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# A Class of Modified Wiener Indices*

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The Wiener index of a tree T obeys the relation $W(\mathrm{T}) = \Sigma_e\, n_1(e) \cdot n_2(e)$ where $n_1(e)$ and $n_2(e)$ are the number of vertices on the two sides of the edge $e$, and where the summation goes over all edges of T. Recently Nikolić, Trinajstić and Randić put forward a novel modification ${}^{\mathrm{m}}W$ of the Wiener index, defined as ${}^{\mathrm{m}}W(\mathrm{T}) = \Sigma_e\, [\, n_1(e) \cdot n_2(e)\, ]^{-1}$. We now extend their definition as ${}^{\mathrm{m}}W_\lambda(\mathrm{T}) = \Sigma_e\, [\, n_1(e) \cdot n_2(e)\, ]^{\lambda}$, and show that some of the main properties of both $W$ and ${}^{\mathrm{m}}W$ are, in fact, properties of ${}^{\mathrm{m}}W_\lambda$, valid for all values of the parameter $\lambda \neq 0$. In particular, if $\mathrm{T}_n$ is any $n$-vertex tree, different from the $n$-vertex path $\mathrm{P}_n$ and the $n$-vertex star $\mathrm{S}_n$, then for any positive $\lambda$, ${}^{\mathrm{m}}W_\lambda(\mathrm{P}_n) > {}^{\mathrm{m}}W_\lambda(\mathrm{T}_n) > {}^{\mathrm{m}}W_\lambda(\mathrm{S}_n)$, whereas for any negative $\lambda$, ${}^{\mathrm{m}}W_\lambda(\mathrm{P}_n) < {}^{\mathrm{m}}W_\lambda(\mathrm{T}_n) < {}^{\mathrm{m}}W_\lambda(\mathrm{S}_n)$. Thus ${}^{\mathrm{m}}W_\lambda$ provides a novel class of structure-descriptors, suitable for modeling branching-dependent properties of organic compounds, applicable in QSPR and QSAR studies. We also demonstrate that if trees are ordered with regard to ${}^{\mathrm{m}}W_\lambda$ then, in the general case, this ordering is different for different $\lambda$.

## INTRODUCTION

The molecular-graph-based quantity $W$, introduced[1] by Harold Wiener in 1947, nowadays known under the name Wiener index or Wiener number, is one of the most thoroughly studied molecular-structure-descriptors.[2,3] Its chemical applications[4–8] and mathematical properties[9,10] are well documented. Of the several review articles on the Wiener index we mention just a few.[11–13]

Already in Wiener's seminal paper[1] the following formula for the calculation of the Wiener number of acyclic (molecular) graphs was reported:

$$W(\mathrm{T}) = \sum_e n_1(e) \cdot n_2(e) \tag{1}$$

where T denotes a tree (= connected and acyclic graph),[2,9] $n_1(e)$ and $n_2(e)$ are the number of vertices of T lying on the two sides of the edge $e$, and where the summation

* Dedicated to Professor Nenad Trinajstić on the occasion of his 65th birthday, in recognition of his 30 years long fruitful research in Chemical Graph Theory.

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goes over all edges of T. [Recall that formula (1) is not the definition of the Wiener index, but a mathematical theorem; the Wiener index is defined as the sum of distances between all pairs of vertices.]

A large number of modifications and extensions of the Wiener index was considered in the chemical literature; an extensive bibliography on this matter can be found in the reviews[14,15] and the recent paper.[16] One of the newest such modifications was put forward by Nikolić, Trinajstić and Randić.[17] They introduced the »modified Wiener index« ${}^{m}W$, defined as

$$ {}^{m}W(\mathrm{T}) = \sum_{e} [\, n_1(e) \cdot n_2(e)]^{-1} \qquad (2)$$

in analogy to formula (1).

An important property of the Wiener index are the inequalities

$$ W(\mathrm{P}_n) > W(\mathrm{T}_n) > W(\mathrm{S}_n) \qquad (3)$$

where $\mathrm{P}_n$, $\mathrm{S}_n$, and $\mathrm{T}_n$ denote respectively the $n$-vertex path, the $n$-vertex star (*cf.* Figure 1), and any $n$-vertex tree different from $\mathrm{P}_n$ and $\mathrm{S}_n$, and $n$ is any integer greater than 4. Because of the relation (3), the Wiener index may be viewed as a »branching index«, namely a topological index capable of measuring the extent of branching of the carbon-atom skeleton of molecules and capable of ordering isomers according to the extent of branching. (For more details on the problem of measuring branching see Ref. 16 and the references quoted therein.)

