MATCH
Communications in Mathematical and in Computer Chemistry

no. 50, February 2004
MATCDY (50) 93- 108 (2004)

ISSN 0340 - 6253

On Modified Wiener Indices of Thorn Graphs*

Damir Vukičević
Department of Mathematics, University of Split,
Nikole Tesle 12, HR-21000, Split, Croatia
damir.vukicevic@pmfst.hr

Ante Graovac
The R. Bošković Institute,
POB 180, HR-10002, Zagreb, Croatia,
and Faculty of Science, University of Split,
Nikole Tesle 12, HR-21000, Split, Croatia
graovac@rudjer.irb.hr

Received: December 30, 2002

Abstract

Considerable attention has been recently paid to thorn graphs as chemical models. Here, we consider, three classes of thorn trees T^*.The recently introduced λ-modified Wiener index ${}^mW_\lambda$, is a reasonable generalization of the well-known Wiener index W, as it fulfills basic requirements to model branching. The explicit formulae are given to calculate ${}^mW_\lambda(T^*)$ in terms of λ-modified Wiener indices of parent tree T for all three classes of thorn trees

*Dedicated to Professor Haruo Hosoya who introduced the notion of topological index 31 years ago and after that made a long lasting contributions to theory and applications of topological indices.

considered. These formulae represent a generalization of Gutman's results on W for the same classes of thorn trees discussed here.

1 Introduction

The connectivity of atoms in a molecule is conveniently described by its molecular graph, $G = G(M)$ [1,2]. The set of vertices $V = V(G) = \{v_1, v_2, ..., v_n\}$, correspond to atoms, and set of edges, $E = E(G) = \{e_1, e_2, ..., e_m\}$, to chemical bonds in molecule, where n and m stand for cardinalities of $V$and E, $n = n(G) = |V(G)|$ and $m = m(G) = |E(G)|$. The number of edges incident to a given vertex v_i is called its vertex degree and is denoted by γ_i. It corresponds to the valence of its corresponding atom.

The information given by graph G could be compressed to a number, so called *molecular descriptor* [3]. Of course, there is an infinite number of ways to do this and only those descriptors which are able to correlate well with physical, chemical and biological properties of molecules are of interest to study. The particular descriptor Z was developed by Hosoya 31 years ago [4] and named *Topological index*. Since then other molecular descriptors as well are called topological indices. These indices have found enormous application in QSPR (Quantitative Structure Property Relationships) and QSAR (Quantitative Structure Activity Relationships) and other studies, and for an overview reader is referred to recent monograph [5].

The first and most studied topological index up to now is Wiener index [6], $W(G)$, which in Hosoya's formulation is defined by (half of) the sum of distances between all possible pairs of vertices in G.However, in the original paper of Wiener $W = W(G)$is defined by:

$$W = \sum_{e} n_{G,1}(e) \cdot n_{G,2}(e), \tag{1}$$

where $n_{G,1}(e)$. $n_{G,2}(e)$ are the numbers of vertices of G lying on two sides of the edge $e$and summation goes over all edges of G. Note, that definition (1) applies only to *trees*, i. e. to (connected) graphs possessing no cycles. Many chemical compounds like alkanes, alkenes and alkynes are conveniently represented by trees.

In recent years, a new class of trees, so called thorn trees have been studied [7,8] as a model to describe dendrimers. Study of dendrimers has become a very active interdisciplinary research area which has an enormous potential for applications ranging from optoelectronics, catalisys up to drug delivery. The classes of dendrimers which have arised a special attention are fullerodendrimers, antibody-dendrimer conjugates, dendryzimes, biodendrimers and similar.

The *thorn graph* $G^{*} = G^{*}(p_1, ..., p_n)$ of G is obtained by attaching p_i new vertices of degree 1 to the vertex v_i of G, 1,2,...,m, and obviously repetition of such a procedure is suited to model a dendritic growth.

For G being a tree T, $G^{*} = T^{*}$is called *a thorn tree* and in the present paper, we consider only torn trees, namely more specifically only the following three classes of thorn trees:

Class 1. The thorn trees where an equal number p of vertices is added to each vertex, i. e. $p_1 = p_2 = ... = p_n = p$.

Class 2. The thorn trees where the number of added vertices to every vertex equals its degree, i. e. $p_i = \gamma_i$, $i = 1, 2, ..., n$.

