MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **70** (2013) 901-919

ISSN 0340 - 6253

Chemical Graphs Constructed from Rooted Product and Their Zagreb Indices

Mahdieh Azari and Ali Iranmanesh*

Department of Pure Mathematics, Faculty of Mathematical Sciences, Tarbiat Modares University, P. O. Box: 14115-137, Tehran, Iran

iranmanesh@modares.ac.ir

(Received March 16, 2013)

Abstract. Rooted product of n vertex graph H by a sequence of n rooted graphs $G_1, G_2, \dots, G_n$, is the graph obtained by identifying the root vertex of G_i with the i-th vertex of H for all $i = 1,2,\dots,n$. In this paper, we show how the first and second Zagreb indices of rooted product of graphs are determined from the respective indices of the individual graphs. The first and second Zagreb indices of cluster of graphs, thorn graphs and bridge graphs as three important special cases of rooted product are also determined. Using these formulae, the first and second Zagreb indices of several important classes of chemical graphs will be computed.

1. Introduction

In this paper, we consider connected finite graphs without any loops or multiple edges. Let G be such a graph with the vertex set $V(G)$ and the edge set $E(G)$. For $u \in V(G)$, we denote by $N_G(u)$ the set of all neighbors of u in G. Cardinality of the set $N_G(u)$ is called the degree of u in G and will be denoted by $\deg_G(u)$. We denote by $\alpha_G(u)$, the sum of degrees of all neighbors of the vertex u in G, i.e., $\alpha_G(u) = \sum_{a \in N_G(u)} \deg_G(a)$. We denote by $|S|$ the cardinality of a set S.

*Corresponding author

In theoretical Chemistry, the physico-chemical properties of chemical compounds are often modeled by the molecular graph based molecular structure descriptors which are also referred to as topological indices [1]. The Zagreb indices belong among the oldest topological indices, and were introduced as early as in 1972 [2,3]. For details on their theory and applications see [4-7], and especially the recent papers [8-11]. The first and second Zagreb indices of G are denoted by $M_1(G)$ and $M_2(G)$, respectively and defined as follows:

$$M_1(G) = \sum_{u\in V(G)} \deg_G(u)^2 \text{ and } M_2(G) = \sum_{uv\in E(G)} \deg_G(u)\deg_G(v).$$

The first Zagreb index can also be expressed as a sum over edges of G:

$$M_1(G) = \sum_{uv\in E(G)} (\deg_G(u) + \deg_G(v)).$$

Let P_n, C_n and S_n denote the path, cycle and star on n vertices. It is easy to that;

$$M_1(P_n) = 4n-6, \qquad (n \geq 2),$$

$$M_2(P_2) = 1, M_2(P_n) = 4n-8, \qquad (n \geq 3),$$

$$M_1(C_n) = M_2(C_n) = 4n, \qquad (n \geq 3),$$

$$M_1(S_n) = n(n-1), M_2(S_n) = (n-1)^2, \quad (n \geq 2).$$

We denote by K_1, the single vertex graph and assume that $P_1 = S_1 = K_1$. Clearly, $M_1(K_1) = M_2(K_1) = 0$.

At this point, we recall the definition of rooted product of graphs. Let H be a labeled graph on n vertices and let G be a sequence of n rooted graphs $G_1, G_2, ..., G_n$. According to [12], the rooted product of H by G, denoted by $H(G) = H(G_1, G_2, ..., G_n)$ is the graph obtained by identifying the root vertex of G_i with the i-th vertex of H for all $i = 1,2,...,n$. In the special case when the components G_i, $i = 1,2,...,n$ are mutually isomorphic to a graph K, the rooted product of H by G is denoted by $H\{K\}$ and called the cluster of H and K.

In this paper, we determine the first and second Zagreb indices of rooted product of graphs. Also, we introduce several classes of chemical graphs which can be considered as the rooted product and apply our results to find the first and second Zagreb indices of them.

2. Zagreb indices of rooted product of graphs

Let H be a labeled graph on n vertices with the vertex set $V(H) = \{1,2,...,n\}$ and let G be a sequence of n rooted graphs $G_1, G_2, ..., G_n$. In this section, we compute the first and second

Zagreb indices of the rooted product of H by G. The first and second Zagreb indices of cluster of graphs, thorn graphs and bridge graphs as three important special cases of rooted product are also determined. For $i=1,2,\ldots,n$, we denote the root vertex of G_i by w_i and the degree of w_i in G_i by ω_i.

Theorem 2.1 The first and second Zagreb indices of the rooted product $H(G)$ are given by:

(i) $M_1(H(G)) = M_1(H) + \sum_{i=1}^{n} M_1(G_i) + 2\sum_{i=1}^{n} \omega_i \deg_H(i)$,

(ii) $M_2(H(G)) = M_2(H) + \sum_{i=1}^{n} M_2(G_i) + \sum_{i=1}^{n} \deg_H(i)\alpha_{G_i}(w_i) + \sum_{ij\in E(H)} [\omega_j \deg_H(i) + \omega_i \deg_H(j) + \omega_i\omega_j]$.

Proof. (i) Using definition of the first Zagreb index, we have:

$$M_1(H(G)) = \sum_{i=1}^{n} \{[\deg_H(i) + \omega_i]^2 + \sum_{u\in V(G_i)-\{w_i\}} \deg_{G_i}(u)^2\} =$$

$$\sum_{i=1}^{n} \deg_H(i)^2 + \sum_{i=1}^{n} [\omega_i^2 + \sum_{u\in V(G_i)-\{w_i\}} \deg_{G_i}(u)^2] + 2\sum_{i=1}^{n} \omega_i \deg_H(i) =$$

$$M_1(H) + \sum_{i=1}^{n} M_1(G_i) + 2\sum_{i=1}^{n} \omega_i \deg_H(i).$$

(ii) Using definition of the second Zagreb index, we have:

$$M_2(H(G)) = \sum_{ij\in E(H)} [\deg_H(i) + \omega_i][\deg_H(j) + \omega_j] +$$

$$\sum_{i=1}^{n} \{ \sum_{uv\in E(G_i);\ u,v\neq w_i} \deg_{G_i}(u)\deg_{G_i}(v) + \sum_{uv\in E(G_i);\ u\in V(G_i), v=w_i} \deg_{G_i}(u)[\deg_H(i) + \omega_i] \} =$$

$$\sum_{ij\in E(H)} \deg_H(i)\deg_H(j) + \sum_{ij\in E(H)} [\omega_j \deg_H(i) + \omega_i \deg_H(j) + \omega_i\omega_j] +$$

$$\sum_{i=1}^{n} \sum_{uv\in E(G_i)} \deg_{G_i}(u)\deg_{G_i}(v) + \sum_{i=1}^{n} \deg_H(i) \sum_{u\in N_{G_i}(w_i)} \deg_{G_i}(u) =$$

$$M_2(H) + \sum_{i=1}^{n} M_2(G_i) + \sum_{i=1}^{n} \deg_H(i)\alpha_{G_i}(w_i) + \sum_{ij\in E(H)} [\omega_j \deg_H(i) + \omega_i \deg_H(j) + \omega_i\omega_j]. \blacksquare$$

