TWMS J. App. and Eng. Math. V.16, N.9, 2026, pp. 1042-1056

STRUCTURAL MATHEMATICS OF DENDRIMERS THROUGH COMPLEMENTARY TOPOLOGICAL INDICES

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Abstract. Topological indices are key molecular descriptors in theoretical chemistry, nanotechnology and molecular modeling, linking structural and physicochemical properties. Recent advances in graph theory have broadened the application of these indices, revealing new mathematical insights and practical uses. This study investigates four complementary topological indices—recently proposed but still underexplored—in a special class of chemical graphs: dendrimers. Using combined approaches from graph theory and mathematical chemistry, we derive closed-form analytical expressions for the complementary Zagreb, Forgotten, geometric-arithmetic, and augmented Zagreb indices across four dendrimer families. These findings not only fill a theoretical gap but also establish quantitative links between dendrimer architecture and molecular properties.

Keywords: Topological indices, Dendrimers, Graph theory, Molecular descriptors.

AMS Subject Classification: 05C09; 05C92; 05C90.

1. Introduction

Molecular descriptors are fundamental mathematical tools that translate molecular structures into quantitative information, essential for predicting physicochemical, toxicological, and biological properties in complex chemical systems [6]. In cheminformatics, molecules can be represented by molecular graphs, where atoms correspond to vertices and chemical bonds correspond to edges. Among the diverse descriptors available, topological indices have emerged as particularly effective in capturing key structural aspects of molecules.

Topological indices have long been applied in theoretical chemistry, drug design, and quantitative structure–activity/property relationship studies (QSAR/QSPR) [5, 18]. Derived from graph theory, they provide numerical representations of molecular structures, enabling computational analysis, reducing experimental costs, and facilitating the prediction of molecular properties.

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§ Manuscript received: May 26, 2025; accepted: September 08, 2025.
TWMS Journal of Applied and Engineering Mathematics, Vol.16, No.9;

Classical topological indices include the Wiener index, Randić index, Zagreb indices, and Hosoya index, each highlighting distinct structural features. The Wiener index sums the shortest paths between all atom pairs, reflecting overall molecular connectivity [20]. The Randić index measures the effect of molecular branching and has been linked to thermodynamic and biological properties [15]. The Zagreb indices quantify vertex-degree interactions, while the Hosoya index relates to molecular stability and aromaticity [4,9,10]. These indices provide valuable insights into molecular topology, yet they may overlook structural asymmetries and subtle differences in vertex degree distributions, particularly in highly branched molecules.

To address these limitations, recent studies introduced complementary topological indices, which capture additional structural nuances not fully described by classical descriptors [7]. Complementary indices emphasize differences between vertex degrees and highlight asymmetrical connectivity patterns. By considering these aspects, complementary indices provide a more detailed characterization of molecular structures, particularly in complex and highly branched systems.

Dendrimers are a suitable class of chemical graphs for exploring complementary indices. These highly branched, regular, and often symmetric macromolecules exhibit unique topological features, making them ideal for testing the sensitivity and informativeness of new descriptors. The structural complexity of dendrimers allows for a comprehensive evaluation of how complementary indices behave compared to classical indices, potentially revealing new insights into the correlation between molecular topology and physicochemical properties.

Several studies have examined topological indices in dendrimeric structures, contributing to the development and application of degree-based descriptors. For example, Ghaleb et al. [8] and Zheng et al. [21] analyzed dendrimer structures using classical indices, while Ovais et al. [19], Rajesh and Saminathan [14], and Mirzaei and Ghorbani [12] focused on entropy-based and degree-oriented descriptors. Ahmad and Ashraf [1], Aslam et al. [2], Kang et al. [11], and Sarkar et al. [17] further explored the relationships between topological indices and molecular properties in dendrimeric networks, providing a solid foundation for subsequent studies on complementary indices [3,16]. Additional studies on topological indices for other families of graphs can be seen in [7, 9, 13, 18, 23–32, 35–54], while studies on extremal graphs are available in [22, 33, 34].

Firstly, let $G = (V, E)$ be a simple undirected graph of order $n = |V|$ and size $m = |E|$. For vertices $u, v \in V(G)$, edge $uv \in E(G)$, and $d(u)$, $d(v)$ being the respective degrees of vertices u and v. Let n_{ij} denote the number of edges $e = uv \in E(G)$ such that $d(u) = i$ and $d(v) = j$. Table 1 summarizes the classical degree-based topological indices considered in this study, the second Zagreb index ($M_2(G)$), the forgotten index ($F(G)$), the geometric-arithmetic index ($GA(G)$), and the augmented Zagreb index ($AZI(G)$) together with their complementary versions proposed by Furtula and Oz [7]. These indices were selected because they are widely used in the literature, represent distinct structural features, and have demonstrated strong correlations with various molecular properties. The complementary versions emphasize structural differences and asymmetries, providing new perspectives on molecular branching and connectivity.

