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Research Article

On Theoretical Study of Zagreb Indices and Zagreb Polynomials of Water-Soluble Perylenediimide-Cored Dendrimers

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Abstract. The topological indices are numerical invariants associated to a graph which describe its molecular topology. In QSAR/QSPR study, the Zagreb indices and Zagreb polynomials are used to predict the bioactivity of different chemical compounds. They also correlate the certain physico-chemical properties of the chemical compounds. In this paper, we compute the closed formulas of the first and second Zagreb indices and their variants and their Zagreb polynomials for the two classes of perylenediimide-cored (PDI-cored) dendrimers.

Keywords. Zagreb index; Zagreb polynomial; PDI-cored dendrimers

MSC. 68Qxx

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1. Introduction

Unlike the other linear polymers, dendrimers can be constructed with a well-defined molecular structure i.e. monodisperse. The dendrimers have a uniform and well-defined size and shape, which are of prominent interest in the biomedical applications and nanotechnology. They have three structural units named as the core, branching units and the terminal end groups.

The charge on end groups plays a vital role in the exploration of the dendrimers as drug delivery vehicles. The dendrimers are currently attracting the interest of a great number of scientists and researchers because of their unusual chemical and physical properties and the wide range of potential application in different fields of applied sciences such as biology, medicine, physics, chemistry and engineering, to name a few [20].

In this paper, G is considered to be a molecular graph with vertex set $V(G)$ and the edge set $E(G)$. The vertices of the graph G correspond to the atoms and an edge between two vertices corresponds to the chemical bond between these vertices. In a graph G, two vertices u and v are called adjacent if they are end vertices of an edge $e \in E(G)$ and we write as $e = uv$ or $e = vu$. For a vertex $u \in V(G)$, the set of neighbor vertices is denoted by N_u and is defined as $N_u = \{v \in V(G) : uv \in E(G)\}$. The *degree* of a vertex $u \in V(G)$ is denoted by d_u and is defined as $d_u = |N_u|$. Similarly, for an edge $e = uv$, the set of neighbor edges is denoted by $\widehat{N}_e$ and is defined as $\widehat{N}_e = \{f \in E(G) : e$ and f share a common end-vertex$\}$. The degree of an edge $e \in E(G)$ is denoted by $\widehat{d}_e$ and is defined as $\widehat{d}_e = |\widehat{N}_e|$.

A whole graph can be uniquely represented by a numeric number, a sequence of numbers, a polynomial, or by a matrix. A *topological index* characterizes the topology of the graph by associated a numeric quantity with a graph and it is invariant under the action of graph automorphism. Among the major and most studied classes of topological indices, the degree based topological indices and counting related polynomials indices have a prominent place and play a vital role in chemical graph theory and particularly in theoretical chemistry. A topological index denoted by $\mathrm{Top}(G)$ of a graph G has a property that if two graphs G and $\widehat{G}$ are isomorphic, then we have $\mathrm{Top}(G) = \mathrm{Top}(\widehat{G})$. In 1947, Harold Wiener [22] introduced a numeric quantity W_e, eventually named *Wiener index* or Wiener number. He showed that there are excellent correlations between the quantity W_e and a variety of physico-chemical properties of the organic compounds.

The *Zagreb indices* are the oldest and most studied molecular structure descriptors and there have been found significant applications of these molecular structure descriptors in theoretical and computational chemistry. Nowadays, there exist hundreds of papers on Zagreb indices, their variants and their related matters. In 1972, Gutman and Trinajstić [9] introduced the first Zagreb index based on the degree of the vertices of a graph G. The first and second Zagreb indices of a graph G can be defined in the following way

$$M_1(G) = \sum_{uv \in E(G)} (d_u + d_v), \tag{1.1}$$

$$M_2(G) = \sum_{uv \in E(G)} (d_u \times d_v). \tag{1.2}$$

For historical background, different properties, efficient ways of computation, relations and bounds of these topological indices, the interested reader can refer to [3, 23] and the references cited therein. Shirdel and his co-authors [19] introduced a new degree-based Zagreb index of a graph G in 2013, and they named it *hyper-Zagreb index* that is defined as follows:

$$HM(G) = \sum_{uv \in E(G)} (d_u + d_v)^2. \tag{1.3}$$

Some properties of this index of different graphs have been discussed in the papers [1,5]. In 2012, the two new versions of Zagreb indices of a graph G which are named as *multiple Zagreb indices* were introduced by Ghorbani and Azimi [8]. These indices are defined as:

