

Zagreb, multiplicative Zagreb Indices and Coindices of graphs

V. Ahmadi ^{*†}, M. R. Darafsheh [‡], J. Hashemi [§]

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Abstract

Let $G=(V,E)$ be a simple connected graph with vertex set V and edge set E . The first, second and third Zagreb indices of G are respectively defined by: $M_1(G) = \sum_{u \in V} d(u)^2$, $M_2(G) = \sum_{uv \in E} d(u).d(v)$ and $M_3(G) = \sum_{uv \in E} |d(u) - d(v)|$, where $d(u)$ is the degree of vertex u in G and uv is an edge of G connecting the vertices u and v . Recently, the first and second multiplicative Zagreb indices of G are defined by: $PM_1(G) = \prod_{u \in V} d(u)^2$ and $PM_2(G) = \prod_{u \in V} d(u)^{d(u)}$. The first and second Zagreb coindices of G are defined by: $\overline{M}_1(G) = \sum_{uv \notin E} (d(u) + d(v))$ and $\overline{M}_2(G) = \sum_{uv \notin E} d(u).d(v)$. The indices $\overline{PM}_1(G) = \prod_{uv \notin E} d(u) + d(v)$ and $\overline{PM}_2(G) = \prod_{uv \notin E} d(u).d(v)$, are called the first and second multiplicative Zagreb coindices of G , respectively. In this article, we compute the first, second and third Zagreb indices and the first and second multiplicative Zagreb indices of some classes of dendrimers. The first and second Zagreb coindices and the first and second multiplicative Zagreb coindices of these graphs are also computed. Also, the multiplicative Zagreb indices are computed using link of graphs.

Keywords : Zagreb indices; Multiplicative Zagreb indices; Zagreb coindices; Multiplicative Zagreb coindices; Link.

1 Introduction

The graphs considered in this paper are simple and connected. Let $G=(V,E)$ be a simple connected graph with vertex set V and edge set E . A topological index is a fixed number under graph automorphisms. Gutman and Trinajstić [4] defined the first and second Zagreb indices. Zagreb indices are defined as follows:

$$M_1(G) = \sum_{u \in V} d(u)^2, \quad (1.1)$$

$$M_2(G) = \sum_{uv \in E} d(u).d(v) \quad (1.2)$$

The alternative expression of $M_1(G)$ is

$$\sum_{uv \in E} (d(u) + d(v)). \quad (1.3)$$

G.H.Fath-Tabar [3] defined the third Zagreb index, by:

$$M_3(G) = \sum_{uv \in E} |d(u) - d(v)|. \quad (1.4)$$

Todeschini et al. [6, 7] have recently proposed to consider multiplicative variants of additive graph invariants, applied to the Zagreb indices, lead to:

$$PM_1(G) = \prod_{u \in V} d(u)^2, \quad (1.5)$$

$$PM_2(G) = \prod_{u \in V} d(u)^{d(u)} \quad (1.6)$$

*Corresponding author. vidaahmadi_math@yahoo.com

[†]Department of Mathematics, Shahid Chamran University, Ahvaz, Iran.

[‡]Department of Mathematics, Tehran University, Tehran, Iran.

[§]Department of Mathematics, Shahid Chamran University, Ahvaz, Iran.

The alternative expression of $PM_2(G)$ is

$$\prod_{uv \in E} d(u).d(v). \tag{1.7}$$

Gutman et al. [5] computed multiplicative Zagreb indices for a class of dendrimers using link of graphs.

Recently, Ashrafi, Doli and Hamzeh [1, 2] defined the first and second Zagreb coindices by:

$$\overline{M}_1(G) = \sum_{uv \notin E} (d(u) + d(v)), \tag{1.8}$$

$$\overline{M}_2(G) = \sum_{uv \notin E} d(u).d(v). \tag{1.9}$$

In 2013 Xu, Das and Tang [8] defined multiplicative Zagreb coindices by:

$$\overline{PM}_1(G) = \prod_{uv \notin E} d(u) + d(v), \tag{1.10}$$

$$\overline{PM}_2(G) = \prod_{uv \notin E} d(u).d(v). \tag{1.11}$$

They define multiplicative sum Zagreb index and the total multiplicative sum Zagreb index by:

$$PM_1^*(G) = \prod_{uv \in E} d(u) + d(v), \tag{1.12}$$

$$PM^T(G) = \prod_{u,v \in V} d(u) + d(v). \tag{1.13}$$

The goal of this article is computing Zagreb indices, multiplicative Zagreb indices, Zagreb coindices, multiplicative Zagreb coindices, multiplicative sum Zagreb index and the total multiplicative sum Zagreb index of some graphs.

2 Preliminaries

Define d_i to be the number of vertices with degrees i and $x_{ij}, i \neq j$, to be the number of edges connecting the vertex of degree i with a vertex of degree j and x_{ii} to be the number of edges connecting two vertices of degree i . Figure 1 shows a first-type nanostar dendrimer which has grown two stages and four similar branches with the same number, d_i of vertices and x'_{ij} of edges connecting a vertex of degree i with a vertex of degree j and x''_{ii} to be the number of edges connecting two vertices of degree i . Define \bar{x}_{ij} to be the number of subsets with vertices of degree i, j , so that \bar{x}_{ij}

does not include the number of edges that connect vertices i, j . Define \bar{x}_{ii} to be the number of subsets with vertices of degree i , so that \bar{x}_{ii} does not include the number of edges which connect two vertices of degree i .

Lemma 2.1 *The amount of $\bar{x}_{ij}, \bar{x}_{ii}$ are equal to:*

$$\bar{x}_{ij} = \binom{d_i}{1} \binom{d_j}{1} - x_{ij} = d_i d_j - x_{ij}, \tag{2.14}$$

$$\bar{x}_{ii} = \binom{d_i}{2} - x_{ii} = \frac{d_i(d_i - 1)}{2} - x_{ii}. \tag{2.15}$$

Proof. straight forward. \square

We use the above formulae to obtain Zagreb and multiplicative Zagreb coindices.

Lemma 2.2 *The number of subsets with vertices of degree i as well as the number of subsets with vertices of degree i, j , are equal to:*

$$\binom{d_i}{2} = \frac{d_i(d_i-1)}{2}, \binom{d_i}{1} \binom{d_j}{1} = d_i d_j. \tag{2.16}$$

Proof. straight forward. \square We use these formulae to obtain $PM^T(G)$.

Definition 2.1 *A link of G and H by vertices u and v is defined as the graph $(G \square H)(u, v)$ obtained by joining u and v by an edge in the union of these graphs.*

Theorem 2.1 *The first and second multiplicative Zagreb indices of the link of G_1 and G_2 satisfies the following relations:*

$$PM^1(G_1 \square G_2)(v_1, v_2) = \frac{(d_{G_1}(v_1)+1)(d_{G_2}(v_2)+1)^2}{d_{G_1}(v_1)d_{G_2}(v_2)}. \tag{2.17}$$

$$PM^2(G_1 \square G_2)(v_1, v_2) = \frac{(d_{G_1}(v_1)+1)^{d_{G_1}(v_1)+1} (d_{G_2}(v_2)+1)^{d_{G_2}(v_2)+1}}{d_{G_1}(v_1)^{d_{G_1}(v_1)} d_{G_2}(v_2)^{d_{G_2}(v_2)}}. \tag{2.18}$$

Proof. See [5] Notice that $d_{G_1}(v_1)$ is defined to be the degree of vertex $v_1 \in V(G_1)$ and $d_{G_2}(v_2)$ is defined similarly. \square

Definition 2.2 Define $PM_1^{(u_i)}(G_1)$ to be the first multiplicative Zagreb index of the graph G_1 , so that $PM_1^{(u_i)}(G_1)$ dose not include the first multiplicative Zagreb index of vertex $u_i \in V(G_1)$ and $PM_2^{(u_i)}(G_1)$ is defined similarly.