The objective of this work is to compute the complementary versions of $M_2(G)$, $F(G)$, $GA(G)$, and $AZI(G)$ for dendrimeric chemical graph structures, specifically: Porphyrin Dendrimer, Propyl Ether Imine (PETIM) Dendrimer, Zinc Porphyrin Dendrimer (DPZ_n), and Poly ethylene amide amine dendrimer (PETAA). This analysis aims to investigate the behavior of these new descriptors in highly branched molecular topologies, with potential applications in modeling molecular properties.

Table 1. Degree-based topological indices and their complementary versions. Consider $d(u) \geq d(v)$ [7].

Definition	Complementary Index
$M_2(G) = \sum_{uv \in E(G)} d(u) \cdot d(v)$	$cM_2(G) = \sum_{uv \in E(G)} (d(u)^2 - d(v)^2)$
$F(G) = \sum_{uv \in E(G)} (d(u)^2 + d(v)^2)$	$cF(G) = 2 \cdot F(G) = 2 \sum_{uv \in E(G)} (d(u)^2 + d(v)^2)$
$GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d(u) \cdot d(v)}}{d(u) + d(v)}$	$cGA(G) = \sum_{uv \in E(G)} \frac{\sqrt{d(u)^2 - d(v)^2}}{d(u)}$
$AZI(G) = \sum_{uv \in E(G)} \left(\frac{d(u) \cdot d(v)}{d(u) + d(v) - 2} \right)^3$	$cAZI(G) = \frac{1}{8} \sum_{uv \in E(G)} \left(\frac{d(u)^2 - d(v)^2}{d(u) - 1} \right)^3$

2. Discussion and main results

In this section, we compute the four complementary topological indices for the dendrimers D_nP_n, $PETIM$, DPZ_n and $PETAA$, shown in Figures $1, \ldots, 4$, respectively.

In Tables 2 through 5, we present the edge partitions for each dendrimer graph: D_nP_n, $PETIM$, DPZ_n and $PETAA$, respectively. Let e_{ij} denote the number of edges of G connecting vertices of degrees i and j. Clearly, $e_{ij} = e_{ji}$.

We now examine the dendrimer D_nP_n represented in Figure 1. Let $n = 2^m$, where $m \geq 2$ denotes the number of branching generations. The molecular graph of D_nP_n is formed by a central core linked to four identical dendritic branches, together with five additional edges in the core region. Each branch contains $24n - 4$ vertices, which can be categorized as follows: $26 \cdot 2^{m-2}$ leaves of degree 1, $17 \cdot 2^{m-1} - 3$ vertices of degree 2, $8 \cdot 2^{m-2}$ vertices of degree 4, and $7n - 1$ vertices of degree 3. Besides this branching structure, the central core contributes four degree-2 vertices and two degree-3 vertices. Collectively, the dendrimer contains $96n - 10$ vertices, partitioned into $26n$ of degree 1, $34n - 8$ of degree 2, $28n - 2$ of degree 3, and $8n$ of degree 4. From these counts, the total number of edges is obtained as $105n - 11$. Since the architecture is based on four equivalent branches connected through the core, the edge partition follows naturally. We find that $e_{31} = 2n$, $e_{41} = 24n$, $e_{22} = 10n - 5$, $e_{32} = 48n - 6$, $e_{33} = 13n$, and $e_{43} = 8n$. These six classes of edges, grouped according to the degrees of their incident vertices, are summarized in Table 2.

Next, consider the PETIM dendrimer shown in Figure 2. This dendrimer originates from an oxygen atom acting as the central core, with growth occurring radially at tertiary nitrogens, each separated by an eight-bond spacer in successive generations. Denote by G the molecular graph of a PETIM dendrimer of generation G_n, with $n \geq 1$. The structure consists of four branches joined at a central unit containing eight edges. Each branch contributes $6 \times 2^n - 8$ edges, so that the total number of edges is $24 \times 2^n - 24$. As G is a tree, it follows that the number of vertices equals $24 \times 2^n - 23$. Among these, the 2^{n+1} leaves correspond to vertices of degree 1, while $2^{n+1} - 2$ vertices are of degree 3, and the remaining $20 \times 2^n - 21$ vertices have degree 2. Regarding the edge distribution, the central part contributes six edges of type $(2, 2)$ and two edges of type $(2, 3)$. In general, we obtain $e_{21} = 2^{n+1}$, $e_{22} = 16 \times 2^n - 18$, and $e_{32} = 6 \times 2^n - 6$. These three edge categories are presented in Table 3 for clarity.