$$PM_1(G) = \prod_{uv \in E(G)} (d_u + d_v), \tag{1.4}$$

$$PM_2(G) = \prod_{uv \in E(G)} (d_u \times d_v). \tag{1.5}$$

The properties of these multiple Zagreb indices have been discussed in [2,4]. The first and second Zagreb polynomials can be defined in the following way:

$$M_1(G,y) = \sum_{uv \in E(G)} y^{|d_u + d_v|}, \tag{1.6}$$

$$M_2(G,y) = \sum_{uv \in E(G)} y^{|d_u \times d_v|}. \tag{1.7}$$

In 2009, Furtula and his co-authors [6] introduced the augmented Zagreb index, which is defined as follow

$$AZI(G) = \sum_{uv \in E(G)} \left(\frac{d_u d_v}{d_u + d_v - 2} \right)^3. \tag{1.8}$$

The different chemical and mathematical properties of this topological index have been studied in [11,21]. Milovanović' et al. [17] introduced the reformulated Zagreb indices in terms of the edge-degrees as follows

$$EM_1(G) = \sum_{e \in E(G)} \widehat{d}(e)^2, \tag{1.9}$$

$$EM_2(G) = \sum_{e \propto f} \widehat{d}(e) \times \widehat{d}(f), \tag{1.10}$$

where $\widehat{d}(e)$ denotes the degree of the edge e in G and $e \propto f$ means that the edges e and f share a common end vertex in G. The various physic-chemical properties, relations and bounds of these indices in terms of other graph-theoretic parameters are explored in [16,18,24]. For detailed discussions of these indices and other well-known topological indices, we refer the interested reader to [7,9,10,12–14,17] and references therein.

The water-soluble PDI-cored dendrimers have broad biological applications, including gene delivery, fluorescence live-cell imaging, and fluorescent labeling. In this paper, we compute the closed formulas of the first and second Zagreb indices and their variants and their Zagreb polynomials for the two classes of PDI-cored dendrimers. First class of PDI-cored dendrimers is *polyglycerol dendronized* (PGD) PDIs, which was developed by Heek and Würthner et al. by using the convergent approachin [10,15]. Let $D_1(n)$ be the molecular graph of first type of PDI-cored dendrimer, where n represents the generation stage of $D_1(n)$. The core and first generation of $D_1(n)$ are shown in Figure 1. $D_1(n)$ with $n = 2$ and $n = 3$ are shown in Figure 2. The second class of PDI-cored dendrimers is fluorescent water-soluble PDI-cored cationic dendrimers that were synthesized by Xu and his co-authors [23].

2. Zagreb Indices and Polynomials of Nanostar Dendrimers $D_1(n)$

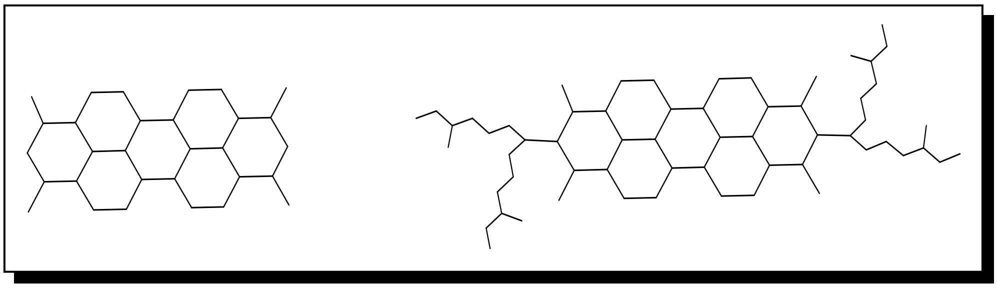

Figure 1. From left to right, the core and first generation of $D_1(n)$, respectively.