Suppose that w is the root vertex of a rooted graph K, and let $G_i = K$ and $w_i = w$ for all $i=1,2,\ldots,n$. Using Theorem 2.1, we easily arrive at:

Corollary 2.2 The first and second Zagreb indices of the cluster $H\{K\}$ are given by:

(i) $M_1(H\{K\}) = M_1(H) + nM_1(K) + 4m\omega$,

(ii) $M_2(H\{K\}) = \omega M_1(H) + M_2(H) + nM_2(K) + m(\omega^2 + 2\alpha_K(w))$,

where $\omega = \deg_K(w)$ and $m = |E(H)|$. $\blacksquare$

Let H be a labeled graph on n vertices. Choose a numbering for vertices of H such that its pendant vertices have numbers $1,2,...,k$ and its non-pendant vertices have numbers $k+1,...,n$. Let G be a sequence of n rooted graphs $G_1, G_2,...,G_n$ with $G_i = K_1$ for $i = k+1, k+2...,n$. Using Theorem 2.1, we can easily get the following result.

Corollary 2.3 The first and second Zagreb indices of the rooted product $H(G) = H(G_1, G_2,...,G_k, K_1, K_1,...,K_1)$ are given by:

(i) $M_1(H(G)) = M_1(H) + \sum_{i=1}^{k} M_1(G_i) + 2\sum_{i=1}^{k} \omega_i$,

(ii) If $H \neq P_2$, then $M_2(H(G)) = M_2(H) + \sum_{i=1}^{k} M_2(G_i) + \sum_{i=1}^{k} \alpha_{G_i}(w_i) + \sum_{i=1}^{k} \omega_i \alpha_H(i)$ and

$M_2(P_2(G_1, G_2)) = M_2(G_1) + M_2(G_2) + \alpha_{G_1}(w_1) + \alpha_{G_2}(w_2) + (\omega_1 + 1)(\omega_2 + 1)$,

where for $i = 1,2,...,k$, w_i denotes the root vertex of G_i and ω_i denotes its degree. ■

In the following Corollary, we consider the special case of Corollary 2.3, when the components G_i, $i = 1,2,...,k$ are mutually isomorphic to a rooted graph K.

Corollary 2.4 Let H be a labeled graph on n vertices whose pendant vertices have numbers $1,2,...,k$ and let K be a rooted graph with the root vertex w. Suppose G is a sequence of n rooted graphs $G_1, G_2,...,G_n$ with $G_i = K$ for $i = 1,2...,k$ and $G_i = K_1$ for $i = k+1, k+2...,n$. Then

(i) $M_1(H(G)) = M_1(H) + kM_1(K) + 2k\omega$,

(ii) If $H \neq P_2$, then $M_2(H(G)) = M_2(H) + k(M_2(K) + \alpha_K(w)) + \omega \sum_{i=1}^{k} \alpha_H(i)$, and

$M_2(P_2(G)) = 2M_2(K) + 2\alpha_K(w) + (\omega + 1)^2$, where $\omega = \deg_K(w)$. ■

Let G be a labeled graph on n vertices and let $p_1, p_2,...,p_n$ be non-negative integers. The thorn graph $G^*(p_1, p_2,...,p_n)$ of the graph G is obtained from G by attaching p_i pendant vertices to the i-th vertex of G, $i = 1,2,...,n$. The concept of thorny graphs was introduced by Ivan Gutman [13] and eventually found a variety of chemical applications [14-17]. The thorn graph $G^*(p_1, p_2,...,p_n)$ can be considered as the rooted product of G by the sequence $\{S_{p_1+1}, S_{p_2+1},...,S_{p_n+1}\}$, where the root vertex of S_{p_i+1} is assumed to be in the vertex of degree p_i, $i = 1,2,...,n$. So we can apply Theorem 2.1 to obtain the first and second Zagreb indices of the thorn graph $G^*(p_1, p_2,...,p_n)$.

Corollary 2.5 The first and second Zagreb indices of the thorn graph $G^*(p_1,p_2,...,p_n)$ are given by:

(i) $M_1(G^*(p_1,p_2,...,p_n)) = M_1(G)+\sum_{i=1}^{n} p_i(p_i+1)+2\sum_{i=1}^{n} p_i \deg_G(i)$,

(ii) If $G \neq P_2$, then

$M_2(G^*(p_1,p_2,...,p_n)) = M_2(G)+\sum_{i=1}^{n} p_i^{\,2}+\sum_{i=1}^{n} p_i \deg_G(i)+\sum_{ij\in E(G)}[p_j \deg_G(i)+p_i \deg_G(j)+p_i p_j]$,

and $M_2(P_2^*(p_1,p_2)) = p_1(p_1+1)+p_2(p_2+1)+(p_1+1)(p_2+1)$.■

Let $\{G_i\}_{i=1}^n$ be a set of finite pairwise disjoint graphs with vertices $w_i \in V(G_i)$. The bridge graph $B = B(G_1,G_2,...,G_n;w_1,w_2,...,w_n)$ of $\{G_i\}_{i=1}^n$ with respect to the vertices $\{w_i\}_{i=1}^n$ is the graph obtained from the graphs $G_1,G_2,...,G_n$ by connecting the vertices w_i and w_{i+1} by an edge for all $i=1,2,...,n-1$. We can consider the bridge graph $B = B(G_1,G_2,...,G_n;w_1,w_2,...w_n)$ as the rooted product of the path P_n and the sequence $\{G_1,G_2,...,G_n\}$, where the root vertex of the graph G_i is assumed to be in the vertex w_i, $i=1,2,...,n$. So using Theorem 2.1, we can reproduce the results of the Theorem 2.2 and Theorem 2.4 of [18].

