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Research Article

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Computing Some Topological Indices of the Molecular Graphs of Benzyl Ether with $C_{60}H$ Core and Benzyl Ether with Porphyrin Core

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Abstract

In this paper, the first, second and third Zagreb indices, the first and second multiplicative Zagreb indices, the F-index and F-polynomial of benzyl ether dendrimer with $C_{60}H$ core and benzyl ether dendrimer with porphyrin core are calculated. In addition, the first and second Zagreb coindices, the first and second multiplicative Zagreb coindices of these graphs are computed as well. Finally, the multiplicative Zagreb index of these graphs is computed through the link of graphs.

Keywords : Zagreb indices; Multiplicative Zagreb indices; Zagreb coindices; Multiplicative Zagreb coindices; F-index; F-polynomial.

1 Introduction

Dendrimers are highly branched nanostructures considered as building blocks in nanotechnology with a variety of appropriate applications. Chemical graph theory is a branch of mathematical chemistry concerned with the study of chemical graphs. The basic idea of chemical graph theory is that physico-chemical properties of molecules can be studied by using the information encoded in their corresponding chemical graphs. A molecular graph is a simple graph, such that its vertices correspond to the atoms and the edges to the bonds. Molecular descriptors play a significant role in chemistry, pharmacology, etc. Among them, topological indices have a prominent place [17]. In organic chemistry, topological indices have been found to be useful in chemical documentation, isomer discrimination, structure-property relationships (SPR), structure-activity relationships (SAR) and pharmaceutical drug design [11]. Throughout this article all graphs are simple and connected. Let $G = (V, E)$ be a simple connected graph with vertex set V and edge set E. The degree $d(u) = d_G(u)$ of a vertex $u \in V$ is the number of vertices of G adjacent to u. The edge connecting the vertices u and v will be expressed by uv. The complement $\overline{G}$ of the graph G is the graph with vertex set V, where two vertices are adjacent if and only if they are not adjacent in G. In 1972, Gutman and Trinajsti [12] defined the first and second Zagreb indices to assess the structure-dependency of the total amount

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of π-electron energy unconjugated systems. Soon after that, it was found that the Zagreb indices provided a measure of the underlying molecules of carbon skeleton branching. The two Zagreb indices belong to the oldest molecular structure descriptors, the properties of which are extensively assessed. The first and second Zagreb indices are defined as follow:

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

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

The alternative expression of the first Zagreb index is $M_1(G) = \sum_{uv\in E}(d(u) + d(v))$. The first general Zagreb index [13, 20] of a graph G is defined as $M_1^{\alpha}(G) = \sum_{u\in V} d(u)^{\alpha} = \sum_{uv\in E}(d(u)^{\alpha-1} + d(v)^{\alpha-1})$, where $\alpha \in \mathbb{R}$ and $\alpha \neq 0, 1$. If $\alpha = 3$, the F-index is neglected. Abdo et al. [1] assessed the extremal trees with respect to F-index . In symbolic notation, the F-index is expressed as $F(G) = \sum_{v\in V} d(v)^3 = \sum_{uv\in E}[d(u)^2 + d(v)^2]$. Analogous to other topological polynomial, the F-Polynomial of graph G is defined as $F(G, x) = \sum_{uv\in E} x^{[d(u)^2+d(v)^2]}$. Ashrafi et al. [4, 5] defined the first and second Zagreb coindices as follows:

$$\overline{M_1}(G) = \sum_{uv \notin E} (d(u) + d(v)),$$

$$\overline{M_2}(G) = \sum_{uv \notin E} (d(u).d(v)).$$

In 2013, Xu. et, al. [19] defined the multiplicative Zagreb coindices by

$$\overline{PM_1}(G) = \prod_{uv \notin E} (d(u) + d(v)),$$

$$\overline{PM_2}(G) = \prod_{uv \notin E} (d(u).d(v)).$$

They defined the multiplicative sum Zagreb index and the total multiplicative sum Zagreb index by

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

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

Gutman and Furtula [10] determine relations between the first Zagreb index and the first Zagreb coindex of graph G and its complement $\bar{G}$ as $M_1(\bar{G}) = M_1(G) + n(n-1)^2 - 4m(n-1)$, $\overline{M}_1(\bar{G}) = 2m(n-1) - M_1(G)$ and $\overline{M}_1(G) = 2m(n-1) - M_1(G)$, where $n = n(G)$ and $m = m(G)$ are the number of vertices and edges of G, respectively. Moreover, there exist known correlations between the first and second Zagreb indices and the second Zagreb coindex of graph G and its complement $\bar{G}$, that expressed as follow:

$$\begin{aligned} M_2(\bar{G}) =& \frac{1}{2}n(n-1)^3 - 3m(n-1)^2 + 2m^2 \\ &+ \frac{2n-3}{2}M_1(G) - M_2(G), \end{aligned}$$

$$\overline{M}_2(\bar{G}) = m(n-1)^2 - (n-1)M_1(G) + M_2(G),$$

$$\overline{M}_2(G) = 2m^2 - \frac{1}{2}M_1(G) - M_2(G).$$

In addition, Fath-Tabar [9] defined the third Zagreb index, as $M_3(G) = \sum_{uv\in E} \mid d(u) - d(v) \mid$. Todeschine et al. [16, 18] defined the first and second multiplicative Zagreb indices as follow:

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

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

The alternative expression of the second multiplicative Zagreb index can be expressed as $PM_2(G) = \prod_{uv\in E} d(u).d(v)$. Iranmaesh et al. [14] computed multiplicative Zagreb indices for a class of dendrimers by applying the link of graphs. In some recent papers [2, 3, 6, 7, 8, 15], the authors calculated the Zagreb indices and coindices of some chemical graphs and nanotubes.

