambda} + (n-1-pk)\,[(k+1)(n-k-1)]^{\lambda} $$

$$ {}^{m}W_{\lambda}(S_{n,p}) = p(n-1)^{\lambda} + \sum_{i=1}^{n-1-p} \left[\left(\left\lfloor \frac{p}{2} \right\rfloor + i\right)\left(n - \left\lfloor \frac{p}{2} \right\rfloor - i\right)\right]^{\lambda} $$

where $k = \lfloor \frac{n-1}{p} \rfloor$.

We point out that the notation in [10] can be used in proof of all our lemmas and theorems.

Vukičević and Žerovnik [13] initiated the study of the variable Wiener indices, defined as

$$ {}_{\lambda}W(T) = \frac{1}{2} \sum_{e \in E(T)} \left[|V(T)|^{\lambda} - n_{T,1}(e)^{\lambda} - n_{T,2}(e)^{\lambda}\right]. $$

Let $T \in \mathcal{T}_{n,p}$ and $T \neq F_{n,p}, S_{n,p}$, where $3 \leq p \leq n-2$. Using the fact that the function $g(t) = t^{\lambda} + (n-t)^{\lambda}$ is decreasing if $\lambda > 1$ and increasing if $\lambda < 1$ for $1 \leq t \leq \frac{n}{2}$ and similar arguments as above, we can obtain the following similar result for variable Wiener indices ${}_{\lambda}W$:

$$ {}_{\lambda}W(F_{n,p}) < {}_{\lambda}W(T) < {}_{\lambda}W(S_{n,p}) \quad \text{if} \quad \lambda > 1 $$

$$ {}_{\lambda}W(S_{n,p}) < {}_{\lambda}W(T) < {}_{\lambda}W(F_{n,p}) \quad \text{if} \quad \lambda < 1\,. $$

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References

[1] H. Wiener, Structural determination of paraffin boiling points, *J. Am. Chem. Soc.* **69** (1947) 17–20.

[2] R. Todeschini, V. Consonni, *Handbook of Molecular Descriptors*, Wiley–VCH, Weinheim, 2000.

[3] I. Gutman, O. E. Polansky, *Mathematical Concepts in Organic Chemistry*, Springer–Verlag, Berlin, 1986.

[4] A. A. Dobrynin, R. Entringer, I. Gutman, Wiener index of trees: theory and applications, *Acta Appl. Math.* **66** (2001) 211–249.

[5] I. Gutman, D. Vukičević, J. Žerovnik, A class of modified Wiener indices, *Croat. Chem. Acta* **77** (2004) 103–109.

[6] S. Nikolić, N. Trinajstić, M. Randić, Wiener index revisited, *Chem. Phys. Lett.* **333** (2001) 319–321.

[7] I. Gutman, J. Žerovnik, Corroborating a modification of the Wiener index, *Croat. Chem. Acta* **75** (2002) 603–612.

[8] D. Vukičević, Distinction between modifications of Wiener indices, *MATCH Commun. Math. Comput. Chem.* **47** (2003) 87–105.

[9] M. Gorše, J. Žerovnik, A remark on modified Wiener indices, *MATCH Commun. Math. Comput. Chem.* **50** (2004) 109–116.

[10] D. Vukičević, I. Gutman, Note on a class of modified Wiener indices, *MATCH Commun. Math. Comput. Chem.* **47** (2003) 107–117.

[11] I. Gutman, I. Vidović, B. Furtula, I. G. Zenkevich, Wiener-type indices and internal molecular energy, *Serb. Chem. Soc.* **68** (2003) 401–408.

[12] B. Lučić, A. Miličević, S. Nikolić, N. Trinajstić, On variable Wiener index, *Indian J. Chem.* **42A** (2003) 1279–1282.

[13] D. Vukičević, J. Žerovnik, Variable Wiener indices, *MATCH Commun. Math. Comput. Chem.* **53** (2005) 385–402.

[14] J. W. Moon, On the total distance between nodes in trees, *Systems Sci. Math. Sci.* **9** (1996) 93–96.