Class 3. The thorn trees where to each vertex of T so many vertices are added to make it of a degree γ, i. e. $p_i = \gamma - \gamma_i$, $i = 1, 2, ..., n$, where of course $\gamma > \gamma_i$, $i = 1, 2, ..., n$

Recently, the original Wiener's Definition 1 was generalized to [9]:

$$^{m}W_{\lambda} = \sum_{e} \{n_{G,1}(e) \cdot n_{G,2}(e)\}^{\lambda}, \quad \lambda \in \mathbb{R}, \tag{2}$$

and $^{m}W_{\lambda}$ is called *λ-modified Wiener index.* A special case for $\lambda = -1$ was put forward by Nikolić *at al.* It has been proven that $^{m}W_{\lambda}$, in parallel with $W = {}^{m}W_1$, satisfies two basic requirements (described in [10]) to represent a proper measure of branching.

Our main result is given in the next chapter and it presents the explicit formulae to calculate $^{m}W_{\lambda}$ in terms of λ-modified Wiener indices of original tree T with T^{*} being thorn trees of *Classes 1-3.* The proof for *Class 1* is given in *Chapter 3* and it shows that $^{m}W_{\lambda}(T^{*})$ is a linear function of $^{m}W_{\lambda}(T)$ for any real value of λ. The *Chapters 4-5* give the proof for *Classes 2-3*, and show that then $^{m}W_{\lambda}(T^{*})$ is a linear function of indices ${}^{m}W_{\mu}$ of T, $\mu = 0, 1, ..., \lambda$, where λ is a natural number and μ runs only over natural numbers and zero.

2 The Main Result

Our paper generalize the results of Gutman [7], i. e. his three Corollaries.

Corollary 1.1 of [7]

$$W(T^{*}) \equiv {}^{m}W_{1}(T^{*}) = (p+1)^{2} \cdot W(T) + np(np+n-1), \quad (3)$$

where T^{*} is a thorn graph of *Class 1*, we generalize to

Theorem 1

$${}^{m}W_{\lambda}(T^{*}) = (p+1)^{2\lambda} \cdot {}^{m}W_{\lambda}(T) + np(np+n-1)^{\lambda}. \quad (4)$$

for any real λ.

Corollary 1.2 of [7]

$$W(T^{*}) \equiv {}^{m}W_{1}(T^{*}) = 9 \cdot W(T) + (n-1)(3n-5). \quad (5)$$

where T^{*} is a thorn graph of *Class 2*, we generalize for λ being a natural number k to

Theorem 2

$${}^{m}W_{k}(T^{*}) = \sum_{i=0}^{k} \left[\binom{k}{i} 9^{i} (1-3n)^{k-i} \cdot {}^{m}W_{i}(T) \right] + (2n-2) \cdot (3n-3)^{k}. \quad (6)$$

Our final generalization concerns

Corollary 1.3 of [7]

$$W(T^{*}) \equiv {}^{m}W_{1}(T^{*}) = (\gamma-1)^{2} \cdot W(T) + [(\gamma-1)n+1]^{2}. \quad (7)$$

where T^* is a thorn graph of *Class 3* and λ is a natural number k, and reads as

Theorem 3

$$\begin{aligned} {}^{k}W(T^*) &= \sum_{i=0}^{k}\left[\binom{k}{i}(\gamma-1)^{2i}\left((\gamma-1)n+1\right)^{k-i}\cdot {}^{i}W(T)\right] + \qquad (8) \\ &\quad + ((\gamma-2)n+2)\cdot((\gamma-1)n+1)^{k}. \end{aligned}$$

3 The λ-Modified Wiener Index for Thorn Trees of Class 1

After noting that

$$[n_{T^*,1}(e)\cdot n_{T^*,2}(e)]^{\lambda} = (p+1)^{2\lambda}\cdot[n_{T,1}(e)\cdot n_{T,2}(e)]^{\lambda}, \text{ for each } e\in E(T). \qquad (9)$$

