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NOTE ON A CLASS OF MODIFIED WIENER INDICES

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Abstract

The *Wiener index* of an n-vertex tree T can be computed by means of the expression $W = \sum_e [n_1(e) \cdot n_2(e)]$, where $n_1(e)$ and $n_2(e) = n - n_1(e)$ are the number of vertices on the two sides of the edge e, and where the summation goes over all edges of T. The *modified Wiener index* is defined as ${}^mW = \sum_e [n_1(e) \cdot n_2(e)]^{-1}$. Both W and ${}^mW$ are special cases of the quantity ${}^mW_\lambda = \sum_e [n_1(e) \cdot n_2(e)]^\lambda$, recently put forward by Žerovnik and the present authors. We now establish a few general properties of ${}^mW_\lambda$, in particular conditions under which for two trees T_1 and T_2 the inequality ${}^mW_\lambda(T_1) > {}^mW_\lambda(T_2)$ holds for all negative or all positive values of the parameter λ.

INTRODUCTION

The topological index W, conceived by Wiener in 1947 [1], is defined as the sum of distances between all pairs of vertices of the molecular graph. It is the oldest and probably the most thoroughly examined molecular-graph-based structure descriptor.

Motivated by the success of the Wiener index, but also attempting to overcome some of its weak points, numerous of its modifications and extensions were proposed in the chemical literature; an extensive bibliography on this matter can be found in the handbook [2], review [3] and the recent papers [4, 5].

In the seminal paper [1], in addition to the vertex–distance–based definition of the Wiener index, a peculiar formula for its calculation was communicated:

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

where T stands for the molecular graph of an alkane, where $n_1(e|T)$ and $n_2(e|T)$ are the number of vertices of T lying on the two sides of the edge e, and where the summation embraces all edges of T. It can be immediately verified [6, p. 127] that formula (1) holds for all trees (= connected acyclic graphs).

One of the newly proposed modifications of the Wiener index [7] is based on formula (1) and reads

$$^{m}W(T) = \sum_e [n_1(e|T) \cdot n_2(e|T)]^{-1} \ . \tag{2}$$

The quantity ^{m}W was named "*modified Wiener index*" [7]. Some of its mathematical properties were recently established [5], and found to be analogous (yet opposite) to the properties of the ordinary Wiener index. These findings motivated us to consider an entire class of Wiener–type indices, defined as [8]

$$^{m}W_\lambda(T) = \sum_e [n_1(e|T) \cdot n_2(e|T)]^\lambda \ . \tag{3}$$

Evidently, for $\lambda = +1$ and $\lambda = -1$ the right–hand side of Eq. (3) reduces to the ordinary and the modified Wiener index, respectively, Eqs. (1) and (2).

It has been shown [8] that there are numerous (chemical) trees whose ordering with respect to $^{m}W_\lambda$ does not depend on the actual value of the parameter λ (except that this ordering is reversed when λ changes sign). This invariant behavior is based on the following elementary result [8]:

Lemma 1a. *Let T_1 and T_2 be two trees with equal number of vertices (and hence with equal number of edges). If their edges can be labeled so that*

$$n_1(e|T_1) \cdot n_2(e|T_1) \leq n_1(e|T_2) \cdot n_2(e|T_2) \tag{4}$$

for all e, then ${}^mW_\lambda(T_1) \leq {}^mW_\lambda(T_2)$ for any $\lambda > 0$ and ${}^mW_\lambda(T_1) \geq {}^mW_\lambda(T_2)$ for any $\lambda < 0$. If at least one of the inequalities (4) is strict, then the inequalities between ${}^mW_\lambda(T_1)$ and ${}^mW_\lambda(T_2)$ are also strict.

In this paper, when ambiguity is not possible, we write n_i instead of $n_i(e|T)$, $i = 1, 2$. Further, we shall always label n_1 and n_2 so that $n_1 \leq n_2$.