Corollary 2.6 The first and second Zagreb indices of the bridge graph $B = B(G_1,G_2,...,G_n;w_1,w_2,...,w_n)$ are given by:

(i) For $n \geq 2$, $M_1(B)=\sum_{i=1}^{n} M_1(G_i)+2\omega_1+4\sum_{i=2}^{n-1}\omega_i+2\omega_n+4n-6$. In particular for $n=2$, $M_1(B)=M_1(G_1)+M_1(G_2)+2(\omega_1+\omega_2+1)$.

(ii) For $n=2$, $M_2(B)=M_2(G_1)+M_2(G_2)+\alpha_{G_1}(w_1)+\alpha_{G_2}(w_2)+(\omega_1+1)(\omega_2+1)$, and for $n \geq 3$,

$M_2(B)=\sum_{i=1}^{n} M_2(G_i)+\alpha_{G_1}(w_1)+\alpha_{G_n}(w_n)+2\sum_{i=2}^{n-1}\alpha_{G_i}(w_i)+\sum_{i=1}^{n-1}\omega_i\omega_{i+1}+2(\omega_1+\omega_n)-(\omega_2+\omega_{n-1})+$
$4\sum_{i=2}^{n-1}\omega_i+4(n-2)$, where $\omega_i=\deg_{G_i}(w_i)$, for $1 \leq i \leq n$.

Also by Corollary 2.2, we can reproduce the results of the Corollary 2.3 and Corollary 2.5 of [18].

Corollary 2.7 The first and second Zagreb indices of the bridge graph $B = B(G,G,...,G;w,w,...,w)$ ($n \geq 2$ times) are given by:

(i) For $n \geq 2$, $M_1(B)=nM_1(G)+4\omega(n-1)+4n-6$,

(ii) For $n=2$, $M_2(B)=2M_2(G)+2\alpha_G(w)+(\omega+1)^2$, and for $n\geq 3$,

$M_2(B_1)=nM_2(G)+(n-1)[(\omega+2)^2+2\alpha_G(w)]-2(\omega+2)$, where $\omega=\deg_G(w)$. ■

3. Corollaries and examples

In this section, we consider several classes of molecular graphs constructed by rooted product and determine their Zagreb indices.

3.1 Caterpillars and Cycle-caterpillars

A caterpillar or caterpillar tree is a tree in which all the vertices are within distance 1 of a central path. If we delete all pendent vertices of a caterpillar tree, we reach to a path. So caterpillars are thorn graphs whose parent graph is a path, see Fig. 1.

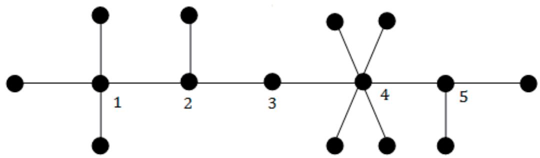


Fig. 1. The caterpillar tree $P_5^*(3,1,0,4,2)$.

Using Corollary 2.5, we can easily get the formulae for the first and second Zagreb indices of caterpillar trees.

Corollary 3.1 Let $p_1, p_2,\ldots,p_n$ be non-negative integers. The first and second Zagreb indices of the caterpillar tree $P_n^*(p_1,p_2,\ldots,p_n)$ are given by:

(i) $M_1(P_n^*(p_1,p_2,\ldots,p_n))=\sum_{i=1}^{n} p_i^2+5\sum_{i=1}^{n} p_i-2(p_1+p_n)+4n-6, \quad n\geq 2$

(ii) $M_2(P_n^*(p_1,p_2,\ldots,p_n))=\begin{cases} p_1(p_1+1)+p_2(p_2+1)+(p_1+1)(p_2+1) & \text{if } n=2 \\ \sum_{i=1}^{n} p_i^2+\sum_{i=1}^{n-1} p_ip_{i+1}+6\sum_{i=1}^{n} p_i-3(p_1+p_n)-(p_2+p_{n-1})+4n-8 & \text{if } n\geq 3 \end{cases}$. ■

Caterpillar trees are used in chemical graph theory to represent the structure of benzenoid hydrocarbon molecules. For example, for positive integer $p\leq 3$, the caterpillar tree $P_n^*(p,2,2,\ldots,2,p)$ is the molecular graph of certain hydrocarbon. Specially, $P_2^*(3,3)$, $P_3^*(3,2,3)$, $P_4^*(3,2,2,3)$ are the molecular graphs of Ethane, Propane and Butane, respectively, see Fig. 2.

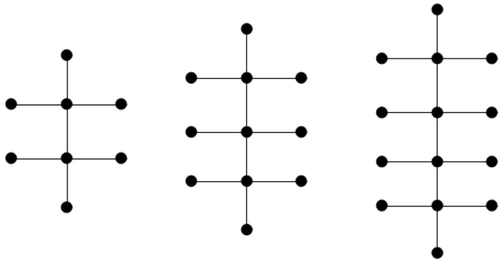


Fig. 2. The molecular graphs of Ethane, Propane and Butane.

Using Corollary 3.1, we can get the formulae for the first and second Zagreb indices of $P_n^*(p,2,2,\ldots,2,p)$.

Corollary 3.2 For positive integer $p \le 3$, the first and second Zagreb indices of $P_n^*(p,2,2,\ldots,2,p)$ are given by:

(i) $M_1(P_n^*(p,2,\ldots,2,p)) = 2p^2 + 6p + 18n - 34$,

(ii) $M_2(P_n^*(p,2,\ldots,2,p)) = \begin{cases} 3p^2 + 4p + 1 & \text{if } n = 2 \\ 2p^2 + 10p + 24n - 56 & \text{if } n \ge 3 \end{cases}$. ■

Specially, for Ethane, Propane and Butane, we easily arrive at:

Corollary 3.3 The first and second Zagreb indices of Ethane, Propane and Butane, are given by:

(i) $M_1(P_2^*(3,3)) = 38$, $M_1(P_2^*(3,2,3)) = 56$, $M_1(P_2^*(3,2,2,3)) = 74$,

(ii) $M_2(P_2^*(3,3)) = 40$, $M_2(P_2^*(3,2,3)) = 64$, $M_2(P_2^*(3,2,2,3)) = 88$. ■

A unicyclic graph is called cycle-caterpillar if deleting all its pendent vertices will reduce it to a cycle. So cycle-caterpillars are thorn graphs whose parent graph is a cycle, see Fig. 3. Using Corollary 2.5, we easily get the following formulae for Zagreb indices of cycle-caterpillars.