We have

$$\begin{aligned} {}^{\lambda}W(T^*) &= \sum_{e\in E(T^*)}[n_{T^*,1}(e)\cdot n_{T^*,2}(e)]^{\lambda} \qquad (10) \\ &= \sum_{e\in E(T)}[n_{T^*,1}(e)\cdot n_{T^*,2}(e)]^{\lambda} + \sum_{e\in E(T^*)\setminus E(T)}[n_{T^*,1}(e)\cdot n_{T^*,2}(e)]^{\lambda} \\ &= (p+1)^{2\lambda}\cdot\sum_{e\in E(T)}[n_{T,1}(e)\cdot n_{T,2}(e)]^{\lambda} + \sum_{e\in E(T^*)\setminus E(T)}[(np+n-1)\cdot 1]^{\lambda} \\ &= (p+1)^{2\lambda}\cdot{}^{\lambda}W(T) + np\cdot(np+n-1)^{\lambda}. \end{aligned}$$

The dependence between ${}^{\lambda}W(T^*)$ and ${}^{\lambda}W(T)$ remains linear no matter what λ we choose.

4 The λ-Modified Wiener Index for Thorn Trees of Class 2

Before proceeding, we shall need some technical results:

Lemma 4 *Let M_0 be the following matrix:*

$$M_0 = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & \ddots & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix}, \tag{11}$$

of the type $(k+1) \times (k+1)$. Its powers shift 1's downwards, and so in its i-th power, $1 \leq i \leq k$, the 1st column starts with i zeros, the 2nd column with $(i+1)$ zeros and so on:

$$M_0^i = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ \vdots & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & \ddots & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \end{bmatrix}. \tag{12}$$

Obviously, M_0^{k+1} is null-matrix.

Lemma 5 *Let M be the following matrix*

$$M = \begin{bmatrix} y & 0 & 0 & 0 \\ x & y & 0 & 0 \\ 0 & \ddots & \ddots & 0 \\ 0 & 0 & x & y \end{bmatrix} \tag{13}$$

of the type $(k+1) \times (k+1)$, and S be the column matrix with the first entry equals z and other k entries equal zero:

$$S = \begin{bmatrix} z \\ 0 \\ \vdots \\ 0 \end{bmatrix}. \tag{14}$$

Then it holds:

$$M^k \cdot S = \begin{bmatrix} y^k z \\ \binom{k}{1} x y^{k-1} z \\ \vdots \\ \binom{k}{k-1} x^{k-1} y z \\ x^k z \end{bmatrix}. \tag{15}$$

Proof. Note that $M = xM_0 + yI$, where I is the unit matrix of the type $(k+1) \times (k+1)$. Therefore,

$$M^k = \sum_{i=0}^{k} \binom{k}{i} x^i y^{k-i} M_0^i. \tag{16}$$

and by use of Lemma 4, one obtains:

$$M^k = \begin{bmatrix} y^k & 0 & 0 & 0 & 0 \\ \binom{k}{1} xy^{k-1} & y^k & 0 & 0 & 0 \\ \ddots & \binom{k}{1} xy^{k-1} & y^k & 0 & 0 \\ \binom{k}{k-1} x^{k-1} y & \ddots & \ddots & \ddots & 0 \\ x^k & \binom{k}{k-1} x^{k-1} y & \ddots & \binom{k}{1} xy^{k-1} & y^k \end{bmatrix}, \tag{17}$$

and by multiplying this with S, we finally get equation (15) . ∎

Lemma 6 *If T^* is the thorn graph of Class 2 of the tree T, i. e. T^* with parameters $p_i = \gamma_i$, $i = 1, 2, .., n$, then ${}^kW(T^*)$ and ${}^iW(T)$, $1 \le i \le k$ are related as*

$$\begin{aligned} {}^kW(T^*) &= \begin{bmatrix} {}^0W(T) \\ {}^1W(T) \\ {}^2W(T) \\ \vdots \\ {}^kW(T) \end{bmatrix}^T \cdot \left(\begin{bmatrix} 1-3n & 0 & 0 & 0 \\ 9 & 1-3n & 0 & 0 \\ 0 & \ddots & \ddots & 0 \\ 0 & 0 & 9 & 1-3n \end{bmatrix}^k \cdot \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} \right) \\ &\quad + (2n-2) \cdot (3n-3)^k . \end{aligned} \tag{18}$$

Proof. We have

$${}^kW(T^*) = \sum_{e \in E(T)} (n_{T^*,1}(e) \cdot n_{T^*,2}(e))^k + \sum_{e \in E(T^*) \setminus E(T)} (n_{T^*,1}(e) \cdot n_{T^*,2}(e))^k \tag{19}$$