We now turn to the dendrimer DPZ_n (Figure 3), where $n \geq 1$ denotes the number of growth steps. Its molecular graph consists of a central core connected symmetrically to four identical branches. The core of DPZ_n is composed of 49 vertices, among which 24 are

of degree 2, 24 are of degree 3, and a single vertex has degree 4. Each branch contributes $14(2^n-1)$ vertices, subdivided into $11\cdot 2^n-9$ vertices of degree 2 and $3\cdot 2^n-5$ vertices of degree 3. Summing the contributions of all branches with the central structure, the graph DPZ_n contains a total of $56\cdot 2^n-7$ vertices. These are distributed as $44\cdot 2^n-12$ vertices of degree 2, $12\cdot 2^n+4$ vertices of degree 3, and one vertex of degree 4. From this distribution, the total number of edges can be computed as $64\cdot 2^n-4$. Furthermore, the partition of edges by endpoint degrees yields four categories: $e_{22}=16\cdot 2^n-4$, $e_{32}=40\cdot 2^n-16$, $e_{33}=8\cdot 2^n+12$, and $e_{43}=4$. These values are summarized in Table 4.

We now turn to the dendrimer $PETAA$ (Figure 4), where $n\geq 1$ denotes the number of growth steps. Its molecular graph consists of a central core symmetrically connected to four identical branches. The total number of vertices and edges of $PETAA$ are given by $|V(PETAA)|=44\cdot 2^n-18$ and $|E(PETAA)|=44\cdot 2^n-19$, respectively. The vertices can be classified into three degree types: $8\cdot 2^n-2$ vertices of degree 1, $28\cdot 2^n-12$ vertices of degree 2, and $8\cdot 2^n-4$ vertices of degree 3. From this distribution, the total number of edges follows directly. Furthermore, the edges can be grouped into four categories according to the degrees of their endpoints: $e_{12}=4\cdot 2^n$, $e_{13}=4\cdot 2^n-2$, $e_{22}=16\cdot 2^n-8$, and $e_{23}=20\cdot 2^n-9$. These values are summarized in Table 5.

Now, we calculate the second complementary Zagreb index for the four types of dendrimers, according to the following theorem.

Theorem 2.1. *The second complementary Zagreb index $cM_2(G)$ for the dendrimer graphs D_nP_n, $PETIM$, DPZ_n and $PETAA$, respectively, is given by:*

$$cM_2(D_nP_n)=672n-30, \tag{1}$$

$$cM_2(PETIM)=36\times 2^n-30, \tag{2}$$

$$cM_2(DPZ_n)=200\times 2^n-52, \tag{3}$$

$$cM_2(PETAA)=9\times 2^{(n+4)}-61. \tag{4}$$

Proof. The graph D_nP_n (Figure 1) has edge types and their respective quantities as presented in Table 2. Therefore, by applying the formula for the $cM_2(G)$ index provided in Table 1, we derive:

$$\begin{aligned} cM_2(D_nP_n) &= \sum_{uv\in E(G)}(d(u)^2-d(v)^2)\\ &= n_{31}(3^2-1^2)+n_{41}(4^2-1^2)+n_{22}(2^2-2^2)+n_{32}(3^2-2^2)+n_{33}(3^2-3^2)\\ &+ n_{43}(4^2-3^2)\\ &= (2n)(8)+(24n)(15)+(48n-6)(5)+(8n)(7)\\ &= 672n-30. \end{aligned}$$

The graph $PETIM$ (Figure 2) has edge types and their respective quantities as presented in Table 3. Therefore, by applying the formula for the $cM_2(G)$ index provided in Table 1, we derive:

$$\begin{aligned} cM_2(PETIM) &= \sum_{uv\in E(G)}(d(u)^2-d(v)^2)\\ &= n_{21}(2^2-1^2)+n_{22}(2^2-2^2)+n_{32}(3^2-2^2)\\ &= (2^{n+1})(3)+(6\cdot 2^n-6)(5)\\ &= 36\times 2^n-30. \end{aligned}$$

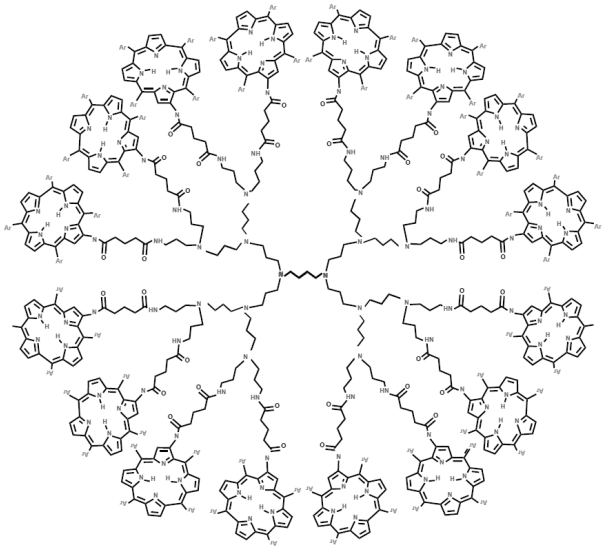

Figure 1. Porphyrin Dendrimer $D_{16}P_{16}$.

