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Retraction

Retracted: Computing Connection-Based Topological Indices of Dendrimers

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This article has been retracted by Hindawi following an investigation undertaken by the publisher [1]. This investigation has uncovered evidence of one or more of the following indicators of systematic manipulation of the publication process:

(1) Discrepancies in scope
(2) Discrepancies in the description of the research reported
(3) Discrepancies between the availability of data and the research described
(4) Inappropriate citations
(5) Incoherent, meaningless and/or irrelevant content included in the article
(6) Peer-review manipulation

The presence of these indicators undermines our confidence in the integrity of the article's content and we cannot, therefore, vouch for its reliability. Please note that this notice is intended solely to alert readers that the content of this article is unreliable. We have not investigated whether authors were aware of or involved in the systematic manipulation of the publication process.

Wiley and Hindawi regrets that the usual quality checks did not identify these issues before publication and have since put additional measures in place to safeguard research integrity.

We wish to credit our own Research Integrity and Research Publishing teams and anonymous and named external researchers and research integrity experts for contributing to this investigation.

The corresponding author, as the representative of all authors, has been given the opportunity to register their agreement or disagreement to this retraction. We have kept a record of any response received.

References

[1] A. Sattar, M. Javaid, and E. Bonyah, "Computing Connection-Based Topological Indices of Dendrimers," *Journal of Chemistry*, vol. 2022, Article ID 7204641, 15 pages, 2022.

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Research Article

Computing Connection-Based Topological Indices of Dendrimers

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Dendrimers are artificially synthesized polymeric macromolecules composed of frequently branching chains called monomers. Topological indices (TIs) are the molecular descriptors which characterize the topology and help to correlate the distinct psychochemical properties such as stability, boiling point, and strain energy of molecular compounds. TIs are classified on the basis of their degrees, distance, and spectrum. Among these TIs, connection-based topological descriptors have great significance. In this study, we initiate the general expressions to compute multiplicative connection Zagreb indices (MZIs), named as first MZCI, second MZCI, third MZCI, fourth MZCI, modified first MZCI, modified second MZCI, and modified third MZCI of two exceptional dendrimers nanostars, namely, poly (propyl) ether imine (PPIE) dendrimer and polypropylenimine octamin (PPIO) dendrimer. Furthermore, in order to check the superiority of our computed results, a comparative analysis is conducted.

1. Introduction

Dendrimers are infinitesimal, hyperbranched radially symmetric macromolecules with monodisperse, well-defined, and homogenous tree-like structure. Dendrimers are characterized by exceptional attributes that make them a propitious contender for a lot of applications in various domains including immunology, medicine delivery, vaccine, and the development of antimicrobials and antivirals; for details, see [1–3]. At present, researchers are paying attention to characterize the molecular structure by applying topological perspectives, involving numerical graph descriptors. These graph invariants have been broadly utilized to study the quantitative structure-activity relationship (QSAR) and quantitative structure property relationships (QSPR) [4]. A graph can be viewed as a drawing, sequence of numbers, a numeric number, polynomial, or a matrix. Topological index (TI) is a numeric measure which characterizes the topology and helps to correlate the distinct psychochemical properties such as volatility, density, stability, flammability, and strain energy of molecular compounds. Topological indices (TIs) are categorized on the bases of distance, degree, and polynomial. A TI which is concerned with a length between two nodes or vertices of a graph is said to be distance-based TI. Wiener [5] initiated the idea of distance-based TI, which is known by the Wiener index. By theoretical and conceptual framework, the Wiener index was the first and most studied TI. Mazorodze et al. [6] utilized the Gutman index, which is distance-based TI, to compute the sharp upper bounds of graphs for the diameter $\delta \geq 2$. Moreover, in 2019, Gao et al. [7] utilized distance-based descriptors to study topological aspects of dendrimers.

In 1972, in order to calculate the π-electron energy of alternant hydrocarbon, Gutman and Trinajstic [8] proposed the innovative conception of first Zagreb index (FZI). In 1975, Gutman et al. [9] investigated the second ZI (SZI). Das and Gutaman [10] discussed some properties of SZI. The FZI and SZI are frequently utilized in the field of chemical graph theory. Furthermore, Furtula and Gutman [11] initiated the idea of third ZI (TZI), which is also called the forgotten index because it was explored after a long time of the introduction of FZI and SZI. All of these degree-based TIs have fruitful application in the field of cheminformatics which is an amalgamation of mathematics, chemistry, and information technology [12–14]. Furthermore, in 2003, the novel conception of modified ZI was initiated by Nikolic et al. [15]. Hao [16] made the comparative analysis of these ZIs and put forwarded the main consequences concerning these indices. These TIs have much importance because they can be employed to study the psychochemical properties of various molecular compounds such as dendrimers, nanotubes, and neural networks. Furthermore, Dhanalakshmi et al. [17] investigated multiplicative ZIs (MZIs) on graph operators.

Recently, a new term called connection number or leap degree of vertex is invented which took the serious consideration of researchers. A number of those vertices which are at distance two from a certain vertex is referred to as CN. Ali and Trinnajstic [18] initiated Zagreb connection indices (ZCIs) and used octane isomers to examine their applicability. According to their research, ZIs on connection basis, as compared to the classical ZIs, provide a better absolute value of the correlation coefficient. Latterly, in 2020, Cao et al. [19] computed ZCIs of molecular graphs. Furthermore, Du et al. [20] used modified FZI on the basis of CN to find the extremal alkanes. Moreover, Tang et al. [21] utilized ZCIs and modified ZCIs to compute the results of T-sum graphs. Recently, Ali et al. [22] calculated the modified ZCIs for T-sum graphs in 2020. Haoer et al. [23] introduced the multiplicative leap ZIs. Javaid et al. [24] calculated multiplicative ZIs of different wheel-related graphs.

Moreover, Bokhary et al. [25] considered the topological properties of some nanostars. Bashir et al. [26] calculated the third ZI of a dendrimer nanostar. Furthermore, Dorosti et al. [27] calculated the cluj index of the first type of dendrimer nanostar. Gharibi et al. [28] developed the conception of Zagreb polynomials of nanotubes and nanocones. Furthermore, in 2016, Siddiqui et al. [29] put forward Zagreb polynomial of dendrimer nanostars.