We compute these indices for the following figures.

3 Results and discussion

Theorem 3.1 Zagreb, multiplicative Zagreb indices and coindices of First-type nanostar dendrimer, $NS_1[2]$ (see Figure 1) are computed as follows:

$$\begin{aligned} M_1 &= 17 \cdot 2^{n+4} - 112, \\ M_2 &= 41 \cdot 2^{n+3} - 140, \\ M_3 &= 2^{n+5} - 16, \\ PM_1 &= 2^{2^{n+6}-20} \cdot 3^{2^{n+5}-16}, \\ PM_2 &= 2^{2^{n+6}-20} \cdot 3^{3 \cdot 2^{n+4}-24}, \\ \overline{M}_1 &= 21 \cdot 2^{2n+8} - 141 \cdot 2^{n+5} + 948, \\ \overline{M}_2 &= 49 \cdot 2^{2n+7} - 337 \cdot 2^{n+4} + 1164, \\ \overline{PM}_1 &= 2^9 \cdot 2^{2n+7} - 53 \cdot 2^{n+4} + 154 \cdot 3^{2^{2n+7}-9 \cdot 2^{n+4}+40} \cdot 5^{2^{2n+9}-7 \cdot 2^{n+6}+96}, \\ \overline{PM}_2 &= 2^3 \cdot 2^{2n+9} - 9 \cdot 2^{n+7} + 210 \cdot 3^{3 \cdot 2^{2n+8}-23 \cdot 2^{n+5}+176}. \end{aligned}$$

Proof. Figure 1, has grown four similar branches and two stages. Now, we compute these indices from the stage n. For the graph of Figure 2 is the central part of Figure 1. For the Figure 2 it is obvious that: $d_2 = 18, d_3 = 12$, so $d_2 = 4d'_2 + 18, d_3 = 4d'_3 + 12$.

For example, for $n = 1$ we have $d_2 = 54, d_3 = 24$. On the other hand, calculations show that: $d'_2 = 2^{n+3} - 7, d'_3 = 2^{n+2} - 5$, therefore, $d_2 = 2^{n+5} - 10, d_3 = 2^{n+4} - 8$. Elementary computation gives:

$$\begin{aligned} M_1 &= 17 \cdot 2^{n+4} - 112, \\ PM_1 &= 2^{2^{n+6}-20} \cdot 3^{2^{n+5}-16}, \\ PM_2 &= 2^{2^{n+6}-20} \cdot 3^{3 \cdot 2^{n+4}-24}. \end{aligned}$$

For the graph of Figure 2, it is obvious that: $x_{22} = 6, x_{23} = 24, x_{33} = 4$, so $x_{22} = 4x'_{22} + 6, x_{23} = 4x'_{23} + 24, x_{33} = 4x'_{33} + 4$. For example, for $n = 1$ we have $x'_{22}=30, x'_{23}=48, x'_{33}=12$.

On the other hand, calculations show that: $x'_{22} = 2^{n+2} - 2, x'_{23} = 2^{n+3} - 10, x'_{33} = 2^{n+1} - 2$, therefore, $x_{22} = 2^{n+4} - 2, x_{23} = 2^{n+5} - 16, x_{33} = 2^{n+3} - 4$.

Elementary computation gives:

$$M_2 = 41 \cdot 2^{n+3} - 140, M_3 = 2^{n+5} - 16.$$

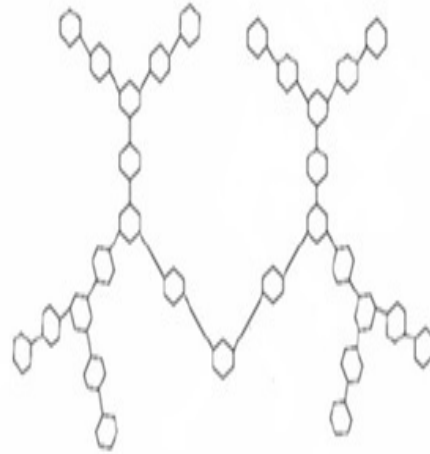


Figure 1: First-type nanostar dendrimer, $NS_1[2]$

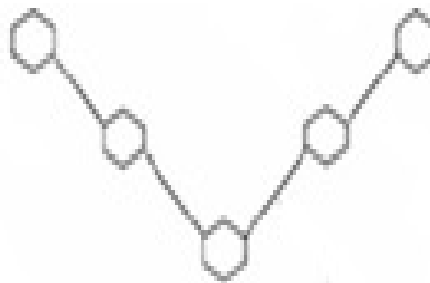


Figure 2: First-type nanostar dendrimer, $NS_1[2]$

Similar calculation shows that:

$$\begin{aligned} \overline{M}_1 &= 21 \cdot 2^{2n+8} - 141 \cdot 2^{n+5} + 948, \\ \overline{M}_2 &= 49 \cdot 2^{2n+7} - 337 \cdot 2^{n+4} + 1164, \\ \overline{PM}_1 &= 2^9 \cdot 2^{2n+7} - 53 \cdot 2^{n+4} + 154 \cdot 3^{2^{2n+7}-9 \cdot 2^{n+4}+40} \cdot 5^{2^{2n+9}-7 \cdot 2^{n+6}+96}, \\ \overline{PM}_2 &= 2^3 \cdot 2^{2n+9} - 9 \cdot 2^{n+7} + 210 \cdot 3^{3 \cdot 2^{2n+8}-23 \cdot 2^{n+5}+176}. \end{aligned}$$

Now, we compute multiplicative Zagreb indices using the link of graphs G_1, G_2 as shown in Figure

3: It is easy to see that:

$$\begin{aligned} PM_1(G_1) &= 2^{20} \cdot 3^4, \\ PM_1^{(u_i)}(G_1) &= 2^{18} \cdot 3^4, \\ PM_1^{(v_j)}(G_1) &= 2^{18} \cdot 3^4, \\ PM_1^{(v_i, u_{i+1})}(G_1) &= 2^{16} \cdot 3^4 \end{aligned}$$

and so, for $1 \leq i \leq n - 1, 1 \leq j \leq n - 1$.