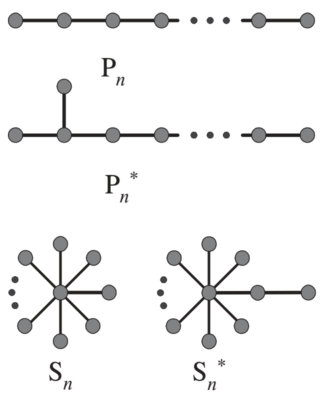



Figure 1. Trees extremal with respect to the modified Wiener indices ${}^{m}W_{\lambda}$, for all non-zero values of the parameter $\lambda$. Among the $n$-vertex trees the path ($\mathrm{P}_n$) and the star ($\mathrm{S}_n$) are extremal, *cf.* Eqs. (6) and (7), and the trees $\mathrm{P}_n^*$ and $\mathrm{S}_n^*$ second-extremal. The path is evidently the least and the star the most branched tree.

It has been demonstrated[16] that also the modified Wiener index ${}^{m}W$ possesses this desired property, *i.e.*, that it satisfies relations fully analogous to (3):

$$ {}^{m}W(\mathrm{P}_n) < {}^{m}W(\mathrm{T}_n) < {}^{m}W(\mathrm{S}_n). \qquad (4)$$

Motivated by the analogy between Eqs. (1) and (2), as well as between the relations (3) and (4), we examined a class of modified Wiener indices ${}^{m}W_{\lambda}$, defined *via*

$$ {}^{m}W_{\lambda}(\mathrm{T}) = \sum_{e} [\, n_1(e) \cdot n_2(e)]^{\lambda} \qquad (5)$$

where $\lambda$ is a parameter that may assume different values. Clearly, for $\lambda = +1$ and $\lambda = -1$, the modified Wiener index ${}^{m}W_{\lambda}$ reduces to the ordinary Wiener index $W$ and the Nikolić-Trinajstić-Randić index ${}^{m}W$, respectively.

As a pleasant surprise we found that ${}^{m}W_{\lambda}$ maintains its branching-index-nature for any (non-zero) value of $\lambda$. This we prove in the subsequent section. In a later section we demonstrate another intriguing property of our class of modified Wiener indices, namely that for $\lambda_1 \neq \lambda_2$, the ordering of trees with respect to ${}^{m}W_{\lambda_1}$ and ${}^{m}W_{\lambda_2}$ is never the same. We prove this result for $\lambda_1, \lambda_2 < 0$.

## ${}^{m}W_{\lambda}$ IS A BRANCHING INDEX FOR ALL $\lambda$

In this section we prove a result implying that for all $\lambda$ the modified Wiener indices ${}^{m}W_{\lambda}$ satisfy the basic requirement for being a branching index.

*Theorem 1.* – If $\mathrm{T}_n$ is an arbitrary tree on $n$ vertices, different from $\mathrm{P}_n$ and $\mathrm{S}_n$, then for any $n \geq 5$,

$$ {}^{m}W_{\lambda}(\mathrm{P}_n) > {}^{m}W_{\lambda}(\mathrm{T}_n) > {}^{m}W_{\lambda}(\mathrm{S}_n) \qquad (6)$$

holds for all positive values of $\lambda$, and

$$ {}^{m}W_{\lambda}(\mathrm{P}_n) < {}^{m}W_{\lambda}(\mathrm{T}_n) < {}^{m}W_{\lambda}(\mathrm{S}_n) \qquad (7)$$

holds for all negative values of $\lambda$.

Clearly, relations (3) and (4) are special cases of (6) and (7), respectively.

In order to demonstrate the validity of Theorem 1 we first state a general property of our class of modified Wiener indices. For brevity $n_1(e) \cdot n_2(e)$, occurring in formulas (1), (2) and (5), will be denoted by $w(e \mid \mathrm{T})$. Then Eq. (5) is rewritten as

$$ {}^{m}W_{\lambda}(\mathrm{T}) = \sum_{e} w(e \mid \mathrm{T})^{\lambda}. \qquad (8)$$

The following result is an immediate consequence of (8) and the fact that $w(e \mid \mathrm{T})$ is greater than unity for all edges $e$ of any tree T, provided T has more than two vertices.