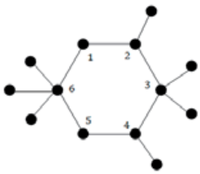


Fig. 3. The cycle-caterpillar $C_6^*(0,1,2,1,0,3)$.

Corollary 3.4 Let $p_1, p_2, ..., p_n$ be non-negative integers. The first and second Zagreb indices of the cycle-caterpillar $C_n^*(p_1, p_2, ..., p_n)$ are given by:

(i) $M_1(C_n^*(p_1, p_2, ..., p_n)) = \sum_{i=1}^{n} p_i^2 + 5\sum_{i=1}^{n} p_i + 4n$,

(ii) $M_2(C_n^*(p_1, p_2, ..., p_n)) = \sum_{i=1}^{n} p_i^2 + 6\sum_{i=1}^{n} p_i + \sum_{i=1}^{n-1} p_i p_{i+1} + p_1 p_n + 4n$. ■

3.2 Sunlike graphs and Starlike trees

Let G be a labeled graph on n vertices with the vertex set $V(G) = \{1,2,...,n\}$ and let $k_1, k_2, ..., k_n$ be positive integers. The sunlike graph $G(k_1, k_2, ..., k_n)$ is the graph obtained by identifying the root vertex of P_{k_i} with the i-th vertex of G for all $i = 1,2,...,n$, see Fig. 4.

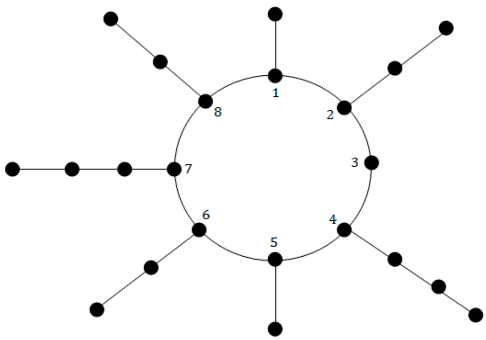


Fig. 4. The sunlike graph $C_8(2,3,1,4,2,3,4,3)$.

Note that in the case that $k_i = 1$, then $P_{k_i} = P_1$ is a single vertex graph and for $k_i > 1$ the root vertex of P_{k_i} is assumed to be in its pendant vertex. The sunlike graph $G(k_1, k_2, ..., k_n)$ can be considered as the rooted product of the graph G with the sequence $\{P_{k_1}, P_{k_2}, ..., P_{k_n}\}$. So, we can apply Theorem 2.1 to compute the first and second Zagreb indices of the sunlike graph $G(k_1, k_2, ..., k_n)$.

Corollary 3.5 Let G be a labeled graph on n vertices with the vertex set $V(G) = \{1,2,...,n\}$ and let $k_1, k_2, ..., k_n$ be positive integers. Set $I_1 = \{i \mid 1 \le i \le n, k_i = 1\}$, $I_2 = \{i \mid 1 \le i \le n, k_i = 2\}$ and

$I_3=\{i\,|\,1\le i\le n, k_i\ge 3\}$ and let $|I_1|=t$, $|I_2|=r$. The first and second Zagreb indices of the sunlike graph $G(k_1,k_2,...,k_n)$ are given by:

(i) $M_1(G(k_1,k_2,...,k_n))=M_1(G)+2\sum_{i\in I_2\cup I_3}\deg_G(i)+4\sum_{i\in I_2\cup I_3}k_i-6(n-t)$,

(ii) $M_2(G(k_1,k_2,...,k_n))=M_2(G)+\sum_{i\in I_2}\deg_G(i)+2\sum_{i\in I_3}\deg_G(i)+\sum_{ij\in E(G);\ i,j\in I_2\cup I_3}[\deg_G(i)+\deg_G(j)+1]+$

$\sum_{ij\in E(G);\ i\in I_1, j\in I_2\cup I_3}\deg_G(i)+4\sum_{i\in I_3}k_i-8n+9r+8t$. ■

If for all $1\le i\le n$, $k_i\ge 2$ then the formulae of Corollary 3.5 can be simplified as follows:

Corollary 3.6 Let G be a labeled graph on n vertices and m edges with the vertex set $V(G)=\{1,2,...,n\}$ and let $k_1,k_2,...,k_n$ be positive integers with $k_i\ge 2$ for all $1\le i\le n$.

(i) The first Zagreb index of the sunlike graph $G(k_1,k_2,...,k_n)$ is given by:

$$M_1(G(k_1,k_2,...,k_n))=M_1(G)+4\sum_{i=1}^{n}k_i+4m-6n,$$

(ii) Suppose $I=\{i\,|\,1\le i\le n, k_i=2\}$ and $I'=\{i\,|\,1\le i\le n, k_i\ge 3\}$ and let $|I|=r$. The second Zagreb index of the sunlike graph $G(k_1,k_2,...,k_n)$ is given by:

$$M_2(G(k_1,k_2,...,k_n))=M_1(G)+M_2(G)-\sum_{i\in I}\deg_G(i)+4\sum_{i\in I'}k_i-8n+9r+5m.$$

If in particular for all $1\le i\le n$, $k_i\ge 3$, then

$$M_2(G(k_1,k_2,...,k_n))=M_1(G)+M_2(G)+4\sum_{i=1}^{n}k_i+5m-8n. \ ■$$

A starlike tree is a tree with exactly one vertex having degree greater than two. We denote by $S(k_1,k_2,...,k_n)$, the starlike tree which has a vertex v of degree $n\ge 3$ and has the property that $S(k_1,k_2,...,k_n)-v=P_{k_1}\cup P_{k_2}\cup...\cup P_{k_n}$, where $k_1\ge k_2\ge...\ge k_n\ge 1$. Clearly, $k_1,k_2,...,k_n$ determine the starlike tree up to isomorphism and $S(k_1,k_2,...,k_n)$ has exactly $k_1+k_2+...+k_n+1$ vertices. For $1\le i\le n$, denote by v_i, the root vertex of P_{k_i} attached to the vertex v, see Fig. 5. Clearly, for $k_i\ge 2$, $\deg_{P_{k_i}}(v_i)=1$. Now consider the subtree T of $S(k_1,k_2,...,k_n)$ with the vertex set $V(T)=\{v,v_1,v_2,...,v_n\}$. Clearly T is isomorphic to $n+1$ vertex star, S_{n+1}. Choose a numbering for vertices of T such that the vertex v_i, $1\le i\le n$, has number i and the vertex v has number $n+1$. So we can consider the starlike tree $S(k_1,k_2,...,k_n)$ as the sunlike graph $T(k_1,k_2,...,k_{n+1})$

where $k_{n+1}=1$ and we can apply Corollary 3.5 to compute the first and second Zagreb indices of the starlike tree $S(k_1,k_2,...,k_n)$.