Denote by n the number of vertices of the tree T. Then, in view of the fact that $n_1(e|T) + n_2(e|T) = n$ holds for all edges e of T, and that

$$1 \cdot (n-1) < 2 \cdot (n-2) < \cdots < \lfloor n/2 \rfloor \cdot \lceil n/2 \rceil \tag{5}$$

we may re-state Lemma 1a as follows:

Lemma 1b. *Let T_1 and T_2 be two trees with equal number of vertices. If their edges can be labeled so that*

$$n_1(e|T_1) \leq n_1(e|T_2) \tag{6}$$

for all e, then ${}^mW_\lambda(T_1) \leq {}^mW_\lambda(T_2)$ for any $\lambda > 0$ and ${}^mW_\lambda(T_1) \geq {}^mW_\lambda(T_2)$ for any $\lambda < 0$. If at least one of the inequalities (6) is strict, then the inequalities between ${}^mW_\lambda(T_1)$ and ${}^mW_\lambda(T_2)$ are also strict.

In what follows we deduce some additional conditions under which the ordering of trees (with respect to ${}^mW_\lambda$) is same for all negative or all positive values of λ. We start with another elementary finding.

Let $\mathcal{T}$ denote the set of all trees.

Lemma 2. *Let $T_1, T_2 \in \mathcal{T}$. If ${}^mW_\lambda(T_1) < {}^mW_\lambda(T_2)$ for all $\lambda < 0$, then T_1 and T_2 have equal number of vertices.*

Before proving Lemma 2 we point out two properties of the Wiener-type index ${}^mW_\lambda$. Let T be a tree with n vertices, of which p vertices are of degree 1. Then

$$\lim_{\lambda \to 0} {}^mW_\lambda(T) = n - 1 \tag{7}$$

$$\lim_{\lambda \to -\infty} \frac{{}^{m}W_\lambda(T)}{p(n-1)^\lambda} = 1 \ . \tag{8}$$

The limit (7) holds because the right-hand side of Eq. (3) has $n-1$ summands. The limit (8) is a direct consequence of (5) and the fact that in T there are p. edges whose contribution to the right-hand side summation in Eq. (3) is equal to $[1 \cdot (n-1)]^\lambda = (n-1)^\lambda$. Note that relation (8) holds for $n \geq 3$. For the (unique) 2-vertex tree, namely the 2-vertex path, $p = 2$ and ${}^{m}W_\lambda \equiv 1$. Therefore, for $n = 2$ the right-hand side of Eq. (8) is equal to $1/2$.

Proof of Lemma 2. Applying the limit (7) we get

$$\lim_{\lambda \to 0^-} [{}^{m}W_\lambda(T_1) - {}^{m}W_\lambda(T_2)] = n(T_1) - n(T_2) \ .$$

It cannot be $n(T_1) > n(T_2)$, because then for near-zero (and negative) values of λ it would be ${}^{m}W_\lambda(T_1) > {}^{m}W_\lambda(T_2)$.

It cannot be $n(T_1) < n(T_2)$, because then from the limit (8) it would follow:

$$\lim_{\lambda \to -\infty} \frac{{}^{m}W_\lambda(T_2)}{{}^{m}W_\lambda(T_1)} = \frac{p(T_2)}{p(T_1)} \lim_{\lambda \to -\infty} \left(\frac{n(T_2)-1}{n(T_1)-1} \right)^\lambda = 0$$

implying ${}^{m}W_\lambda(T_2) < {}^{m}W_\lambda(T_1)$ for sufficiently large (and negative) λ.

Therefore, if ${}^{m}W_\lambda(T_1) < {}^{m}W_\lambda(T_2)$ holds for all negative values of the parameter λ, then it must be $n(T_1) = n(T_2)$. □

There is no analog of Lemma 2 for $\lambda > 0$. Namely, there exist pairs of trees T_1 and T_2 with unequal number of vertices, such that ${}^{m}W_\lambda(T_1) < {}^{m}W_\lambda(T_2)$ holds for all $\lambda > 0$. Example: the 2-vertex path (${}^{m}W_\lambda = 1$) and the 3-vertex path ${}^{m}W_\lambda = 2 \cdot 2^\lambda$.

In order to become able to formulate and prove further results of the same kind we need to introduce a few more notions.

PREPARATIONS

Consider an n-vertex tree T. As before, $n_1(e|T) = n_1$ denotes the number of vertices of T that lie on one side of the edge e, assuming that not fewer vertices lie on the other side of e. The minimal value of n_1 is 1, because any tree possesses vertices of degree 1. The maximal possible value of n_1 is $\lfloor n/2 \rfloor$.