We define G_n as follows:

$$\begin{aligned} G_n &= (G_{n-1} \square G_1)(v_1, u_1) \\ G_{n-1} &= (G_{n-2} \square G_1)(v_2, u_2) \\ &\vdots \\ &\vdots \\ G_2 &= (G_1 \square G_1)(v_{n-1}, u_{n-1}) \end{aligned}$$

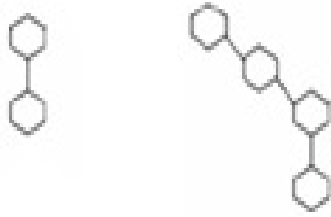


Figure 3: G_1 and G_2

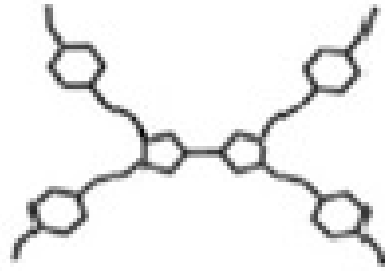


Figure 5: The central part of Figure 4

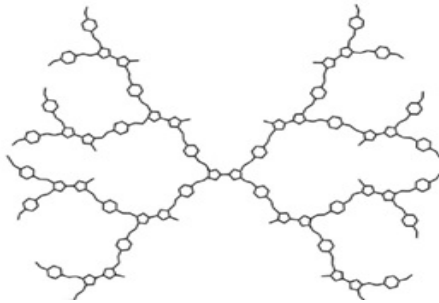


Figure 4: Molecular graph of dendrimers using tetrathiafulvalene units as branching centers, D [2]

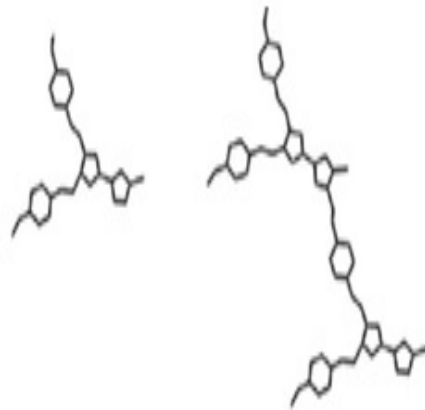


Figure 6: G_1 and G_2

According to Theorem 3.1 we have the following relations:

$$\begin{aligned}
 &PM_1(G_n) = \\
 &PM_1^{(v_1)}(G_{n-1})PM_1^{(u_1)}(G_1).3^4 \\
 &PM_1^{(v_1)}(G_{n-1}) = \\
 &PM_1^{(v_2)}(G_{n-2})PM_1^{(v_1, u_2)}(G_1).3^4 \\
 &\cdot \\
 &\cdot \\
 &\cdot \\
 &PM_1^{(v_{n-2})}(G_2) = \\
 &PM_1^{(v_{n-1})}(G_1)PM_1^{(v_{n-2}, u_{n-1})}(G_1).3^4 \\
 &\text{Therefore:} \\
 &PM_1(G_n) = PM_1^{(v_{n-1})}(G_1)PM_1^{(u_1)}(G_1) \\
 &\prod_{i=2}^{n-1} PM_1^{(v_{i-1}, u_i)}(G_1).3^{4(n-1)} = \\
 &PM_1^{(v_{n-1})}(G_1)PM_1^{(u_1)}(G_1) \\
 &(PM_1^{(v_1, u_2)}(G_1))^{n-2}.3^{4(n-1)} = \\
 &2^{16n+4}.3^{8n-4}.
 \end{aligned}$$

A branch is added in the second layer such as G_1 and three branches are added in the third layer that its first multiplicative Zagreb index is $2^{-2}.2^{18}.3^{18}$. The total number of added branches in all layers are equal to $2^n - n - 1$.

The first multiplicative Zagreb index for a main branch of the graph of Figure 1 is equal to $2^{2n+4-12}.3^{2n+3-12}$.

Since the graph has four main branches then we obtain high values for four main branches and

we consider the obtained number with the first multiplicative Zagreb index which has the central part value of figure that is $2^{-8}.2^{36}.3^{32}$. Therefore:

$$PM_1(G) = 2^{2n+6-20}.3^{2n+5-16}.$$

It is easy to see that:

$$\begin{aligned}
 &PM_2(G_1) = 2^{20}.3^6, PM_2^{(u_i)}(G_1) = 2^{18}.3^6, \\
 &PM_2^{(v_j)}(G_1) = 2^{18}.3^6, PM_2^{(v_i, u_{i+1})}(G_1) = \\
 &2^{16}.3^6
 \end{aligned}$$

and so, for $1 \leq i \leq n - 1, 1 \leq j \leq n - 1$.

According to Theorem 3.1 we have the following relations:

$$\begin{aligned}
 &PM_2(G_n) = \\
 &PM_2^{(v_1)}(G_{n-1})PM_2^{(u_1)}(G_1).(3^3.3^3) \\
 &PM_2^{(v_1)}(G_1) = \\
 &PM_2^{(v_2)}(G_{n-2})PM_2^{(v_1, u_2)}(G_1).(3^3.3^3) .
 \end{aligned}$$

$$\begin{aligned}
 &\cdot \\
 &\cdot \\
 &PM_2^{(v_{n-2})}(G_2) = \\
 &PM_2^{(v_{n-1})}(G_1)PM_2^{(v_{n-2}, u_{n-1})}(G_1).(3^3.3^3)
 \end{aligned}$$

$$\begin{aligned}
 &\text{Therefore:} \\
 &PM_2(G_n) = PM_2^{(v_{n-1})}(G_1)PM_2^{(u_1)}(G_1) \\
 &(PM_2^{(v_1, u_2)}(G_1))^{n-2}.(3^3.3^3)^{(n-1)} =
 \end{aligned}$$

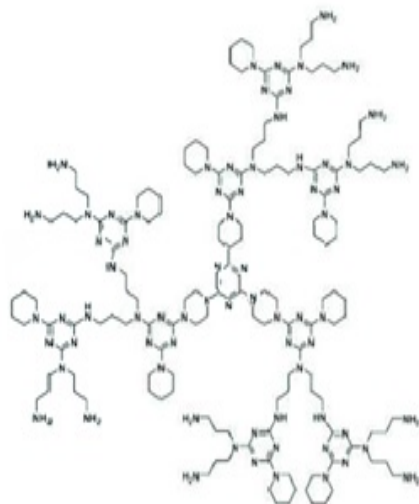


Figure 7: Polymer dendrimer, P [2]

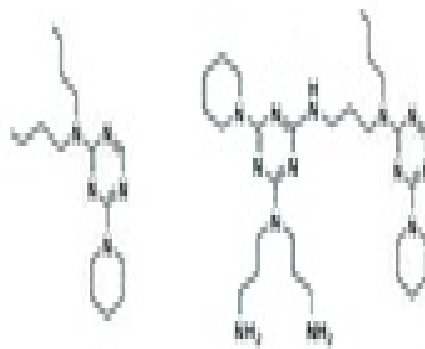


Figure 9: G_1 and G_2

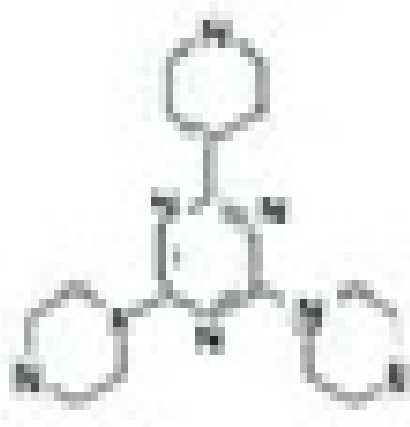


Figure 8: The central part of Figure 7

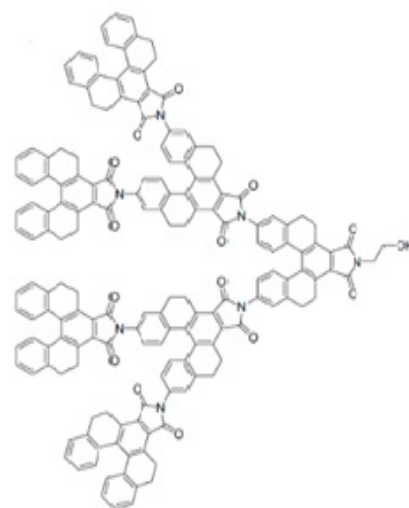


Figure 10: Helicene-based dendrimers, H [2]

$$2^{16n+4} \cdot 3^{12n-6}.$$

The second multiplicative Zagreb index for a main branch of the graph G is equal to $2^{2n+4-12} \cdot 3^{3 \cdot 2^{n+2}-18}$.