In this article, we compute the Zagreb indices, the first and second multiplicative Zagreb indices, the first and second Zagreb coindices, the first and second multiplicative Zagreb coindices, the multiplicative sum Zagreb index and the total multiplicative sum Zagreb index of benzyl ether dendrimer with $C_{60}H$ core and benzyl ether dendrimer with porphyrin core.

2 Preliminaries

Let G be a simple connected graph. The number of vertices with degree i, expressed d_i and e_{ij}, $i \neq$

j, constitutes the number of edges connecting the vertex of degree i with a vertex of degree j and e_{ii} constitutes the number of edges connecting two vertices of degree i. The symbol d'_i is the number of vertices with degree i in a branch and e'_{ij}, $i \neq j$, constitutes the number of edges connecting the vertex of degree i with a vertex of degree j in a branch. The symbol n' constitutes the number of vertices in a branch and m' is the number of edges in a branch.

Lemma 2.1. *The number of two element subsets with vertices of degree i is $\binom{d_i}{2} = \frac{d_i(d_i-1)}{2}$ and the number of subsets with vertices of degrees i and j is $\binom{d_i}{1}\binom{d_j}{1} = d_i d_j$.*

Proof. For $i \neq j$, let D_i and D_j be the sets of vertices of degrees i and j, respectively. Then $|D_i|= d_i$, $|D_j|= d_j|$ and the number of two element subsets with vertices of degrees i and j is $|D_i||D_j|= d_i d_j = \binom{d_i}{1}\binom{d_j}{1}$. In addition, D_i has $\binom{d_i}{2}$ two element subsets. Thus the number of two element subsets with vertices of degree i is $\binom{d_i}{2} = \frac{d_i(d_{i-1})}{2}$. □

Lemma 2.2. *Let $\overline{e}_{ij}$ be the number of two element subsets of not adjacent vertices of degrees i and j, so that $\overline{e}_{ij}$ does not include the number of edges that connect vertices i and j and $\overline{e}_{ii}$ be the number of two element subsets of not adjacent vertices of degrees i, so that $\overline{e}_{ii}$ does not include the number of edges that connect two vertices of degree i. Then the following relations are hold:*

$$\overline{e}_{ij} = \binom{d_i}{1}\binom{d_j}{1} - e_{ij} = d_i d_j - e_{ij},$$

$$\overline{e}_{ii} = \binom{d_i}{2} - e_{ii} = \frac{d_i(d_i-1)}{2} - e_{ii}.$$

Proof. By definition, the number of two element subsets of adjacent vertices of degree i is e_{ii} and the number of two element subsets of adjacent vertices of degrees i and j is e_{ij}. In addition, $\overline{e}_{ii}$ is the number of two element subsets of not adjacent vertices of degree i and $\overline{e}_{ij}$ is the number of two element subsets of not adjacent vertices of degrees i and j. Therefore, by Lemma 2.1 $\overline{e}_{ij} = \binom{d_i}{1}\binom{d_j}{1} - e_{ij}$ and $\overline{e}_{ii} = \binom{d_i}{2} - e_{ii}$. □

The above lemmas are applied to obtain $PM^T(G)$, the Zagreb and the multiplicative Zagreb coindices .

Definition 2.1. *Let G and H be the two graphs, $u \in V(G)$ and $v \in V(H)$. 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.*

Lemma 2.3. *[12] Let G_1 and G_2 be the two graphs. The first and second Zagreb indices of G_1 and G_2 link satisfies the following relations:*

$$PM_1(G_1 \square G_2)(v_1, v_2) =$$

$$\left(\frac{(d_{G_1}(v_1)+1)(d_{G_2}(v_2)+1)}{d_{G_1}(v_1)d_{G_2}(v_2)}\right)^2$$

$$\times PM_1(G_1)PM_1(G_2),$$

$$PM_2(G_1 \square G_2)(v_1, v_2) =$$

$$\frac{(d_{G_1}(v_1)+1)^{d_{G_1}(v_1)+1}(d_{G_2}(v_2)+1)^{d_{G_2}(v_2)+1}}{(d_{G_1}(v_1))^{d_{G_1}(v_1)}(d_{G_2}(v_2))^{d_{G_2}(v_2)}}$$

$$\times PM_2(G_1)PM_2(G_2).$$

3 Main results

In this section, we derive the main results of this paper. If G is a graph and $u_1, ..., u_n \in V$, then we use the truncated versions of two multiplicative Zagreb indices as

$$PM_1^{(u_1,...,u_n)}(G) = \prod_{\substack{u \in V \\ u \neq u_1,...u_n}} d(u)^2,$$

$$PM_2^{(u_1,...,u_n)}(G) = \prod_{\substack{u \in V \\ u \neq u_1,...u_n}} d(u)^{d(u)}.$$