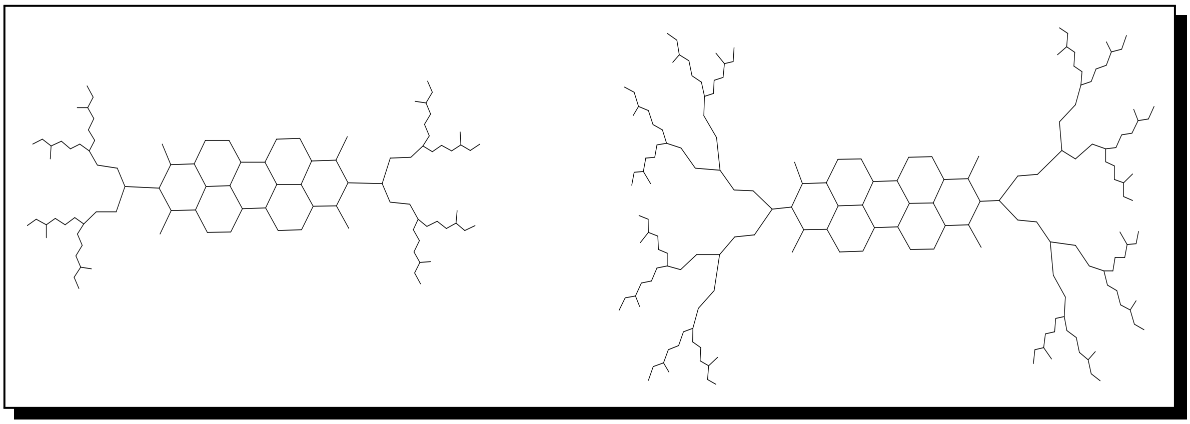

Figure 2. From left to right, $D_(n)$ with $n = 2$ and $n = 3$, respectively.

Now, we compute the first and second Zagreb indices, hyper-Zagreb index, first and second multiple Zagreb indices, first and second Zagreb polynomials and the augmented Zagreb index of $D_1(n)$ in the following theorem.

Theorem 2.1. *For the molecular graph $D_1(n)$ we have*

- $M_1(D_1(n)) = 2^{n-1} \times 100 + 2^{n+1} \times 19 + 148.$
- $M_2(D_1(n)) = 2^{n+2} + 2^{n-1} \times 120 + 2^{n+1} \times 15 + 210.$
- $HM(D_1(n)) = 2^{n-1} \times 500 + 2^{n+1} \times 73 + 856.$
- $PM_1(D_1(n)) = 3^{2^{n+1}} \times 4^{(2^{n+1}+1)4} \times 5^{5\times 2^{n+1}} \times 6^{22}.$
- $PM_2(D_1(n)) = 2^{2^{n+1}} \times 6^{5\times 2^{n+1}} \times 64^{2^{n+1}} \times 81^{(1+2^{n-1})} \times 9^{22}.$
- $M_1(D_1(n), y) = 2y^3(11y^3 + 2^n \times 5y^2 + 2y + 2^n \times 4y + 2^n).$
- $M_2(D_1(n), y) = 2y^2(11y^7 + 2^n \times 5y^4 + 2y + 2^n \times 3y^2 + 2^n y + 2^n).$
- $AZI(D_1(n)) = \dfrac{2^{n+4} \times 128 + 2^{n+2} \times 640 + 2^{n-1} \times 432 + 8451}{32}.$

Proof. The total number of edges of the molecular graph $D_1(n)$ is $5 \times 2^{n+2} + 26$. Now, we define $d^1_{ij}(n)$ to be the number of edges connecting a vertex of degree i with a vertex of degree j in $D_1(n)$.

Now, we get the edge partition based on the degree of the end vertices. For this molecular graph, we have the following five edge partitions. The first partition $E_1^1(D_1(n))$ consists of 2^{n+1} edges that have end vertices of degree 1 and 2. The second partition $E_2^1(D_1(n))$ has $4(2^{n-1}+1)$ edges that have end vertices of degree 1 and 3. The third partition $E_3^1(D_1(n))$ consists of $3\times 2^{n+1}$ edges that have both end vertices of degree 2. The forth partition $E_4^1(D_1(n))$ has $20\times 2^{n-1}$ edges that have end vertices of degree 2 and 3. The fifth partition $E_5^1(D_1(n))$ consists of 22 edges that have both end vertices of degree 3. It is easy to see that $|E_1^1(D_1(n))| = d_{12}^1(n)$, $|E_2^1(D_1(n))| = d_{13}^1(n)$, $|E_3^1(D_1(n))| = d_{22}^1(n)$, $|E_4^1(D_1(n))| = d_{23}^1(n)$ and $|E_5^1(D_1(n))| = d_{33}^1(n)$. Now by using equations (1.1)-(1.8), we get