Table 2. Edge partition of dendrimer D_nP_n, based on $(d(u), d(v))$.

$(d(u), d(v))$, where $uv \in E(D_nP_n)$	Number of edges (n_{ij})
$(3, 1)$	$2n$
$(4, 1)$	$24n$
$(2, 2)$	$10n - 5$
$(3, 2)$	$48n - 6$
$(3, 3)$	$13n$
$(4, 3)$	$8n$

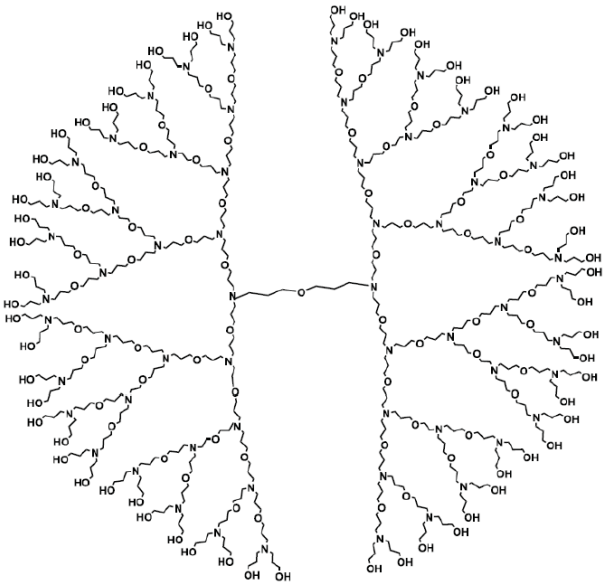

Figure 2. Propyl Ether Imine (PETIM) Dendrimer, with $n = 5$.

Table 3. Edge partition of graph $PETIM$, based on $(d(u), d(v))$.

$(d(u), d(v))$, where $uv \in E(PETIM)$	Number of edges (n_{ij})
$(2, 1)$	2^{n+1}
$(2, 2)$	$2^{n+4} - 18$
$(3, 2)$	$6 \cdot 2^n - 6$

Table 4. Edge partition of graph DPZ_n, based on $(d(u), d(v))$.

$(d(u), d(v))$, where $uv \in E(DPZ_n)$	Number of edges (n_{ij})
$(2, 2)$	$16 \cdot 2^n - 4$
$(3, 2)$	$40 \cdot 2^n - 16$
$(3, 3)$	$8 \cdot 2^n + 12$
$(4, 3)$	4

The graph DPZ_n (Figure 3) has edge types and their respective quantities as presented in Table 4. Therefore, by applying the formula for the $cM_2(G)$ index provided in Table 1, we derive:

$$\begin{aligned} cM_2(DPZ_n) &= \sum_{uv \in E(G)} (d(u)^2 - d(v)^2) \\ &= n_{22}(2^2 - 2^2) + n_{32}(3^2 - 2^2) + n_{33}(3^2 - 3^2) + n_{43}(4^2 - 3^2) \\ &= (40 \times 2^n - 16)(5) + (4)(7) \\ &= 200 \times 2^n - 52. \end{aligned}$$

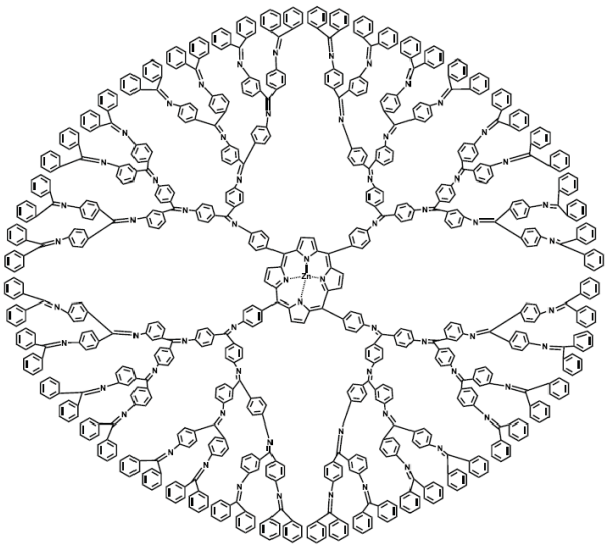

Figure 3. Zinc Porphyrin Dendrimer DPZ_n.