In this study, we work on calculating multiplicative ZCIs of two special types of dendrimer nanostars, namely, PPEI dendrimer and PPIO dendrimer. We also compare the results of both types of dendrimers to check the superiority of proposed expressions.

This research article is structured as follows. In Section 2, we discuss the preliminaries which are compulsory to fully understand the main idea of this article. In Section 3, we compute multiplicative ZCIs for PPEI dendrimer. Section 4 covers the main results for PPIO dendrimer in a comprehensive way. In Section 5, we compare the computed values of both types of dendrimers with each other. Section 6 holds the conclusions.

2. Preliminaries

This section states the some primary definitions which are mandatory to understand the idea of this research article. Moreover, Definition 1 presents the degree based Zagreb indices (first, sercond and forgotten), Definition 2 to Definition 5 present the connection number based topological indices. In Definition 6, all the multiplicative connection number based topological indices are re-written where the connection number θ moves from 0 to $\widehate{t}-2$.

Definition 1 (see [8, 9, 11]). Let $\widetilde{C} = (\mathcal{J}(\widetilde{C}), \mathcal{K}(\widetilde{C}))$ be a graph, where $\mathcal{J}(\widetilde{C})$ is the vertex set and $\mathcal{K}(\widetilde{C})$ is the edge set. Then, the first Zagreb index (FZI), second Zagreb index (SZI), and third Zagreb index (TZI) can be defined as

(1) $\widehat{\mathfrak{Z}}_1(\widetilde{C}) = \sum_{z\in\mathcal{J}(\widetilde{C})} (\widehat{d_{\widetilde{C}}}(z))^2 = \sum_{zp\in\mathcal{K}(\widetilde{C})} (\widehat{d_{\widetilde{C}}}(z) + d_{\widetilde{C}}(p))$

(2) $\widehat{\mathfrak{Z}}_2(\widetilde{C}) = \sum_{zp\in\mathcal{K}(\widetilde{C})} (\widehat{\mathbf{d}}_{\widetilde{C}}(z) \times \widehat{\mathbf{d}}_{\widetilde{C}}(p))$

(3) $\widehat{\mathfrak{Z}}_3(\widetilde{C}) = \sum_{zp\in\mathcal{K}(\widetilde{C})} (\widehat{d_{\widetilde{C}}}(z) + \widehat{d_{\widetilde{C}}}(p))$

where $\widehat{d_{\widetilde{C}}}(z)$ and $\widehat{d_{\widetilde{C}}}(p)$ represent the degree of the vertex z and p, respectively.

Definition 2 (see [18]). For a graph $\widetilde{C}$, the first Zagreb connection index (FZCI) and second Zagreb connection index (SZCI) can be defined as

(1) $\widehat{\mathfrak{Z}\mathfrak{C}}_1(\widetilde{C}) = \sum_{z\in\mathcal{J}(\widetilde{C})} (\widetilde{\chi_{\widetilde{C}}}(z))^2$

(2) $\widehat{\mathfrak{Z}\mathfrak{C}}_2(\widetilde{C}) = \sum_{zp\in\mathcal{K}(\widetilde{C})} (\widetilde{\chi_{\widetilde{C}}}(z) \times \widetilde{\chi_{\widetilde{C}}}(p))$

where $\widetilde{\chi_{\widetilde{C}}}(z)$ and $\widetilde{\chi_{\widetilde{C}}}(p)$ indicate the connection number (CN) of the vertex z and p, respectively.

Definition 3 (see [18, 22]). For a graph $\widetilde{C}$, the modified FZCI, modified SZCI, and modified TZCI can be given as

(1) $\widehat{\mathfrak{Z}\mathfrak{C}}_1^*(\widetilde{C}) = \sum_{zp\in\mathcal{K}(\widetilde{C})} (\widetilde{\chi_{\widetilde{C}}}(z) + \widetilde{\chi_{\widetilde{C}}}(p)) = \sum_{zp\in\mathcal{K}(\widetilde{C})} (\widehat{d_{\widetilde{C}}}(z)\chi_{\widetilde{C}}(z))$

(2) $\widehat{\mathfrak{Z}\mathfrak{C}}_2^*(\widetilde{C}) = \sum_{zp\in\mathcal{K}(\widetilde{C})} [\widehat{d}_{\widetilde{C}}(z)\widetilde{\chi_{\widetilde{C}}}(p) + \widehat{d}_{\widetilde{C}}(p)\widetilde{\chi_{\widetilde{C}}}(z)]$

(3) $\widehat{\mathfrak{Z}\mathfrak{C}}_3^*(\widetilde{C}) = \sum_{zp\in\mathcal{K}(\widetilde{C})} [\widehat{\mathbf{d}}_{\widetilde{C}}(z)\widetilde{\chi_{\widetilde{C}}}(z) + \widehat{\mathbf{d}}_{\widetilde{C}}(p)\widetilde{\chi_{\widetilde{C}}}(p)]$

Definition 4 (see [24]). For a graph $\widetilde{C}$, first multiplicative ZCI (FsMZCI), second multiplicative ZCI (SMZCI), third multiplicative ZCI (TMZCI), and fourth multiplicative ZCI (FrMZCI) can be defined as

(1) $M\widehat{\mathfrak{Z}\mathfrak{C}}_1(\widetilde{C}) = \prod_{z\in\mathcal{J}(\widetilde{C})} (\widetilde{\chi_{\widetilde{C}}}(z))^2$

(2) $M\widehat{\mathfrak{Z}\mathfrak{C}}_2(\widetilde{C}) = \prod_{zp\in\mathcal{K}(\widetilde{C})} (\widetilde{\chi_{\widetilde{C}}}(z) \times \widetilde{\chi_{\widetilde{C}}}(p))$

(3) $M\widehat{\mathfrak{Z}\mathfrak{C}}_3(\widetilde{C}) = \prod_{z\in\mathcal{J}(\widetilde{C})} (\widehat{d_{\widetilde{C}}}(z)\chi_{\widetilde{C}}(z))$