Theorem 3.1. *Let G be the Molecular graph of benzyl ether dendrimers with $C_{60}H$ core (see Fig. 1). Then the following relations are hold:*

$$M_1(G) = 21.2^{k+2} + 500,$$

$$M_2(G) = 3.2^{k+5} + 779,$$

$$M_3(G) = 3.2^{k+2} - 6,$$

$$PM_1(G) = 2^{3.2^{k+3}-6}.3^{2^{k+3}+110},$$

$$PM_2(G) = 2^{3.2^{k+3}+2}.3^{3.2^{k+2}+165},$$

$$\overline{M_1}(G) = 9.2^{2k+6} + 1069.2^{k+2} + 7500,$$

$$\overline{M_2}(G) = 1089.2^{2k+1} - 1719.2^{k+1} + 1356,$$

$$\overline{PM_1}(G) = 2^{19.2^{2k+3}+29.2^{k+1}+1550} .3^{2^{2k+3}+127.2^{k+1}+1377} .5^{3.2^{2k+4}+155.2^{k+2}-370}.7^{2^{k+3}+105},$$

$$\overline{PM_2}(G) = 2^{3.2^{2k+6}+33.2^{k+4}-152} .3^{2^{2k+6}+267.2^{k+2}+2585},$$

$$PM_1^*(G) = 2^{3.2^{k+2}+90}.3^{87}.5^{3.2^{k+2}-13}.7^5,$$

$$PM^T(G) = 2^{19.2^{2k+3}+35.2^{k+1}+1637} .3^{2^{2k+3}+127.2^{k+1}+1464} .5^{3.2^{2k+4}+158.2^{k+2}-383}.7^{2^{k+3}+110}.$$

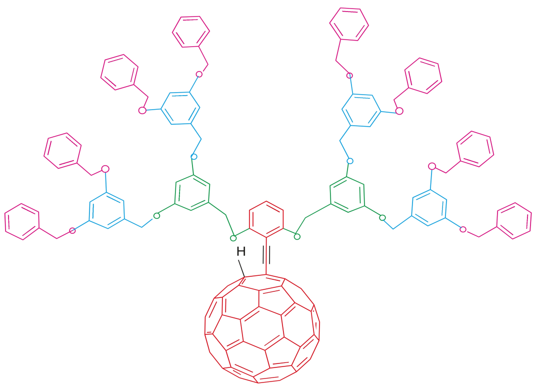

Figure 1: Molecular graph of benzyl-ether type dendrimers from the first to three generations having a fullerene cage as an electroactive core $G_kC_{60}H(k = 1 - 3)$

Proof. The growth of two similar branches and three stages are shown in Fig. 1. These indices are computed from the stage k. The central part of Fig. 1 is shown in Fig. 2 and it is easy to see that $d_1 = 1, d_2 = 3, d_3 = 61, d_4 = 2$. Thus $d_1 = 1$, $d_2 = 2d_2' + 3$, $d_3 = 2d_3' + 61$, $d_4 = 2$. For example, for $k = 1$, the $d_1 = 1$, $d_2 = 17$, $d_3 = 63$, $d_4 = 2$ are yield. Now, calculations indicate that $d_2' = 3.2^{k+1} - 5$, $d_3' = 2^{k+1} - 3$. Therefore, $d_1 = 1$,

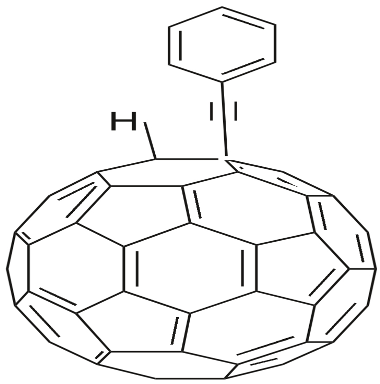

Figure 2: The central part of Fig. 1

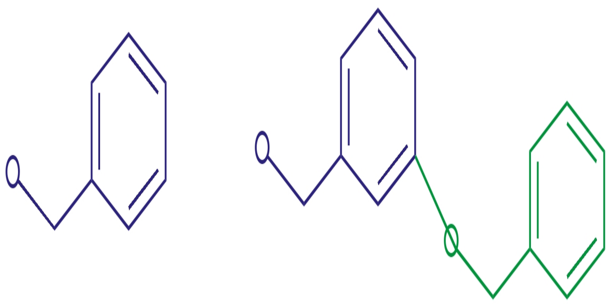

Figure 3: G_1 and $G_2 = G_1 \square G_1$

$d_2 = 3.2^{k+2} - 7$, $d_3 = 2^{k+2} + 55$ and $d_4 = 2$. The following relations are yield now:

$$M_1(G) = 21.2^{k+2} + 500,$$

$$PM_1(G) = 2^{3.2^{k+3}-6}.3^{2^{k+3}+110},$$

$$PM_2(G) = 2^{3.2^{k+3}+2}.3^{3.2^{k+2}+165}.$$

As to Fig. 2, it is obvious that $e_{14} = 1$, $e_{22} = 2$, $e_{23} = 2$, $e_{33} = 87$, $e_{34} = 5$, $e_{44} = 1$. So $e_{22} = 2e_{22}' + 2$, $e_{23} = 2e_{23}' + 2$. For example, for $k = 1$, $e_{14} = 1$, $e_{22} = 12$, $e_{23} = 10$, $e_{33} = 87$, $e_{34} = 5$, $e_{44} = 1$ are yield. Here, calculations show that $e_{22}' = 3.2^k - 1$, $e_{23}' = 3.2^{k+1} - 8$. Therefore, $e_{14} = 1$, $e_{22} = 3.2^{k+1}$, $e_{23} = 3.2^{k+2} - 14$, $e_{33} = 87$, $e_{34} = 5$, $e_{44} = 1$. The followings are derived now:

$$M_2(G) = 3.2^{k+5} + 779,$$

$$M_3(G) = 3.2^{k+2} - 6.$$

We apply Lemma 2.1 and Lemma 2.2, then similar calculations indicate that

$$\overline{M_1}(G) = 9.2^{2k+6} + 1069.2^{k+2} + 7500,$$

$$\overline{M_2}(G) = 81.2^{2k+3} + 2811.2^{k+1} + 11771,$$

$$\overline{PM_1}(G) = 2^{19.2^{2k+3}+29.2^{k+1}+1550} .3^{2^{2k+3}+127.2^{k+1}+1377} .5^{3.2^{2k+4}+155.2^{k+2}-370}.7^{2^{k+3}+105},$$

$$\overline{PM_2}(G) = 2^{3.2^{2k+6}+33.2^{k+4}-152} .3^{2^{2k+6}+267.2^{k+2}+2585},$$

$$PM_1^*(G) = 2^{3.2^{k+2}+90}.3^{87}.5^{3.2^{k+2}-13}.7^5,$$

$$PM^T(G) = 2^{19.2^{2k+3}+35.2^{k+1}+1637} .3^{2^{2k+3}+127.2^{k+1}+1464} .5^{3.2^{2k+4}+158.2^{k+2}-383}.7^{2^{k+3}+110}.$$

Now, the multiplicative Zagreb indices are computed through the link of graph G_1 and G_1 as observe in Fig. 3. It is easy to see that for $1 \le i \le k-1$, $1 \le j \le k-1$ the followings are hold:

$$PM_1(G_1) = 2^{14}.3^2,$$

$$PM_1^{(u_i)}(G_1) = PM_1^{(v_j)}(G_1) = 2^{12}.3^2,$$

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

We define G_k, $k \ge 2$ as follow:

$$G_k = (G_{k-1} \square G_1)(v_1, u_1),$$

$$G_{k-1} = (G_{k-2} \square G_1)(v_2, u_2),$$

$$\vdots$$

$$G_2 = (G_1 \square G_1)(v_{k-1}, u_{k-1}).$$

According to Lemma 2.3, the following relations are derived:

$$PM_1(G_k) = PM_1^{(v_1)}(G_{k-1}) .PM_1^{(u_1)}(G_1).2^2.3^2,$$

$$PM_1^{(v_1)}(G_{k-1}) = PM_1^{(v_2)}(G_{k-2}) .PM_1^{(v_1,u_2)}(G_1).2^2.3^2,$$

$$\vdots$$

$$PM_1^{(v_{k-2})}(G_2) = PM_1^{(v_{k-1})}(G_1) .PM_1^{(v_{k-2},u_{k-1})}(G_1).2^2 3^2.$$

Therefore the following relations are yield:

$$PM_1(G_k) = PM_1^{(v_{k-1})}(G_1).PM_1^{(u_1)}(G_1) \prod_{i=2}^{k-1} PM_1^{(v_{i-1},u_i)}(G_1).2^{2(k-1)}.3^{2(k-1)}$$
$$= PM_1^{(v_{k-1})}(G_1).PM_1^{(u_1)}(G_1) .(PM_1^{(v_1,u_2)}(G_1))^{k-2}.2^{2(k-1)}.3^{2(k-1)}$$
$$= 2^{8k}3^{8k-2}.$$

One branch like G_1 is added in the second layer and three branches are added in the third layer. The total number of added branches in all layers is equal to $2^k - k - 1$. The first multiplicative Zagreb index for a branch of graph of Fig. 1 is equal to $2^{3.2^{k+2}-10}.3^{2^{k+2}-6}$. As the graph has two main branches, 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 $1^2.2^6.3^{122}.4^4$. Therefore $PM_1(G) = 2^{3.2^{k+3}-6}.3^{2^{k+3}+110}$. Now, it is easy to see that for $1 \le i \le k-1$ and $1 \le j \le k-1$, we have

$$PM_2(G_1) = 2^{14}.3^3,$$

$$PM_2^{(u_i)}(G_1) = PM_2^{(v_j)}(G_1) = 2^{12}.3^3,$$

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

Again Lemma 2.3 show that the following relations are hold too:

$$PM_2(G_k) = PM_2^{(v_1)}(G_{k-1}) .PM_2^{(u_1)}(G_1).2^2.3^3,$$

$$PM_2^{(v_1)}(G_{k-1}) = PM_2^{(v_2)}(G_{k-2}) .PM_2^{(v_1,u_2)}(G_1).2^2.3^3,$$

$$\vdots$$

$$PM_2^{(v_{k-2})}(G_2) = PM_2^{(v_{k-1})}(G_1) .PM_2^{(v_{k-2},u_{k-1})}(G_1).2^2.3^3.$$