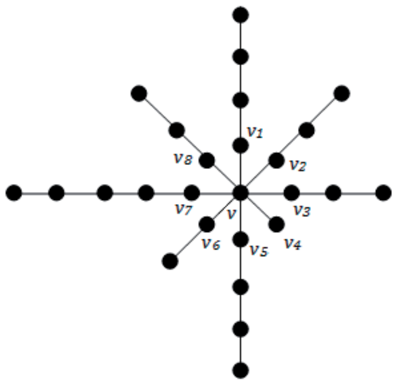


Fig. 5. The starlike tree $S(4,3,3,1,4,2,5,3)$ with vertex v of degree $n=8$.

Corollary 3.7 Let $k_1,k_2,...,k_n$ be n positive integers. Set $I_1=\{i\,|\,1\le i\le n, k_i=1\}$, $I_2=\{i\,|\,1\le i\le n, k_i=2\}$ and $I_3=\{i\,|\,1\le i\le n, k_i\ge 3\}$ and let $|I_1|=t$, $|I_2|=r$. The first and second Zagreb indices of the starlike tree $S(k_1,k_2,...,k_n)$ are given by:

(i) $M_1(S(k_1,k_2,...,k_n))=n^2-3n+4t+4\sum_{i\in I_2\cup I_3}k_i$,

(ii) $M_2(S(k_1,k_2,...,k_n))=2n^2-6n+8r-t(n-6)+4\sum_{i\in I_3}k_i$. ■

The starlike tree $S(k_1,k_2,...,k_n)$ is said to be regular, if $k_1=k_2=...=k_n=k$. Clearly $S(\underbrace{1,1,...,1}_{n\ times})=S_{n+1}$. Using Corollary 3.7, we can get the following formulae for Zagreb indices of regular starlike trees.

Corollary 3.8 Let k be a positive integer. The first and second Zagreb indices of the regular starlike tree $S(\underbrace{k,k,...,k}_{n\ times})$ are given by:

(i) $M_1(S(\underbrace{k,k,...,k}_{n\ times}))=n^2-3n+4nk$,

(ii) $M_2(S(\underbrace{k,k,...,k}_{n\ times}))=\begin{cases} n^2 & if\ \ k=1 \\ 2n^2-6n+4nk & if\ \ k\ge 2 \end{cases}$. ■

Let $S(k_1,k_2,...,k_n)$ denote the starlike tree which has a vertex v of degree greater than two and has the property $S(k_1,k_2,...,k_n)-v=P_{k_1}\cup P_{k_2}\cup...\cup P_{k_n}$. Also let $S(k'_1,k'_2,...,k'_{n'})$ denote the starlike tree which has a vertex v' of degree greater than two and has the property $S(k'_1,k'_2,...,k'_{n'})-v'=P_{k'_1}\cup P_{k'_2}\cup...\cup P_{k'_{n'}}$. The graph $S(k_1,k_2,...,k_n;k'_1,k'_2,...,k'_{n'})$ obtained by joining the vertex v of the graph $S(k_1,k_2,...,k_n)$ to the vertex v' of the graph $S(k'_1,k'_2,...,k'_{n'})$ by an edge is called double starlike tree, see Fig. 6. It has exactly two adjacent vertices v and v' of degree greater than three and has the property $S(k_1,k_2,...,k_n;k'_1,k'_2,...,k'_{n'})-\{v,v'\}=P_{k_1}\cup P_{k_2}\cup...\cup P_{k_n}\cup P_{k'_1}\cup P_{k'_2}\cup...\cup P_{k'_{n'}}$. We can consider the double starlike tree $S(k_1,k_2,...,k_n;k'_1,k'_2,...,k'_{n'})$, as the bridge graph $B(S(k_1,k_2,...,k_n),S(k'_1,k'_2,...,k'_{n'});v,v')$. So using Corollary 2.6 for the case $n=2$, and then Corollary 3.7, we can easily get the following result.

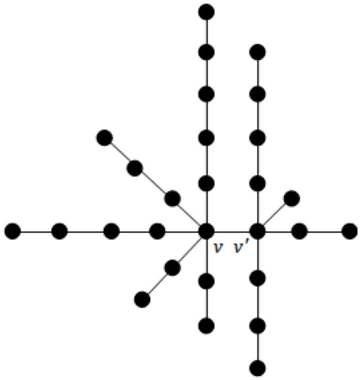


Fig. 6. The double starlike tree $S(5,3,4,2,2;4,1,2,3)$.

Corollary 3.9 Let $\{k_1,k_2,...,k_n\}$ and $\{k'_1,k'_2,...,k'_{n'}\}$ be two sequences of positive integers. Set $I_1=\{i\,|\,1\le i\le n, k_i=1\}$, $I_2=\{i\,|\,1\le i\le n, k_i=2\}$, $I_3=\{i\,|\,1\le i\le n, k_i\ge 3\}$, $I'_1=\{i\,|\,1\le i\le n', k'_i=1\}$, $I'_2=\{i\,|\,1\le i\le n', k'_i=2\}$ and $I'_3=\{i\,|\,1\le i\le n', k'_i\ge 3\}$. Also let $|I_1|=t$, $|I_2|=r$, $|I'_1|=t'$ and $|I'_2|=r'$. The first and second Zagreb indices of the double starlike tree $S(k_1,k_2,...,k_n;k'_1,k'_2,...,k'_{n'})$ are given by:

(i) $M_1(S(k_1,k_2,...,k_n;k'_1,k'_2,...,k'_m))=4(\sum_{i\in I_2\cup I_3}k_i+\sum_{i\in I'_2\cup I'_3}k'_i)+n(n-1)+n'(n'-1)+4(t+t')+2$,

(ii) $M_2(S(k_1,k_2,...,k_n;k'_1,k'_2,...,k'_m)) = 4(\sum_{i\in I_3} k_i + \sum_{i\in I'_3} k'_i) + n(2n-t-3) + n'(2n'-t'-3) + 8(r+r') +$

$5(t+t') + nn' + 1$.■

If $n = n'$ and $k_i = k'_i$ for $1 \le i \le n$, then the double starlike tree $S(k_1,k_2,...,k_n;k_1,k_2,...,k_n)$ is called symmetric double starlike. Using Corollary 3.9, we get the following formula for the first and second Zagreb indices of symmetric double starlike trees.