The graph $PETAA$ (Figure 4) has edge types and their respective quantities as presented in Table 5. Therefore, by applying the formula for the $cM_2(G)$ index provided in

Table 1, we derive:

$$\begin{aligned} cM_2(PETAA) &= \sum_{uv\in E(G)} (d(u)^2 - d(v)^2) \\ &= n_{21}(2^2-1^2) + n_{31}(3^2-1^2) + n_{22}(2^2-2^2) + n_{32}(3^2-2^2) \\ &= (4\times 2^n)3 + (4\times 2^n - 2)8 + (16\times 2^n - 8)(0) + (20\times 2^n - 9)5 \\ &= 9\times 2^{(n+4)} - 61. \end{aligned}$$

Table 5. Edge partition of dendrimer PETAA, based on $(d(u), d(v))$.

$(d(u), d(v))$, where $uv \in E\,(PETAA)$	Number of edges (n_{ij})
$(2,1)$	$4\cdot 2^n$
$(3,1)$	$4\cdot 2^n - 2$
$(2,2)$	$16\cdot 2^n - 8$
$(3,2)$	$20\cdot 2^n - 9$

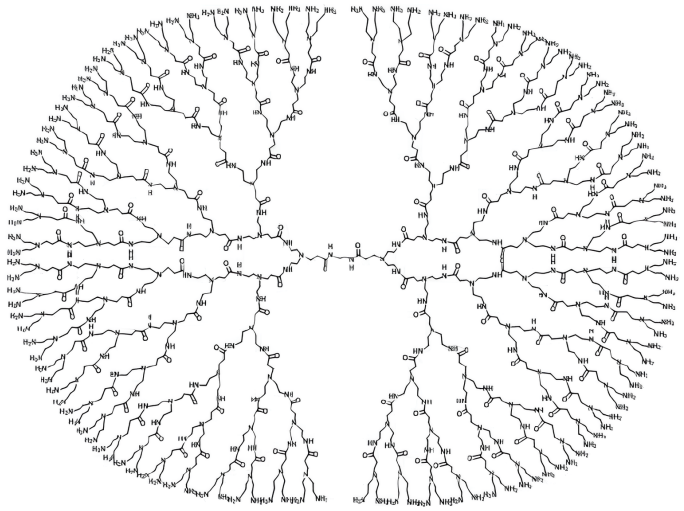

Figure 4. Poly ethylene amide amine dendrimer PETAA.

Thus, we conclude the results. □

In the next theorem, we calculate the complementary Forgotten index $cF(G)$ for the respective dendrimers.

Theorem 2.2. *The complementary Forgotten index $cF(G)$ for the dendrimer graphs D_nP_n, $PETIM$, DPZ_n and $PETAA$, respectively, is given by:*

$$cF(D_nP_n) = 3132n - 236, \tag{5}$$

$$cF(PETIM) = 432\times 2^n - 444, \tag{6}$$

$$cF(DPZ_n) = 1584\times 2^n + 152, \tag{7}$$

$$cF(PETAA) = 896\times 2^n - 402. \tag{8}$$

Proof. The graph D_nP_n (Figure 1) has edge types and their respective quantities as presented in Table 2. Therefore, by applying the formula for the $cF(G)$ index provided in Table 1, we derive:

$$\begin{aligned}
cF(D_nP_n) &= \sum_{uv\in E(G)} 2(d(u)^2 + d(v)^2) \\
&= 2\left[n_{31}(3^2+1^2) + n_{41}(4^2+1^2) + n_{22}(2^2+2^2)\right] \\
&+ 2\left[n_{32}(3^2+2^2) + n_{33}(3^2+3^2) + n_{34}(3^2+4^2)\right] \\
&= 2\left[(2n)(10) + (24n)(17) + (10n-5)(8) + (48n-6)(13) + (13n)(18) + (8n)(25)\right] \\
&= 3132n - 236.
\end{aligned}$$

The graph $PETIM$ (Figure 2) has edge types and their respective quantities as presented in Table 3. Therefore, by applying the formula for the $cF(G)$ index provided in Table 1, we derive:

$$\begin{aligned}
cF(PETIM) &= \sum_{uv\in E(G)} 2(d(u)^2 + d(v)^2) \\
&= 2\left[n_{21}(2^2+1^2) + n_{22}(2^2+2^2) + n_{32}(3^2+2^2)\right] \\
&= 2\left[(2^{n+1})(5) + (2^{n+4}-18)(8) + (6\times 2^n - 6)(13)\right] \\
&= 432\times 2^n - 444.
\end{aligned}$$

