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Computing entire Zagreb indices of some dendrimer structures

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Abstract: Topological indices are numerical numbers associated to molecular graphs and are invariant of a graph. In QSAR/QSPR study, Zagreb indices are used to explain the different properties of chemical compounds at the molecular level mathematically. They have been studied extensively due to their ease of calculation and numerous applications in place of the existing chemical methods which needed more time and increased the costs. In this paper, we compute precise values of new versions of Zagreb indices for two classes of dendrimers.

Keywords: first entire Zagreb index; second entire Zagreb index; molecular graph; dendrimer

1 Introduction

Dendrimers are discrete nanostructures with the well-defined, homogeneous and monodisperse structure having tree-like arms with low polydispersity and high functionality. The structure of these materials has a great impact on their physical and chemical properties. Due to their singular behaviour, these are acceptable for a wide range of potential applications in several areas of research, technology and treatment. With bettered synthesis, additional understandings of their unique characteristics and recognition of new applications, dendrimers will become hopeful candidates for further exploitation in drug discovery and clinical applications. Developing of commercial implementations of dendrimer technology will provide strength for its functionality in the future (Abbasi et al., 2014; Boad et al., 2006; Klajnert and Bryszewska, 2001).

Throughout the paper we consider G to be a finite, simple and connected molecular graph. The vertex set and the edge set of G are denoted by $V(G)$ and $E(G)$, respectively. In a molecular graph, the vertices correspond to atoms and the edges correspond to chemical bonds between the atoms. For an element in a molecular graph $G = (V, E)$, we mean either a vertex or an edge. Two vertices u and v are called adjacent if there is an edge between them and we write it as $e = uv$ or $e = vu$. Similarly, two edges e and f are called adjacent if they have a common vertex. The degree of a vertex u $V(G)$ is the cardinality of the set of edges incident to u and is denoted by d_u. For a given edge $e = uv$ $E(G)$, the degree of e is defined as $d_{uv} = d_u + d_v - 2$.

The topological index is a numerical number linked with chemical constitutions. This number claims to correlate the chemical structures with its many physical/chemical properties, biological activity or chemical reactivity. Many topological indices have been introduced based on the transformation of a molecular graph into a number that examines the relationship between the structure, properties, and activity of chemical compounds in molecular modelling. These topological indices are invariant under graph isomorphism, If A and B are two molecular graphs such that A B, then we have $Top(A) = Top(B)$, where $Top(A)$ and $Top(B)$ denote the topological indices of A and B, respectively. In the field of nanotechnology, biochemistry, and chemistry, different topological indices are observed to be useful in structure-property relationship, isomer discrimination, and structure-activity relationship. In recent decades, many topological indices have been

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defined and utilized for chirality, similarity/dissimilarity, study of molecular complexity, chemical documentation, isomer discrimination, structure-property relationship and structure-activity relationship, lead optimization, drug design, and database selection, etc. There are three main types of topological indices: distance-based, degree-based, and counting-related. For further studies of numerous kinds of topological indices of graphs and chemical structures (Aslam et al., 2017, 2018; Gao et al., 2018; Iqbal et al., 2017, 2019; Kang et al., 2018).

Among the degree-based Topological indices the Zagreb indices are the oldest and most studied molecular structure descriptors and they found significant applications in chemistry. Nowadays, there exist hundreds of papers on Zagreb indices and related matters. Gutman and Trinajstić (1972) introduced the first and second Zagreb index based on the degree of vertices of a graph G. The first and second Zagreb index of a molecular graph G are denoted and defined as:

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

$$M_2(G)=\sum_{uv\in E(G)} d_u d_v$$

These formulas were obtained analyzing the structural dependency of total π electron energy. It was observed that these terms increase with the increase extent of branching of carbon-atom Skelton. This shows that these formulas provide the quantitative measures of molecular branching.