*Fundamental Observation.* – Let $\mathrm{T}^*$ and $\mathrm{T}^{**}$ be two trees with equal number of vertices (and hence equal number of edges). If their edges can be labeled so that

$$ w(e \mid \mathrm{T}^*) \leq w(e \mid \mathrm{T}^{**}) \qquad (9)$$

for all $e$, then ${}^{m}W_{\lambda}(\mathrm{T}^*) \leq {}^{m}W_{\lambda}(\mathrm{T}^{**})$ for any $\lambda > 0$ and ${}^{m}W_{\lambda}(\mathrm{T}^*) \geq {}^{m}W_{\lambda}(\mathrm{T}^{**})$ for any $\lambda < 0$. If at least one of the inequalities (9) is strict, then the inequalities between ${}^{m}W_{\lambda}(T^{*})$ and ${}^{m}W_{\lambda}(T^{**})$ are also strict.

The proof of the left-hand side inequalities in (6) and (7) is now easy: Because $n_1(e) + n_2(e) = n$ and $n_1(e)$, $n_2(e) \geq 1$, the product $w(e \mid T) = n_1(e) \cdot n_2(e)$ cannot be less than $1{\cdot}(n-1) = n-1$. In the case of the star $S_n$, all $w(e \mid S_n)$-values are equal to $n-1$. For all other $n$-vertex trees, at least one $w(e \mid T)$-value is greater than $n-1$.

This proves one half of Theorem 1.

Instead of directly verifying the right-hand side inequalities in (6) and (7) we prove a somewhat more general statement, namely Theorem 2. For this, consider the trees T′ and T″, depicted in Figure 2.

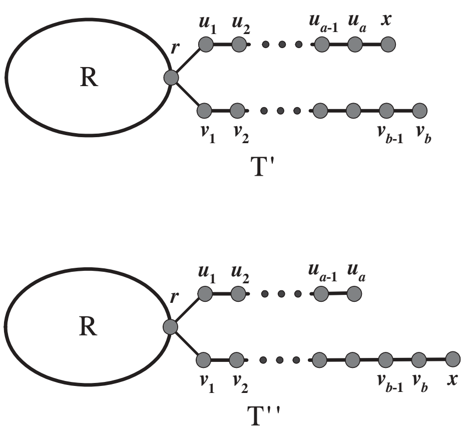



Figure 2. The trees considered in Theorem 2.

By R is denoted an arbitrary fragment with $n_R$ vertices, and $a \geq 0$, $b \geq 1$. Hence both T′ and T″ possess $n_R + a + b + 1$ vertices. Note that the vertex $r$ belongs to the fragment R. If $r$ would be the only vertex of R, then it would be T′ = T″. Therefore, the only interesting case is when $n_R \geq 2$.

*Theorem 2.* – Let T′ and T″ be trees the structure of which is shown in Figure 2. Then the transformation T′ $\rightarrow$ T″, increases ${}^{m}W_{\lambda}$ if $\lambda > 0$ and decreases ${}^{m}W_{\lambda}$ if $\lambda < 0$.

*Proof of Theorem 2*. The edge connecting the vertices $x$ and $y$ is denoted by $(x,y)$.

*Lemma 1*. – The edges of the trees T′ and T″, depicted in Figure 2, can be labeled so that equality $w(e \mid T') = w(e \mid T'')$ holds for all edges except one. These exceptional edges are $(r,u_1)$ in T′ and $(r,v_1)$ in T″.

*Proof of Lemma 1*. Evidently, $w(e \mid T') = w(e \mid T'')$ holds for all edges belonging to R. Also evidently,

$$w((x,u_a) \mid T') = w((u_a,u_{a-1}) \mid T'')$$

$$w((u_a,u_{a-1}) \mid T') = w((u_{a-1},u_{a-2}) \mid T'')$$

$$w((u_2,u_1) \mid T') = w((u_1,r) \mid T'')$$

and

$$w((v_b,v_{b-1}) \mid T') = w((x,v_b) \mid T'')$$

$$w((v_{b-1},v_{b-2}) \mid T') = w((v_b,v_{b-1}) \mid T'')$$

$$\cdots \qquad \cdots$$

$$w((v_1,r) \mid T') = w((v_2,v_1) \mid T'')$$

*Lemma 2*. – If for the trees T′ and T″, depicted in Figure 2, $a + 1 \leq b$, then $w((r,u_1) \mid T') < w((r,v_1) \mid T'')$.

*Proof of Lemma 2.*

$$w((r,u_1) \mid T') = (a + 1) \cdot (b + n_R)$$

$$w((r,v_1) \mid T'') = (b + 1) \cdot (a + n_R)$$

and therefore

$$w((r,v_1) \mid T'') - w((r,u_1) \mid T') = (b - a)(n_R - 1)$$

which necessarily is positive.