(4) $M\widehat{\mathfrak{Z}\mathfrak{C}}_4(\widetilde{C}) = \prod_{zp\in\mathcal{K}(\widetilde{C})} (\widetilde{\chi_{\widetilde{C}}}(z) + \widetilde{\chi_{\widetilde{C}}}(p))$

Definition 5 (see [24]). For a graph $\widetilde{C}$, modified first multiplicative ZCI (FMZCI), modified second multiplicative ZCI (SMZCI), and modified third multiplicative ZCI (TMZCI) can be defined as

(1) $M\widehat{\mathfrak{Z}\mathfrak{C}}_1^*(\widetilde{C}) = \prod_{zp\in\mathcal{K}(\widetilde{C})} [\widehat{\mathbf{d}}_{\widetilde{C}}(z)\widetilde{\chi_{\widetilde{C}}}(p) + \widehat{\mathbf{d}}_{\widetilde{C}}(p)\widetilde{\chi_{\widetilde{C}}}(z)]$

(2) $M\widehat{\mathfrak{Z}\mathfrak{C}}_2^*(\widetilde{C}) = \prod_{zp\in\mathcal{K}(\widetilde{C})} [\widehat{\mathbf{d}}_{\widetilde{C}}(z)\widetilde{\chi_{\widetilde{C}}}(z) + \widehat{\mathbf{d}}_{\widetilde{C}}(p)\widetilde{\chi_{\widetilde{C}}}(p)]$

(3) $M\widehat{\mathfrak{Z}\mathfrak{C}}_3^*(\widetilde{C}) = \prod_{zp\in\mathcal{K}(\widetilde{C})} [\widehat{\mathbf{d}}_{\widetilde{C}}(z)\widetilde{\chi_{\widetilde{C}}}(z) \times \widehat{\mathbf{d}}_{\widetilde{C}}(p)\widetilde{\chi_{\widetilde{C}}}(p)]$

Definition 6 For a graph $\widetilde{C}$, the FsMZCI can be rewritten as

$$M\hat{\mathfrak{Z}}\mathfrak{C}_1(\widetilde{C}) = \prod_{0\le\theta\le\hat{t}-2} [\theta^2]^{|\mathfrak{N}_\theta(\widetilde{C})|}, \quad (1)$$

where $|\mathfrak{N}_\theta(\widetilde{C})|$ is the total amount of vertices in $\widetilde{C}$ with CN θ.

The SMZCI is rewritten as

$$M\hat{\mathfrak{Z}}\mathfrak{C}_2(\widetilde{C}) = \prod_{0\le\theta\le\kappa\le\hat{t}-2} [\theta\times\kappa]^{|\mathfrak{N}_{(\theta,\kappa)}(\widetilde{C})|}, \quad (2)$$

where $|\mathfrak{N}_{(\theta,\kappa)}(\widetilde{C})|$ is the total amount of edges with CNs θ and κ.

The TMZCI can be rewritten as

$$M\hat{\mathfrak{Z}}\mathfrak{C}_3(\widetilde{C}) = \prod_{0\le\gamma\le\theta\le\hat{t}-2} [\gamma\times\theta]^{|\mathfrak{N}'_{((\gamma,\theta))}(\widetilde{C})|}, \quad (3)$$

where $|\mathfrak{N}_{((\gamma,\theta))}(\widetilde{C})|$ is the total amount of vertices with degree γ and CN θ.

Similarly, the FrMZCI can be rewritten as

$$M\hat{\mathfrak{Z}}\mathfrak{C}^*_4(\widetilde{C}) = \prod_{0\le\theta\le\kappa\le\hat{t}-2} [\theta+\kappa]^{|\mathfrak{N}_{(\theta,\kappa)}(\widetilde{C})|}, \quad (4)$$

where $|\mathfrak{N}_{(\theta,\kappa)}(\widetilde{C})|$ is the total amount of edges in $\widetilde{C}$ with CNs (θ,κ).

Furthermore, we can rewrite the modified FMZCI as

$$M\hat{\mathfrak{Z}}\mathfrak{C}^*_1(\widetilde{C}) = \prod_{\substack{0\le\theta\le\kappa\le\hat{t}-2,\\ 0\le\mu\le\nu\le\hat{t}-2}} [\mu\kappa+\nu\theta]^{|\mathfrak{N}_{(\mu,\nu)(\theta,\kappa)}(\widetilde{C})|}. \quad (5)$$

The modified SMZCI can be rewritten as

$$M\hat{\mathfrak{Z}}\mathfrak{C}^*_2(\widetilde{C}) = \prod \prod_{\substack{0\le\theta\le\kappa\le\hat{t}-2\\ 0\le\mu\le\nu\le\hat{t}-2}} [\mu\theta+\nu\kappa]^{|\mathfrak{N}_{(\mu,\nu)(\theta,\kappa)}(\widetilde{C})|}. \quad (6)$$

The modified TMZCI can be rewritten as

$$M\hat{\mathfrak{Z}}\mathfrak{C}^*_3(\widetilde{C}) = \prod_{\substack{0\le\theta\le\kappa\le\hat{t}-2\\ 0\le\mu\le\nu\le\hat{t}-2}} [\mu\theta\times\nu\kappa]^{|\mathfrak{N}_{(\mu,\nu)(\theta,\kappa)}(\widetilde{C})|}, \quad (7)$$

where $|\mathfrak{N}_{(\mu,\nu)(\theta,\kappa)}(\widetilde{C})|$ is the total amount of edges in $\widetilde{C}$ with degrees (μ,ν) and CNs (θ,κ).

3. MZCIs of Poly (Propyl) Ether Imine Dendrimer

In this section, we compute MZCIs, namely, FsMZCI, SMZCI, TMZCI, FrMZCI, modified FMZCI, modified SMZCI, and modified TZCI of PPEI dendrimer. Let $\widetilde{C}(t)$ be a molecular graph of PPEI dendrimer, where $t\ge 1$ is the growth of the dendrimer. The formation of PPEI dendrimer up to five generations is displayed in Figure 1. From Figure 1, we can see that the structure of PPEI dendrimer have eight edges in central core and four branches outside.