Simple calculation shows that $n(T^*) = 3n - 2$, $n = n(T)$,and from here it easily follows

$$\sum_{e \in E(T^*) \setminus E(T)} (n_{T^*,1}(e) \cdot n_{T^*,2}(e))^k = (2n-2) \cdot (3n-3)^k . \tag{20}$$

It remains to prove that:

$$\sum_{e\in E(T)} \left(n_{T^*,1}(e)\cdot n_{T^*,2}(e)\right)^k =$$

$$= \begin{bmatrix} {}^0W(T) \\ {}^1W(T) \\ {}^2W(T) \\ \vdots \\ {}^kW(T) \end{bmatrix}^{\tau} \cdot \left(\begin{bmatrix} 1-3n & 0 & 0 & 0 \\ 9 & 1-3n & 0 & 0 \\ 0 & \ddots & \ddots & 0 \\ 0 & 0 & 9 & 1-3n \end{bmatrix}^k \cdot \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} \right) \tag{21}$$

and prior to doing that, we shall prove:

$$n_{T^*,1}(e) = 3\cdot n_{T,1}(e)-1, \text{ for each } e\in E(T) \tag{22}$$

$$n_{T^*,2}(e) = 3\cdot n_{T,2}(e)-1, \text{ for each } e\in E(T). \tag{23}$$

Note that

$$\sum_{u\in N_{T,1}(e)} \gamma_T(u) = 2\cdot\left(n_{T^*,1}(e)-1\right)+1, \tag{24}$$

where $\gamma_T(u)$ is the degree of vertex u in T, and so:

$$n_{T^*,1}(e) = 3\cdot n_{T,1}(e)-1, \text{ for each } e\in E(T). \tag{25}$$

The relation (23) is proved completely analogously.

Now, we shall prove (21) by the induction on k. First, assume that $k=1$. We have

$$\begin{bmatrix} {}^0W(T) \\ {}^1W(T) \\ {}^2W(T) \\ \vdots \\ {}^kW(T) \end{bmatrix}^{\tau} \cdot \left(\begin{bmatrix} 1-3n & 0 & 0 & 0 \\ 9 & 1-3n & 0 & 0 \\ 0 & \ddots & \ddots & 0 \\ 0 & 0 & 9 & 1-3n \end{bmatrix} \cdot \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} \right) =$$

$$\begin{aligned}
&= (1-3n)(n-1)+9\cdot{}^1W(T) = \\
&= \sum_{e\in E(T)} \left(1-3\left(n_{T,1}(e)+n_{T,2}(e)\right)+9\cdot n_{T,1}(e)\cdot n_{T,2}(e)\right) = \\
&= \sum_{e\in E(T)} \left(3n_{T,1}(e)-1\right)\cdot\left(3n_{T,2}(e)-1\right) \\
&= \sum_{\in e\in E(T)} \left(n_{T^*,1}(e)\cdot n_{T^*,2}(e)\right)^1.
\end{aligned} \tag{26}$$

Now, let us prove the inductive step. Suppose that claim is true for each $k < k_0$ and let us prove it for $k = k_0$. Denote:

$$\begin{bmatrix} \alpha_0 \\ \alpha_1 \\ \vdots \\ \alpha_k \end{bmatrix} = \begin{bmatrix} 1-3n & 0 & 0 & 0 \\ 9 & 1-3n & 0 & 0 \\ 0 & \ddots & \ddots & 0 \\ 0 & 0 & 9 & 1-3n \end{bmatrix}^{k-1} \cdot \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}. \tag{27}$$

From the inductive hypothesis, it follows that:

$$\sum_{e \in E(T)} (n_{T^\bullet,1}(e) \cdot n_{T^\bullet,2}(e))^{k-1} = \sum_{i=0}^{k-1} \left(\alpha_i \cdot \sum_{e \in E(T)} (n_{T,1}(e) \cdot n_{T,2}(e))^i \right). \tag{28}$$