After this, many new extended and reformulated versions of Zagreb indices have been introduced, e.g. see: Ali et al. (2018), Ashrafi et al. (2010), Borovicanin et al. (2017), Braun et al. (2005), Das and Ali (2019), Gutman and Trinajstić (1972), Gutman and Das (2004), Javaid et al. (2019), Khalifeh et al. (2009), Kok et al. (2017), Liu et al. (2020), Zhou (2004), and Zhou and Gutman (2004, 2005). Recently, a new version of Zagreb indices has been introduced by Alwardi et al. (2018) and they named it as entire Zagreb indices. In addition these indices take into account the relations between the vertices and edges between vertices. The first and second entire Zagreb indices are defined by Alwardi et al. (2018).

$$M_1^{\varepsilon}(G)=\sum_{x\in V(G)\cup E(G)} [d_x]^2$$

$$M_2^{\epsilon}(G)=\sum_{x \text{ is either adjacent or incident to } y} d_x\times d_y$$

This article is organized as follows: in Section 2, we compute the entire Zagreb indices for a class of Trizane based dendrimer, whereas Section 3 contains computation of these indices for water soluble PDI cored sendrimers. Conclusion and references will close this article.

2 The entire Zagreb indices for molecular graph of Trizane based dendrimer

In this section, we will compute the entire Zagreb indices for the molecular graph of Triazine based dendrimer (Gajjar et al., 2015). Let $D_1(n)$ be the molecular graph of this dendrimer, where n represents the generation stage of $D_1(n)$. The number of vertices and edges in $D_1(n)$ is $\frac{2(20\times 2^{2n}+1)}{3}$ and $14\times 2^{2n}+1$, respectively. To compute the entire Zagreb indices of $D_1(n)$ it is sufficient to determine the desired data for the sets of representatives of $V(D_1(n))$. We will compute the required information by using the computational arguments. Now, we partition the vertex set $V(D_1(n))$ into two sets A and B. For the set A, these representatives are labelled by β_k, where $1\le k\le 5$, and for the set B, these representatives are labelled by $a_j, b_j, c_j, d_j, e_j, f_j, g_j, h_j$, where $1\le j\le n$. Table 1 shows the sets of representatives, their degrees and frequencies of occurrence. The labelled molecular graphs of $D_1(n)$ with $n=1$ and $n=2$ are shown in Figure 1.

In Table 2, we find the edge partition with respect to the pairs of end vertices of sets A and B, degree of each edge and their frequencies of occurrence.

Theorem 2.1

For $D_1(n)$, the first entire Zagreb index is given by:

$$M_1^{\varepsilon}(D_1(n))=\frac{58+500\times 4^n}{3}.$$

Proof. Followed by values depicted in Tables 1 and 2, and the expression of first entire Zagreb index, $M_1^{\varepsilon}(D_1(n))$ can be calculated as follows:

Table 1: Representatives, degrees, and frequencies used.

Representatives	Degree	Frequency	Representatives	Degree	Frequency	Representatives	Degree	Frequency
β_1	3	2	a_j	3	2^{2j-1}	f_j	2	2^{2j+1}
β_2	2	4	b_j	2	2^{2j}	g_n	2	2^{2n+1}
β_3	2	4	c_j	3	2^{2j}	$g_j, j \neq n$	2	2^{2j+1}
β_4	3	2	d_j	2	2^{2j-1}	h_n	1	2^{2n+1}
β_5	2	2	e_j	3	2^{2j}	$h_j, j \neq n$	2	2^{2j+1}

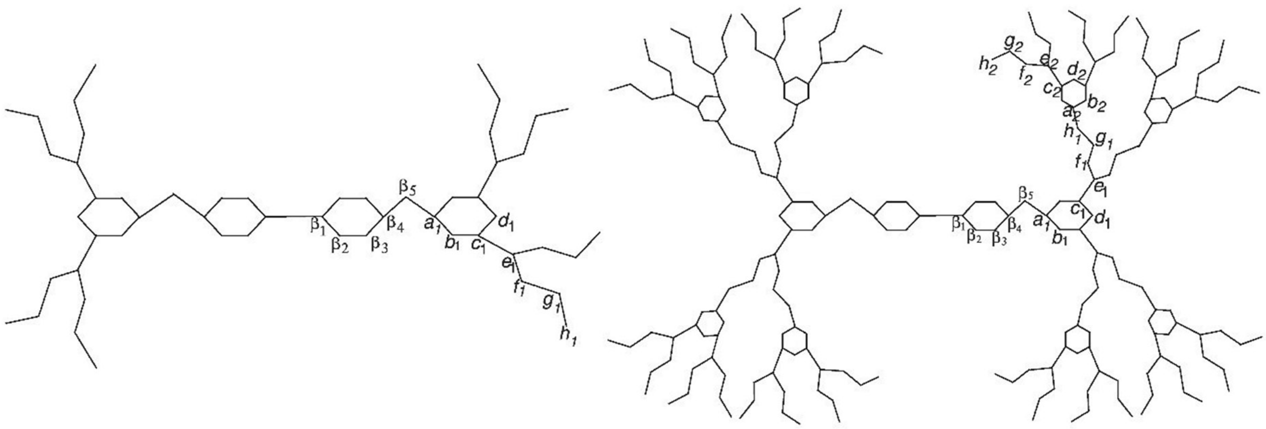

Figure 1: From left to right, $D_1(n)$ with $n = 1$ and $n = 2$.