Therefore,

$$PM_2(G) = 2^{2n+6-20} \cdot 3^{3 \cdot 2^{n+4}-24}. \quad \square$$

Theorem 3.2 Zagreb, multiplicative Zagreb indices and coindices of Molecular graph of dendrimers using tetrathiafulvalene units as branching centers, D [2] (see Figure 4) are computed as follows:

$$\begin{aligned} M_1 &= 21 \cdot 2^{n+5} - 414, \\ M_2 &= 99 \cdot 2^{n+3} - 493, \\ M_3 &= 13 \cdot 2^{n+3} - 64, \\ PM_1 &= 2^{19 \cdot 2^{n+3}-88} \cdot 3^{5 \cdot 2^{n+4}-52}, \\ PM_2 &= 2^{19 \cdot 2^{n+3}-88} \cdot 3^{15 \cdot 2^{n+3}-78}, \end{aligned}$$

$$\begin{aligned} \overline{M}_1 &= 1085 \cdot 2^{2n+5} - 5344 \cdot 2^{n+3} + 13164, \\ \overline{M}_2 &= 1225 \cdot 2^{2n+5} - 6091 \cdot 2^{n+3} + 15150, \\ \overline{PM}_1 &= 2^{453 \cdot 2^{2n+4}-271 \cdot 2^{n+5}+2598} \cdot 3^{11 \cdot 2^{2n+7}-433 \cdot 2^{n+2}+536}, \\ &595 \cdot 2^{2n+5} - 957 \cdot 2^{n+2} + 1200, \\ \overline{PM}_2 &= 2^{589 \cdot 2^{2n+4}-2827 \cdot 2^{n+2}+3388} \cdot 3^{155 \cdot 2^{2n+5}-793 \cdot 2^{n+3}+2028}. \end{aligned}$$

Proof. Figure 4, has grown four similar branches and two stages. Now, we compute these indices from the stage n . Figure 5 is the central part of Figure 4. For the graph of Figure 5 it is obvious that: $d_2 = 36, d_3 = 14$ so $d_2 = 4d'_2 + 36, d_3 = 4d'_3 + 14$.

For example, for $n = 1$ we have $d_1 = 12, d_2 = 108, d_3 = 54$. On the other hand, calculations show that: $d'_1 = 4 \cdot 2^{n-1} - 1, d'_2 = 19 \cdot 2^n - 20, d'_3 =$



Figure 11: The central part of Figure 10

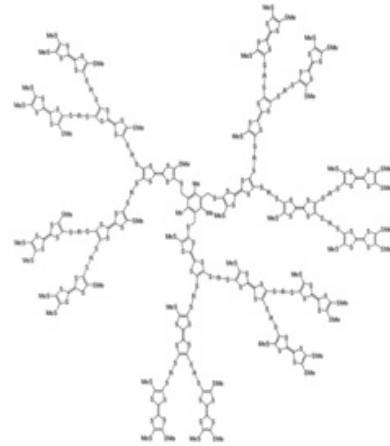


Figure 13: Tetrathiafulvalene [TTF]₂₁-glycol dendrimer, T [3]

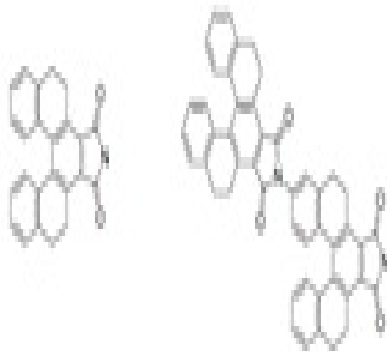


Figure 12: G_1 and G_2

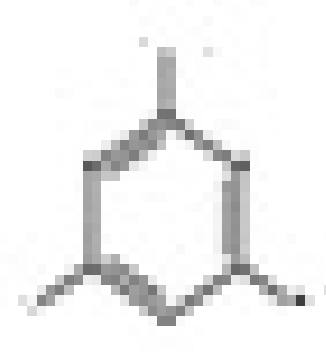


Figure 14: The central part of Figure 14

$5 \cdot 2^{n+1} - 10$, therefore, $d_1 = 2^{n+3} - 4, d_2 = 19 \cdot 2^{n+2} - 44, d_3 = 5 \cdot 2^{n+3} - 26$. Elementary computation gives:

$$\begin{aligned} M_1 &= 21 \cdot 2^{n+5} - 414, \\ PM_1 &= 2^{19 \cdot 2^{n+3} - 88} \cdot 3^{5 \cdot 2^{n+4} - 52}, \\ PM_2 &= 2^{19 \cdot 2^{n+3} - 88} \cdot 3^{15 \cdot 2^{n+3} - 78}. \end{aligned}$$

For the graph of Figure 5, it is obvious that: $x_{22} = 16, x_{23} = 36, x_{33} = 3$, so $x_{22} = 4x'_{22} + 16, x_{23} = 4x'_{23} + 36, x_{33} = 4x'_{33} + 3$. For example, for $n = 1$ we have $x_{13} = 4, x_{12} = 8, x_{22} = 40, x_{23} = 128, x_{33} = 15$.

On the other hand, calculations show that: $x'_{13} = 2^n - 1, x'_{12} = 2^n, x'_{22} = 7 \cdot 2^n - 8, x'_{23} = 23 \cdot 2^n - 23, x'_{33} = 3 \cdot 2^n - 3$, therefore, $x_{13} = 2^{n+2} - 4, x_{12} = 2^{n+2}, x_{22} = 7 \cdot 2^{n+2} - 16, x_{23} = 23 \cdot 2^{n+2} - 56, x_{33} = 3 \cdot 2^{n+2} - 9$.