Therefore the following relations are yield:

$$\begin{aligned}PM_2(G_k) &= PM_2^{(v_{k-1})}(G_1).PM_2^{(u_1)}(G_1)\\ &\prod_{i=2}^{k-1} PM_2^{(v_{i-1},u_i)}(G_1).(2^2.3^3)^{(k-1)}\\ &=PM_2^{(v_{k-1})}(G_1).PM_2^{(u_1)}(G_1)\\ &.(PM_2^{(v_1,u_2)}(G_1))^{k-2}.(2^2.3^3)^{(k-1)}\\ &=2^{12k+2}.3^{6k-3}.\end{aligned}$$

One branch like G_1 is added in the second layer and three branches are added in the third layer. The total number of added branches in all layers is equal to $2^k - k - 1$. The second multiplicative Zagreb index for a branch of graph of Fig. 1 is equal to $2^{3.2^{k+1}-10}.3^{3.2^{k+1}-9}$. As the graph has two main branches then we obtain high values for two main branches and we consider the obtained number with the second multiplicative Zagreb index which has the central part value of figure is $1^1.2^6.3^{183}.4^8$. Thus

$$PM_2(G) = 2^{3.2^{k+3}+2}.3^{3.2^{k+2}+165}.$$

□

Theorem 3.2. *Let G be the benzyl ether dendrimer with $C_{60}H$ core (see Fig. 1). Then the first Zagreb index and the first Zagreb coindex of $\bar{G}$ are computed as follow:*

$$\begin{aligned}M_1(\bar{G}) &=2^{3k+12} + 293.2^{2k+7}\\ &+ 28241.2^{k+2} + 112000,\\ \overline{M}_1(\bar{G}) &=9.2^{2k+6} + 1069.2^{k+2} + 7500.\end{aligned}$$

Proof. For the graph of Fig. 2, it is obvious that $n = 67$ and $m = 98$. Thus $n = 2n' + 67$ and $m = 2m' + 98$. For example, if $k = 1$, then $n = 83$, $m = 116$. Now, calculations indicate that $n' = 2^{k+3} - 8$ and $m' = 9.2^k - 9$. Therefore, $n = 2^{k+4} + 51$ and $m = 9.2^{k+1} + 80$. Thus, we obtain

$$\begin{aligned}M_1(\bar{G}) &=2^{3k+12} + 293.2^{2k+7}\\ &+ 28241.2^{k+2} + 112000,\\ \overline{M}_1(\bar{G}) &=9.2^{2k+6} + 1069.2^{k+2} + 7500.\end{aligned}$$

□

Theorem 3.3. *Suppose G be the benzyl ether dendrimer with $C_{60}H$ core (see Fig. 1). Then*

$$\begin{aligned}F(G) &=51.2^{k+2} + 1558,\\ F(G,x) &=x^{17} + (3.2^{k+1}).x^8\\ &+ (3.2^{k+2} - 14).x^{13}\\ &+ 87.x^{18} + 5.x^{25} + x^{32}.\end{aligned}$$

Proof. Let the edge set of G be divided into six classes based on the degree of the end vertices as $e_{14} = 1$, $e_{22} = 3.2^{k+1}$, $e_{23} = 3.2^{k+2} - 14$, $e_{33} = 87$, $e_{34} = 5$, $e_{44} = 1$. In the following, we calculate the F-index of benzyl ether dendrimer with $C_{60}H$ core (see Fig. 1) as:

$$\begin{aligned}F(G) &=17.e_{14} + 8.e_{22} + 13.e_{23}\\ &+ 18.e_{33} + 25.e_{34} + 32.e_{44}\\ &=51.2^{k+2} + 1558.\end{aligned}$$

The F-Polynomial is calculated as

$$\begin{aligned}F(G,x) &=e_{14}.x^{17} + e_{22}.x^8 + e_{23}.x^{13}\\ &+ e_{33}.x^{18} + e_{34}.x^{25} + e_{44}.x^{32}.\end{aligned}$$

So, we obtain

$$\begin{aligned}F(G,x) &=x^{17} + (3.2^{k+1}).x^8\\ &+ (3.2^{k+2} - 14).x^{13}\\ &+ 87.x^{18} + 5.x^{25} + x^{32}.\end{aligned}$$

□

Theorem 3.4. *Let G be the benzyl ether dendrimers with porphyrin core. Then the first and second Zagreb, multiplicative Zagreb indices and coindices are computed as follow:*