Table 2: The edge partition with respect to the pairs of end vertices of sets A and B, degree of each edge and their frequencies of occurrence.

Edge	Degree	Frequency	Edge	Degree	Frequency	Edge	Degree	Frequency
$[\beta_1,\beta_1]$	4	1	$[\beta_5,a_1]$	3	2	$[e_j,f_j]$	3	2^{2j+1}
$[\beta_1,\beta_2]$	3	4	$[a_j,b_j]$	3	2^{2j}	$[f_j,g_j]$	2	2^{2j+1}
$[\beta_2,\beta_3]$	2	4	$[b_j,c_j]$	3	2^{2j}	$[g_n,h_n]$	1	2^{2n+1}
$[\beta_3,\beta_4]$	3	4	$[c_j,d_j]$	3	2^{2j}	$[g_j,h_j]\ j \neq n$	2	2^{2j+1}
$[\beta_4,\beta_5]$	3	2	$[c_j,e_j]$	4	2^{2j}	$[h_j,a_{j+1}]\ j \neq n$	3	2^{2j+1}

$$
\begin{aligned}
M_1^{\varepsilon}(D_1(n)) = M_1^{\varepsilon}(A)+M_1^{\varepsilon}(B) &= \sum_{v\in V(A)\cup E(A)} [d_v]^2 + \sum_{v\in V(B)\cup E(B)} [d_v]^2 \\
&= 2(3)^2+4(2)^2+4(2)^2+2(3)^2+2(2)^2+2^{2n+1}(1)^2+2^{2n+1}(2)^2+\sum_{i=1}^{n}2^{2i-1}((3)^2+(2)^2)+\sum_{i=1}^{n}2^{2i}((2)^2++(3)^2+(3)^2+2(2)^2) \\
&+\sum_{i=1}^{n-1}2^{2i+1}((2)^2+(2)^2)+1(4)^2+4(3)^2+4(2)^2+4(3)^2+2(3)^2+2(3)^2+2^{2n+1}(1)^2 \\
&+\sum_{i=1}^{n}2^{2i}((3)^2+(3)^2+(3)^2+(4)^2+2(3)^2+2(2)^2)+\sum_{i=1}^{n-1}2^{2i+1}((2)^2+(3)^2).
\end{aligned}
$$

After several calculational steps, we obtain the following:

$$M_1^{\varepsilon}(D_1(n)) = \frac{58+500\times 4^n}{3}.$$

To compute the second entire Zagreb index, at first, we compute the non-repeated collection of representatives with corresponding adjacent vertices and their frequencies of occurrence as shown in Table 3. Secondly, we find the edge partition with respect to the

Table 3: Representatives with corresponding adjacent vertices and their frequencies of occurrence for $n \geq 1$.

Representatives	Adjacent vertices	Frequency	Representatives	Adjacent vertices	Frequency
β_1	β_1, β_2	1,4	b_j	c_j	2^{2j}
β_2	β_3	4	c_j	d_j, e_j	$2^{2j}, 2^{2j}$
β_3	β_4	4	e_j	f_j	2^{2j+1}
β_4	β_5	2	$f_j, j \neq n$	g_j	2^{2j+1}
β_5	a_1	2	g_n	f_n, h_n	$2^{2n+1}, 2^{2n+1}$
a_j	b_j	2^{2j}	$g_j, j \neq n$	h_j	2^{2j+1}
$h_j, j \neq n$	a_{j+1}	2^{2j+1}			

Table 4: Edge partition with respect to the pairs of end vertices of sets A and B, their corresponding adjacent edges and frequencies of occurrence for $n \geq 1$.