$$\begin{aligned}
M_1(D_1(n)) &= \sum_{uv\in E(D_1(n))} (d_u+d_v)\\
&= 3|E_1^1(D_1(n))|+4|E_2^1(D_1(n))|+4|E_3^1(D_1(n))|+5|E_4^1(D_1(n))|+6|E_5^1(D_1(n))|\\
&= 2^{n-1}\times 100+2^{n+1}\times 19+148.\\
M_2(D_1(n)) &= \sum_{uv\in E(D_1(n))} (d_u\times d_v)\\
&= 2|E_1^1(D_1(n))|+3|E_2^1(D_1(n))|+4|E_3^1(D_1(n))|+6|E_4^1(D_1(n))|+9|E_5^1(D_1(n))|\\
&= 2^{n+2}+2^{n-1}\times 120+2^{n+1}\times 15+210.\\
HM(D_1(n)) &= \sum_{uv\in E(D_1(n))} (d_u+d_v)^2\\
&= 9|E_1^1(D_1(n))|+16|E_2^1(D_1(n))|+16|E_3^1(D_1(n))|+25|E_4^1(D_1(n))|+36|E_5^1(D_1(n))|\\
&= 2^{n-1}\times 500+2^{n+1}\times 73+856.\\
PM_1(D_1(n)) &= \prod_{uv\in E(D_1(n))} (d_u+d_v)\\
&= 3^{|E_1^1(D_1(n))|}\times 4^{|E_2^1(D_1(n))|}\times 4^{|E_3^1(D_1(n))|}\times 5^{|E_4^1(D_1(n))|}\times 6^{|E_5^1(D_1(n))|}\\
&\quad = 3^{2^{n+1}}\times 4^{(2^{n+1}+1)4}\times 5^{5\times 2^{n+1}}\times 6^{22}.\\
PM_2(D_1(n)) &= \prod_{uv\in E(D_1(n))} (d_u\times d_v)\\
&= 2^{|E_1^1(D_1(n))|}\times 3^{|E_2^1(D_1(n))|}\times 4^{|E_3^1(D_1(n))|}\times 6^{|E_4^1(D_1(n))|}\times 9^{|E_5^1(D_1(n))|}\\
&= 2^{2^{n+1}}\times 6^{5\times 2^{n+1}}\times 64^{2^{n+1}}\times 81^{(1+2^{n-1})}\times 9^{22}.\\
M_1(D_1(n),y) &= \sum_{uv\in E(G)} y^{|d_u+d_v|}\\
&= y^3|E_1^1(D_1(n))|+y^4|E_2^1(D_1(n))|+y^4|E_3^1(D_1(n))|+y^5|E_4^1(D_1(n))|+y^6|E_5^1(D_1(n))|\\
&= 2y^3(11y^3+2^n\times 5y^2+2y+2^n\times 4y+2^n).\\
M_2(D_1(n),y) &= \sum_{uv\in E(G)} y^{|d_u\times d_v|}
\end{aligned}$$

$$= y^2|E_1^1(D_1(n))| + y^3|E_2^1(D_1(n))| + y^4|E_3^1(D_1(n))| + y^6|E_4^1(D_1(n))| + y^9|E_5^1(D_1(n))|$$
$$= 2y^2(11y^7 + 2^n \times 5y^4 + 2y + 2^n \times 3y^2 + 2^n y + 2^n).$$

$$AZI(D_1(n)) = \sum_{uv\in E(D_1(n))} \left(\frac{d_u d_v}{d_u + d_v - 2}\right)^3$$
$$= 8|E_1^1(D_1(n))| + \frac{27}{8}|E_2^1(D_1(n))| + 8|E_3^1(D_1(n))| + 8|E_4^1(D_1(n))| + \frac{729}{64}|E_5^1(D_1(n))|$$
$$= \frac{2^{n+4} \times 128 + 2^{n+2} \times 640 + 2^{n-1} \times 432 + 8451}{32}.$$

In the next theorem, we will compute a closed formula for the first reformulated Zagreb index of molecular graph $D_1(n)$.

Theorem 2.2. *For the molecular graph $D_1(n)$, the first reformulated Zagreb index is given by*

$$EM_1(D_1(n)) = 2^{n-1} \times 180 + 2^{n+1} \times 17 + 368.$$

Proof. In the molecular graph $D_1(n)$, there are total $5 \times 2^{n+2} + 26$ edges among which 2^{n+1} edges of degree 1, $4(2^{n+1} + 1)$ edges having degree 2, $20 \times 2^{n-1}$ edges of degree 3 and 22 edges of degree 4. Now by using this information in equation (1.9), we can obtain the required result, which completes the proof. □

Let $E(p_{ij}^1(n)) \subseteq E(D_1(n))$ be the set of edges of degrees i and j that share a common end vertex in the $D_1(n)$. By using the computational arguments, we have $|E(p_{13}^1(n))| = 2^{n+1} = |E(p_{22}^1(n))|$, $|E(p_{23}^1(n))| = 6 \times 2^{n+1}$, $|E(p_{24}^1(n))| = 8$, $|E(p_{33}^1(n))| = 2^{n+3} - 10$, $|E(p_{34}^1(n))| = 20$ and $|E(p_{44}^1(n))| = 30$. Now by using this information, we compute the second reformulated Zagreb index in the following theorem.