Theorem 2 is a direct consequence of Lemmas 1 and 2 and the »Fundamental Observation«.

Repeating the transformation T′ $\rightarrow$ T″ $a + 1$ times, the entire a-branch of T′ will be transferred to the b-branch and the degree of the vertex $r$ reduced by one. Repeating such transformations sufficiently many times we will finally obtain the path $P_n$.

This proves the right-hand side inequalities in (6) and (7).

The proof of Theorem 1 is thus completed.

The same reasoning gives us the structure of the second maximal and second minimal trees. These are also shown in Figure 1 as $P_n^{*}$ and $S_n^{*}$.

## MORE APPLICATIONS OF THE »FUNDAMENTAL OBSERVATION«

Theorem 2 implies that there exist molecular graphs whose order with regard to the modified Wiener indices is independent of the parameter $\lambda$. Indeed, there are numerous pairs of trees obeying the relations (9). We illustrate this on the example of the 7-vertex trees.

In Figure 3 are depicted the eleven distinct trees on 7 vertices. The first nine of them are molecular graphs, representing the nine isomeric heptanes $C_7H_{16}$. In Table I are given the respective $w(e \mid T)$-values.

An inspection of Table 1 shows that the molecular graphs of 2,2-dimethylpentane (**6**) and 2,3-dimethylpentane (**7**) have equal $w(e \mid T)$-sequences, *i. e.*, for them all relations (9) reduce to equalities. Consequently, neither the ordinary Wiener index $W$ nor the Nikolić-Trinajstić-Randić index ${}^{m}W$ nor any of the presently considered

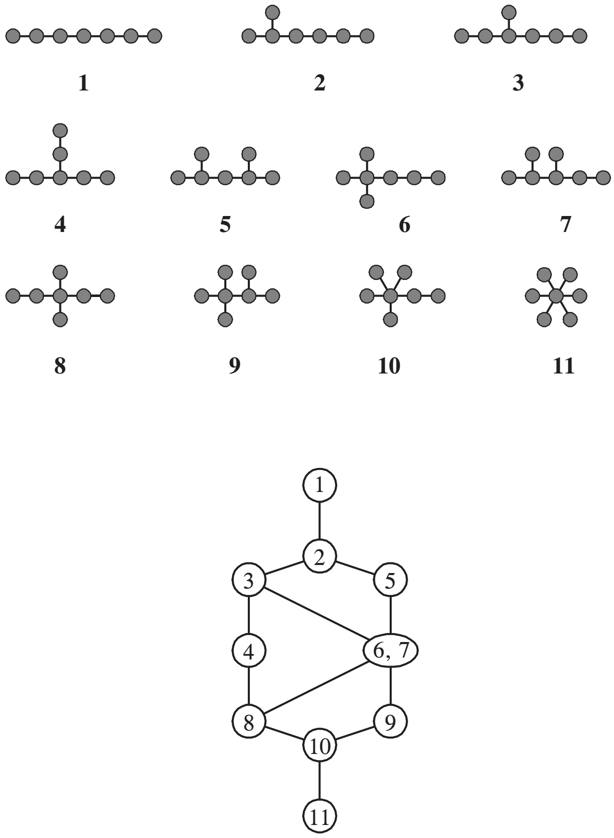



Figure 3. The 7-vertex trees and the comparability (Hasse) diagram pertaining to their $w(e \mid T)$-values, *cf.* Table I.

TABLE I. The 7-vertex trees (numbered as in Figure 3) and their $w(e \mid T)$-values

| tree T | $w(1\|T)$ | $w(2\|T)$ | $w(3\|T)$ | $w(4\|T)$ | $w(5\|Y)$ | $w(6\|T)$ |
|---|---|---|---|---|---|---|
| 1 | 6 | 6 | 10 | 10 | 12 | 12 |
| 2 | 6 | 6 | 6 | 10 | 12 | 12 |
| 3 | 6 | 6 | 6 | 10 | 10 | 12 |
| 4 | 6 | 6 | 6 | 10 | 10 | 10 |
| 5 | 6 | 6 | 6 | 6 | 12 | 12 |
| 6 | 6 | 6 | 6 | 6 | 10 | 12 |
| 7 | 6 | 6 | 6 | 6 | 10 | 12 |
| 8 | 6 | 6 | 6 | 6 | 10 | 10 |
| 9 | 6 | 6 | 6 | 6 | 6 | 12 |
| 10 | 6 | 6 | 6 | 6 | 6 | 10 |
| 11 | 6 | 6 | 6 | 6 | 6 | 6 |

modified Wiener indices ${}^{m}W_{\lambda}$ can distinguish these two isomers.