Theorem 1. *Let $\widetilde{C}(t)$ be a molecular graph of PPEI dendrimer (see Figure 2). Then, FsMZCI, SMZCI, TMZCI, and FrMZCI are given in the following:*

(1) $M\hat{\mathfrak{Z}}\mathfrak{C}_1(\widetilde{C}) = [4]^{12r-15}\times[9]^{8(r-1)}$

(2) $M\hat{\mathfrak{Z}}\mathfrak{C}_2(\widetilde{C}) = [2]^{2r}\times[4]^{8r-12}\times[54]^{6(r-1)}$

(3) $M\hat{\mathfrak{Z}}\mathfrak{C}_3(\widetilde{C}) = [2]^{2r}\times[2]^{12r-15}\times[6]^{6(r-1)}\times[9]^{2(r-1)}$

(4) $M\hat{\mathfrak{Z}}\mathfrak{C}_4(\widetilde{C}) = [6]^{2r}\times[4]^{8r-12}\times[30]^{6(r-1)}$

where $r=2^t$.

Proof. (1) First, we calculate the number of vertices and edges of $\widetilde{C}$ as the graph $\widetilde{C}$ has total four branches and one central core which have eight edges. Then, the total amount of edges in $\widetilde{C}$ will be equal to number of edges in central core plus the quadruple of number of edges in each branch. Therefore,

$$\begin{aligned}
\text{Number of edges in each branch} &= \left(8+(2\times 8)+\left(2^2\times 8\right)+\cdots+\left(2^{t-2}\times 8\right)+\left(2^{t-1}\times 4\right)\right),\\
&= 6\left(2^t\right)-8,\\
\text{Total number of edges in all branches} &= 4\left(6\times 2^t-8\right),\\
&= 24\left(2^t\right)-32,\\
\text{Total edges in }\widetilde{C} &= 8+\left(24\times 2^t-32\right),\\
&= 24\left(2^t-1\right).
\end{aligned} \quad (8)$$

Total amount of vertices in $\widetilde{C}$ is $24(2^t)-23$ as $\widetilde{C}$ is a tree.

In order to find the general expressions to compute the ZCIs in $\widetilde{C}$, we make the partition of the number of vertices

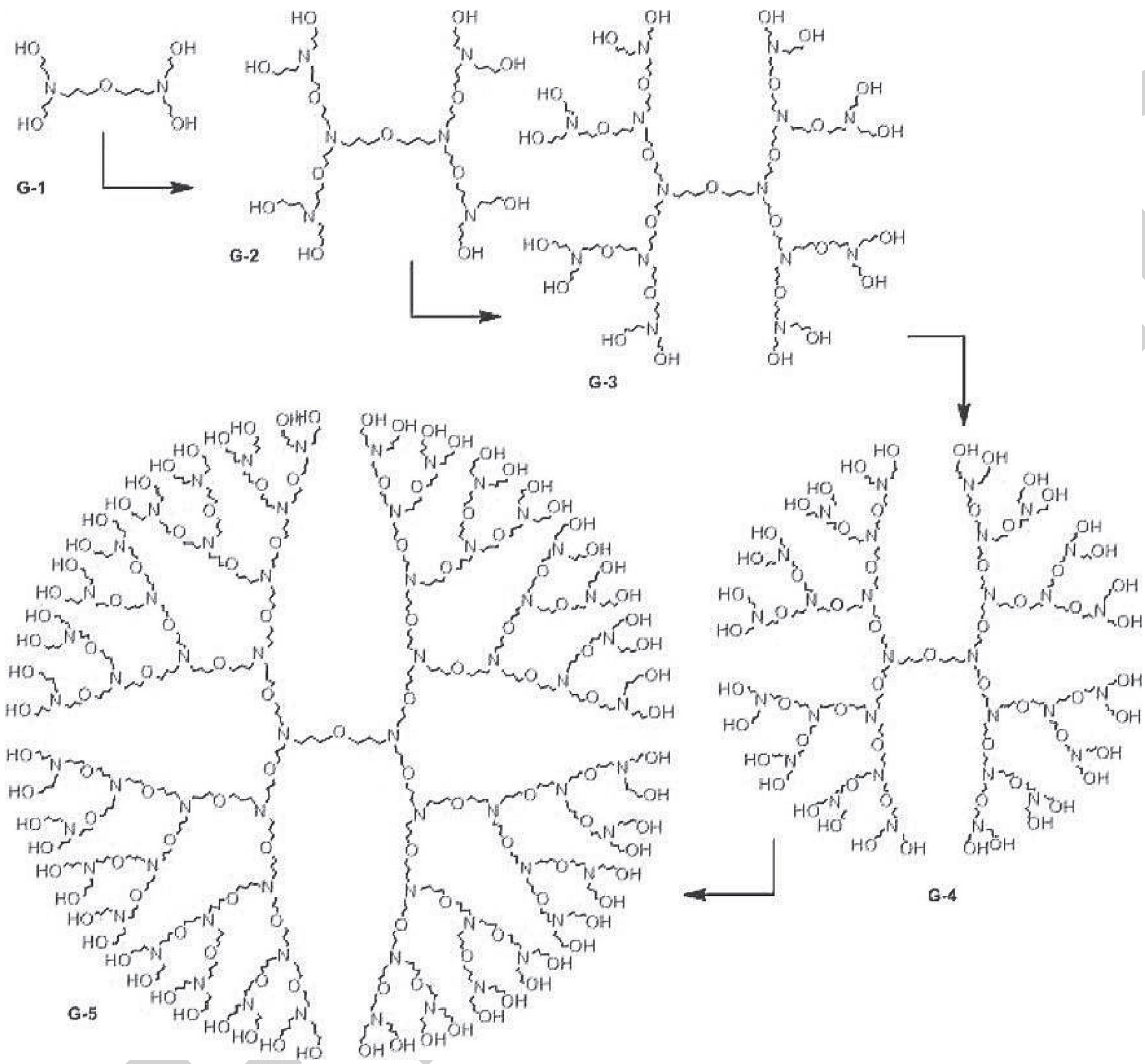

Figure 1: Chemical structural formula of PPEI dendrimer.