Let $\nu(T, k)$ be the number of times the n_1-values of the tree T are equal to k. Let $\nu(T)$ stand for the $(\lfloor n/2 \rfloor)$-tuple

$$(\nu(T,1), \nu(T,2), \ldots, \nu(T, \lfloor n/2 \rfloor)) \ .$$

Note that

$$\sum_{k=1}^{\lfloor n/2 \rfloor} \nu(T,k) = n(T) - 1 \qquad (9)$$

and

$${}^{m}W_{\lambda}(T) = \sum_{k=1}^{\lfloor n/2 \rfloor} \nu(T,k) \ [k\,(n-k)]^{\lambda} \ . \qquad (10)$$

The *lexicographic order* of n-tuples of real numbers, denoted by $<_{lex}$ is defined as usual:

$$(a_1, a_2, \ldots, a_n) <_{lex} (b_1, b_2, \ldots, b_n) \Leftrightarrow$$

$$\Leftrightarrow \quad (\exists i)[(a_i < b_i) \wedge (\forall j) j < i \Longrightarrow a_j = b_j] \ .$$

We say that $(a_1, a_2, \ldots, a_n) = (b_1, b_2, \ldots, b_n)$ if $a_i = b_i$ for all $i = 1, 2, \ldots, n$. If $(a_1, a_2, \ldots, a_n) \neq (b_1, b_2, \ldots, b_n)$, then either $(a_1, a_2, \ldots, a_n) <_{lex} (b_1, b_2, \ldots, b_n)$ or $(b_1, b_2, \ldots, b_n) <_{lex} (a_1, a_2, \ldots, a_n)$.

The *inverse lexicographic order* $<_{lex^*}$ is determined analogously:

$$(a_1, a_2, \ldots, a_n) <_{lex^*} (b_1, b_2, \ldots, b_n) \Leftrightarrow$$

$$\Leftrightarrow \quad (\exists i)[(a_i < b_i) \wedge (\forall j) j > i \Longrightarrow a_j = b_j] \ .$$

We introduce a further relation $<_{slex}$ as follows:

$$(a_1, a_2, \ldots, a_n) <_{slex} (b_1, b_2, \ldots, b_n) \Leftrightarrow$$

$$\Leftrightarrow \quad (\forall j) \left(\sum_{i=1}^{j} a_i \leq \sum_{i=1}^{j} b_i \right) \wedge [(a_1, a_2, \ldots, a_n) \neq (b_1, b_2, \ldots, b_n)] \ .$$

For the elements of the set $\mathcal{T}$ of all trees, three binary relations, $\prec$, $\prec^*$, and $\prec_s$ can now be defined.

Let $T_1, T_2 \in \mathcal{T}$. Then

$$T_1 \prec T_2 \quad \Leftrightarrow \quad (n(T_1) = n(T_2)) \wedge [\nu(T_1) <_{lex} \nu(T_2)]$$

$$T_1 \prec^* T_2 \quad \Leftrightarrow \quad (n(T_1) = n(T_2)) \wedge [\nu(T_1) <_{lex^*} \nu(T_2)]$$

$$T_1 \prec_s T_2 \quad \Leftrightarrow \quad (n(T_1) = n(T_2)) \wedge [\nu(T_1) <_{slex} \nu(T_2)] \ .$$

THE MAIN RESULTS

Theorem 3. *Let T_1 and T_2 be any trees. If ${}^mW_\lambda(T_1) < {}^mW_\lambda(T_2)$ holds for all $\lambda < 0$ then $T_1 \prec T_2$.*

Proof. From Lemma 2 follows that $n(T_1) = n(T_2)$. In order to simplify the below notation, denote $n(T_1) = n(T_2)$ by n.

Let the index i, $1 \leq i \leq \lfloor n/2 \rfloor$, be determined by the conditions $\nu(T_1, i) \neq \nu(T_2, i)$ and $\nu(T_1, j) = \nu(T_2, j)$ for all $j < i$. Because $\nu(T_1) \neq \nu(T_2)$, such i always exists.