Elementary computation gives:

$$\begin{aligned} M_2 &= 99 \cdot 2^{n+3} - 493, \\ M_3 &= 13 \cdot 2^{n+3} - 64. \end{aligned}$$

Similar calculation shows that:

$$\begin{aligned} \overline{M_1} &= 1085 \cdot 2^{2n+5} - 5344 \cdot 2^{n+3} + 13164, \\ \overline{M_2} &= 1225 \cdot 2^{2n+5} - 6091 \cdot 2^{n+3} + 15150, \\ \overline{PM_1} &= 2^{453 \cdot 2^{2n+4} - 271 \cdot 2^{n+5} + 2598} \cdot \\ & 3^{11 \cdot 2^{2n+7} - 433 \cdot 2^{n+2} + 536} \cdot \\ & 5^{95 \cdot 2^{2n+5} - 957 \cdot 2^{n+2} + 1200}, \\ \overline{PM_2} &= 2^{589 \cdot 2^{2n+4} - 2827 \cdot 2^{n+2} + 3388} \cdot \\ & 3^{155 \cdot 2^{2n+5} - 793 \cdot 2^{n+3} + 2028}. \end{aligned}$$

Now, we compute multiplicative Zagreb indices using the link of graphs G_1, G_2 as shown in Figure 6:

It is easy to see that:

$$\begin{aligned} PM_1(G_1) &= 2^{38} \cdot 3^{18}, \\ PM_1^{(u_i)}(G_1) &= 2^{38} \cdot 3^{18}, \\ PM_1^{(v_j)}(G_1) &= 2^{36} \cdot 3^{18}, \\ PM_1^{(v_i, u_{i+1})}(G_1) &= 2^{36} \cdot 3^{18} \end{aligned}$$

and so, for $1 \leq i \leq n - 1, 1 \leq j \leq n - 1$.

Therefore:

$$PM_1(G_n) = PM_1^{(v_{n-1})}(G_1) PM_1^{(u_1)}(G_1)$$

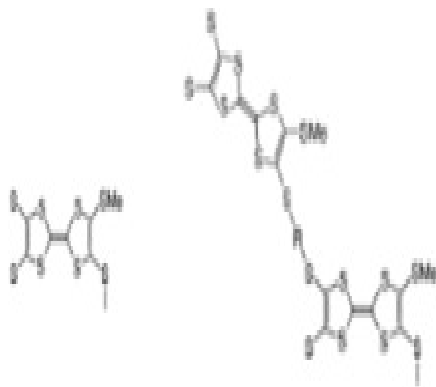


Figure 15: G_1 and G_2

$$(PM_1^{(v_1, u_2)}(G_1))^{n-2} \cdot 6^{2(n-1)} = 2^{38n} \cdot 3^{20n-2}.$$

A branch is added in the second layer such as G_1 and three branches are added in the third layer that its first multiplicative Zagreb index is $2^{38} \cdot 3^{20}$. The total number of added branches in all layers are equal to $2^n - n - 1$.

The first multiplicative Zagreb index for a main branch of the graph of Figure 4 is equal to $2^{38} \cdot 2^{n-38} \cdot 3^{20} \cdot 2^{n-22}$.

Since the graph has four main branches then we obtain high values for four main branches and we consider the obtained number with the first multiplicative Zagreb index which has the central part value of figure that is $2^{-8} \cdot 2^{72} \cdot 3^{36}$.

Therefore:

$$PM_1(G) = 2^{152 \cdot 2^n - 88} \cdot 3^{80 \cdot 2^n - 52}.$$

It is easy to see that:

$$PM_2(G_1) = 2^{38} \cdot 3^{27},$$

$$PM_2^{(u_i)}(G_1) = 2^{38} \cdot 3^{27},$$

$$PM_2^{(v_j)}(G_1) = 2^{36} \cdot 3^{27},$$

$$PM_2^{(v_i, u_{i+1})}(G_1) = 2^{36} \cdot 3^{27}$$

and so, for $1 \leq i \leq n - 1, 1 \leq j \leq n - 1$.

Therefore:

$$PM_2(G_n) = PM_2^{(v_{n-1})}(G_1) PM_2^{(u_1)}(G_1)$$

$$(PM_2^{(v_1, u_2)}(G_1))^{n-2} \cdot (2^2 \cdot 3^3)^{n-1} = 2^{38n} \cdot 3^{30n-3}.$$

The second multiplicative Zagreb index for a main branch of the graph G is equal to $2^{38} \cdot 2^{n-38} \cdot 3^{30} \cdot 2^{n-33}$.

Therefore,

$$PM_2(G) = 2^{152 \cdot 2^n - 88} \cdot 3^{120 \cdot 2^n - 78}. \quad \square$$

Theorem 3.3 Zagreb, multiplicative Zagreb indices and coindices of Molecular graph of Poly-

mer dendrimer, $P[2]$ (see Figure 7) are computed as follows:

$$M_1 = 159 \cdot 2^{n+1} - 186,$$

$$M_2 = 183 \cdot 2^{n+1} - 204,$$

$$M_3 = 18 \cdot 2^{n+1} - 18,$$

$$PM_1 = 2^{45 \cdot 2^{n+1} - 66} \cdot 3^{15 \cdot 2^{n+1} - 12},$$

$$PM_2 = 2^{45 \cdot 2^{n+1} - 66} \cdot 3^{45 \cdot 2^n - 18},$$

$$\overline{M}_1 = 8694 \cdot 2^{2n} - 11130 \cdot 2^n + 3546,$$

$$\overline{M}_2 = 4761 \cdot 2^{2n+1} - 12117 \cdot 2^n + 3825,$$

$$\overline{PM}_1 = 2^{279 \cdot 2^{2n+3} - 1605 \cdot 2^{n+1} + 1191}.$$

$$3^{495 \cdot 2^{2n-1} - 411 \cdot 2^{n-1} + 21} \cdot 5^{675 \cdot 2^{2n} - 399 \cdot 2^{n+1} + 216},$$

$$\overline{PM}_2 = 2^{2835 \cdot 2^{2n} - 3969 \cdot 2^n + 1386}.$$

$$3^{945 \cdot 2^{2n} - 1023 \cdot 2^n + 258}.$$

Proof. Figure 7, has grown three similar branches and two stages. Now, we compute these indices from the stage n . Figure 8 the central part of Figure 7. For the graph of Figure 8 it is obvious that: $d_2 = 15, d_3 = 9$, so $d_2 = 3d_2 + 15, d_3 = 3d_3 + 9$.

For example, for $n = 1$ we have $d_1 = 6, d_2 = 57, d_3 = 24$. On the other hand, calculations show that: $d_1 = 2^n, d_2 = 15 \cdot 2^n - 16, d_3 = 5 \cdot 2^n - 5$, therefore, $d_1 = 3 \cdot 2^n, d_2 = 45 \cdot 2^n - 33, d_3 = 15 \cdot 2^n - 6$.

Elementary computation gives:

$$M_1 = 159 \cdot 2^{n+1} - 186,$$

$$PM_1 = 2^{45 \cdot 2^{n+1} - 66} \cdot 3^{15 \cdot 2^{n+1} - 12},$$

$$PM_2 = 2^{45 \cdot 2^{n+1} - 66} \cdot 3^{45 \cdot 2^n - 18}.$$

For the graph of Figure 8, it is obvious that: $x_{22} = 6, x_{23} = 18, x_{33} = 3$. so $x_{22} = 3x_{22} + 6, x_{23} = 3x_{23} + 18, x_{33} = 3x_{33} + 3$. For example, for $n = 1$ we have $x_{12} = 6, x_{22} = 30, x_{23} = 48, x_{33} = 12$.