on connection basis. It is clear that there are three partitions of vertices:

$$
\begin{aligned}
\mathfrak{N}_1 &= \left\{z \in \mathscr{J} : \widetilde{\chi_C}(z) = 1\right\},\\
\mathfrak{N}_2 &= \left\{z \in \mathscr{J} : \widetilde{\chi_C}(z) = 2\right\},\\
\mathfrak{N}_3 &= \left\{z \in \mathscr{J} : \widetilde{\chi_C}(z) = 3\right\},\\
\left|\mathfrak{N}_1\right| &= 4\left(2 \times 2^{t-1}\right)\\
&= 4\left(2^t\right),\\
\left|\mathfrak{N}_2\right| &= 5 + 4\left[5 + (2 \times 5) + \left(2^2 \times 5\right) + \left(2^3 \times 5\right) + \cdots \left(2^{t-1} \times 1\right)\right]\\
&= 12\left(2^t\right) - 15,\\
\left|\mathfrak{N}_3\right| &= (24 \times 2t - 23) - \left(12 \times 2^t - 15\right) - 4\left(2^t\right),\\
&= 8\left(2^t - 1\right).
\end{aligned}
\tag{9}
$$

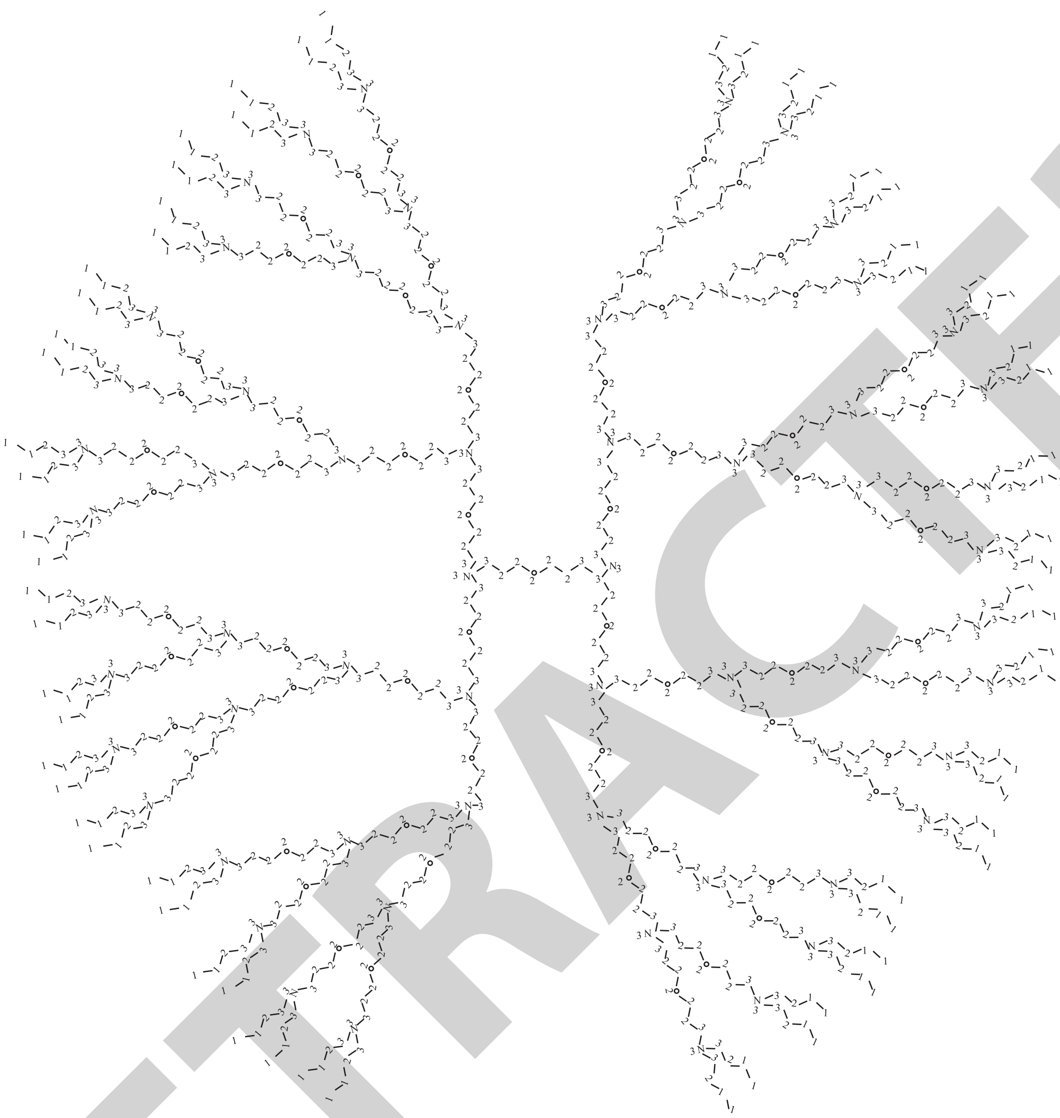

Figure 2: Structural formula of PPEI dendrimer for $t = 5$ along with CNs.

From equation (1), we have

$$
\begin{aligned}
M\widehat{\mathfrak{Z}}\mathfrak{C}_1(\widetilde{C}) &= \prod_{0\le\theta\le3}\left[\theta^2\right]^{\left|\mathfrak{N}_\theta(\widetilde{C})\right|}\\
&= \left[1^2\right]^{\left|\mathfrak{N}_1(\widetilde{C})\right|}\times\left[2^2\right]^{\left|\mathfrak{N}_2(\widetilde{C})\right|}\times\left[3^2\right]^{\left|\mathfrak{N}_3(\widetilde{C})\right|}\\
&= [1]^{4\left(2^t\right)}\times\left[2^2\right]^{\left(12\left(2^t\right)-15\right)}\times\left[3^2\right]^{8\left(2^t-1\right)}\\
&= [4]^{12r-15}\times[9]^{8(r-1)}.
\end{aligned}
\tag{10}
$$