The inequalities (9) are fulfilled in a non-trivial manner for several pairs of molecular graphs, *e.g.*, between 2-methylhexane (**2**) and 3-methyhexane (**3**), between 3-methylhexane and 3-ethylepentane (**4**) or between 3-ethylpentane and 3,3-dimethylpentane (**8**). Then, in view of the »Fundamental Observation«, the ordering of these molecular graphs is independent of the actual value of the parameter $\lambda$.

On the other hand, some pairs of molecular graphs do not satisfy the inequalities (9) by all edges. Such are 3-methylhexane and 2,4-dimethylpentane (**5**) or 3,3-dimethylpentane and 2,2,3-trimethylbutane (**9**). The ordering of these isomers with regard to the modified Wiener indices ${}^{m}W_{\lambda}$ does depend on the actual value of $\lambda$.

In Figure 3 is shown the comparability (Hasse) diagram of the mutual relations of the 7-vertex trees, in view of the inequalities (9). Whenever these inequalities are obeyed for all edges, there is a descending path between the circles representing the respective two trees. Then the »Fundamental Observation« is applicable and these two trees are equally ordered by all ${}^{m}W_{\lambda}$. Otherwise the ordering of these trees is $\lambda$-dependent.

Analogous relations are encountered also for $n$-vertex trees and $n$-vertex chemical trees when $n > 7$. Their study will be communicated elsewhere. In what follows we show that no matter what the values of $\lambda_1$ and $\lambda_2$ are, there always exist trees that are oppositely ordered with regard to ${}^{m}W_{\lambda_1}$ and ${}^{m}W_{\lambda_2}$. The proof of this result is difficult and we restrict our considerations to the case of $\lambda_1$, $\lambda_2 < 0$.

## ON THE $\lambda$-DEPENDENCE OF ORDERING OF TREES BY MEANS OF ${}^{m}W_{\lambda}$

The set of all trees is denoted by $\mathfrak{T}$. The set of some topological indices (*e.g.* the set of the modified Wiener indices ${}^{m}W_{\lambda}$ for all values of $\lambda$) is denoted by $\mathfrak{I}$. We define an equivalence relation $\equiv$ on the set $\mathfrak{I}$ as

$$(i_1 \equiv i_2) \Leftrightarrow [\ (\forall \mathrm{T}_a, \mathrm{T}_b \in \mathfrak{T})\ (i_1(\mathrm{T}_a) \leq i_1(\mathrm{T}_b)) \Leftrightarrow (i_2(\mathrm{T}_a) \leq i_2(\mathrm{T}_b))\ ].$$

In words: two topological indices $i_1$ and $i_2$ are considered to be equivalent if they order all trees in the exactly same manner.

*Theorem 3.* – For each two numbers $\lambda_1, \lambda_2 < 0$ the modified Wiener indices ${}^{m}W_{\lambda_1}$ and ${}^{m}W_{\lambda_2}$ are not equivalent.

Before proving Theorem 3, we state an auxiliary result:

*Lemma 3.* – Let $\lambda_1, \lambda_2 \in \langle -\infty, 0 \rangle \setminus \{-1\}$, $\lambda_1 \neq \lambda_2$. There is a rational number $q \in \langle 1, \infty \rangle$, such that

$$\sqrt[\lambda_1+1]{\frac{q+1+2^{\lambda_1}}{q+2}} \neq \sqrt[\lambda_2+1]{\frac{q+1+2^{\lambda_2}}{q+2}}.$$

*Proof.* Suppose, to the contrary, that such number does not exist. Then, for each rational $x \in \langle 1, \infty \rangle$, we have

$$\frac{1}{\lambda_1+1} \ln\left(\frac{x+1+2^{\lambda_1}}{x+2}\right) = \frac{1}{\lambda_2+1} \ln\left(\frac{x+1+2^{\lambda_2}}{x+2}\right).$$

Since both functions are continuous this equality holds for any $x \in \langle 1,\infty \rangle$. Then also the first derivatives of these functions coincide. Replacing $y = x + 2$ and computing the first derivatives we get

$$\frac{1}{\lambda_1+1} \cdot \frac{1}{1+(2^{\lambda_1}-1)/y} \cdot (2^{\lambda_1}-1) \cdot \left(-\frac{1}{y^2}\right) =$$