We also have

$$\begin{aligned} &\begin{bmatrix} 1-3n & 0 & 0 & 0 \\ 9 & 1-3n & 0 & 0 \\ 0 & \ddots & \ddots & 0 \\ 0 & 0 & 9 & 1-3n \end{bmatrix}^{k} \cdot \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} = \\ = &\begin{bmatrix} 1-3n & 0 & 0 & 0 \\ 9 & 1-3n & 0 & 0 \\ 0 & \ddots & \ddots & 0 \\ 0 & 0 & 9 & 1-3n \end{bmatrix} \cdot \begin{bmatrix} \alpha_0 \\ \alpha_1 \\ \vdots \\ \alpha_k \end{bmatrix} \\ = &\begin{bmatrix} (1-3n) \cdot \alpha_0 \\ 9\alpha_0 + (1-3n) \cdot \alpha_1 \\ \vdots \\ 9\alpha_{k-1} + (1-3n) \cdot \alpha_k \end{bmatrix}, \end{aligned} \tag{29}$$

and so it remains to prove that

$$\sum_{e \in E(T)} (n_{T^\bullet,1}(e) \cdot n_{T^\bullet,2}(e))^k = \tag{30}$$

$$= (1-3n) \cdot \alpha_0 \cdot (n-1) + \sum_{i=1}^{k-1} \left((9\alpha_{i-1} + (1-3n) \cdot \alpha_i) \cdot \sum_{e \in E(T)} (n_{T,1}(e) \cdot n_{T,2}(e))^i \right)$$

i.e. that

$$\sum_{e\in E(T)}\left[\begin{array}{c}((3\cdot n_{T,1}(e)-1)\cdot(3\cdot n_{T,2}(e)-1))^{k-1}\cdot\\(9\cdot n_{T,1}(e)\cdot n_{T,2}(e)+(1-3n))\end{array}\right]=$$
$$=(1-3n)\cdot\alpha_0\cdot(n-1)+$$
$$+\sum_{i=1}^{k-1}\left((9\alpha_{i-1}+(1-3n)\cdot\alpha_i)\cdot\sum_{e\in E(T)}(n_{T,1}(e)\cdot n_{T,2}(e))^i\right)\quad(31)$$

Note that

$$\sum_{e\in E(T)}\left[((3\cdot n_{T,1}(e)-1)\cdot(3\cdot n_{T,2}(e)-1))^{k-1}\cdot(1-3n)\right]=$$
$$=(1-3n)\cdot\sum_{e\in E(T)}((3\cdot n_{T,1}(e)-1)\cdot(3\cdot n_{T,2}(e)-1))^{k-1}$$
$$=(1-3n)\cdot\left(\alpha_0\cdot(n-1)+\sum_{i=1}^{k-1}\left(\alpha_i\cdot\sum_{e\in E(T)}(n_{T,1}(e)\cdot n_{T,2}(e))^i\right)\right)\quad(32)$$

Also, we have

$$\sum_{e\in E(T)}\left[((3\cdot n_{T,1}(e)-1)\cdot(3\cdot n_{T,2}(e)-1))^{k-1}\cdot(n_{T,1}(e)\cdot n_{T,2}(e))\right]=$$
$$=\sum_{i=0}^{k-1}\left(\alpha_i\cdot\sum_{e\in E(T)}(n_{T,1}(e)\cdot n_{T,2}(e))^{i+1}\right)$$
$$=\sum_{i=1}^{k}\left(\alpha_{i-1}\cdot\sum_{e\in E(T)}(n_{T,1}(e)\cdot n_{T,2}(e))^i\right)\quad(33)$$

By multiplying relation (33) with 9 and summing the result with (32), we get (31). So, the claim is proved. ■

By combining *Lemma 6* and *Lemma 5*, we get finally *Theorem 2*. This is indeed a generalization of *Corollary 1.2*, because linear dependence is preserved.

5 The λ-Modified Wiener Index for Thorn Graphs of Class 3

Lemma 7 *Let γ be an integer with the property $\gamma \geqslant \gamma_i$, $i = 1, ..., n$ and $k \in \mathbb{N}$ be any integer. If T^* is the thorn graph of Class 3, i. e. T^* with parameters $p_i = \gamma - \gamma_i$, $i = 1, ..., n$, then ${}^kW(T^*)$ and ${}^iW(T)$, $1 \le i \le k$, are related as*

$$
{}^kW(T^*) = \begin{bmatrix} {}^0W(T) \\ {}^1W(T) \\ {}^2W(T) \\ \vdots \\ {}^kW(T) \end{bmatrix}^T \cdot \left(\begin{bmatrix} y & 0 & 0 & 0 \\ (\gamma-1)^2 & y & 0 & 0 \\ 0 & \ddots & \ddots & 0 \\ 0 & 0 & (\gamma-1)^2 & y \end{bmatrix}^k \cdot \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} \right) +
$$
$$
+ ((\gamma-2)n+2) \cdot ((\gamma-1)n+1)^k . \qquad (34)
$$

where $y = (\gamma - 1)n + 1$.