$$M_1(G) = 13.2^{2k+6} - 512,$$

$$M_2(G) = 119.2^{2k+3} - 564,$$

$$M_3(G) = 9.2^{2k+4} - 88,$$

$$PM_1(G) = 2^{13.2^{2k+4}-160}.3^{\frac{17.2^{2k+4}-128}{3}},$$

$$PM_2(G) = 2^{13.2^{2k+4}-160}3^{17.2^{2k+3}-64},$$

$$\overline{M_1}(G) = \frac{649.2^{4k+8} - 6759.2^{2k+5} + 70304}{3},$$

$$\overline{M_2}(G) = 121.2^{4k+9} - 10027.2^{2k+3} + 25908,$$

$$\begin{aligned}\overline{PM_1}(G) =& 2^{\frac{443.2^{4k+8}+20447.2^{2k+3}+61004}{9}} \\ & .3^{\frac{523.2^{4k+5}-3667.2^{2k+2}+2036}{9}} \\ & .5^{\frac{221.2^{4k+6}-35.2^{2k+9}+5384}{3}}, \\ \overline{PM_2}(G) =& 2^{\frac{767.2^{4k+6}-8789.2^{2k+3}+25040}{3}} \\ & .3^{\frac{1003.2^{4k+6}-2287.2^{2k+5}+20224}{9}}, \\ PM_1^*(G) =& 2^{3.2^{2k+5}-60}.3^{12}.5^{2^{2k+7}-88}, \\ PM^T(G) =& 2^{\frac{443.2^{4k+8}-20339.2^{2k+3}+60464}{9}} \\ & .3^{\frac{523.2^{4k+5}-3667.2^{2k+2}+2144}{9}} \\ & .5^{\frac{221.2^{4k+6}-137.2^{2k+7}+5120}{3}}.\end{aligned}$$

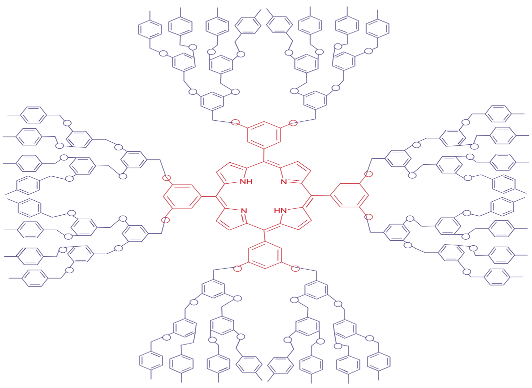

Figure 4: Molecular graph of benzyle ether dendrimers with porphyrin core

Proof. The growth of eight similar branches and one stages are shown in Fig. 4. Now these indices can be computed from the stage k. The graph in Fig. 5 shows the central part of Fig. 4. Form the graph of Fig. 5, it is obvious that $d_2 = 32$ and $d_3 = 24$. Thus $d_1 = 8d_1'$, $d_2 = 8d_2' + 32$ and $d_3 = 8d_3' + 24$. For example, for $k = 1$, the $d_1 = 32$, $d_2 = 336$ and $d_3 = 160$ are yield. Now, calculations show that $d_1' = 2^{2k}$, $d_2' = 13.2^{2k} - 14$, $d_3' = \frac{17.2^{2k}-17}{3}$. Therefore, $d_1 = 2^{2k+3}$, $d_2 = 13.2^{2k+3} - 80$ and $d_3 = \frac{17.2^{2k+3}-64}{3}$. On the other

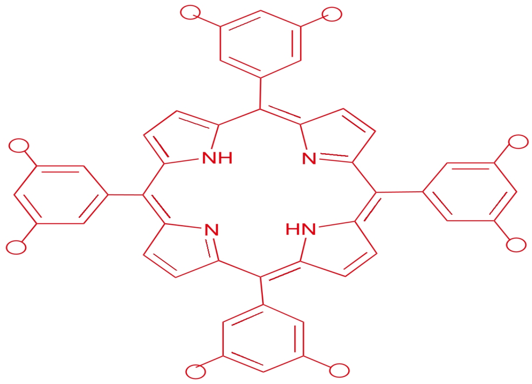

Figure 5: The central part of Fig. 4

hand, elementary computation gives

$$\begin{aligned}M_1(G) =& 13.2^{2k+6} - 512, \\ PM_1(G) =& 2^{13.2^{2k+4}-160}.3^{\frac{17.2^{2k+4}-128}{3}}, \\ PM_2(G) =& 2^{13.2^{2k+4}-160}.3^{17.2^{2k+3}-64}.\end{aligned}$$

For the graph in Fig. 5, it is obvious that $e_{22} = 4$, $e_{23} = 48$ and $e_{33} = 12$. Thus $e_{13} = 8.e_{13}'$, $e_{22} = 8.e_{22}' + 4$, $e_{23} = 8.e_{23}' + 48$ and $e_{33} = 8.e_{33}' + 12$. For example, if $k = 1$, then $e_{13} = 32$, $e_{22} = 124$, $e_{23} = 424$ and $e_{33} = 12$ are yield. Now, calculations show that $e_{13}' = 2^{2k}$, $e_{22}' = 5.2^{2k} - 5$, $e_{23}' = 2^{2k+4} - 17$ and $e_{33}' = 0$. Therefore, $e_{13} = 2^{2k+3}$, $e_{22} = 5.2^{2k+3} - 36$, $e_{23} = 2^{2k+7} - 88$ and $e_{33} = 12$. So elementary computation gives

$$\begin{aligned}M_2(G) =& 119.2^{2k+3} - 564, \\ M_3(G) =& 9.2^{2k+4} - 88.\end{aligned}$$