Edge	Adjacent edges	Frequency	Edge	Adjacent edges	Frequency
$[\beta_1,\beta_1]$	$[\beta_1,\beta_2]$	4	$[b_j,c_j]$	$[c_j,d_j]$, $[c_j,e_j]$	$2^{2j}, 2^{2j}$
$[\beta_1,\beta_2]$	$[\beta_1,\beta_2]$, $[\beta_2,\beta_3]$	2,4	$[c_j,d_j]$	$[c_j,d_j]$, $[c_j,e_j]$	$2^{2j-1}, 2^{2j}$
$[\beta_2,\beta_3]$	$[\beta_3,\beta_4]$	4	$[c_j,e_j]$	$[e_j,f_j]$	2^{2j+1}
$[\beta_3,\beta_4]$	$[\beta_3,\beta_4]$, $[\beta_4,\beta_5]$	2,4	$[e_j,f_j]$	$[e_j,f_j]$, $[f_j,g_j]$	$2^{2j}, 2^{2j+1}$
$[\beta_4,\beta_5]$	$[\beta_5,a_1]$	2	$[f_j,g_j]$	$[g_j,h_j]$	2^{2j+1}
$[\beta_5,a_1]$	$[a_1,b_1]$	4	$[g_j,h_j]$ $j \neq n$	$[h_j,a_{j+1}]$	2^{2j+1}
$[a_j,b_j]$	$[a_j,b_j]$, $[b_j,c_j]$	$2^{2j-1}, 2^{2j}$	$[h_j,a_{j-1}]$ $j \neq n$	$[a_{j+1},b_{j+1}]$	2^{2j+2}

Table 5: Representatives with corresponding edges on which these are incident and their frequencies of occurrence for $n \geq 1$.

Representatives	Edges on which representatives are incident	Frequency	Representatives	Edges on which representatives are incident	Frequency
β_1	$[\beta_1,\beta_1]$, $[\beta_1,\beta_2]$	1,4	c_j	$[b_j,c_j]$, $[c_j,d_j]$, $[c_j,e_j]$	$2^{2j}, 2^{2j}, 2^{2j}$
β_2	$[\beta_1,\beta_2]$, $[\beta_2,\beta_3]$	4,4	d_j	$[c_j,d_j]$	2^{2j}
β_3	$[\beta_2,\beta_3]$, $[\beta_3,\beta_4]$	4,4	e_j	$[c_j,e_j]$, $[e_j,f_j]$	$2^{2j}, 2^{2j+1}$
β_4	$[\beta_3,\beta_4]$, $[\beta_4,\beta_5]$	4,2	f_j	$[e_j,f_j]$, $[f_j,g_j]$	$2^{2j+1}, 2^{2j+1}$
β_5	$[\beta_4,\beta_5]$, $[\beta_5,a_1]$	2,2	g_n	$[g_n,h_n]$, $[f_n,g_n]$	$2^{2n+1}, 2^{2n+1}$
a_j	$[\beta_5,a_1]$, $[a_j,b_j]$	$2, 2^{2j}$	g_j $j \neq n$	$[f_j,g_j]$, $[g_j,h_j]$	$2^{2j+1}, 2^{2j+1}$
b_j	$[a_j,b_j]$, $[b_j,c_j]$	$2^{2j}, 2^{2j}$	h_j $j \neq n$	$[g_j,h_j]$, $[h_j,a_{j+1}]$	$2^{2j+1}, 2^{2j+1}$
h_n	$[g_n,h_n]$	2^{2n+1}			

pairs of end vertices of sets A and B, their corresponding adjacent edges and frequencies of occurrence. These calculations are shown in Table 4. Finally, we find all the edges on which a specific vertex is incident and their frequencies of occurrence for $n \geq 1$. These computations are shown in Table 5.

Now, we are ready to compute the second entire Zagreb index.

Theorem 2.2

For $D_1(n)$ the second entire Zagreb index is given by:

$$M_2^{\varepsilon}(D_1(n)) = \frac{181+1190\times 4^n}{3}.$$

Proof. By using the values of Tables 1-5 and the definition of second entire Zagreb index, we calculate $M_2^{\varepsilon}(D_1(n))$ in the following way:

$$M_2^{\varepsilon}(D_1(n)) = M_2^{\varepsilon}(A)+M_2^{\varepsilon}(B) = 1(3)^2+4(3\times2)+4(2\times2)+4(3\times2)+2(3\times2)+2(3\times2)+2^{2n+1}(2\times1)+2^{2n+1}(2\times2)$$
$$+\sum_{i=1}^{n}2^{2i}((3\times2)+(3\times2)+(3\times3)+(3\times2)+2(3\times2))+\sum_{i=1}^{n-1}2^{2i+1}((2)^2+(2)^2+(3\times2))+4(3\times4)+2(3)^2+4(3\times2)+4(3\times2)$$
$$+2(3)^2+4(3)^2+2(3)^2+4(3\times3)+\sum_{i=1}^{n}2^{2i-1}(2(3)^2)+\sum_{i=1}^{n}2^{2i}((3)^2+(3)^2+(3\times4)+(3\times4)+2(3\times4)+(3)^2+2(3\times2)$$
$$+2(2\times2))+\sum_{i=1}^{n-1}2^{2i+1}((3\times2)+2(3)^2)+1(3\times4)+4(3\times3)+4(3\times2)+4(3\times3)+2(3\times3)+2(3\times2)+2(3\times2)+2(3\times3)$$
$$+\sum_{i=1}^{n}2^{2i}((3)^2+(3\times2)+(3\times2)+(3\times3)+(3\times3)+(3\times4)+(3\times2)+(3\times4)+2(3\times3)+2(3\times2)+2(2\times2))$$
$$+2^{2n+1}(2)+2^{2n+1}(2\times2)+2^{2n+1}+\sum_{i=1}^{n-1}2^{2i+1}((2\times2)+(2\times2)+(2\times2)+(2\times3)).$$

By means of simple calculations, we derive:

$$M_2^{\varepsilon}(D_1(n)) = \frac{181+1190\times4^n}{3}.$$

3 The entire Zagreb indices for molecular graph of water soluble PDI cored dendrimer

The water-soluble perylenediimide (PDI)-cored dendrimers have an important place among the other dendrimers due to their wide range of potential applications and have many advantages include low cytotoxicity, excellent photo stability, versatile surface modification, high quantum yield, strong red fluorescence, and biological applications including fluorescence live-cell imaging, gene delivery, and fluorescent labelling (Kok et al., 2017). Here we will calculate the entire Zagreb indices for the molecular graph of one class of water-soluble PDI-cored.

Let $D_2(n)$ be the molecular graph of this dendrimer, where n represents the generation stage of $D_2(n)$. It is easy to see that the number of vertices and edges in $D_2(n)$ are $20(2^n + 1)$ and $20 \times 2^n + 26$, respectively. To compute the entire Zagreb indices of $D_2(n)$, we will compute the required information for the sets of representatives of $V(D_2(n))$. We will use computational arguments for this computation. First we partition the molecular graph $D_2(n)$ into two sets C and D. For the set C, we label the representatives by γ_l, where $1 \le l \le 9$, and for the set D, these representatives are labelled by a_i, b_i, c_i, d_n, e_n, f_n, g_n, h_n, where $1 \le i \le n$. Table 6 shows these representatives, their degrees and frequencies of their occurrence. The labelled molecular graphs with $n = 1$ and $n = 2$ are shown in Figure 2.

In Table 7, we find theedge partition with respect to the pairs of end vertices of sets C and D, degree of each edge and their frequencies of occurrence.

Now, in the following theorem we compute the first entire Zagreb index.

Theorem 3.1

For $D_2(n)$, the first entire Zagreb index is given by:

$$M_1^{\varepsilon}(D_2(n)) = 516+212\times2^n.$$

Proof. According to values in Tables 6 and 7, and the definition of first entire Zagreb index the value of $M_1^{\varepsilon}(D_2(n))$ can be computed as:

Table 6: Representatives with their degrees and frequencies of occurrence for $n \ge 1$.

Representatives	Degree	Frequency	Representatives	Degree	Frequency	Representatives	Degree	Frequency
γ_1	3	4	γ_7	3	4	d_n	2	2^{n+1}
γ_2	3	2	γ_8	1	4	e_n	3	2^{n+1}
γ_3	2	4	γ_9	3	2	f_n	1	2^{n+1}
γ_4	3	2	a_i	3	2^i	g_n	2	2^{n+1}
γ_5	2	4	b_i	2	2^{i+1}	h_n	1	2^{n+1}
γ_6	3	4	c_i	2	2^{i+1}			