Proof. We have

$$
{}^kW(T^*) = \sum_{e \in E(T)} (n_{T^*,1}(e) \cdot n_{T^*,2}(e))^k + \sum_{e \in E(T^*) \setminus E(T)} (n_{T^*,1}(e) \cdot n_{T^*,2}(e))^k . \qquad (35)
$$

Simple calculation shows that $n(T^*) = (\gamma - 1)n + 2$, $n = n(T)$, and from here, it easily follows that:

$$
\sum_{e \in E(T^*) \setminus E(T)} (n_{T^*,1}(e) \cdot n_{T^*,2}(e))^k = ((\gamma-2)n+2) \cdot ((\gamma-1)n+1)^k . \qquad (36)
$$

It remains to prove that:

$$
\sum_{e \in E(T)} (n_{T^*,1}(e) \cdot n_{T^*,2}(e))^k =
$$
$$
= \begin{bmatrix} {}^0W(T) \\ {}^1W(T) \\ {}^2W(T) \\ \vdots \\ {}^kW(T) \end{bmatrix}^T \cdot \left(\begin{bmatrix} y & 0 & 0 & 0 \\ (\gamma-1)^2 & y & 0 & 0 \\ 0 & \ddots & \ddots & 0 \\ 0 & 0 & (\gamma-1)^2 & y \end{bmatrix}^k \cdot \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} \right) \qquad (37)
$$

Before proving the above we should prove that:

$$\begin{aligned} n_{T^{\bullet},1}(e) &= (\gamma-1)\cdot n_{T,1}(e)+1, \text{ for each } e\in E(T) & (38)\\ n_{T^{\bullet},2}(e) &= (\gamma-1)\cdot n_{T,2}(e)+1, \text{ for each } e\in E(T), & (39)\end{aligned}$$

Note that

$$\sum_{x\in N_{T,1}(e)}(\gamma-d_T(e))=\gamma n_{T,1}(e)-(2\cdot(n_{T^{\bullet},1}(e)-1)+1), \tag{40}$$

and so

$$n_{T^{\bullet},1}(e)=(\gamma-1)\cdot n_{T,1}(e)+1, \text{ for each } e\in E(T) \tag{41}$$

holds. The relation (39) can be proved completely analogously.

Now, we shall prove (37) by the induction on k. First, assume that $k=1$. We have

$$\begin{aligned}
&\begin{bmatrix} {}^0W(T)\\ {}^1W(T)\\ {}^2W(T)\\ \vdots\\ {}^kW(T)\end{bmatrix}^T\cdot\left(\begin{bmatrix} y & 0 & 0 & 0\\ (\gamma-1)^2 & y & 0 & 0\\ 0 & \ddots & \ddots & 0\\ 0 & 0 & (\gamma-1)^2 & y\end{bmatrix}\cdot\begin{bmatrix}1\\0\\ \vdots\\0\end{bmatrix}\right)=\\
&= (n-1)\cdot((\gamma-1)n+1)+(\gamma-1)^2\cdot{}^1W(T)\\
&= \sum_{e\in E(T)}\left[(\gamma-1)(n_{T,1}(e)+n_{T,2}(e))+1+(\gamma-1)^2\cdot n_{T,1}(e)\cdot n_{T,2}(e)\right]\\
&= \sum_{e\in E(T)}\left[(\gamma-1)\cdot n_{T,1}(e)+1\right]\cdot\left[(\gamma-1)\cdot n_{T,2}(e)+1\right]\\
&= \sum_{e\in E(T)}\left(n_{T^{\bullet},1}(e)\cdot n_{T^{\bullet},2}(e)\right)^1. \qquad (42)
\end{aligned}$$