(2) Now, we make the partition of edge set of $\widetilde{C}$. There are five partitions of edge set as given below:

$$
\begin{aligned}
\mathfrak{N}_{(1,1)} &= \left\{e = zp \in \mathscr{K}\colon \chi_{\widetilde{C}}(z) = 1, \chi_{\widetilde{C}}(p) = 1\right\},\\
\mathfrak{N}_{(1,2)} &= \left\{e = zp \in \mathscr{K}\colon \chi_{\widetilde{C}}(z) = 1, \chi_{\widetilde{C}}(p) = 2\right\},\\
\mathfrak{N}_{(2,2)} &= \left\{e = zp \in \mathscr{K}\colon \chi_{\widetilde{C}}(z) = 2, \chi_{\widetilde{C}}(p) = 2\right\},\\
\mathfrak{N}_{(2,3)} &= \left\{e = zp \in \mathscr{K}\colon \chi_{\widetilde{C}}(z) = 2, \chi_{\widetilde{C}}(p) = 3\right\},\\
\mathfrak{N}_{(3,3)} &= \left\{e = zp \in \mathscr{K}\colon \chi_{\widetilde{C}}(z) = 3, \chi_{\widetilde{C}}(p) = 3\right\}.
\end{aligned}
\tag{11}
$$

Now,

$$
\begin{aligned}
|\mathfrak{N}_{(1,1)}| &= 4\left(2^{t-1}\right)\\
|\mathfrak{N}_{(1,2)}| &= 4\left(2^{t-1}\right)\\
|\mathfrak{N}_{(2,2)}| &= 4 + 4\left(4 + (2\times 4) + \left(2^2\times 4\right) + \left(2^3\times 4\right) + \cdots + \left(2^{t-2}\times 4\right)\right)\\
&= 4 + 4/\text{time}\, 4\left(1 + 2 + 2^2 + 2^3 + \cdots + 2^{t-2}\right)\\
&= 8\left(2^t\right) - 12,\\
|\mathfrak{N}_{(2,3)}| &= 2 + 4\left(2 + (2\times 2) + \left(2^2\times 2\right) + \left(2^3\times 2\right) + \cdots + \left(2^{t-2}\times 2\right) + \left(2^{t-1}\times 1\right)\right)\\
&= 2 + 4\left(2\left(1 + 2 + 2^2 + 2^3 + \cdots + 2^{t-2}\right)\right) + 4\left(2^{t-1}\right)\\
&= 6\left(2^t - 1\right),\\
|\mathfrak{N}_{(3,3)}| &= 6\left(2^t - 1\right).
\end{aligned}
\tag{12}
$$

Here, we have used the following sum series formula to find the sum of the series:

$$
S = \frac{a\left(1 - b^t\right)}{1 - b}, \tag{13}
$$

where a is the first term and b is the common difference between two consecutive terms of the series.

From equation (2), we have

$$
\begin{aligned}
M\hat{\mathfrak{Z}}\mathfrak{C}_2(\tilde{C}) &= \prod_{0\le\theta\le\kappa\le 3} |\mathfrak{N}_{(\theta,\kappa)}(\tilde{C})|[\theta\times\kappa]\\
&= [1\times 1]^{|\mathfrak{N}_{(1,1)}(\tilde{C})|} \times [1\times 2]^{|\mathfrak{N}_{(1,2)}(\tilde{C})|} \times [2\times 2]^{|\mathfrak{N}_{(2,2)}(\tilde{C})|} \times [2\times 3]^{|\mathfrak{N}_{(2,3)}(\tilde{C})|} \times [3\times 3]^{|\mathfrak{N}_{(3,3)}(\tilde{C})|}\\
&= [1]^{\left(2\times 2^t\right)} \times [2]^{2\left(2^t\right)} \times [4]^{8\left(2^t\right)-12} \times [6]^{6\left(2^t-1\right)} \times [9]^{6\left(2^t-1\right)}\\
&= [2]^{2r} \times [4]^{8r-12} \times [54]^{6(r-1)}.
\end{aligned}
\tag{14}
$$

(3) In order to find $M\hat{\mathfrak{Z}}\mathfrak{C}_3(\tilde{C})$, we have to calculate the number of vertices which have degree γ and CN θ, i.e., $|\mathfrak{N}'_{((\gamma,\theta))}(\tilde{C})|$:

$$
\begin{aligned}
|\mathfrak{N}'_{((1,1))}(\tilde{C})| &= 4\left(1\times 2^{t-1}\right) = 2\left(2^t\right),\\
|\mathfrak{N}'_{((2,1))}(\tilde{C})| &= 4\left(1\times 2^{t-1}\right) = 2\left(2^t\right),\\
|\mathfrak{N}'_{((2,2))}(\tilde{C})| &= 5 + 4\left(5 + (5\times 2) + \left(5\times 2^2\right) + \cdots + \left(5\times 2^{t-2}\right) \times \left(1\times 2^{t-1}\right)\right)\\
&= 5 + 20\left(1 + 2 + 2^2 + 2^3 + \cdots + 2^{t-2}\right) + 4\left(2^{t-1}\right) = 12\left(2^t\right) - 15,\\
|\mathfrak{N}'_{((2,3))}(\tilde{C})| &= 2 + 4\left(2 + (2\times 2) + \left(2\times 2^2\right) + \cdots + \left(2\times 2^{t-2}\right) \times \left(1\times 2^{t-1}\right)\right)\\
&= 2 + 8\left(1 + 2 + 2^2 + 2^3 + \cdots + 2^{t-2}\right) + 4\left(2^{t-1}\right) = 6\left(2^t - 1\right),\\
|\mathfrak{N}'_{((3,3))}(\tilde{C})| &= 2 + 4\left(1 + (1\times 2) + \left(1\times 2^2\right) + \cdots + \left(1\times 2^{t-2}\right)\right)\\
&= 2 + 4\left(1 + 2 + 2^2 + 2^3 + \cdots + 2^{t-2}\right) = 2\left(2^t - 1\right).
\end{aligned}
\tag{15}
$$