Theorem 2.3. *For the molecular graph $D_1(n)$, the second reformulated Zagreb index is given by*

$$EM_2(D_1(n)) = 2^{n+3} \times 9 + 2^{n+1} \times 43 + 694.$$

Proof. By using the equation (1.10), we get

$$EM_2(D_1(n)) = \sum_{e\propto f} \widehat{d}(e) \times \widehat{d}(f)$$
$$= 2^{n+1}(1\times 3) + 2^{n+1}(2\times 2) + 6\times 2^{n+1}(2\times 3)$$
$$+ 8(2\times 4) + (2^{n+3} - 10)(3\times 3) + 20(3\times 4) + 30(4\times 4)$$
$$= 2^{n+3} \times 9 + 2^{n+1} \times 43 + 694.$$ □

3. Zagreb Indices and Polynomials of $D_2(n)$

Let $D_2(n)$ be the molecular graph of second type of PDI-cored dendrimer, where $D_2(n)$ represents the generation stage of $D_2(n)$. The core and first generation of $D_2(n)$ are shown in Figure 3. $D_2(n)$ with $n = 2$ is shown in Figure 4.

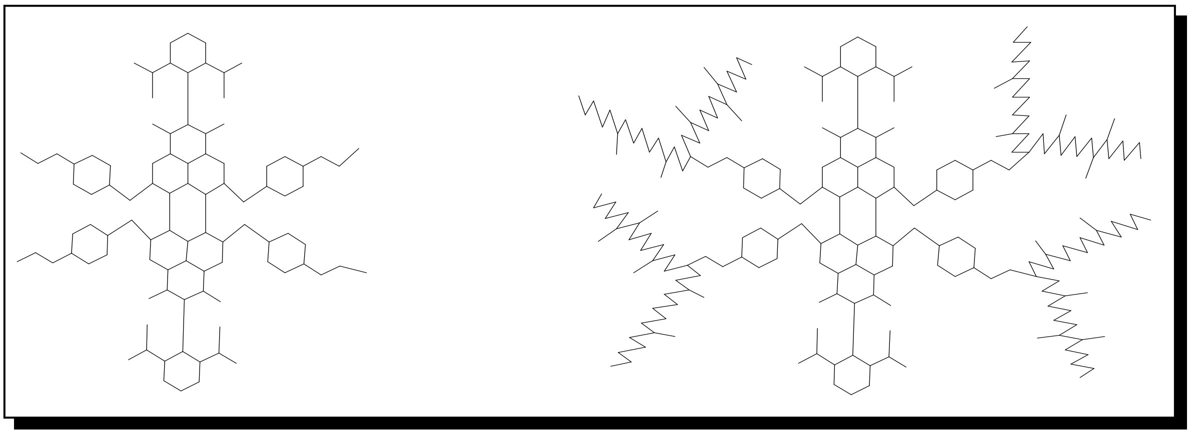

Figure 3. From left to right, the core and first generation of $D_2(n)$, respectively.