Now, in view of relation (10), ${}^mW_\lambda(T_1) < {}^mW_\lambda(T_2)$ is tantamount to

$$\sum_{k=1}^{\lfloor n/2 \rfloor} [\nu(T_1, k) - \nu(T_2, k)] \, [k\,(n-k)]^\lambda < 0 \tag{11}$$

After cancellation in Eq. (11) we get

$$\sum_{k=i}^{\lfloor n/2 \rfloor} [\nu(T_1, k) - \nu(T_2, k)] \, [k\,(n-k)]^\lambda < 0$$

i. e.,

$$\frac{\sum_{k=i}^{\lfloor n/2 \rfloor} \nu(T_1, k) \, [k\,(n-k)]^\lambda}{\sum_{k=i}^{\lfloor n/2 \rfloor} \nu(T_2, k) \, [k\,(n-k)]^\lambda} < 1$$

which holds for all $\lambda < 0$. On the other hand,

$$\lim_{\lambda \to -\infty} \frac{\sum_{k=i}^{\lfloor n/2 \rfloor} \nu(T_1, k) \, [k\,(n-k)]^\lambda}{\sum_{k=i}^{\lfloor n/2 \rfloor} \nu(T_2, k) \, [k\,(n-k)]^\lambda} = \frac{\nu(T_1, i)}{\nu(T_2, i)}$$

and therefore $\nu(T_1, i)/\nu(T_2, i) < 1$, implying $T_1 \prec T_2$. □

In a fully analogous manner we prove:

Theorem 4. *Let T_1 and T_2 be trees with equal number of vertices. If ${}^mW_\lambda(T_1) < {}^mW_\lambda(T_2)$ holds for all $\lambda > 0$ then $T_1 \prec^* T_2$.*

The converses of Theorems 3 and 4 are not true. Namely, there exist pairs of trees, such that $T_1 \prec T_2$, but ${}^mW_\lambda(T_1) > {}^mW_\lambda(T_2)$ for some $\lambda < 0$. Also, there exist pairs of trees, such that $T_1 \prec^* T_2$, but ${}^mW_\lambda(T_1) > {}^mW_\lambda(T_2)$ for some $\lambda > 0$.

A counterexample to the converse of Theorem 3 are the $(2a+1)$-vertex trees $T_1(a)$ and $T_2(a)$ for sufficiently large value of the parameter a.

$T_1(a)$ is obtained from a copies of 2-vertex paths, by joining a vertex of each copy to a new vertex. $T_2(a)$ is obtained from an $(a+1)$-vertex path, by attaching to its terminal vertex a new vertices of degree 1.

We have

$$\begin{aligned} \nu(T_1(a)) &= (a, a, 0, 0, 0, \ldots, 0) \\ \nu(T_2(a)) &= (a+1, 1, 1, 1, 1, \ldots, 1) \end{aligned}$$

and, consequently, $T_1(a) \prec T_2(a)$.

Note that

$$\lim_{a\to\infty} \left((a+1)\cdot\frac{1}{2a} + \frac{1}{2(2a-1)} + (a-1)\cdot\frac{1}{3(2a-2)} \right) = \frac{2}{3}$$

and that

$$\lim_{a\to\infty} \left(a\cdot\frac{1}{2a} + a\cdot\frac{1}{2(2a-1)} \right) = \frac{3}{4}.$$

Therefore, for a sufficiently large value of a

$$a\cdot\frac{1}{2a} + a\cdot\frac{1}{2(2a-1)} > (a+1)\cdot\frac{1}{2a} + \frac{1}{2(2a-1)} + (a-1)\cdot\frac{1}{3(2a-2)}.$$

Bearing this inequality in mind, we now have

$$\begin{aligned} W_{-1}(T_1(a)) &= a\cdot\frac{1}{2a} + a\cdot\frac{1}{2(2a-1)} \\ &> (a+1)\cdot\frac{1}{2a} + \frac{1}{2(2a-1)} + (a-1)\cdot\frac{1}{3(2a-2)} \\ &\ge (a+1)\cdot\frac{1}{2a} + \frac{1}{2(2a-1)} + \sum_{k=3}^{a}\frac{1}{k(2a+1-k)} \\ &= W_{-1}(T_2(a)). \end{aligned}$$

Hence, in spite of $T_1(a) \prec T_2(a)$, for sufficiently large values of the parameter a, the modified Wiener index of $T_1(a)$ exceeds the modified Wiener index of $T_2(a)$.

A counterexample to the converse of Theorem 4 are the $(6b+4)$-vertex trees $T_1(b)$ and $T_2(b)$ for sufficiently large value of the parameter b.