Corollary 3.10 Let $k_1,k_2,...,k_n$ be positive integers. Set $I_1 = \{i \mid 1 \le i \le n, k_i = 1\}$, $I_2 = \{i \mid 1 \le i \le n, k_i = 2\}$ and $I_3 = \{i \mid 1 \le i \le n, k_i \ge 3\}$ and let $|I_1| = t$, $|I_2| = r$. The first and second Zagreb indices of the symmetric double starlike tree $S(k_1,k_2,...,k_n;k_1,k_2,...,k_n)$ are given by:

(i) $M_1(S(k_1,k_2,...,k_n;k_1,k_2,...,k_n)) = 8\sum_{i\in I_2 \cup I_3} k_i + 2n(n-1) + 8t + 2$,

(ii) $M_2(S(k_1,k_2,...,k_n;k_1,k_2,...,k_n)) = 8\sum_{i\in I_3} k_i + 5n^2 - 2n(t+3) + 16r + 10t + 1$. ■

3.3 Generalized Bethe trees

The level of a vertex in a rooted tree is one more than its distance from the root vertex. A generalized Bethe tree of k levels, $k > 1$ is a rooted tree in which vertices at the same level have the same degree [19]. Let B_k be a generalized Bethe tree of k levels. For $i = 1,2,...,k$, we denote by d_{k-i+1} and n_{k-i+1} the degree of the vertices at the level i of B_k and their number, respectively. Also, suppose $e_k = d_k$ and $e_i = d_i - 1$ for $i = 1,2,...,k-1$. Thus, $d_1 = 1$ is the degree of the vertices at the level k (pendent vertices) and d_k is the degree of the root vertex. On the other hand, $n_k = 1$ is pertaining to the single vertex at the first level, the root vertex. For $i = 1,2,...,k-1$, suppose β_{k-i+1} denotes the subtree of B_k which is also a generalized Bethe tree of $k-i+1$ levels and its root is any vertex of the level i of B_k, as shown in Fig. 7 and let $\beta_1 = K_1$. Now consider the subtree of β_{k-i+1}, $i = 1,2,...,k-1$ which is isomorphic to the star graph $S_{e_{k-i+1}+1}$ and choose a numbering for its vertices such that its e_{k-i+1} pendant vertices have numbers $1,...,e_{k-i+1}$ and its vertex of degree e_{k-i+1} has number $e_{k-i+1}+1$. We can consider the generalized Bethe tree $\beta_{k-i+1}, i = 1,2,...,k-1$ as the rooted product of $S_{e_{k-i+1}+1}$ by the sequence $\{\underbrace{\beta_{k-i},...,\beta_{k-i}}_{e_{k-i+1}\ times}, K_1\}$, i.e.,

$$\beta_{k-i+1} = S_{e_{k-i+1}+1}\{\underbrace{\beta_{k-i},...,\beta_{k-i}}_{e_{k-i+1}\ times}, K_1\},\ i = 1,2,...,k-1.$$

Clearly, $\beta_2 = S_{e_2} + 1$, $\beta_k = B_k$.

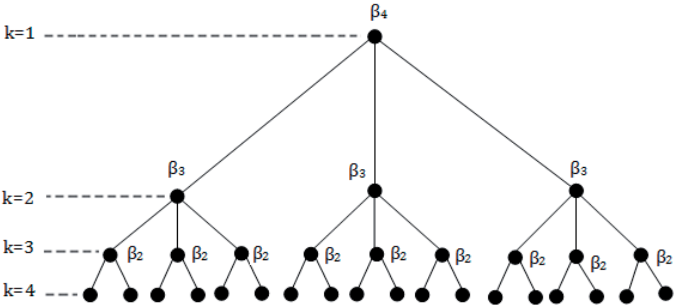


Fig. 6. A generalized Bethe tree of 4 levels with its subtrees β_2, β_3, β_4.

Now using Corollary 2.4, we can get the following recurrence relations for the first and second Zagreb indices of the generalized Bethe tree β_{k-i+1}, $i = 1,2,\ldots,k-1$.

Corollary 3.11 The first and second Zagreb indices of the generalized Bethe tree β_{k-i+1}, $i = 1,2,\ldots,k-1$ are given by:

(i) $M_1(\beta_1) = 0$, $M_1(\beta_{k-i+1}) = e_{k-i+1} M_1(\beta_{k-i}) + e_{k-i+1}(e_{k-i+1} + 2e_{k-i} + 1)$, $1 \le i \le k-1$,

(ii) $M_2(\beta_2) = e_2^{\,2}$, $M_2(\beta_{k-i+1}) = e_{k-i+1} M_2(\beta_{k-i}) + e_{k-i+1}^{\,2} d_{k-i} + e_{k-i+1} e_{k-i} d_{k-i-1}$, $1 \le i \le k-2$. ■

Note that the formulae of Corollary 3.11 hold for all $1 \le i \le k-1$. So using Corollary 3.11, we can get the following explicit relations for computing the first and second Zagreb indices of the generalized Bethe tree B_k.

Corollary 3.12 The first and second Zagreb indices of the generalized Bethe tree B_k are given by:

(i) $M_1(B_k) = \sum_{i=1}^{k} d_i^{\,2} \prod_{j=i+1}^{k} e_j$,

(ii) $M_2(B_k) = \sum_{i=1}^{k-1} e_{i+1} d_{i+1} d_i \prod_{j=i+2}^{k} e_j$. ■

The ordinary Bethe tree $B_{d,k}$ is a rooted tree of *k* levels whose root vertex has degree *d*, the vertices from levels 2 to $k-1$ have degree $d+1$, and the vertices at level k have degree 1, see Fig. 8.

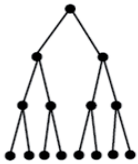


Fig. 7. The ordinary Bethe tree $B_{2,4}$.

Note that $B_{1,k} = P_k$ and $B_{d,2} = S_{d+1}$. Using Corollary 3.12, we get the following relations for computing the first and second Zagreb indices of ordinary Bethe tree $B_{d,k}$.