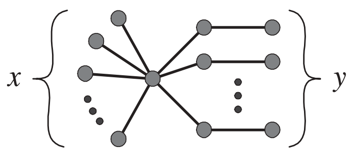
$$\frac{1}{\lambda_2+1} \cdot \frac{1}{1+(2^{\lambda_2}-1)/y} \cdot (2^{\lambda_2}-1) \cdot \left(-\frac{1}{y^2}\right).$$

Therefrom,

$$\left(\frac{\lambda_1+1}{2^{\lambda_1}-1} - \frac{\lambda_2+1}{2^{\lambda_2}-1}\right) y^2 + (\lambda_1 - \lambda_2)\, y = 0$$

for each $y \in \langle 3,\infty \rangle$. All the coefficients of the last polynomial are equal to zero, because otherwise it would have at most two zero-points. Therefore $\lambda_1 = \lambda_2$. This is a contradiction, so our claim is proved.

*Proof of Theorem 3*. Denote by T($x$,$y$) the tree depicted in Figure 4. This tree has $x + 2y + 1$ vertices.




T($x$, $y$)

Figure 4. The tree considered in Theorem 3.

It is sufficient to find trees G and H such that

$${}^{\mathrm{m}}W_{\lambda_1}(\mathrm{G}) \geq {}^{\mathrm{m}}W_{\lambda_1}(\mathrm{H}) \text{ and } {}^{\mathrm{m}}W_{\lambda_2}(\mathrm{G}) < {}^{\mathrm{m}}W_{\lambda_2}(\mathrm{H})$$

or trees G and H such that

$${}^{\mathrm{m}}W_{\lambda_1}(\mathrm{G}) > {}^{\mathrm{m}}W_{\lambda_1}(\mathrm{H}) \text{ and } {}^{\mathrm{m}}W_{\lambda_2}(\mathrm{G}) \leq {}^{\mathrm{m}}W_{\lambda_2}(\mathrm{H}).$$

We have to distinguish between three cases:

*Case 1*. $(\lambda_1+1)(\lambda_2+1) < 0$.

Without loss of generality, we may assume that $\lambda_1 < -1$ and $\lambda_2 > -1$. Then,

$${}^{\mathrm{m}}W_{\lambda_1}(\mathrm{P}_2) = 1$$

$${}^{\mathrm{m}}W_{\lambda_1}(\mathrm{S}_4) = 3 \cdot 3^{\lambda_1} < 1$$

$${}^{\mathrm{m}}W_{\lambda_2}(\mathrm{P}_2) = 1$$

$${}^{\mathrm{m}}W_{\lambda_2}(\mathrm{S}_4) = 3 \cdot 3^{\lambda_2} > 1$$

and therefore

$${}^{\mathrm{m}}W_{\lambda_1}(\mathrm{P}_2) > {}^{\mathrm{m}}W_{\lambda_1}(\mathrm{S}_4)$$

$${}^{\mathrm{m}}W_{\lambda_2}(\mathrm{P}_2) < {}^{\mathrm{m}}W_{\lambda_2}(\mathrm{S}_4).$$

*Case 2*. One of the numbers $\lambda_1$ and $\lambda_2$ is equal to –1. Without loss of generality, we may assume that $\lambda_1 = -1$. Distinguish two subcases:

*Subcase 2.1.* $\lambda_2 > -1$.

Let $a$ be the smallest natural number such that

$$a^{\lambda_1+1}\left[4 \cdot 7^{\lambda_2} + 3 \cdot \left(14 - \frac{2}{a}\right)^{\lambda_2}\right] > 1 .$$

Such a certainly exists, because $\lambda_2 + 1 > 0$. Let $b = 3a$. Then,

$${}^{\mathrm{m}}W_{\lambda_1}(\mathrm{P}_2) = 1$$

$${}^{\mathrm{m}}W_{\lambda_1}(\mathrm{T}(a,b)) = (a+b)(a+2b)^{-1} + b\,[\,2\,(a+2b-1)\,]^{-1} < \frac{4}{7} + \frac{1}{4} < 1$$

$$\mathrm{m}W_{\lambda_2}(\mathrm{P}_2) = 1$$

$${}^{\mathrm{m}}W_{\lambda_2}(\mathrm{T}(a,b)) = (a+b)(a+2b)^{\lambda_2} + b\,[2\,(a+2b-1)]^{\lambda_2} = a^{\lambda_1}\left[4 \cdot 7^{\lambda_2} + 3 \cdot \left(14 - \frac{2}{a}\right)^{\lambda_2}\right] > 1$$

and therefore

$${}^{\mathrm{m}}W_{\lambda_1}(\mathrm{P}_2) > {}^{\mathrm{m}}W_{\lambda_1}(\mathrm{T}(a,b))$$

$${}^{\mathrm{m}}W_{\lambda_2}(\mathrm{P}_2) \leq {}^{\mathrm{m}}W_{\lambda_2}(\mathrm{T}(a,b)) .$$

*Subcase 2.2.* $\lambda_2 < -1$.