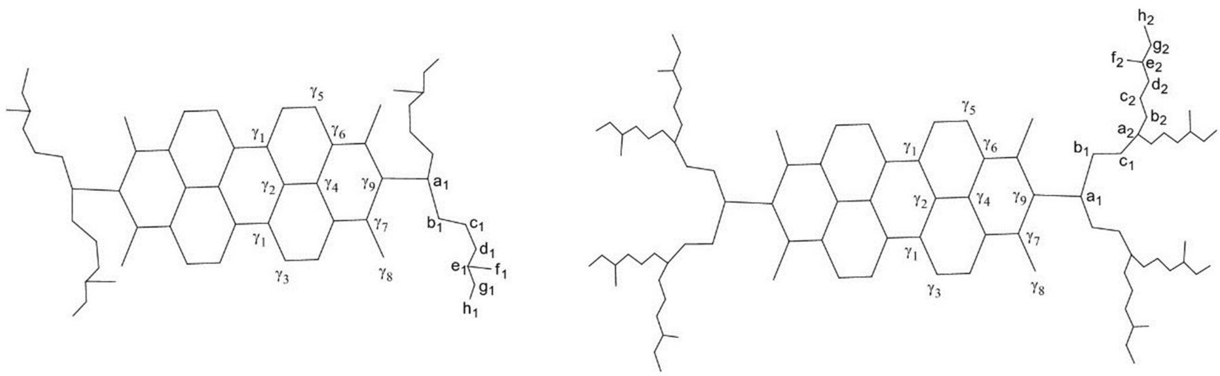

Figure 2: From left to right, $D_2(n)$ with $n = 1$ and $n = 2$.

Table 7: The edge partition with respect to the pairs of end vertices of sets *C* and *D*, degree of each edge and their frequency of occurrence.

Edge	Degree	Frequency	Edge	Degree	Frequency	Edge	Degree	Frequency
$[\gamma_1,\gamma_1]$	4	2	$[\gamma_6,\gamma_7]$	4	4	$[c_i,a_{i+1}]$ $i \neq n$	3	2^{i+1}
$[\gamma_1,\gamma_2]$	4	4	$[\gamma_7,\gamma_8]$	2	4	$[c_n,d_n]$	2	2^{n+1}
$[\gamma_1,\gamma_3]$	3	4	$[\gamma_7,\gamma_9]$	4	4	$[d_n,e_n]$	3	2^{n+1}
$[\gamma_2,\gamma_4]$	4	2	$[\alpha_9,a_1]$	4	2	$[e_n,f_n]$	2	2^{n+1}
$[\gamma_3,\gamma_5]$	2	4	$[a_i,b_i]$	3	2^{i+1}	$[e_n,g_n]$	3	2^{n+1}
$[\gamma_4,\gamma_6]$	4	4	$[b_i,c_i]$	2	2^{i+1}	$[g_n,h_n]$	1	2^{n+1}
$[\gamma_5,\gamma_6]$	3	4						

Table 8: Representatives with corresponding adjacent vertices and their frequencies of occurrence for $n \geq 1$.

Representatives	Adjacent vertices	Frequency	Representatives	Adjacent vertices	Frequency
γ_1	$\gamma_1,\gamma_2,\gamma_3$	2,4,4	γ_9	a_1	2
γ_2	γ_4	2	a_i	b_i	2^{i+1}
γ_3	γ_5	4	b_i, $i \neq n$	c_i	2^{i+1}
γ_4	γ_6	4	c_n	d_n	2^{n+1}
γ_5	γ_6	4	d_n	e_n	2^{n+1}
γ_6	γ_7	4	e_n	f_n, g_n	$2^{n+1}, 2^{n+1}$
γ_7	γ_8,γ_9	4,4	g_n	h_n	2^{n+1}

$$M_1^{\varepsilon}(D_2(n)) = M_1^{\varepsilon}(C)+M_1^{\varepsilon}(D) = \sum_{v\in V(C)\cup E(C)} [d_v]^2 + \sum_{u\in V(D)\cup E(D)} [d_u]^2$$
$$= 4(3)^2+2(3)^2+4(2)^2+2(3)^2+4(2)^2+4(3)^2+4(3)^2+4(1)^2+2(3)^2+2^{n+1}(2)^2+2^{n+1}(3)^2+2^{n+1}(1)^2+2^{n+1}(2)^2$$
$$+2^{n+1}(1)^2+\sum_{i=1}^{n}2^i((3)^2+2(2)^2+2(2)^2)+2(4)^2+4(4)^2+4(3)^2+2(4)^2+4(2)^2+4(4)^2+4(3)^2+4(4)^2+4(2)^2$$
$$+4(4)^2+2(4)^2+2^{n+1}(2)^2+2^{n+1}(3)^2+2^{n+1}(2)^2+2^{n+1}(3)^2+2^{n+1}(1)^2+\sum_{i=1}^{n}2^i(2(3)^2+2(2)^2)+\sum_{i=1}^{n-1}2^{i+1}((3)^2).$$