$T_1(b)$ is obtained from a $(4b+3)$-vertex path, by attaching to its central vertex the terminal vertex of a $(2b+1)$-vertex path. $T_2(b)$ is obtained from the 2-vertex path, by attaching to each of its vertices $3b+1$ new vertices of degree 1.

We have

$$\nu(T_1(b)) = (3,3,\ldots,3,0,0,\ldots,0)$$
$$\nu(T_2(b)) = (6b+2,0,0,\ldots,0,1)$$

and, consequently, $T_1(b) \prec^* T_2(b)$.

Direct calculation yields

$$^mW_\lambda(T_1(b)) = \sum_{k=1}^{2b+1} 3\,[k(6b+4-k)]^\lambda$$
$$^mW_\lambda(T_2(b)) = (6b+2)\,(6b+3)^\lambda + (3b+2)^{2\lambda}$$

which for $\lambda = +1$ results in

$$W(T_1(b)) = (b+1)(2b+1)(14\,b+9)$$
$$W(T_2(b)) = 45\,b^2 + 42\,b + 10\,.$$

Thus, for $\lambda = +1$ and sufficiently large b, $^mW_\lambda(T_1(b))$ exceeds $^mW_\lambda(T_2(b))$.

On the other hand, in the limit case $\lambda \to +\infty$,

$$^mW_\lambda(T_1(b)) \sim 3\,(8\,b^2 + 10\,b + 3)^\lambda$$
$$^mW_\lambda(T_2(b)) \sim (9\,b^2 + 12\,b + 4)^\lambda$$

and therefore, for sufficiently large values of b and λ, $^mW_\lambda(T_1(b)) < {}^mW_\lambda(T_2(b))$.

Hence, in spite of $T_1(b) \prec^* T_2(b)$, if b is sufficiently large, then the value of $^mW_\lambda(T_1(b))$ is sometimes smaller and sometimes greater than $^mW_\lambda(T_2(b))$, depending on the actual value of the parameter $\lambda > 0$.

In what follows we need an auxiliary result:

Lemma 5. *Let $a_1, a_2, \ldots, a_m$ be numbers, not all of which being equal to zero, such that*

$$\sum_{k=1}^{j} a_k \geq 0 \tag{12}$$

holds for all $j = 1, 2, \ldots, m$. Let $b_1, b_2, \ldots, b_m$ be numbers, such that $b_1 > b_2 > \cdots > b_m > 0$. Then

$$\sum_{k=1}^{m} a_k b_k > 0 . \tag{13}$$

Proof. For $j = 1, 2, \ldots, m-1$, multiply the inequality (12) by $b_j - b_{j+1} > 0$. For $j = m$, multiply (12) by $b_m > 0$. This yields

$$a_1 (b_1 - b_2) \geq 0$$

$$a_1 (b_2 - b_3) + a_2 (b_2 - b_3) \geq 0$$

$$a_1 (b_3 - b_4) + a_2 (b_3 - b_4) + a_3 (b_3 - b_4) \geq 0$$

$$\ldots \qquad \ldots \qquad \ldots$$

$$a_1 (b_{m-1} - b_m) + a_2 (b_{m-1} - b_m) + a_3 (b_{m-1} - b_m) + \cdots + a_{m-1} (b_{m-1} - b_m) \geq 0$$

$$a_1 b_m + a_2 b_m + a_3 b_m + \cdots + a_{m-1} b_m + a_m b_m \geq 0 .$$

Because not all a_k's are equal to zero, at least one of the above inequalities is strict. By summing them we arrive at (13). □

Theorem 6. *Let $T_1, T_2 \in \mathcal{T}$. If $T_1 \prec_s T_2$, then ${}^mW_\lambda(T_1) < {}^mW_\lambda(T_2)$ for all values of $\lambda < 0$.*

Proof. $T_1 \prec_s T_2$ implies that T_1 and T_2 have equal number of vertices, which (as before) we denote by n. Further, $T_1 \prec_s T_2$ means that the inequalities

$$\sum_{k=1}^{j} [\nu(T_2, k) - \nu(T_1, k)] \geq 0$$

are obeyed for all $j = 1, 2, \ldots, \lfloor n/2 \rfloor$.