Frome equation (3), we have

$$
\begin{aligned}
M\widehat{\mathfrak{Z}}\mathfrak{C}_3(\widetilde{C}) &= \prod_{0\leq\gamma\leq\theta\leq\widehat{t}-2} [\gamma\times\theta]^{\left|\mathfrak{N}'_{(\gamma,\theta)}(\widetilde{C})\right|}\\
&= [1]^{\left|\mathfrak{N}'_{((1,1))}(\widetilde{C})\right|}\times[2\times 1]^{\left|\mathfrak{N}'_{((2,1))}(\widetilde{C})\right|}\times[2\times 2]^{\left|\mathfrak{N}'_{((2,2))}(\widetilde{C})\right|}\times[2\times 3]^{\left|\mathfrak{N}'_{((2,3))}(\widetilde{C})\right|}\times[3\times 3]^{\left|\mathfrak{N}'_{((3,3))}(\widetilde{C})\right|}\\
&= [1]^{2(2^t)}\times[2]^{2(2^t)}\times[4]^{12(2^t)-15}\times[6]^{6(2^t-1)}\times[9]^{2(2^t-1)}\\
&= [2]^{2r}\times[4]^{12r-15}\times[6]^{6(r-1)}\times[9]^{2(r-1)}.
\end{aligned}
\tag{16}
$$

(4) By putting all the above calculated values of $|\mathfrak{N}_{(\theta,\kappa)}(\widetilde{C})|$ in equation (4), we have

$$
\begin{aligned}
M\widehat{\mathfrak{Z}}\mathfrak{C}_3(\widetilde{C}) &= \prod_{0\leq\theta\leq\kappa\leq 3}\left|\mathfrak{N}_{(\theta,\kappa)}(\widetilde{C})\right|[\theta+\kappa]\\
&= [1+1]^{\left|\mathfrak{N}_{(1,1)}(\widetilde{C})\right|}\times[1+2]^{\left|\mathfrak{N}_{(1,2)}(\widetilde{C})\right|}\times[2+2]^{\left|\mathfrak{N}_{(2,2)}(\widetilde{C})\right|}\times[2+3]^{\left|\mathfrak{N}_{(2,3)}(\widetilde{C})\right|}\times[3+3]^{\left|\mathfrak{N}_{(3,3)}(\widetilde{C})\right|}\\
&= [2]^{2(2^t)}\times[3]^{2(2^t)}\times[4]^{8(2^t)-12}\times[5]^{6(2^t-1)}\times[6]^{6(2^t-1)}\\
&= [6]^{2r}\times[4]^{8r-12}\times[30]^{6(r-1)}.
\end{aligned}
\tag{17}
$$

This proves the theorem. □

Theorem 2. *Let $\widetilde{C}$ be a molecular graph of PPEI dendrimer, see Figure 2. Then, modified FMZCI, modified SMZCI, and modified TMZCI are given in the following*:

(1) $M\widehat{\mathfrak{Z}}\mathfrak{C}_1^*(\widetilde{C}) = [18]^{2r}\times[8]^{8r-12}\times[150]^{6(r-1)}$

(2) $M\widehat{\mathfrak{Z}}\mathfrak{C}_2^*(\widetilde{C}) = [18]^{2r}\times[8]^{8r-12}\times[150]^{6(r-1)}$

(3) $M\widehat{\mathfrak{Z}}\mathfrak{C}_3^*(\widetilde{C}) = [18]^{2r}\times[8]^{8r-12}\times[1296]^{6(r-1)}$

Proof. (1) First, we do the partitioning of edges on the basis of their degrees of incident vertices. Clearly, $|\mathfrak{N}_{(1,2)}(\widetilde{C})| = 2(2^t)$, $|\mathfrak{N}_{(2,2)}(\widetilde{C})| = 16(2^t)-18$, and $|\mathfrak{N}_{(2,3)}(\widetilde{C})| = 6(2^t-1)$. In order to compute the modified FMZCI, modified SMZCI, and modified TMZCI, we split the partitioned number of edges on degree basis with respect to the number of edges on connection basis.

From row 1 of Table 1, it can be seen that the number of edges $zp\in\widetilde{C}$, where vertex z has degree 1 and CN 1 is adjacent to the vertex p having degree 2 and CN 1 is $2(2^t)$, i.e., $|\mathfrak{N}_{(1,2)(1,1)}(\widetilde{C})| = 2(2^t)$. Similarly for the others edges, we have

$$
\begin{aligned}
&\left|\mathfrak{N}_{(2,2)(1,2)}(\widetilde{C})\right| = 2\left(2^t\right), \left|\mathfrak{N}_{(2,2)(2,2)}(\widetilde{C})\right| = 8\left(2^t\right)-12,\\
&\left|\mathfrak{N}_{(2,2)(2,3)}(\widetilde{C})\right| = 6\left(2^t-1\right), \left|\mathfrak{N}_{(2,3)(3,3)}(\widetilde{C})\right| = 6\left(2^t-1\right).
\end{aligned}
\tag{18}
$$

By putting the values of $|\mathfrak{N}_{(\mu,\nu)(\theta,\kappa)}(\widetilde{C})|$ in equation (5), we have

$$
\begin{aligned}
M\widehat{\mathfrak{Z}}\mathfrak{C}_1^*(\widetilde{C}) &= \prod_{\substack{0\leq\theta\leq\kappa\leq\widehat{t}-2,\\ 0\leq\mu\leq\nu\leq\widehat{t}-2}}[\mu\kappa+\nu\theta]^{\left|\mathfrak{N}_{(\mu,\nu)(\theta,\kappa)}(\widetilde{C})\right|}\\
&= [(1)(1)+(2)(1)]^{\left|\mathfrak{N}_{(1,2)(1,1)}(\widetilde{C})\right|}\times[(2)(2)+(2)(1)]^{\left|\mathfrak{N}_{(2,2)(1,2)}(\widetilde{C})\right|}+[(2)(2)+(2)(2)]^{\left|\mathfrak{N}_{(2,2)(2,2)}(\widetilde{C})\right|}\\
&\quad\times[(2)(3)+(2)(2)]^{\left|\mathfrak{N}_{(2,2)(2,3)}(\widetilde{C})\right|}\times[(2)(3)+(3)(3)]^{\left|\mathfrak{N}_{(2,3)(3,3)}(\widetilde{C})\right|}\\
&= [3]^{2(2^t)}\times[6]^{2(2^t)}\times[8]^{8(2^t)-12}\times[10]^{6(2^t)-1}\times[15]^{6(2^t-1)}\\
&= [18]^{2r}\times[8]^{8r-12}\times[150]^{6(r-1)}.
\end{aligned}
\tag{19}
$$

Table 1: Total amount of edges on degree and connection basis.