Now, we apply Lemma 2.1 and Lemma 2.2, then Similar calculations reveal that

$$\overline{M_1}(G) = \frac{649.2^{4k+8} - 6759.2^{2k+5} + 70304}{3},$$

$$\overline{M_2}(G) = 121.2^{4k+9} - 10027.2^{2k+3} + 25908,$$

$$\begin{aligned}\overline{PM_1}(G) =& 2^{\frac{443.2^{4k+8}+20447.2^{2k+3}+61004}{9}}\\ &.3^{\frac{523.2^{4k+5}-3667.2^{2k+2}+2036}{9}}\\ &.5^{\frac{221.2^{4k+6}-35.2^{2k+9}+5384}{3}},\\ \overline{PM_2}(G) =& 2^{\frac{767.2^{4k+6}-8789.2^{2k+3}+25040}{3}}\\ &.3^{\frac{1003.2^{4k+6}-2287.2^{2k+5}+20224}{9}},\\ PM_1^*(G) =& 2^{3.2^{2k+5}-60}.3^{12}.5^{2^{2k+7}-88},\\ PM^T(G) =& 2^{\frac{443.2^{4k+8}-20339.2^{2k+3}+60464}{9}}\\ &.3^{\frac{523.2^{4k+5}-3667.2^{2k+2}+2144}{9}}\\ &.5^{\frac{221.2^{4k+6}-137.2^{2k+7}+5120}{3}}.\end{aligned}$$

Now, the multiplicative Zagreb indices can be computed through the link of graph G_1 and G_1 as shown in Fig. 6. It is easy to observe that for $1 \le i \le k-1$, $1 \le j \le k-1$ we have

$$PM_1(G_1) = 2^{78}.3^{34},$$

$$PM_1^{(u_i)}(G_1) = PM_1^{(v_j)}(G_1) = 2^{76}.3^{34},$$

$$PM_1^{(v_i,u_{i+1})}(G_1) = 2^{74}.3^{34}.$$

We define G_k, $k \ge 2$ as follow:

$$G_k = (G_{k-1}\Box G_1)(v_1,u_1),$$

$$G_{k-1} = (G_{k-2}\Box G_1)(v_2,u_2),$$

$$\vdots$$

$$G_2 = (G_1\Box G_1)(v_{k-1},u_{k-1}).$$

According to Lemma 2.3, the following relations are derived:

$$\begin{aligned}PM_1(G_k) =& PM_1^{(v_1)}(G_{k-1})\\ &.PM_1^{(u_1)}(G_1).2^4,\\ PM_1^{(v_1)}(G_{k-1}) =& PM_1^{(v_2)}(G_{k-2})\\ &.PM_1^{(v_1,u_2)}(G_1).2^4,\\ &\vdots\\ PM_1^{(v_{k-2})}(G_2) =& PM_1^{(v_{k-1})}(G_1)\\ &.PM_1^{(v_{k-2},u_{k-1})}(G_1).2^4.\end{aligned}$$

Therefore

$$\begin{aligned}PM_1(G_k) =& PM_1^{(v_{k-1})}(G_1).PM_1^{(u_1)}(G_1)\\ &\prod_{i=2}^{k-1} PM_1^{(v_{i-1},u_i)}(G_1).2^{4(k-1)}\\ =& PM_1^{(v_{k-1})}(G_1).PM_1^{(u_1)}(G_1)\\ &.(PM_1^{(v_1,u_2)}(G_1))^{k-2}.2^{4(k-1)}\\ =& 2^{78k}.3^{34k}.\end{aligned}$$

Three branches like G_1 are added in the second layer and fifteen branches are added in the third layer. The total number of added branches in all layers is equal to $\frac{4^k-3k-1}{3}$. The first multiplicative Zagreb index for a branch of graph of Fig. 4 is equal to $2^{13.2^{2k+1}-26}.3^{\frac{17.2^{2k+1}-34}{3}}$. As this graph has eight main branches, high values for eight main branches are obtained and the obtained number with the first multiplicative Zagreb index which has the central part value of figure is $2^{-16}.2^{64}.3^{48}$. Therefore $PM_1(G) = 2^{(13.2^{2k+4}-160)}.3^{\frac{17.2^{2k+4}-128}{3}}$. Now, it is easy to observe that for $1 \le i \le k-1$ and $1 \le j \le k-1$ the followings are hold:

$$PM_2(G_1) = 2^{78}.3^{51},$$

$$PM_2^{(u_i)}(G_1) = PM_2^{(v_j)}(G_1) = 2^{76}.3^{51},$$

$$PM_2^{(v_i,u_{i+1})}(G_1) = 2^{74}.3^{51}.$$

Once again Lemma 2.3 show that the following relations are hold:

$$\begin{aligned}PM_2(G_k) =& PM_2^{(v_1)}(G_{k-1})\\ &.PM_2^{(u_1)}(G_1).2^2.2^2,\\ PM_2^{(v_1)}(G_{k-1}) =& PM_2^{(v_2)}(G_{k-2})\\ &.PM_2^{(v_1,u_2)}(G_1).2^2.2^2,\\ &\vdots\\ PM_2^{(v_k-2)}(G_2) =& PM_2^{(v_{k-1})}(G_1)\\ &.PM_2^{(v_{k-2},u_{k-1})}(G_1).2^2.2^2.\end{aligned}$$