Corollary 3.13 The first and second Zagreb indices of the ordinary Bethe tree $B_{d,k}$ are given by:

(i) $M_1(B_{d,k}) = d^2 + d^{k-1} + d(d+1)^2 \sum_{s=0}^{k-3} d^s$,

(ii) $M_2(B_{d,k}) = \begin{cases} d^2 & \text{if } k = 2 \\ 2d^2(d+1)\sum_{s=0}^{k-3} d^s & \text{if } k \geq 3 \end{cases}$. ■

Denote by $C(d,k,n)$, the unicyclic graph obtained by attaching the root vertex of $B_{d,k}$ to the vertices of n vertex cycle C_n, see Fig. 9. For more information about this graph, see [18].

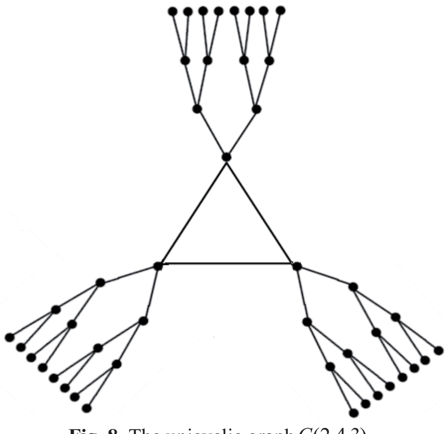


Fig. 8. The unicyclic graph $C(2,4,3)$.

It is easy to see that $C(d,k,n)$ is the cluster of C_n and $B_{d,k}$. So we can apply Corollary 2.2 and then Corollary 3.13, to get the following formulae for the first and second Zagreb indices of $C(d,k,n)$.

Corollary 3.14 The first and second Zagreb indices of $C(d,k,n)$ are given by:

(i) $M_1(C(d,k,n)) = 4n(d+1) + nd^2 + nd^{k-1} + nd(d+1)^2 \sum_{s=0}^{k-3} d^s$,

(ii) $M_2(C(d,k,n)) = \begin{cases} 2n(d^2+3d+2) & \text{if } k=2 \\ n(3d^2+6d+4) + 2nd^2(d+1)\sum_{s=0}^{k-3} d^s & \text{if } k \geq 3 \end{cases}$. ■

Denote by $P(d,k,n)$, the tree obtained by attaching the root vertex of $B_{d,k}$ to the vertices of n vertex path P_n, see Fig. 10. For more information about this classes of trees, see [20]. The graph $P(d,k,n)$ can be considered as the bridge graph $B(B_{d,k}, B_{d,k}, \ldots, B_{d,k}; w, w, \ldots, w)$, where w denotes the root vertex of $B_{d,k}$. So we can apply Corollary 2.7 and then Corollary 3.13, to get the formulae for the first and second Zagreb indices of the tree $P(d,k,n)$.

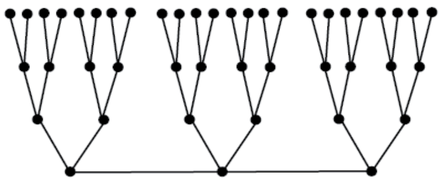


Fig. 9. The tree $P(2,4,3)$.

Corollary 3.15 The first and second Zagreb indices of $P(d,k,n)$ are given by:

(i) $M_1(P(d,k,n)) = 4d(n-1) + 4n - 6 + nd^2 + nd^{k-1} + nd(d+1)^2 \sum_{s=0}^{k-3} d^s$,

(ii) $M_2(P(d,k,2)) = 3d^2 + 4d + 1 + 4d^2(d+1)\sum_{s=0}^{k-3} d^s$, and

$$M_2(P(d,k,n)) = \begin{cases} (2n-1)d^2 + 6nd + 4n - 8d - 8 & \text{if } k=2 \\ 3(n-1)(d+1)^2 + n - 2d - 5 + 2nd^2(d+1)\sum_{s=0}^{k-3} d^s & \text{if } k \geq 3 \end{cases}. ■$$

Dendrimers are hyperbranched molecules, synthesized by repeatable steps, either by adding branching blocks around a central core (thus obtaining a new, larger orbit or generation-the “divergent growth” approach) or by building large branched blocks starting from the periphery and then attaching them to the core (the “convergent growth” [21]). Details on dendrimers, an important and recently much studied class of nano-materials, and especially on their topological properties can be found in the books [22-23] and the references quoted therein. A dendrimer tree $T_{d,k}$ is a rooted tree such that the degree of its non-pendent vertices is equal to d and the distance between the rooted (central) vertex and the pendent vertices is equal to k [24], see Fig. 11. So $T_{d,k}$ can be considered as a generalized Bethe tree with $k+1$ levels, such that whose non-pendent vertices have equal degrees. Note that $T_{2,k} = P_{2k+1}$ and $T_{d,1} = S_{d+1}$. Using Corollary 3.12, we get the following relations for the first and second Zagreb indices of the dendrimer tree $T_{d,k}$.

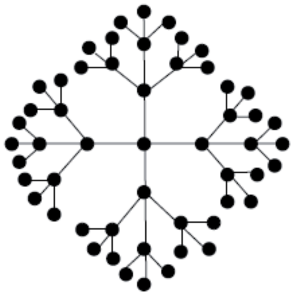


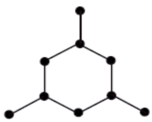
Fig. 10. The dendrimer tree $T_{4,3}$.

Corollary 3.16 The first and second Zagreb indices of the dendrimer tree $T_{d,k}$ are given by:

(i) $M_1(T_{d,k}) = d^2 + d(d-1)^{k-1} + d^3\sum_{s=0}^{k-2}(d-1)^s$,

(ii) $M_2(T_{d,k}) = d^2(d-1)^{k-1} + d^3\sum_{s=0}^{k-2}(d-1)^s$. ■

Now we introduce a class of dendrimers for which Corollary 2.4 is applicable. This molecular structure can be seen in some of the dendrimer graphs such as tertiary phosphine dendrimers. Let D_0 be the graph of Fig. 12.



D_0

Fig. 12. The dendrimer graph D_0.

For positive integers d and k, suppose $D_{d,k}$ be a series of dendrimer graphs obtained by attaching d pendent vertices to each pendent vertex of $D_{d,k-1}$ and set $D_{d,0} = D_0$. Some examples of this class of dendrimer graphs are shown in Fig. 13 and Fig. 14.