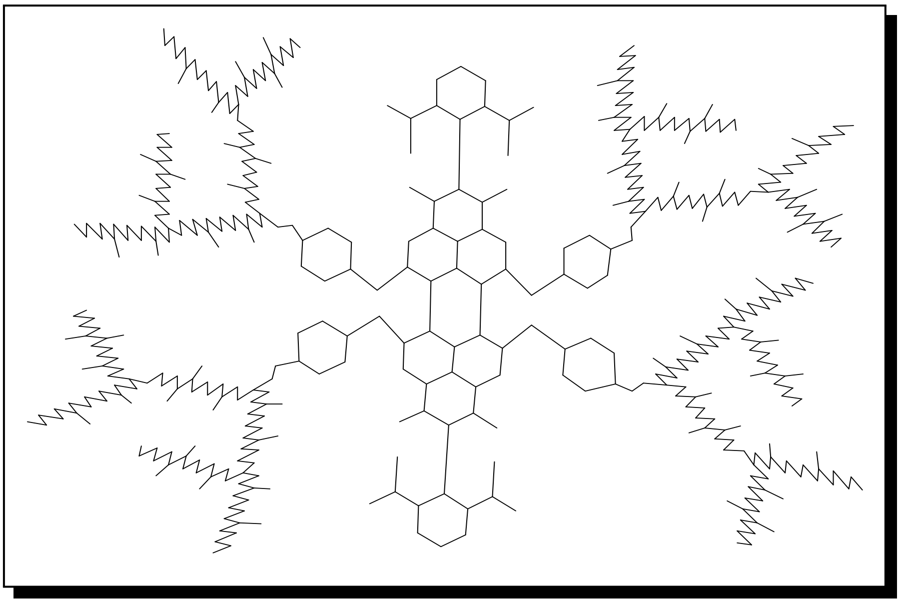

Figure 4. $D_2(n)$ with $n = 2$.

The molecular graph $D_2(n)$ has four similar branches and one core. So we can partition the molecular graph $D_2(n)$ into two parts; one of them is the core C^2 and other is the maximal subgraph $T^2(n)$ of $D_2(n)$ which has four similar branches with vertex set $V(D_2(n)) - V(C^2)$. Now, we define $d^2_{ij}(n)$ to be the number of edges connecting a vertex of degree i with a vertex of degree j in $D_2(n)$. Also, we define c^2_{ij}, b^2_{ij} and t^2_{ij} to be the number of edges connecting a vertex of degree i with a vertex of degree j in core, one branch of $T^2(n)$ and $T^2(n)$, respectively. A simple calculation shows that $c^2_{12} = 0$, $b^2_{12} = 2^n$, thus $t^2_{12} = 2^{n+2}$, therefore we have $d^2_{12}(n) = c^2_{12} + t^2_{12} = 2^{n+2}$. Similarly, $c^2_{13} = 12$, $b^2_{13} = 6(2^n - 1)$, thus $t^2_{13} = 24(2^n - 1)$, therefore $d^2_{13}(n) = 24 \times 2^n - 12$. On same lines, $c^2_{22} = 16$, $b^2_{22} = 14(2^n - 1)$, thus $t^2_{22} = 56(2^n - 1)$, therefore $d^2_{22}(n) = 8(7 \times 2^n - 5)$. Also, we have $c^2_{23} = 44$, $b^2_{23} = 11 \times 2^n - 12$, thus $t^2_{23} = 4(11 \times 2^n - 12)$, therefore $d^2_{23}(n) = 4(11 \times 2^n - 1)$ and finally $c^2_{33} = 34$, $b^2_{33} = 2(2^n - 1)$, thus $t^2_{33} = 8(2^n - 1)$, therefore $d^2_{33}(n) = 8 \times 2^n + 26$. Now, we compute the first and second Zagreb indices, hyper-Zagreb index, first and second multiple Zagreb indices, first and second Zagreb polynomials and augmented Zagreb index of $D_2(n)$ in the following theorem.

Theorem 3.1. *For the molecular graph $D_2(n)$, we have the following results*

- $M_1(D_2(n)) = 2^n \times 540 + 2^{n+3} \times 6 + 2^{n+2} \times 3 - 72.$
- $M_2(D_2(n)) = 2^n \times 560 + 2^{n+3} \times 10 + 14..$
- $HM(D_2(n)) = 2^n \times 2380 + 2^{n+2} \times 9 + 2^{n+3} \times 36 + 4.$
- $PM_1(D_2(n)) = 3^{2^{n+2}} \times 36^{(2^{n+2}+13)} \times 256^{(5\times 2^{n+2}-13)} \times 625^{(2^n\times 11-1)}.$
- $PM_2(D_2(n)) = 2^{2^{n+2}} \times 81^{(2^{n+2}+13)} \times 1296^{(11\times 2^n-1)} \times 531441^{(2^{n+1}-1)} \times 65536^{(7\times 2^n-5)}.$
- $M_1(D_2(n), y) = 2y^3(13y^3 + 2^n \times 4y^3 + 2^n \times 22y^2 + 2^n \times 40y - 2y^2 - 26y + 2^{n+1}).$
- $M_2(D_2(n), y) = 2y^2(13y^7 + 2^n \times 4y^7 + 2^n \times 22y^4 + 2^n \times 28y^2 + 12y \times 2^n - 2y^4 - 20y^2 - 6y + 2^{n+1}).$
- $AZI((D_2(n))) = \dfrac{2^{n+5} \times 32 + 2^{n+1} \times 1296 + 2^n \times 28516 - 3083}{32}.$