On the other hand, calculations show that: $x_{12} = 2^n, x_{22} = 9 \cdot 2^n - 10, x_{23} = 11 \cdot 2^n - 12, x_{33} = 2^{n+1} - 1$.

therefore, $x_{12} = 3 \cdot 2^n, x_{22} = 27 \cdot 2^n - 24, x_{23} = 33 \cdot 2^n - 18, x_{33} = 3 \cdot 2^{n+1}$.

Elementary computation gives:

$$M_2 = 183 \cdot 2^{n+1} - 204,$$

$$M_3 = 18 \cdot 2^{n+1} - 18.$$

Similar calculation shows that:

$$\overline{M}_1 = 8694 \cdot 2^{2n} - 11130 \cdot 2^n + 3546,$$

$$\overline{M}_2 = 4761 \cdot 2^{2n+1} - 12117 \cdot 2^n + 3825,$$

$$\overline{PM}_1 = 2^{279 \cdot 2^{2n+3} - 1605 \cdot 2^{n+1} + 1191}.$$

$$3^{495 \cdot 2^{2n-1} - 411 \cdot 2^{n-1} + 21} \cdot 5^{675 \cdot 2^{2n} - 399 \cdot 2^{n+1} + 216},$$

$$\overline{PM}_2 = 2^{2835 \cdot 2^{2n} - 3969 \cdot 2^n + 1386}.$$

$$3^{945 \cdot 2^{2n} - 1023 \cdot 2^n + 258}.$$

Now, we compute multiplicative Zagreb indices using the link of graphs G_1, G_2 as shown in Figure 9:

It is easy to see that:

$$PM_1(G_1) = 2^{30} \cdot 3^8,$$

$$PM_1^{(u_i)}(G_1) = 2^{30} \cdot 3^8,$$

$$PM_1^{(v_j)}(G_1) = 2^{28} \cdot 3^8,$$

$$PM_1^{(v_i, u_{i+1})}(G_1) = 2^{28} \cdot 3^8$$

and so, for $1 \leq i \leq n - 1, 1 \leq j \leq n - 1$.

Therefore:

$$PM_1(G_n) = PM_1^{(v_{n-1})}(G_1)PM_1^{(u_1)}(G_1)$$

$$(PM_1^{(v_1, u_2)}(G_1))^{n-2} \cdot 6^{2(n-1)} =$$

$$2^{30n} \cdot 3^{10n-2}.$$

A branch is added in the second layer such as G_1 and three branches are added in the third layer that its first multiplicative Zagreb index is $2^{30} \cdot 3^{10}$. The total number of added branches in all layers are equal to $2^n - n - 1$.

The first multiplicative Zagreb index for a main branch of the graph of Figure 7 is equal to $2^{30 \cdot 2^n - 30} \cdot 3^{10 \cdot 2^n - 12}$.

Since the graph has three main branches then we obtain high values for three main branches and we consider the obtained number with the first multiplicative Zagreb index which has the central part value of figure that is $2^{-6} \cdot 2^{30} \cdot 3^{24}$. Therefore:

$$PM_1(G) = 2^{90 \cdot 2^n - 66} \cdot 3^{30 \cdot 2^n - 12}.$$

It is easy to see that:

$$PM_2(G_1) = 2^{30} \cdot 3^{12},$$

$$PM_2^{(u_i)}(G_1) = 2^{30} \cdot 3^{12},$$

$$PM_2^{(v_j)}(G_1) = 2^{28} \cdot 3^{12},$$

$$PM_2^{(v_i, u_{i+1})}(G_1) = 2^{28} \cdot 3^{12}$$

and so, for $1 \leq i \leq n - 1, 1 \leq j \leq n - 1$.

Therefore:

$$PM_2(G_n) = PM_2^{(v_{n-1})}(G_1)PM_2^{(u_1)}(G_1)$$

$$(PM_2^{(v_1, u_2)}(G_1))^{n-2} \cdot (2^2 \cdot 3^3)^{n-1} =$$

$$2^{30n} \cdot 3^{15n-3}.$$

The second multiplicative Zagreb index for a main branch of the graph G is equal to $2^{30 \cdot 2^n - 30} \cdot 3^{15 \cdot 2^n - 18}$.

$$PM_2(G) = 2^{90 \cdot 2^n - 66} \cdot 3^{45 \cdot 2^n - 18}. \quad \square$$

Theorem 3.4 *Zagreb, multiplicative Zagreb indices and coindices of Helicene-based dendrimers, H[2] (see Figure 10) are computed as follows:*

$$M_1 = 43 \cdot 2^{n+3} - 168,$$

$$M_2 = 225 \cdot 2^{n+1} - 226,$$

$$M_3 = 7 \cdot 2^{n+2} - 14,$$

$$PM_1 = 2^{11 \cdot 2^{n+2} - 16} \cdot 3^{7 \cdot 2^{n+3} - 30},$$

$$PM_2 = 2^{11 \cdot 2^{n+2} - 16} \cdot 3^{21 \cdot 2^{n+2} - 45},$$

$$\overline{M}_1 = 891 \cdot 2^{2n+3} - 874 \cdot 2^{n+3} + 1718,$$

$$\overline{M}_2 = 1089 \cdot 2^{2n+3} - 4403 \cdot 2^{n+1} + 2232,$$

$$\overline{PM}_1 = 2^{277 \cdot 2^{2n+2} - 263 \cdot 2^{n+2} + 249} \cdot$$

$$3^{15 \cdot 2^{2n+5} - 259 \cdot 2^{n+1} + 143} \cdot$$

$$5^{77 \cdot 2^{2n+3} - 287 \cdot 2^{n+1} + 131},$$

$$\overline{PM}_2 = 2^{297 \cdot 2^{2n+2} - 513 \cdot 2^{n+1} + 216} \cdot$$

$$3^{189 \cdot 2^{2n+3} - 797 \cdot 2^{n+1} + 420}.$$

Proof. Figure 10, has grown two similar branches and two stages. Now, we compute these indices from the stage n. Figure 11 is the central part of Figure 10. For the graph of Figure 11 it is obvious that: $d_1 = 3, d_2 = 12, d_3 = 15$ so $d_1 = 2d'_1 + 3, d_2 = 2d'_2 + 12, d_3 = 2d'_3 + 15$.

For example, for $n = 1$ we have $d_1 = 7, d_2 = 36, d_3 = 41$. On the other hand, calculations show that: $d'_1 = 2^{n+1} - 2, d'_2 = 11 \cdot 2^n - 10, d'_3 = 7 \cdot 2^{n+1} - 15$, therefore, $d_1 = 2^{n+2} - 1, d_2 = 11 \cdot 2^{n+1} - 8, d_3 = 7 \cdot 2^{n+2} - 15$.

Elementary computation gives:

$$M_1 = 43 \cdot 2^{n+3} - 168,$$

$$PM_1 = 2^{11 \cdot 2^{n+2} - 16} \cdot 3^{7 \cdot 2^{n+3} - 30},$$

$$PM_2 = 2^{11 \cdot 2^{n+2} - 16} \cdot 3^{21 \cdot 2^{n+2} - 45}.$$

For the graph of Figure 11, it is obvious that: $x_{12} = 1, x_{13} = 2, x_{22} = 5, x_{23} = 13, x_{33} = 14$ so $x_{12} = 2x'_{12} + 1, x_{13} = 2x'_{13} + 2, x_{22} = 2x'_{22} + 5, x_{23} = 2x'_{23} + 13, x_{33} = 2x'_{33} + 14$. For example, for $n = 1$ we have $x_{12} = 1, x_{13} = 6, x_{22} = 21, x_{23} = 29, x_{33} = 44$.