The graph DPZ_n (Figure 3) has edge types and their respective quantities as presented in Table 4. Therefore, by applying the formula for the $cF(G)$ index provided in Table 1, we derive:

$$\begin{aligned}
cF(DPZ_n) &= \sum_{uv\in E(G)} 2(d(u)^2 + d(v)^2) \\
&= 2\left[n_{22}(2^2+2^2) + n_{32}(3^2+2^2) + n_{33}(3^2+3^2) + n_{43}(4^2+3^2)\right] \\
&= 2\left[(16\times 2^n - 4)(8) + (40\times 2^n - 16)(13) + (8\times 2^n + 12)(18) + (4)(25)\right] \\
&= 1584\times 2^n + 152.
\end{aligned}$$

The graph $PETAA$ (Figure 4) has edge types and their respective quantities as presented in Table 5. Therefore, by applying the formula for the $cF(G)$ index provided in Table 1, we derive:

$$\begin{aligned}
cF(PETAA) &= \sum_{uv\in E(G)} 2(d(u)^2 + d(v)^2) \\
&= 2\left[n_{21}(2^2+1^2) + n_{31}(3^2+1^2) + n_{22}(2^2+2^2) + n_{32}(3^2+2^2)\right] \\
&= 2\left[(4\times 2^n)(5) + (4\times 2^n - 2)(10) + (16\times 2^n - 8)(8) + (20\times 2^n - 9)(13)\right] \\
&= 2\left[20\times 2^n + 40\times 2^n - 20 + 128\times 2^n - 64 + 260\times 2^n - 117\right] \\
&= 2\left[(20+40+128+260)\times 2^n - (20+64+117)\right] \\
&= 2\left[448\times 2^n - 201\right] \\
&= 896\times 2^n - 402.
\end{aligned}$$

Thus, we conclude the results. □

In the next theorem, we calculate the complementary geometric-arithmetic index ($cGA(G)$) for the dendrimer graph families.

Theorem 2.3. *The complementary geometric-arithmetic index ($cGA(G)$) for the dendrimer graphs D_nP_n, $PETIM$, DPZ_n and $PETAA$, respectively, is given by:*

$$cGA(D_nP_n) = \left(\frac{4\sqrt{2}}{3} + 6\sqrt{15} + 16\sqrt{5} + 2\sqrt{7}\right) n - 2\sqrt{5}, \tag{9}$$

$$cGA(PETIM) = \left(\sqrt{3} + 2\sqrt{5}\right) 2^n - 2\sqrt{5}, \tag{10}$$

$$cGA(DPZ_n) = \frac{40\sqrt{5}}{3}2^n - \frac{16\sqrt{5}}{3} + \sqrt{7}, \tag{11}$$

$$cGA(PETAA) = \left(2\sqrt{3} + \frac{8\sqrt{2}}{3} + \frac{20\sqrt{5}}{3}\right) 2^n - \frac{4\sqrt{2}}{3} - 3\sqrt{5}. \tag{12}$$

Proof. The graph D_nP_n (Figure 1) has edge types and their respective quantities as presented in Table 2. Therefore, by applying the formula for the $cGA(G)$ index provided in Table 1, we derive:

$$\begin{aligned}
cGA(D_nP_n) &= \sum_{uv\in E(G)} \frac{\sqrt{d(u)^2 - d(v)^2}}{d(u)} \\
&= n_{31}\frac{\sqrt{3^2-1^2}}{3} + n_{41}\frac{\sqrt{4^2-1^2}}{4} + n_{22}\frac{\sqrt{2^2-2^2}}{2} \\
&+ n_{32}\frac{\sqrt{3^2-2^2}}{3} + n_{33}\frac{\sqrt{3^2-3^2}}{3} + n_{43}\frac{\sqrt{4^2-3^2}}{4} \\
&= (2n)\frac{\sqrt{8}}{3} + (24n)\frac{\sqrt{15}}{4} + (10n-5)\frac{\sqrt{0}}{2} + (48n-6)\frac{\sqrt{5}}{3} \\
&+ (13n)\frac{\sqrt{0}}{3} + (8n)\frac{\sqrt{7}}{4} \\
&= \left(\frac{4\sqrt{2}}{3} + 6\sqrt{15} + 16\sqrt{5} + 2\sqrt{7}\right) n - 2\sqrt{5}.
\end{aligned}$$