After some calculations, we obtain the following:

$$M_1^{\varepsilon}(D_2(n)) = 516+212\times 2^n.$$

To compute the second entire Zagreb index, we will have to find three things, firstly in Table 8, we compute the non-repeated collection of representatives with corresponding adjacent vertices and their frequencies of occurrence. Secondly, we find the edge partition with respect to the pairs of end vertices of sets *C* and *D*, their corresponding adjacent edges and frequencies of

Table 9: Edge partition with respect to the pairs of end vertices of sets *C* and *D*, their corresponding adjacent edges and frequencies of occurrence for $n \geq 1$.

Edge	Adjacent edges	Frequency	Edge	Adjacent edges	Frequency
$[\gamma_1,\gamma_1]$	$[\gamma_1,\gamma_2]$, $[\gamma_1,\gamma_3]$	4,4	$[\gamma_7,\gamma_9]$	$[\gamma_7,\gamma_9]$, $[\gamma_9,a_1]$	2,4
$[\gamma_1,\gamma_2]$	$[\gamma_1,\gamma_2]$, $[\gamma_1,\gamma_3]$, $[\gamma_2,\gamma_4]$	2,4,4	$[\gamma_9,a_1]$	$[a_1,b_1]$	4
$[\gamma_1,\gamma_3]$	$[\gamma_3,\gamma_5]$	4	$[a_i,b_i]$	$[a_i,b_i]$, $[b_i,c_i]$	2^i, 2^{i+1}
$[\gamma_2,\gamma_4]$	$[\gamma_4,\gamma_6]$	4	$[b_i,c_i]$ $i \neq n$	$[c_i,a_{i+1}]$	2^{i+1}
$[\gamma_3,\gamma_5]$	$[\gamma_5,\gamma_6]$	4	$[c_i,a_{i+1}]$ $i \neq n$	$[a_{i+1},b_{i+1}]$	2^{i+2}
$[\gamma_4,\gamma_6]$	$[\gamma_4,\gamma_6]$, $[\gamma_5,\gamma_6]$, $[\gamma_6,\gamma_7]$	2,4,4	$[b_n,c_n]$	$[c_n,d_n]$	2^{n+1}
$[\gamma_5,\gamma_6]$	$[\gamma_6,\gamma_7]$	4	$[c_n,d_n]$	$[d_n,e_n]$	2^{n+1}
$[\gamma_6,\gamma_7]$	$[\gamma_7,\gamma_8]$, $[\gamma_7,\gamma_9]$	4,4	$[d_n,e_n]$	$[e_n,f_n]$, $[e_n,g_n]$	2^{n+1}, 2^{n+1}
$[\gamma_7,\gamma_8]$	$[\gamma_7,\gamma_9]$	4	$[e_n,g_n]$	$[e_n,f_n]$, $[g_n,h_n]$	2^{n+1}, 2^{n+1}

Table 10: Representatives with corresponding edges on which these are incident and their frequencies of occurrence for $n \geq 1$.

Representatives	Edges on which representatives are incident	Frequency	Representatives	Edges on which representatives are incident	Frequency
γ_1	$[\gamma_1,\gamma_1]$, $[\gamma_1,\gamma_2]$, $[\gamma_1,\gamma_3]$	2,4,4	a_i	$[\gamma_9,a_1]$, $[a_i,b_i]$	2,2^{i+1}
γ_2	$[\gamma_1,\gamma_2]$, $[\gamma_2,\gamma_4]$	4,2,4	b_i	$[a_i,b_i]$, $[b_i,c_i]$	2^{i+1}, 2^{i+1}
γ_3	$[\gamma_1,\gamma_3]$, $[\gamma_3,\gamma_5]$	4,4	c_i	$[b_i,c_i]$	2^{i+1}
γ_4	$[\gamma_2,\gamma_4]$, $[\gamma_4,\gamma_6]$	2,4	c_i, $i \neq n$	$[b_i,c_i]$, $[c_i,a_{i+1}]$	2^{i+1}, 2^{i+1}
γ_5	$[\gamma_3,\gamma_5]$, $[\gamma_5,\gamma_6]$	4,4	f_n	$[e_n,f_n]$	2^{n+1}
γ_6	$[\gamma_4,\gamma_6]$, $[\gamma_5,\gamma_6]$, $[\gamma_6,\gamma_7]$	2,4,4	e_n	$[d_n,e_n]$, $[e_n,g_n]$, $[e_n,f_n]$	2^{n+1}, 2^{n+1}, 2^{n+1}
γ_7	$[\gamma_6,\gamma_7]$, $[\gamma_7,\gamma_8]$, $[\gamma_7,\gamma_9]$	4,4,4	g_n	$[e_n,g_n]$, $[g_n,h_n]$	2^{n+1}, 2^{n+1}
γ_8	$[\gamma_7,\gamma_8]$	4	h_n	$[g_n,h_n]$	2^{n+1}
γ_9	$[\gamma_7,\gamma_9]$, $[\gamma_9,a_1]$	4,2	d_n	$[c_n,d_n]$, $[d_n,e_n]$	2^{n+1}, 2^{n+1}