On the other hand, calculations show that: $x'_{13} = 2^{n+1} - 2, x'_{22} = x'_{22} = 3 \cdot 2^{n+1} - 4, x'_{23} = 5 \cdot 2^{n+1} - 12, x'_{33} = 15 \cdot 2^n - 15$, therefore $x_{12} = 1, x_{13} = 2^{n+2} - 2, x_{22} = 3 \cdot 2^{n+2} - 3, x_{23} = 5 \cdot 2^{n+2} - 11, x_{33} = 15 \cdot 2^{n+1} - 16$.

Elementary computation gives:

$$M_2 = 225 \cdot 2^{n+1} - 226,$$

$$M_3 = 7 \cdot 2^{n+2} - 14.$$

Similar calculation shows that:

$$\overline{M}_1 = 891 \cdot 2^{2n+3} - 874 \cdot 2^{n+3} + 1718,$$

$$\overline{M}_2 = 1089 \cdot 2^{2n+3} - 4403 \cdot 2^{n+1} + 2232,$$

$$\overline{PM}_1 = 2^{277 \cdot 2^{2n+2} - 263 \cdot 2^{n+2} + 249} \cdot$$

$$3^{15 \cdot 2^{2n+5} - 259 \cdot 2^{n+1} + 143} \cdot$$

$$5^{77 \cdot 2^{2n+3} - 287 \cdot 2^{n+1} + 131},$$

$$\overline{PM}_2 = 2^{297 \cdot 2^{2n+2} - 513 \cdot 2^{n+1} + 216} \cdot$$

$$3^{189 \cdot 2^{2n+3} - 797 \cdot 2^{n+1} + 420}.$$

Now, we compute multiplicative Zagreb indices using the link of graphs G_1, G_2 as shown in Figure 12:

It is easy to see that:

$$PM_1(G_1) = 1^4 \cdot 2^{26} \cdot 3^{24},$$

$$PM_1^{(u_i)}(G_1) = 1^4 \cdot 2^{24} \cdot 3^{24},$$

$$PM_1^{(v_j)}(G_1) = 1^4 \cdot 2^{24} \cdot 3^{24},$$

$$PM_1^{(v_i, u_{i+1})}(G_1) = 1^4 \cdot 2^{22} \cdot 3^{24}$$

and so, for $1 \leq i \leq n - 1, 1 \leq j \leq n - 1$.

Therefore:

$$PM_1(G_n) = PM_1^{(v_{n-1})}(G_1)PM_1^{(u_1)}(G_1)$$

$$(PM_1^{(v_1, u_2)}(G_1))^{n-2} \cdot 3^{4(n-1)} =$$

$$2^{22n+4} \cdot 3^{28n-4}.$$

A branch is added in the second layer such as G_1 and three branches are added in the third layer that its first multiplicative Zagreb index is $2^{22} \cdot 3^{28}$. The total number of added branches in all layers are equal to $2^n - n - 1$.

The first multiplicative Zagreb index for a main branch of the graph of Figure 10 is equal to $2^{11 \cdot 2^{n+1} - 18} \cdot 3^{7 \cdot 2^{n+2} - 32}$.

Since the graph has two main branches then we obtain high values for two main branches and we consider the obtained number with the first multiplicative Zagreb index which has the central part value of figure that is $2^{-4} \cdot 2^{24} \cdot 3^{34}$. Therefore:

$$PM_1(G) = 2^{11 \cdot 2^{n+2} - 16} \cdot 3^{7 \cdot 2^{n+3} - 30}.$$

It is easy to see that:

$$PM_2(G_1) = 1^2 \cdot 2^{26} \cdot 3^{36},$$

$$PM_2^{(u_i)}(G_1) = 1^2 \cdot 2^{24} \cdot 3^{36},$$

$$PM_2^{(v_j)}(G_1) = 1^2 \cdot 2^{24} \cdot 3^{36},$$

$$PM_2^{(v_i, u_{i+1})}(G_1) = 1^2 \cdot 2^{22} \cdot 3^{36}$$

and so, for $1 \leq i \leq n - 1, 1 \leq j \leq n - 1$.

Therefore:

$$PM_2(G_n) = PM_2^{(v_{n-1})}(G_1)PM_2^{(u_1)}(G_1)$$

$$(PM_2^{(v_1, u_2)}(G_1))^{n-2} \cdot 3^{6(n-1)} =$$

$$2^{22n+4} \cdot 3^{42n-6}.$$

The second multiplicative Zagreb index for a main branch of the graph G is equal to $2^{11 \cdot 2^n - 18} \cdot 3^{21 \cdot 2^{n+1} - 48}$.

$$PM_2(G) = 2^{11 \cdot 2^{n+1} - 16} \cdot 3^{21 \cdot 2^{n+2} - 45}. \square$$

Theorem 3.5 *Zagreb, multiplicative Zagreb indices and coindices of Tetrathiafulvalene [TTF]₂₁-glycol Dendrimer (see Figure 13) are computed as follows:*

$$M_1 = 63 \cdot 2^{n+2} - 204,$$

$$M_2 = 303 \cdot 2^n - 243,$$

$$M_3 = 21 \cdot 2^{n+1} - 30,$$

$$PM_1 = 2^{21 \cdot 2^{n+1} - 48} \cdot 3^{9 \cdot 2^{n+2} - 24},$$

$$PM_2 = 2^{21 \cdot 2^{n+1} - 48} \cdot 3^{27 \cdot 2^{n+1} - 36},$$

$$\overline{M}_1 = 2295 \cdot 2^{2n+1} - 3903 \cdot 2^{n+1} + 3312,$$

$$\overline{M}_2 = 2601 \cdot 2^{2n+1} - 8997 \cdot 2^n + 3873,$$

$$\overline{PM}_1 = 2^{837 \cdot 2^{2n} - 717 \cdot 2^{n+1} + 699} \cdot$$

$$3^{9 \cdot 2^{2n+5} - 189 \cdot 2^{n+1} + 81},$$

$$5^{189 \cdot 2^{2n+1} - 357 \cdot 2^{n+1} + 318},$$

$$\overline{PM}_2 = 2^{945 \cdot 2^{2n} - 1899 \cdot 2^n + 936} \cdot$$

$$3^{405 \cdot 2^{2n+1} - 315 \cdot 2^{n+2} + 480}.$$

Proof. Figure 13, has grown three similar branches and three stages. Now, we compute these indices from the stage n. Figure 14 is the central part of Figure 13. For the graph of Figure 14 it is obvious that: $d_1 = 3, d_3 = 6$, so $d_1 = 3d'_1 + 3, d_3 = 2d'_3 + 6$.