Let $a$ be the smallest natural number, divisible by 4, such that

$$a^{\lambda_2+1}\left[\frac{5}{4} \cdot \left(\frac{3}{2}\right)^{\lambda_2} + \frac{1}{4} \cdot \left(3 - \frac{2}{a}\right)^{\lambda_2}\right] < 3^{\lambda_2} + 4^{\lambda_2} + 3^{\lambda_2} .$$

Such a certainly exists, because $\lambda_2 + 1 < 0$. Let $b = [a/4]$. Then we have

$${}^{\mathrm{m}}W_{\lambda_1}(\mathrm{P}_4) = \frac{1}{3} + \frac{1}{4} + \frac{1}{3} = \frac{11}{12}$$

$${}^{\mathrm{m}}W_{\lambda_1}(\mathrm{T}(a,b)) = (a+b)(a+2b)^{-1} + b\,[2\,(a+2b-1)]^{-1} > \frac{5}{6} + \frac{1}{10} > \frac{11}{12}$$

$${}^{\mathrm{m}}W_{\lambda_2}(\mathrm{P}_4) = 3^{\lambda_2} + 4^{\lambda_2} + 3^{\lambda_2}$$

$${}^{\mathrm{m}}W_{\lambda_2}(\mathrm{T}(a,b)) = (a+b)(a+2b)^{\lambda_2} + b\,[2\,(a+2b-1)]^{\lambda_2}$$

$$= a^{\lambda_2+1}\left[\frac{5}{4}\cdot\left(\frac{3}{2}\right)^{\lambda_2} + \frac{1}{4}\cdot\left(3-\frac{2}{a}\right)^{\lambda_2}\right] <$$

$$3^{\lambda_2} + 4^{\lambda_2} + 3^{\lambda_2}$$

implying

$$^{\mathrm{m}}W_{\lambda_1}(\mathrm{P}_4) < {}^{\mathrm{m}}W_{\lambda_1}(\mathrm{T}(a,b))$$

$$^{\mathrm{m}}W_{\lambda_2}(\mathrm{P}_4) > {}^{\mathrm{m}}W_{\lambda_2}(\mathrm{T}(a,b)).$$

*Case 3*. $(\lambda_1+1)\cdot(\lambda_2+1) > 0$.
By Lemma 3, there is a rational number $q \in \langle 1,\infty\rangle$, such that

$$\sqrt[\lambda_1+1]{\frac{q+1+2^{\lambda_1}}{q+2}} \neq \sqrt[\lambda_2+1]{\frac{q+1+2^{\lambda_2}}{q+2}}.$$

Therefore

$$\sqrt[\lambda_1+1]{(q+1)(q+2)^{\lambda_1} + 2^{\lambda_1}(q+2)^{\lambda_1}} \neq$$

$$\sqrt[\lambda_2+1]{(q+1)(q+2)^{\lambda_2} + 2^{\lambda_2}(q+2)^{\lambda_2}} \;.$$

Thus, either there is a positive rational number $k$ such that

$$(q+1)(q+2)^{\lambda_1} + 2^{\lambda_1}(q+2)^{\lambda_1} < k^{\lambda_1+1}$$

$$(q+1)(q+2)^{\lambda_2} + 2^{\lambda_2}(q+2)^{\lambda_2} > k^{\lambda_2+1}$$

or there is a positive rational number $k$ such that

$$(q+1)(q+2)^{\lambda_1} + 2^{\lambda_1}(q+2)^{\lambda_1} > k^{\lambda_1+1}$$

$$(q+1)(q+2)^{\lambda_2} + 2^{\lambda_2}(q+2)^{\lambda_2} < k^{\lambda_2+1}.$$

Without loss of generality, we may assume that the first of these two options applies.