Now, let us prove the inductive step. Suppose that claim is true for each $k<k_0$ and let us prove it for $k=k_0$. Denote

$$\begin{bmatrix}\alpha_0\\ \alpha_1\\ \vdots\\ \alpha_k\end{bmatrix}=\begin{bmatrix} y & 0 & 0 & 0\\ (\gamma-1)^2 & y & 0 & 0\\ 0 & \ddots & \ddots & 0\\ 0 & 0 & (\gamma-1)^2 & y\end{bmatrix}^{k-1}\cdot\begin{bmatrix}1\\0\\ \vdots\\0\end{bmatrix}. \tag{43}$$

From the inductive hypothesis, it follows that:

$$\sum_{e\in E(T)} \left(n_{T^*,1}(e)\cdot n_{T^*,2}(e)\right)^{k-1} = \sum_{i=0}^{k-1}\left(\alpha_i \cdot \sum_{e\in E(T)} \left(n_{T,1}(e)\cdot n_{T,2}(e)\right)^i\right). \tag{44}$$

We also have:

$$\begin{aligned}
&\begin{bmatrix} y & 0 & 0 & 0 \\ (\gamma-1)^2 & y & 0 & 0 \\ 0 & \ddots & \ddots & 0 \\ 0 & 0 & (\gamma-1)^2 & y \end{bmatrix}^k \cdot \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} = \\
= &\begin{bmatrix} y & 0 & 0 & 0 \\ (\gamma-1)^2 & y & 0 & 0 \\ 0 & \ddots & \ddots & 0 \\ 0 & 0 & (\gamma-1)^2 & y \end{bmatrix} \cdot \begin{bmatrix} \alpha_0 \\ \alpha_1 \\ \vdots \\ \alpha_k \end{bmatrix} = \\
= &\begin{bmatrix} y\cdot\alpha_0 \\ (\gamma-1)^2\cdot\alpha_0 + y\cdot\alpha_1 \\ \vdots \\ (\gamma-1)^2\cdot\alpha_{k-1} + y\cdot\alpha_k \end{bmatrix}.
\end{aligned} \tag{45}$$

so it remains to prove that

$$\begin{aligned}
&\sum_{e\in E(T)} \left(n_{T^*,1}(e)\cdot n_{T^*,2}(e)\right)^{k-1} = \\
= \; & y\cdot\alpha_0\cdot(n-1) + \\
&+\sum_{i=1}^{k-1}\left(\left((\gamma-1)^2\alpha_{i-1} + y\cdot\alpha_i\right)\cdot \sum_{e\in E(T)} \left(n_{T,1}(e)\cdot n_{T,2}(e)\right)^i\right)
\end{aligned} \tag{46}$$

i.e. that

$$\begin{aligned}
&\sum_{e\in E(T)} \begin{bmatrix} \left[\left((\gamma-1)\cdot n_{T,1}(e)+1\right)\cdot\left((\gamma-1)\cdot n_{T,1}(e)+1\right)\right]^{k-1}\cdot \\ \left((\gamma-1)^2\cdot n_{T,1}(e)\cdot n_{T,2}(e) + \left((\gamma-1)n+1\right)\right) \end{bmatrix} = \\
= \; & y\cdot\alpha_0\cdot(n-1) + \\
&+\sum_{i=1}^{k-1}\left(\left((\gamma-1)^2\alpha_{i-1} + y\cdot\alpha_i\right)\cdot \sum_{e\in E(T)} \left(n_{T,1}(e)\cdot n_{T,2}(e)\right)^i\right).
\end{aligned} \tag{47}$$

Note that

$$\sum_{e\in E(T)}\left[\left(\left((\gamma-1)\cdot n_{T,1}(e)+1\right)\cdot\left((\gamma-1)\cdot n_{T,1}(e)+1\right)\right]^{k-1}\cdot\left((\gamma-1)n+1\right)\right]=$$

$$=\ \left((\gamma-1)n+1\right)\cdot\sum_{e\in E(T)}\left[\left(\left((\gamma-1)\cdot n_{T,1}(e)+1\right)\cdot\left((\gamma-1)\cdot n_{T,1}(e)+1\right)\right]^{k-1}\right]$$

$$=\ y\cdot\left[\alpha_0\cdot(n-1)+\sum_{i=1}^{k-1}\left(\alpha_i\cdot\sum_{e\in E(T)}\left(n_{T,1}(e)\cdot n_{T,2}(e)\right)^i\right)\right]. \tag{48}$$