For example, for $n = 1$ we have $d_1 = 12, d_2 = 18, d_3 = 24$. On the other hand, calculations show that: $d'_1 = 4 \cdot 2^n - 1, d'_2 = 7 \cdot 2^n - 8, d'_3 = 6 \cdot 2^n - 6$, therefore, $d_1 = 6 \cdot 2^n, d_2 = 21 \cdot 2^n - 24, d_3 = 18 \cdot 2^n - 12$.

Elementary computation gives:

$$M_1 = 63 \cdot 2^{n+2} - 204,$$

$$PM_1 = 2^{21 \cdot 2^{n+1} - 48} \cdot 3^{9 \cdot 2^{n+2} - 24},$$

$$PM_2 = 2^{21 \cdot 2^{n+1} - 48} \cdot 3^{27 \cdot 2^{n+1} - 36}.$$

For the graph of Figure 14, it is obvious that: $x_{13} = 3, x_{33} = 6$. so $x_{13} = 3x'_{13} + 3, x_{33} = 3x'_{33} + 6$. For example, for $n = 1$ we have $x_{22} = 3, x_{23} = 30, x_{13} = 12, x_{33} = 15$.

On the other hand, calculations show that: $x'_{22} = 2^{n+1} - 3, x'_{23} = 5 \cdot 2^{n+1} - 10, x'_{13} = 2^{n+1} - 1, x'_{33} = 3 \cdot 2^n - 3$, therefore, $x_{22} = 3 \cdot 2^{n+1} - 9, x_{23} = 15 \cdot 2^{n+1} - 30, x_{13} = 3 \cdot 2^{n+1}, x_{33} = 9 \cdot 2^n - 3$.

Elementary computation gives:

$$M_2 = 303 \cdot 2^n - 243,$$

$$M_3 = 21 \cdot 2^{n+1} - 30.$$

Similar calculation shows that:

$$\overline{M}_1 = 2295 \cdot 2^{2n+1} - 3903 \cdot 2^{n+1} + 3312,$$

$$\overline{M}_2 = 2601 \cdot 2^{2n+1} - 8997 \cdot 2^n + 3873,$$

$$\overline{PM}_1 = 2^{837 \cdot 2^{2n} - 717 \cdot 2^{n+1} + 699} \cdot$$

$$3^{9 \cdot 2^{2n+5} - 189 \cdot 2^{n+1} + 81},$$

$$5^{189 \cdot 2^{2n+1} - 357 \cdot 2^{n+1} + 318},$$

$$\overline{PM}_2 = 2^{945 \cdot 2^{2n} - 1899 \cdot 2^n + 936} \cdot$$

$$3^{405 \cdot 2^{2n+1} - 315 \cdot 2^{n+2} + 480}.$$

Now, we compute multiplicative Zagreb indices using the link of graphs G_1, G_2 as shown in Figure 15:

It is easy to see that:

$$PM_1(G_1) = 2^{10} \cdot 3^{12},$$

$$PM_1^{(u_i)}(G_1) = 2^{10} \cdot 3^{12},$$

$$PM_1^{(v_j)}(G_1) = 2^{10} \cdot 3^{12},$$

$$PM_1^{(v_i, u_{i+1})}(G_1) = 2^{10} \cdot 3^{12}$$

and so, for $1 \leq i \leq n-1, 1 \leq j \leq n-1$.

Therefore:

$$PM_1(G_n) = PM_1^{(v_{n-1})}(G_1)PM_1^{(u_1)}(G_1) \\ (PM_1^{(v_1, u_2)}(G_1))^{n-2} \cdot 2^{4(n-1)} = \\ 2^{14n-4} \cdot 3^{12n}.$$

A branch is added in the second layer such as G_1 and three branches are added in the third layer that its first multiplicative Zagreb index is $2^{14} \cdot 3^{12}$. The total number of added branches in all layers are equal to $2^n - n - 1$.

The first multiplicative Zagreb index for a main branch of the graph of Figure 13 is equal to $2^{14} \cdot 2^{n-18} \cdot 3^{12} \cdot 2^{n-12}$.

Since the graph has three main branches then we obtain high values for three main branches and we consider the obtained number with the first multiplicative Zagreb index which has the central part value of figure that is $2^6 \cdot 3^{12}$. Therefore:

$$PM_1(G) = 2^{42} \cdot 2^{n-48} \cdot 3^{36} \cdot 2^{n-24}.$$

It is easy to see that:

$$PM_2(G_1) = 2^{10} \cdot 3^{18},$$

$$PM_2^{(u_i)}(G_1) = 2^{10} \cdot 3^{18},$$

$$PM_2^{(v_j)}(G_1) = 2^{10} \cdot 3^{18},$$

$$PM_2^{(v_i, u_{i+1})}(G_1) = 2^{10} \cdot 3^{18}$$

and so, for $1 \leq i \leq n-1, 1 \leq j \leq n-1$.

Therefore:

$$PM_2(G_n) = PM_2^{(v_{n-1})}(G_1)PM_2^{(u_1)}(G_1) \\ (PM_2^{(v_1, u_2)}(G_1))^{n-2} \cdot 2^{4(n-1)} = \\ 2^{14n-4} \cdot 3^{18n}.$$

The second multiplicative Zagreb index for a main branch of the graph G is equal to $2^{14} \cdot 2^{n-18} \cdot 3^{18} \cdot 2^{n-18}$.

$$PM_2(G) = 2^{42} \cdot 2^{n-48} \cdot 3^{54} \cdot 2^{n-36}. \quad \square$$

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Vida Ahmadi was born in Masjed-soleyman in 1974. She is a tenured lecturer at Mathematics Department of Abadan Islamic Azad University, Abadan, Iran. Ms. Ahmadi graduated from Shahid-Chamran University of Ahvaz, Ahvaz, Iran, where she got her BSs, MSs, and Ph.D. in Mathematics. She has published two books and two articles in Iranian journals and one of her articles has been published in a foreign journal out of Iran.



Mohammad Reza Derafshe, Ph.D born in Abadan is a full professor at the faculty of Mathematics, Computer and Statistics of Tehran University, Tehran, Iran. He graduated from Tehran University and University of Birmingham, England. After completing his Ph.D. in 1978, he began his working at Ahvaz University. During

all his 37 years of teaching, Dr. Derafshe gained enormous honors and awards including Abuds Salam Award from Theoretical Physics and Trieste Mathematics, Italy and Kharazmi International Award, the 10th Kharazmi International Award. Dr. Derafshe has run three terms as the member of the Executive Council of The Iranian Mathematical Society and is also the member of both The American and The London Mathematical Societies. He has compiled and translated eight books which have been published. It is worth mentioning that Dr. Derafshe has supervised 88 Ph.D. candidates dissertations as their advisors and has been elected as the Researcher of the Year in Tehran University in 2008 and 2011 as well as the Professor of the Year in Tehran University in 2003.



Seyed Jamal Hashemizadeh, Ph.D. born in Ahvaz in 1974 is an assistant professor at the faculty of Mathematics, Computer, and Statistics of Shahid Chamran University of Ahvaz, Ahvaz, Iran.

He graduated from Shahid Chamran University of Ahvaz in Mathematics and started his teaching in that university after completing his Ph.D. Dr. Hashemizadeh has published two articles in foreign journals out of Iran. He has also supervised 3 Ph.D. candidates dissertations and 33 MSs students theses as their advisors.