Let $a$, $b$, $c$ be positive integers, such that $a = qc/k$ and $b = c/k$. Multiplying the above two inequalities by $(c/k)^{\lambda_1+1}$ and $(c/k)^{\lambda_2+1}$, respectively, we get

$$(a+b)(a+2b)^{\lambda_1} + b\,(2^{\lambda_1}(a+2b)^{\lambda_1}) < c\cdot c^{\lambda_1}$$

$$(a+b)(a+2b)^{\lambda_2} + b\,(2^{\lambda_2}(a+2b)^{\lambda_2}) > c\cdot c^{\lambda_2}$$

*i.e.*,

$$\frac{(a+b)(a+2b)^{\lambda_1} + b(2^{\lambda_1}(a+2b)^{\lambda_1})}{c\cdot c^{\lambda_1}} < 1$$

$$\frac{(a+b)(a+2b)^{\lambda_2} + b(2^{\lambda_2}(a+2b)^{\lambda_2})}{c\cdot c^{\lambda_2}} > 1 \;.$$

It follows that

$$\lim_{m\to\infty}\frac{(ma+mb)(ma+2mb)^{\lambda_1} + mb(2^{\lambda_1}(ma+2mb-1)^{\lambda_1})}{mc\cdot(mc)^{\lambda_1}} < 1$$

$$\lim_{m\to\infty}\frac{(ma+mb)(ma+2mb)^{\lambda_2} + mb(2^{\lambda_2}(ma+2mb-1)^{\lambda_2})}{mc\cdot(mc)^{\lambda_2}} > 1.$$

So, there is some sufficiently large integer $m$, such that

$$(ma+mb)(ma+2mb)^{\lambda_1} + mb(2^{\lambda_1}(ma+2mb-1)^{\lambda_1}) < mc\cdot(mc)^{\lambda_1}$$

$$(ma+mb)(ma+2mb)^{\lambda_2} + mb(2^{\lambda_2}(ma+2mb-1)^{\lambda_2}) > mc\cdot(mc)^{\lambda_2}$$

This, finally, yields

$$^{\mathrm{m}}W_{\lambda_1}(\mathrm{T}(ma,mb)) < {}^{\mathrm{m}}W_{\lambda_2}(\mathrm{S}_{mc+1})$$

$$^{\mathrm{m}}W_{\lambda_1}(\mathrm{T}(ma,mb)) > {}^{\mathrm{m}}W_{\lambda_2}(\mathrm{S}_{mc+1}).$$

By this all the cases are exhausted and the proof of Theorem 3 is complete.

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## SAŽETAK

### Jedna klasa modificiranih Wienerovih indeksa

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Wienerov indeks stabla T zadovoljava relaciju $W(\mathrm{T}) = \Sigma_e\, n_1(e) \cdot n_2(e)$ gdje su $n_1(e)$ i $n_2(e)$ broj čvorova na dvije strane grane $e$, i gdje sumiranje ide preko svih grana stabla T. Nedavno su Nikolić, Trinajstić i Randić predložili modifikaciju ${}^{\mathrm{m}}W$ Wienerovog indeksa, definiranu kao ${}^{\mathrm{m}}W(\mathrm{T}) = \Sigma_e\, [\, n_1(e) \cdot n_2(e)\, ]^{-1}$. Mi sada proširujemo njihovu definiciju na ${}^{\mathrm{m}}W_\lambda(\mathrm{T}) = \Sigma_e\, [\, n_1(e) \cdot n_2(e)\, ]^\lambda$, i pokazujemo da neka od važnijih svojstava kako $W$ tako i ${}^{\mathrm{m}}W$ važe za ${}^{\mathrm{m}}W_\lambda$, za svaku vrijednost parametra $\lambda \neq 0$. Ako je $\mathrm{T}_n$ bilo koje stablo s $n$ čvorova, različito od puta $\mathrm{P}_n$ i zvijezde $\mathrm{S}_n$, onda za svaku pozitivnu $\lambda$, ${}^{\mathrm{m}}W_\lambda(\mathrm{P}_n) > {}^{\mathrm{m}}W_\lambda(\mathrm{T}_n) > {}^{\mathrm{m}}W_\lambda(\mathrm{S}_n)$, dok za svaku negativnu $\lambda$, ${}^{\mathrm{m}}W_\lambda(\mathrm{P}_n) < {}^{\mathrm{m}}W_\lambda(\mathrm{T}_n) < {}^{\mathrm{m}}W_\lambda(\mathrm{S}_n)$. Na taj način ${}^{\mathrm{m}}W_\lambda$ predstavlja novu klasu strukturnih deskriptora, pogodnih za modeliranje o razgranatosti ovisnih svojstava organskih spojeva i učinkovitih u QSPR i QSAR studijama. Također pokazujemo da ako su stabla uređena prema ${}^{\mathrm{m}}W_\lambda$, tada se, u općem slučaju, ovaj uređaj razlikuje za različite $\lambda$.