The graph $PETIM$ (Figure 2) has edge types and their respective quantities as presented in Table 3. Therefore, by applying the formula for the $cGA(G)$ index provided in Table 1, we derive:

$$\begin{aligned}
cGA(PETIM) &= \sum_{uv\in E(G)} \frac{\sqrt{d(u)^2 - d(v)^2}}{d(u)} \\
&= n_{21}\frac{\sqrt{2^2-1^2}}{2} + n_{22}\frac{\sqrt{2^2-2^2}}{2} + n_{32}\frac{\sqrt{3^2-2^2}}{3} \\
&= (2^{n+1})\frac{\sqrt{3}}{2} + (2^{n+4}-18)\frac{\sqrt{0}}{2} + (6\times 2^n - 6)\frac{\sqrt{5}}{3} \\
&= \left(\sqrt{3} + 2\sqrt{5}\right) 2^n - 2\sqrt{5}.
\end{aligned}$$

The graph DPZ_n (Figure 3) has edge types and their respective quantities as presented in Table 4. Therefore, by applying the formula for the $cGA(G)$ index provided in Table

1, we derive:

$$\begin{aligned} cGA(DPZ_n) &= \sum_{uv\in E(G)} \frac{\sqrt{d(u)^2 - d(v)^2}}{d(u)} \\ &= n_{22}\frac{\sqrt{2^2-2^2}}{2} + n_{32}\frac{\sqrt{3^2-2^2}}{3} + n_{33}\frac{\sqrt{3^2-3^2}}{3} + n_{43}\frac{\sqrt{4^2-3^2}}{4} \\ &= (16\times 2^n - 4)\frac{\sqrt{0}}{2} + (40\times 2^n - 16)\frac{\sqrt{5}}{3} + (8\times 2^n + 12)\frac{\sqrt{0}}{3} + (4)\frac{\sqrt{7}}{4} \\ &= \frac{40\sqrt{5}}{3}2^n - \frac{16\sqrt{5}}{3} + \sqrt{7}. \end{aligned}$$

The graph $PETAA$ (Figure 4) has edge types and their respective quantities as presented in Table 5. Therefore, by applying the formula for the $cGA(G)$ index provided in Table 1, we derive:

$$\begin{aligned} cGA(PETAA) &= \sum_{uv\in E(G)} \frac{\sqrt{d(u)^2 - d(v)^2}}{d(u)} \\ &= n_{21}\frac{\sqrt{2^2-1^2}}{2} + n_{31}\frac{\sqrt{3^2-1^2}}{3} + n_{22}\frac{\sqrt{2^2-2^2}}{2} + n_{32}\frac{\sqrt{3^2-2^2}}{3} \\ &= (4\times 2^n)\frac{\sqrt{3}}{2} + (4\times 2^n - 2)\frac{\sqrt{8}}{3} + (16\times 2^n - 8)\frac{\sqrt{0}}{2} + (20\times 2^n - 9)\frac{\sqrt{5}}{3} \\ &= \left(2\sqrt{3} + \frac{8\sqrt{2}}{3} + \frac{20\sqrt{5}}{3}\right)2^n - \frac{4\sqrt{2}}{3} - 3\sqrt{5}. \end{aligned}$$

Thus, we conclude the results. □

In the next theorem, we calculate the complementary augmented Zagreb index ($cAZI(G)$) for the dendrimer graph families.

Theorem 2.4. *The complementary augmented Zagreb index ($cAZI(G)$) for the dendrimer graphs D_nP_n, $PETIM$, DPZ_n, and $PETAA$, respectively, is given by:*

$$cAZI(D_nP_n) = \frac{53725n}{108} - \frac{375}{32}, \tag{13}$$

$$cAZI(PETIM) = \frac{591}{32}\times 2^n - \frac{375}{32}, \tag{14}$$

$$cAZI(DPZ_n) = \frac{625}{8}\times 2^n - \frac{2689}{108}, \tag{15}$$

$$cAZI(PETAA) = \frac{1353\times 2^n}{16} - \frac{2149}{64}. \tag{16}$$

Proof. The graph D_nP_n (Figure 1) has edge types and their respective quantities as presented in Table 2. Therefore, by applying the formula for the $cAZI(G)$ index provided in Table 1, we derive:

$$\begin{aligned}
cAZI(D_nP_n) &= \frac{1}{8}\sum_{uv\in E(G)}\left(\frac{d(u)^2-d(v)^2}{d(u)-1}\right)^3 \\
&= n_{31}\frac{1}{8}\left(\frac{3^2-1^2}{3-1}\right)^3 + n_{41}\frac{1}{8}\left(\frac{4^2-1^2}{4-1}\right)^3 + n_{22}\frac{1}{8}\left(\frac{2^2-2^2}{2-1}\right)^3 \\
&\quad + n_{32}\frac{1}{8}\left(\frac{3^2-2^2}{3-1}\right)^3 + n_{33}\frac{1}{8}\left(\frac{3^2-3^2}{3-1}\right)^3 + n_{43}\frac{1}{8}\left(\frac{4^2-3^2}{4-1}\right)^3 \\
&= (2n)(8) + (24n)\frac{125}{8} + (10n-5)(0) + (48n-6)\frac{125}{64} \\
&\quad + (13n)(0) + (8n)\frac{343}{216} \\
&= 16n + 375n + \frac{375}{4}n - \frac{375}{32} + \frac{343}{27}n \\
&= \frac{53725n}{108} - \frac{375}{32}.
\end{aligned}$$