Also, we have

$$\sum_{e\in E(T)}\left[\left(\left((\gamma-1)\cdot n_{T,1}(e)+1\right)\cdot\left((\gamma-1)\cdot n_{T,1}(e)+1\right)\right]^{k-1}\cdot n_{T,1}(e)\cdot n_{T,2}(e)\right]$$

$$=\ \sum_{i=0}^{k-1}\left(\alpha_i\cdot\sum_{e\in E(T)}\left(n_{T,1}(e)\cdot n_{T,2}(e)\right)^{i+1}\right)$$

$$=\ \sum_{i=1}^{k}\left(\alpha_{i-1}\cdot\sum_{e\in E(T)}\left(n_{T,1}(e)\cdot n_{T,2}(e)\right)^{i}\right) \tag{49}$$

By multiplying relation (49) with $(\gamma-1)^2$ and summing the result with (48), we get (47). So, the claim is proved. ■

By combining Lemma 7 and Lemma 5, we get *Theorem 3.* This is indeed a generalization of *Corollary 1.3,* because linear dependence is preserved.

6 Conclusions

Special cases of thorn graphs have been already considered by Cayley [11] and later by Polya [12], as means to proceed from hydrogen suppressed to full molecular graphs. Recently, they have raised a renewed interest in chemistry, e. g. as a model to represent organic molecules [14] and to describe dendrimers [8]. Here, we have studied three special classes of thorn trees.

We have been able to derive explicit formulae for λ-modified Winer index, ${}^{m}W_{\lambda}$, for these three special classes of thorn trees. For the *Class 1,* the formula linearly relates ${}^{m}W_{\lambda}(T^{*})$ with a single ${}^{m}W_{\lambda}(T)$ of the parent tree T, and it holds for all real values of λ. The formulae for *Classes 2-3* give ${}^{m}W_{\lambda}(T^{*})$ as a linear function of indices ${}^{m}W_{\mu}(T)$, $\mu = 0, 1, ..., \lambda$, but now the formulae hold only for λ being a natural number. The above results are formulated in three theorems which are a generalization of analogous ones derived by Gutman for the Wiener index W of the thorn graphs.

The above fact leads to the problem of deriving explicit formulae for ${}^{m}W_{\lambda}(T^{*})$ for real values of λ, where T^{*} is a thorn graph of *Class 2 or Class 3*.

Although there is enormous proliferation of topological indices, the λ-modified Wiener indices considered here should be of chemical interest as they satisfy the basic requirements imposed on an index to be of use in modelling molecular branching. However, the ordering of molecules induced by these novel indices changes with a change in value of λ [13], what gives a framework to model a variety of different properties of molecules, but it remains an open question which λ is the most suitable to model a particular molecular property.

7 Acknowledgements

The partial support of the Ministry of Science and Technology of Republic Croatia (Grant No. 0037117 and Grant No. 009839) is gratefully acknowledged.

8 References

[1] A. Graovac, I. Gutman, and N. Trinajstić, Topological Approach to the Chemistry of Conjugated Molecules. *Springer-Verlag*, Berlin 1977.

[2] N. Trinajstić, Chemical Graph Theory. *CRC Press*, Boca Raton, 1983; 2nd revised ed. 1992.

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

[4] H. Hosoya, *Bull. Chem. Jpn.* **44** (1971) 2332-2339.

[5] R. Todeschini and V. Consonni, Handbook of Molecular Descriptors,

Wiley-VCH, Weinheim, 2000.

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

[7] I. Gutman, *Publ. Inst. Math. (Beograd)* **63** (1998) 31-36.

[8] D. Bonchev and D. J. Klein, Croat. Chem. Acta. **75** **(2)** (2002), 613-620.

[9] I. Gutman, D. Vukičević, and J. Žerovnik, Croat. Chem. Acta., in press.

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

[11] A. Cayley, *Phil. Magazine* **47** (1874) 444-446.

[12] G. Polya, *Acta Math.* **68** (1937) 145-254.

[13] D. Vukičević, *MATCH - Commun. Math. Comput. Chem.*. **47** (2003) 87-105. .

[14] I. Gutman, D. Vidović, and L. Popović, *J. Chem. Soc. Faraday Trans* **94** (1998) 857-860