We may now identify $\lfloor n/2 \rfloor$ and $\nu(T_2, k) - \nu(T_1, k)$ with m and a_k in Lemma 5, and choose $b_k = [k(n-k)]^\lambda$. Because $\nu(T_1) \neq \nu(T_2)$ and because for $\lambda < 0$,

$$[1\,(n-1)]^\lambda > [2\,(n-2)]^\lambda > \cdots > [\lfloor n/2 \rfloor) \cdot \lceil n/2 \rceil]^\lambda$$

all the conditions of Lemma 5 are fulfilled, and therefore

$$\sum_{k=1}^{\lfloor n/2 \rfloor} [\nu(T_2, k) - \nu(T_1, k)] \, [k(n-k)]^\lambda > 0$$

i. e.,

$$\sum_{k=1}^{\lfloor n/2 \rfloor} \nu(T_1, k) \, [k(n-k)]^\lambda < \sum_{k=1}^{\lfloor n/2 \rfloor} \nu(T_2, k) \, [k(n-k)]^\lambda$$

and, in view of (10),

$${}^mW_\lambda(T_1) < {}^mW_\lambda(T_2) \; . \quad \square$$

Lemma 7. *Let $a_1, a_2, \ldots, a_m$ be numbers, not all of which being equal to zero, such that*

$$\sum_{k=1}^{j} a_k \; \geq \; 0 \tag{14}$$

holds for all $j = 1, 2, \ldots, m-1$, and

$$\sum_{k=1}^{m} a_k \; = \; 0 \; . \tag{15}$$

Let $b_1, b_2, \ldots, b_m$ be numbers, such that $0 < b_1 < b_2 < \cdots < b_m$,. Then

$$\sum_{k=1}^{m} a_k \, b_k \; < \; 0 \; .$$

Proof. For $j = 1, 2, \ldots, m-1$, multiply (14) by $b_j - b_{j+1} < 0$, and multiply (15) by $b_m > 0$. Then proceed in an analogous manner as in the proof of Lemma 5. $\square$

Theorem 8. *Let $T_1, T_2 \in \mathcal{T}$. If $T_1 \prec_s T_2$, then ${}^mW_\lambda(T_1) > {}^mW_\lambda(T_2)$ for all values of $\lambda > 0$.*

Proof is analogous as of Theorem 6. We have again

$$\sum_{k=1}^{j} [\nu(T_2, k) - \nu(T_1, k)] \geq 0$$

for $j = 1, 2, \ldots, \lfloor n/2 \rfloor - 1$, whereas for $j = \lfloor n/2 \rfloor$,

$$\sum_{k=1}^{j} [\nu(T_2, k) - \nu(T_1, k)] = 0$$

because of (9).

Identifying $\lfloor n/2 \rfloor$ and $\nu(T_2, k) - \nu(T_1, k)$ with m and a_k in Lemma 7, choosing $b_k = [k(n-k)]^\lambda$, and bearing in mind that for $\lambda > 0$,

$$[1\,(n-1)]^\lambda < [2\,(n-2)]^\lambda < \cdots < [\lfloor n/2 \rfloor) \cdot \lceil n/2 \rceil]^\lambda$$

we see that all the conditions of Lemma 7 are fulfilled. Therefore, for $\lambda > 0$

$$\sum_{k=1}^{\lfloor n/2 \rfloor} [\nu(T_2, k) - \nu(T_1, k)]\,[k(n-k)]^\lambda < 0$$

resulting in ${}^m W_\lambda(T_1) > {}^m W_\lambda(T_2)$. □

References

[1] H. Wiener, *J. Am. Chem. Soc.* **69** (1947) 17–20.

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

[3] M. V. Diudea and I. Gutman, *Croat. Chem. Acta* **71** (1998) 21–51.

[4] O. Ivanciuc and D. J. Klein, *J. Chem. Inf. Comput. Sci.* **42** (2002) 8–22.

[5] I. Gutman and J. Žerovnik, *Croat. Chem. Acta* **75** (2002) 603–612.

[6] I. Gutman and O. E. Polansky, *Mathematical Concepts in Organic Chemistry*, Springer-Verlag, Berlin, 1986.

[7] S. Nikolić, N. Trinajstić and M. Randić, *Chem. Phys. Lett.* **333** (2001) 319–321.

[8] I. Gutman, D. Vukičević and J. Žerovnik, *Croat. Chem. Acta*, submitted.