The graph $PETIM$ (Figure 2) has edge types and their respective quantities as presented in Table 3. Therefore, by applying the formula for the $cAZI(G)$ index provided in Table 1, we derive:

$$\begin{aligned}
cAZI(PETIM) &= \frac{1}{8}\sum_{uv\in E(G)}\left(\frac{d(u)^2-d(v)^2}{d(u)-1}\right)^3 \\
&= n_{21}\frac{1}{8}\left(\frac{2^2-1^2}{2-1}\right)^3 + n_{22}\frac{1}{8}\left(\frac{2^2-2^2}{2-1}\right)^3 + n_{32}\frac{1}{8}\left(\frac{3^2-2^2}{3-1}\right)^3 \\
&= (2^{n+1})\frac{27}{8} + (2^{n+4}-18)(0) + (6\times 2^n - 6)\frac{125}{64} \\
&= \frac{591}{32}\times 2^n - \frac{375}{32}.
\end{aligned}$$

The graph DPZ_n (Figure 3) has edge types and their respective quantities as presented in Table 4. Therefore, by applying the formula for the $cAZI(G)$ index provided in Table 1, we derive:

$$\begin{aligned}
cAZI(DPZ_n) &= \frac{1}{8}\sum_{uv\in E(G)}\left(\frac{d(u)^2-d(v)^2}{d(u)-1}\right)^3 \\
&= n_{22}\frac{1}{8}\left(\frac{2^2-2^2}{2-1}\right)^3 + n_{32}\frac{1}{8}\left(\frac{3^2-2^2}{3-1}\right)^3 \\
&\quad + n_{33}\frac{1}{8}\left(\frac{3^2-3^2}{3-1}\right)^3 + n_{43}\frac{1}{8}\left(\frac{4^2-3^2}{4-1}\right)^3 \\
&= (16\times 2^n - 4)(0) + (40\times 2^n - 16)\frac{125}{64} \\
&\quad + (8\times 2^n + 12)(0) + (4)\frac{343}{216} \\
&= \frac{625}{8}\times 2^n - \frac{2689}{108}.
\end{aligned}$$

The graph $PETAA$ (Figure 4) has edge types and their respective quantities as presented in Table 5. Therefore, by applying the formula for the $cAZI(G)$ index provided in Table 1, we derive:

$$\begin{aligned}
cAZI(PETAA) &= \frac{1}{8}\sum_{uv\in E(G)}\left(\frac{d(u)^2-d(v)^2}{d(u)-1}\right)^3 \\
&= n_{21}\frac{1}{8}\left(\frac{2^2-1^2}{2-1}\right)^3 + n_{31}\frac{1}{8}\left(\frac{3^2-1^2}{3-1}\right)^3 \\
&\quad + n_{22}\frac{1}{8}\left(\frac{2^2-2^2}{2-1}\right)^3 + n_{32}\frac{1}{8}\left(\frac{3^2-2^2}{3-1}\right)^3 \\
&= (4\times 2^n)\frac{27}{8} + (4\times 2^n-2)(8) + (16\times 2^n-8)(0) \\
&\quad + (20\times 2^n-9)\frac{125}{64} \\
&= \frac{27}{2}2^n + 32\times 2^n - 16 + \frac{625}{16}2^n - \frac{1125}{64} \\
&= \frac{1353\times 2^n}{16} - \frac{2149}{64}.
\end{aligned}$$

Thus, we conclude the results. □

3. Conclusions

In this work, we conducted a comprehensive analysis of four complementary topological indices applied to dendrimeric structures, contributing novel insights to the mathematical and chemical understanding of these highly branched macromolecules. The closed-form analytical expressions obtained for the complementary Zagreb, Forgotten, geometric-arithmetic, and augmented Zagreb indices provide precise quantitative tools for the structural characterization of four representative dendrimer families.

These complementary indices allow researchers to quantitatively assess asymmetries and branching patterns in dendrimers, which can be correlated with properties such as solubility, molecular recognition, and stability. By analyzing how variations in these indices reflect structural modifications, the results can directly inform the rational design of dendrimers with tailored properties for applications in nanotechnology, pharmacology, and materials science.

Thus, this study strengthens the link between discrete mathematics and molecular modeling, opening promising perspectives for future investigations involving other complex macromolecular architectures.

4. Acknowledgement

The authors are grateful to the editor and anonymous referees for their insightful comments and valuable suggestions.

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