Therefore, we obtain the following relations:

$$\begin{aligned} PM_2(G_k) =& PM_2^{(v_{k-1})}(G_1).PM_2^{(u_1)}(G_1) \\ & \prod_{i=2}^{k-1} PM_2^{(v_{i-1},u_i)}(G_1).2^{4(k-1)} \\ =& PM_2^{(v_{k-1})}(G_1).PM_2^{(u_1)}(G_1) \\ & .(PM_2^{(v_1,u_2)}(G_1))^{k-2}(2^2.2^2)^{(k-1)} \\ =& 2^{78k}.3^{51k}. \end{aligned}$$

Three branches like G_1 are added in the second layer and fifteen branches are added in the third layer. The total number of added branches in all layers is equal to $\frac{4^k-3k-1}{3}$. The second multiplicative Zagreb index for a branch of graph of Fig. 4 is equal to $2^{13.2^{2k+1}-26}.3^{17.2^{2k}-17}$. As the graph has eight main branches, high values for eight main branches are obtained, where the obtained number with the second multiplicative Zagreb index which has the central part value of figure that is $2^{-16}.2^{64}.3^{72}$. Therefore $PM_2 = 2^{13.2^{2k+4}-160}.3^{17.2^{2k+3}-64}$. □

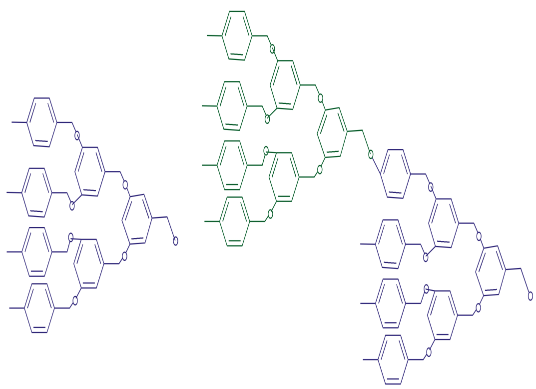

Figure 6: G_1 and $G_2 = G_1 \square G_1$

Theorem 3.5. *Let G be the benzyl ether dendrimers with porphyrin core. Then*

$$\begin{aligned} M_1(\bar{G}) =& \frac{1}{27}(205379.2^{6k+9} - 1621143.2^{4k+7} \\ & + 17057235.2^{2k+3} - 29903344), \\ \overline{M}_1(\bar{G}) =& \frac{649.2^{4k+8} - 6759.2^{2k+5} + 70304}{3}. \end{aligned}$$

Proof. For the graph in Fig. 5, it is obvious that $n = 56, m = 64$. So $n = 8n' + 56$ and $m = 8m' + 64$. For example, if $k = 1$, then $n = 528$, $m = 592$. Now, the calculations show that $n' = \frac{59.2^{2k}-59}{3}$ and $m' = 11.2^{2k+1} - 22$. Therefore, $n = \frac{59.2^{2k+3}-304}{3}$, $m = 11.2^{2k+4} - 112$ and elementary computations yield

$$\begin{aligned} M_1(\bar{G}) =& \frac{1}{27}(205379.2^{6k+9} - 1621143.2^{4k+7} \\ & + 17057235.2^{2k+3} - 29903344), \end{aligned}$$

$$\overline{M}_1(\bar{G}) = \frac{649.2^{4k+8} - 6759.2^{2k+5} + 70304}{3}.$$

□

Theorem 3.6. *Let G be the benzyl ether dendrimers with porphyrin core. Then*

$$F(G) = 129.2^{2k+4} - 1216,$$

$$\begin{aligned} F(G, x) =& 2^{2k+3}.x^{10} + (5.2^{2k+3} - 36).x^8 \\ & + (2^{2k+7} - 88).x^{13} + 12.x^{18}. \end{aligned}$$

Proof. Let the edge set of G be divided into four classes based on the degree of the end vertices $e_{13} = 2^{2k+3}$, $e_{22} = 5.2^{2k+3} - 36$, $e_{23} = 2^{2k+7} - 88$ and $e_{33} = 12$. The F-index of benzyl ether dendrimers with porphyrin core is calculated as follow:

$$F(G) = 10e_{13} + 8e_{22} + 13e_{23} + 18e_{33}$$

$$= 129.2^{2k+4} - 1216.$$

The F-polynomial of benzyl ether dendrimers with porphyrin core is calculated as follow:

$$F(G, x) = e_{13}.x^{10} + e_{22}.x^8 + e_{23}.x^{13} + e_{33}.x^{18}.$$

So, we obtain the following relation:

$$\begin{aligned} F(G, x) =& 2^{2k+3}.x^{10} + (5.2^{2k+3} - 36).x^8 \\ & + (2^{2k+7} - 88).x^{13} + 12.x^{18}. \end{aligned}$$

□

4 Conclusion

In this paper, we considered two different dendrimers. We found the first, second and third

Zagreb indices and the first and second multiplicative Zagreb indices and the F-index and F-polynomial of benzyl ether dendrimer with $C_{60}H$ core and benzyl ether dendrimers with porphyrin core. In addition, the first and second Zagreb coindices and the first and second multiplicative Zagreb coindices and first Zagreb index and Zagreb coindices of complement of this graphs are also computed. Finally, the multiplicative Zagreb indices are computed by the link of graphs.

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