Proof. The total number of edges of the molecular graph $D_2(n)$ is $136 \times 2^n - 30$. Now, we get the edge partition based on the degree of the end vertices. For this molecular graph, we have the following five edge partitions. The first partition $E_1^2(D_2(n))$ consists of 2^{n+2} edges that have end vertices of degree 1 and 2. The second partition $E_2^2(D_2(n))$ has $24 \times 2^n - 12$ edges that have end vertices of degree 1 and 3. The third partition $E_3^2(D_2(n))$ consists of $8(7 \times 2^n - 5)$ edges that have both end vertices of degree 2. The forth partition $E_4^2(D_2(n))$ has $4(11 \times 2^n - 1)$ edges that have end vertices of degree 2 and 3. The fifth partition $E_5^2(D_2(n))$ consists of $8 \times 2^n + 26$ edges that have both end vertices of degree 3. It is easy to see that $|E_1^2(D_2(n))| = d_{12}^2(n)$, $|E_2^2(D_2(n))| = d_{13}^2(n)$, $|E_3^2(D_2(n))| = d_{22}^2(n)$, $|E_4^2(D_2(n))| = d_{23}^2(n)$ and $|E_5^2(D_2(n))| = d_{33}^2(n)$. Now by using the equations (1.1)-(1.8), we get

$$\begin{aligned}
M_1(D_2(n)) &= \sum_{uv\in E(D_2(n))} (d_u + d_v) \\
&= 3|E_1^2(D_2(n))| + 4|E_2^2(D_2(n))| + 4|E_3^2(D_2(n))| + 5|E_4^2(D_2(n))| + 6|E_5^2(D_2(n))| \\
&= 2^n \times 540 + 2^{n+3} \times 6 + 2^{n+2} \times 3 - 72.
\end{aligned}$$

$$\begin{aligned}
M_2(D_2(n)) &= \sum_{uv\in E(D_2(n))} (d_u \times d_v) \\
&= 2|E_1^2(D_2(n))| + 3|E_2^2(D_2(n))| + 4|E_3^2(D_2(n))| + 6|E_4^2(D_2(n))| + 9|E_5^2(D_2(n))| \\
&= 2^n \times 560 + 2^{n+3} \times 10 + 14.
\end{aligned}$$

$$\begin{aligned}
HM(D_2(n)) &= \sum_{uv\in E(D_2(n))} (d_u + d_v)^2 \\
&= 9|E_1^2(D_2(n))| + 16|E_2^2(D_2(n))| + 16|E_3^2(D_2(n))| + 25|E_4^2(D_2(n))| + 36|E_5^2(D_2(n))| \\
&= 2^n \times 2380 + 2^{n+2} \times 9 + 2^{n+3} \times 36 + 4.
\end{aligned}$$

$$\begin{aligned}
PM_1(D_2(n)) &= \prod_{uv\in E(D_2(n))} (d_u + d_v) \\
&= 3^{|E_1^2(D_2(n))|} \times 4^{|E_2^2(D_2(n))|} \times 4^{|E_3^2(D_2(n))|} \times 5^{|E_4^2(D_2(n))|} \times 6^{|E_5^2(D_2(n))|}
\end{aligned}$$

$$= 3^{2^{n+2}} \times 36^{(2^{n+2}+13)} \times 256^{(5\times 2^{n+2}-13)} \times 625^{(2^n \times 11-1)}.$$

$$PM_2(D_2(n)) = \prod_{uv\in E(D_2(n))} (d_u \times d_v)$$
$$= 2^{|E_1^2(D_2(n))|} \times 3^{|E_2^2(D_2(n))|} \times 4^{|E_3^2(D_2(n))|} \times 6^{|E_4^2(D_2(n))|} \times 9^{|E_5^2(D_2(n))|}$$
$$= 2^{2^{n+2}} \times 81^{(2^{n+2}+13)} \times 1296^{(11\times 2^n-1)} \times 531441^{(2^{n+1}-1)} \times 65536^{(7\times 2^n-5)}.$$