occurrence. These calculations are shown in Table 9. Finally, we find all the edges on which a specific vertex is incident and their frequencies of occurrence for $n \geq 1$. These computations are shown in Table 10.

Now, we are ready to compute the second entire Zagreb index.

Theorem 3.2

For $D_2(n)$, the second entire Zagreb index is given by:

$$M_2^{\varepsilon}(D_2(n)) = 1548 + 432 \times 2^n.$$

Proof. Using Tables 6-10 and the definition of second entire Zagreb index, the value of $M_2^{\varepsilon}(D_2(n))$ can be calculated as:

$$\begin{aligned}
M_2^{\varepsilon}(D_2(n)) &= M_2^{\varepsilon}(C) + M_2^{\varepsilon}(D) \\
&= 2(3\times3)+4(3\times3)+4(3\times2)+2(3\times3)+4(2\times2)+4(3\times3)+4(3\times2)+4(3\times3)+4(3\times3)+4(1\times3)+2(3\times3) \\
&\quad +2^{n+1}(2\times2+2\times3+3\times1+3\times2+2\times1)+\sum_{i=1}^{n}2^{2i+1}(3\times2)+\sum_{i=1}^{n-1}2^{2i+1}(2\times2)+4(4\times4)+4(3\times4)+2(4\times4) \\
&\quad +4(3\times4)+4(4\times4)+4(2\times3)+4(4\times4)+4(3\times2)+2(4\times4)+4(3\times4)+4(4\times4)+4(3\times4)+4(2\times4) \\
&\quad +4(4\times4)+4(2\times4)+4(4\times4)+2(4\times4)+4(4\times4)+4(3\times4)+\sum_{i=1}^{n}2^{i}((3\times3)+2(3\times2)) \\
&\quad +\sum_{i=1}^{n-1}2^{i+1}((2\times3)+2(3\times3))+2^{n+1}((2\times2)+(2\times3)+(2\times3)+(3\times3)+(2\times3)+(1\times3))+4(3\times4)+4(3\times4) \\
&\quad +4(3\times3)+4(3\times4)+2(4\times3)+4(2\times3)+4(2\times2)+2(3\times4)+4(3\times4)+4(2\times2)+4(3\times2)+2(3\times4)+4(3\times3) \\
&\quad +4(3\times4)+4(3\times4)+4(4\times4)+4(2\times3)+4(1\times2)+4(3\times4)+2(3\times4)+2(3\times4) \\
&\quad +\sum_{i=1}^{n}2^{i+1}((3\times3)+(3\times2)+(2\times2)+(2\times2))+\sum_{i=1}^{n-1}2^{i+1}((2\times2)+(2\times3)) \\
&\quad +2^{n+1}((2\times1)+(3\times3)+(2\times3)+(2\times3)+(2\times2)+(2\times1)+(1\times1)+(2\times3)+(2\times2)).
\end{aligned}$$

After some simplifications, we obtain the following:

$$M_2^\varepsilon(D_2(n)) = 1548 + 432 \times 2^n.$$

4 Conclusion

In this rapid era of technological improvement, a large number of new chemical structures emerge every year. To find out the chemical properties of such a large number of compounds and drugs requires a large amount of chemical experiments. In this regard, computing different types of topological indices has supplied the evidence of such medicinal behaviour of several compounds and drugs.We considered two classes of dendrimers and studied entire Zagreb indices for their molecular graphs. It will be interesting to compute these indices for other chemical structures, which may be helpful to understand their underlying topologies.

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