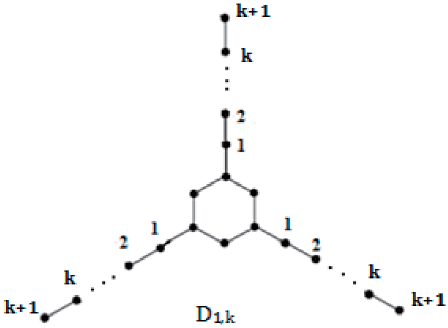


Fig. 13. Dendrimer graph $D_{1,k}$.

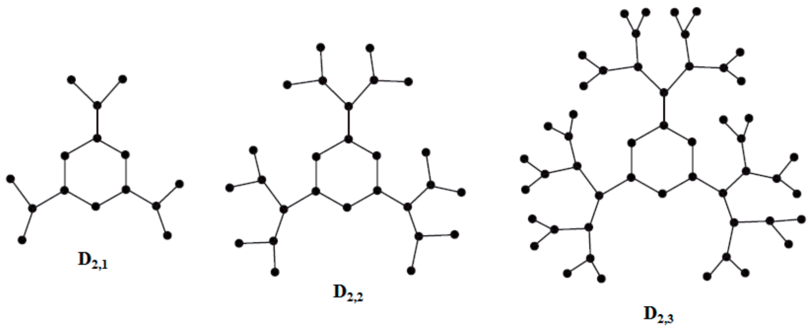


Fig. 14. Dendrimer graphs $D_{d,k}$, for d=2, k=1,2,3.

It is easy to check that, $M_1(D_0) = 42$ and $M_2(D_0) = 45$. Choose a numbering for vertices of D_0 such that its pendant vertices have numbers 1,2,3 and its non-pendant vertices have numbers $4,5,\ldots,9$. It is easy to see that, $D_{d,k}$ is the rooted product of D_0 by the sequence $\{B_{d,k+1}, B_{d,k+1}, B_{d,k+1}, \underbrace{K_1, K_1, \ldots, K_1}_{6\ times}\}$. So by Corollary 2.4, we can get the following relations for the first and second Zagreb indices of the dendrimer graph $D_{d,k}$, $k \geq 1$.

Corollary 3.17 The first and second Zagreb indices of the dendrimer graph $D_{d,k}$, $k \geq 1$ are given by:

(i) $M_1(D_{d,k}) = 42 + 3d(d+3)\sum_{s=0}^{k-1} d^s$,

(ii) $M_2(D_{d,k}) = 3d^2 + 12d + 45 + 6d^2(d+1)\sum_{s=0}^{k-2} d^s$. ■

Acknowledgement. The authors would like to thank the referees for a number of helpful comments and suggestions. This work was partially supported by Center of Excellence of Algebraic Hyperstructures and its Applications of Tarbiat Modares University (CEAHA).

References

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

[2] I. Gutman, N. Trinajstic, Graph theory and molecular orbitals. Total π-electron energy of alternant hydrocarbons, *Chem. Phys. Lett.* **17** (1972) 535–538.

[3] I. Gutman, B. Ruščić, N. Trinajstić, C. F. Wilcox, Graph theory and molecular orbitals. XII. Acyclic polyenes, *J. Chem. Phys.* **62** (1975) 3399–3405.

[4] K. C. Das, I. Gutman, Some properties of the second Zagreb index, *MATCH Commun. Math. Comput. Chem.* **52** (2004) 103–112.

[5] I. Gutman, K. C. Das, The first Zagreb index 30 years after, *MATCH Commun. Math. Comput. Chem.* **50** (2004) 83–92.

[6] B. Zhou, Zagreb indices, *MATCH Commun. Math. Comput. Chem.* **52** (2004) 113–118.

[7] M. Azari, A. Iranmanesh, Generalized Zagreb index of graphs, *Studia Univ. Babes Bolyai Chem.* **3** (2011) 59–70.

[8] K. C. Das, I. Gutman, B. Horoldagva, Comparing Zagreb indices and coindices of trees, *MATCH Commun. Math. Comput. Chem.* **68** (2012) 189–198.

[9] M. Milošević, T. Réti, D. Stevanović, On the constant difference of Zagreb indices, *MATCH Commun. Math. Comput. Chem.* **68** (2012) 157–168.

[10] T. Réti, On the relationships between the first and second Zagreb indices, *MATCH Commun. Math. Comput. Chem.* **68** (2012) 169–188.

[11] D. Stevanović, M. Milanič, Improved inequality between Zagreb indices of trees, *MATCH Commun. Math. Comput. Chem.* **68** (2012) 147–156.

[12] C. D. Godsil, B. D. McKay, A new graph product and its spectrum, *Bull. Austral. Math. Soc*. **18** (1978) 21-28.

[13] I. Gutman, Distance in thorny graph, *Publ. Inst. Math.* (Beograd) **63** (1998) 31-36.

[14] L. Bytautas, D. Bonchev, D. J. Klein, On the generation of mean Wiener numbers of thorny graphs, *MATCH Commun. Math. Comput. Chem.* **44** (2001) 31-40.

[15] D. Vukičević, A. Graovac, On modified Wiener indices of thorn graphs, *MATCH Commun. Math. Comput. Chem.* **50** (2004) 93-108.

[16] A. Heydari, I. Gutman*,* On the terminal Wiener index of thorn graphs, *Kragujevac J. Sci.* **32** (2010) 57-64.

[17] H. B. Walikar, H. S. Ramane, L. Sindagi, S. S. Shirakol, I. Gutman, Hosoya polynomial of thorn trees, rods, rings, and stars, *Kragujevac J. Sci.* **28** (2006), 47-56.

[18] M. Azari, A. Iranmanesh, I. Gutman, Zagreb indices of bridge and chain graphs, *MATCH Commun. Math. Comput. Chem.*, in press.

[19] O. Rojo, The spectra of a graph obtained from copies of a generalized Bethe tree, *Lin. Algebra Appl*. **420** (2007) 490-507.

[20] M. Robbiano, I. Gutman, R. Jimenez, B. San Martin, Spectra of copies of Bethe trees attached to path and applications, *Bull. Acad. Serbe Sci. Arts* (Cl. Sci. Math. Natur.) **137** (2008) 59-81.

[21] M. V. Diudea, Wiener index of dendrimers, *MATCH Commun. Math. Comput. Chem.* **32** (1995) 71–83.

[22] M. V. Diudea (Ed.), *Nanostructures: Novel Architecture*, Nova, New York, 2006.

[23] M. V. Diudea, C. L. Nagy, *Periodic Nanostructures*, Springer, Amsterdam, 2007.

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