$$M_1(D_2(n),y) = \sum_{uv\in E(G)} y^{|d_u+d_v|}$$
$$= y^3|E_1^2(D_2(n))| + y^4|E_2^2(D_2(n))| + y^4|E_3^2(D_2(n))| + y^5|E_4^2(D_2(n))| + y^6|E_5^2(D_2(n))|$$
$$= 2y^3(13y^3 + 2^n \times 4y^3 + 2^n \times 22y^2 + 2^n \times 40y - 2y^2 - 26y + 2^{n+1}).$$

$$M_2(D_2(n),y) = \sum_{uv\in E(G)} y^{|d_u\times d_v|}$$
$$= y^2|E_1^2(D_2(n))| + y^3|E_2^2(D_2(n))| + y^4|E_3^2(D_2(n))| + y^6|E_4^2(D_2(n))| + y^9|E_5^2(D_2(n))|$$
$$= 2y^2(13y^7 + 2^n \times 4y^7 + 2^n \times 22y^4 + 2^n \times 28y^2 + 12y \times 2^n - 2y^4 - 20y^2 - 6y + 2^{n+1}).$$

$$AZI(D_2(n)) = \sum_{uv\in E(D_2(n))} \left(\frac{d_u d_v}{d_u + d_v - 2}\right)^3$$
$$= 8|E_1^2(D_2(n))| + \frac{27}{8}|E_2^2(D_2(n))| + 8|E_3^2(D_2(n))| + 8|E_4^2(D_2(n))| + \frac{729}{64}|E_5^2(D_2(n))|$$
$$= \frac{2^{n+5} \times 32 + 2^{n+1} \times 1296 + 2^n \times 28516 - 3083}{32}. \qquad \square$$

In the following theorem, we compute the closed formula for the first reformulated Zagreb index of the molecular graph $D_2(n)$.

Theorem 3.2. *For the molecular graph $D_2(n)$, the first reformulated Zagreb index is given by* $EM_1(D_2(n)) = 2^n \times 848 + 172$.

Proof. In $D_2(n)$, there are total $136 \times 2^n - 30$ edges among which 2^{n+2} edges of degree 1, $4(20 \times 2^n - 13)$ edges of degree 2, $4(11 \times 2^n - 1)$ edges having degree 3, $2^{n+3} + 26$ edges of degree 4. Now by using this information in equation (1.9), we can obtain the required result, which completes the proof. $\square$

Let $E(p_{ij}^2(n)) \subseteq E(D_2(n))$ be the set of edges of degrees i and j that share a common end vertex in $D_2(n)$. By using the computational arguments, we have $|E(p_{12}^2(n))| = 2^{n+2}$, $|E(p_{22}^2(n))| = 2^{n+5} - 26$, $|E(p_{23}^2(n))| = 4(19 \times 2^n - 13)$, $|E(p_{24}^2(n))| = 2^{n+4}$, $|E(p_{33}^2(n))| = 4(5 \times 2^n + 4)$, $|E(p_{34}^2(n))| = 2^{n+4} + 8$ and $|E(p_{44}^2(n))| = 48$.

Now, by using this information, we compute the second reformulated Zagreb index in the following theorem.

Theorem 3.3. *For the molecular graph $D_2(n)$, the second reformulated Zagreb index is given by* $EM_2(D_2(n)) = 2^n \times 1092 + 592$.

Proof. By using the equation (1.10), we have

$$\begin{aligned}
EM_2(D_2(n)) &= \sum_{e \propto f} \widehat{d}(e) \times \widehat{d}(f) \\
&= 2(9 \times 2^{n+1} - 13)(2 \times 2) + 4(19 \times 2^n - 13)(2 \times 3) + 2^{n+4}(2 \times 4) \\
&\quad + 4(5 \times 2^n + 4)(3 \times 3) + (2^{n+4} + 8)(3 \times 4) + 48(4 \times 4) \\
&= 2^n \times 1092 + 592.
\end{aligned}$$

□

4. Conclusion

The Zagreb indices and their alternative forms have been used to investigate the molecular complexity, ZE-isomerism, heterosystems and chirality, whereas the overall Zagreb indices presented a promising applicability for deducing the multilinear regression models. Zagreb indices are also used by many investigators in their QSPR and QSAR studies. In this paper, we have computed certain Zagreb indices and polynomials for two new classes of dendrimers. For further study, some other topological indices can be computed for the considered structures $D_1(n)$ and $D_2(n)$, which will be helpful to understand their underlying topologies in more details.

Competing Interests

The authors declare that they have no competing interests.

Authors' Contributions

All the authors contributed significantly in writing this article. The authors read and approved the final manuscript.

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