Degree wise	Connection wise
$\lvert\mathfrak{N}_{(1,2)}(\tilde{C})\rvert = 2(2^t)$	$\lvert\mathfrak{N}_{(1,1)}(\tilde{C})\rvert = 2(2^t)$
$\lvert\mathfrak{N}_{(2,2)}(\tilde{C})\rvert = 2(2^t)$	$\lvert\mathfrak{N}_{(1,2)}(\tilde{C})\rvert = 2(2^t)$
$\lvert\mathfrak{N}_{(2,2)}(\tilde{C})\rvert = 8(2^t) - 12$	$\lvert\mathfrak{N}_{(2,2)}(\tilde{C})\rvert = 8(2^t) - 12$
$\lvert\mathfrak{N}_{(2,2)}(\tilde{C})\rvert = 6(2^t - 1)$	$\lvert\mathfrak{N}_{(2,3)}(\tilde{C})\rvert = 6(2^t - 1)$
$\lvert\mathfrak{N}_{(2,3)}(\tilde{C})\rvert = 6(2^t - 1)$	$\lvert\mathfrak{N}_{(3,3)}(\tilde{C})\rvert = 6(2^t - 1)$

(2) By putting the values of $|\mathfrak{N}_{(\mu,\nu)(\theta,\kappa)}(\tilde{C})|$ in equation (6), we have

$$
\begin{aligned}
M\hat{\mathfrak{Z}}\mathfrak{C}_2^*(\tilde{C}) &= \prod_{\substack{0\le\theta\le\kappa\le\hat{t}-2,\\ 0\le\mu\le\nu\le\hat{t}-2}} [\mu\theta+\nu\kappa]^{|\mathfrak{N}_{(\mu,\nu)(\theta,\kappa)}(\tilde{C})|} \\
&= [(1)(1)+(2)(1)]^{|\mathfrak{N}_{(1,2)(1,1)}(\tilde{C})|} \times [(2)(1)+(2)(2)]^{|\mathfrak{N}_{(2,2)(1,2)}(\tilde{C})|} + [(2)(2)+(2)(2)]^{|\mathfrak{N}_{(2,2)(2,2)}(\tilde{C})|} \\
&\quad \times [(2)(2)+(2)(3)]^{|\mathfrak{N}_{(2,2)(2,3)}(\tilde{C})|} \times [(2)(3)+(3)(3)]^{|\mathfrak{N}_{(2,3)(3,3)}(\tilde{C})|} \\
&= [3]^{2(2^t)} \times [6]^{2(2^t)} \times [8]^{(8(2^t)-12)} \times [10]^{6(2^t-1)} \times [15]^{6(2^t-1)} \\
&= [18]^{2r} \times [8]^{8r-12} \times [150]^{6(r-1)}.
\end{aligned} \tag{20}
$$

(3) By putting the values of $|\mathfrak{N}_{(\mu,\nu)(\theta,\kappa)}(\tilde{C})|$ in equation (7), we have

$$
\begin{aligned}
M\hat{\mathfrak{Z}}\mathfrak{C}_3^*(\tilde{C})\& &= \sum_{\substack{0\le\theta\le\kappa\le\hat{t}-2\\ 0\le\mu\le\nu\le\hat{t}-2}} [\mu\theta+\nu\kappa]^{|\mathfrak{N}_{(\mu,\nu)(\theta,\kappa)}(\tilde{C})|} \\
&= [(1)(1)\times(2)(1)]^{|\mathfrak{N}_{(1,2)(1,1)}(\tilde{C})|} \times [(2)(1)\times(2)(2)]^{|\mathfrak{N}_{(2,2)(1,2)}(\tilde{C})|} \times [(2)(2)\times(2)(2)]^{|\mathfrak{N}_{(2,2)(2,2)}(\tilde{C})|} \\
&\quad \times [(2)(2)\times(2)(3)]^{|\mathfrak{N}_{(2,2)(2,3)}(\tilde{C})|} \times [(2)(3)\times(3)(3)]^{|\mathfrak{N}_{(2,3)(3,3)}(\tilde{C})|} \\
&= [2]^{2(2^t)} \times [8]^{2(2^t)} \times [16]^{(8(2^t)-12)} \times [24]^{6(2^t-1)} \times [54]^{6(2^t-1)} \\
&= [18]^{2r} \times [8]^{8r-12} \times [1296]^{6(r-1)}.
\end{aligned} \tag{21}
$$

This proves the theorem. □

4. MZCIs of Polypropylenimine Octamin Dendrimer

In this section, we compute MZCIs, namely, FsMZCI, SMZCI, TMZCI, FrMZCI, modified FMZCI, modified SMZCI, and modified TMZCI of PPIO dendrimer. PPIO dendrimer grows in three dimensions, and it has five bonds in the core. The structural formula of PPIO dendrimer up to five generations is depicted in Figure 3.

Theorem 3. *Let $\tilde{C}$ be a molecular graph of PPIO dendrimer, as given in Figure 4. Then, FsMZCI, SMZCI, TMZCI, and FrMZCI are given in the following:*

(1) $\hat{\mathfrak{Z}}\mathfrak{C}_1(\tilde{C}) = 4[2]^{2r} \times [54]^{6(r-1)}$

(2) $\hat{\mathfrak{Z}}\mathfrak{C}_2(\tilde{C}) = [16]^{2r-1} \times [9]^{8(r-1)}$

(3) $\hat{\mathfrak{Z}}\mathfrak{C}_3(\tilde{C}) = [2]^{2r} \times [4]^{4r-2} \times [6]^{6(r-1)} \times [9]^{2(r-1)}$

(4) $\hat{\mathfrak{Z}}\mathfrak{C}_4(\tilde{C}) = 4[6]^{2r} \times [30]^{6(r-1)}$

where $r = 2^t$.

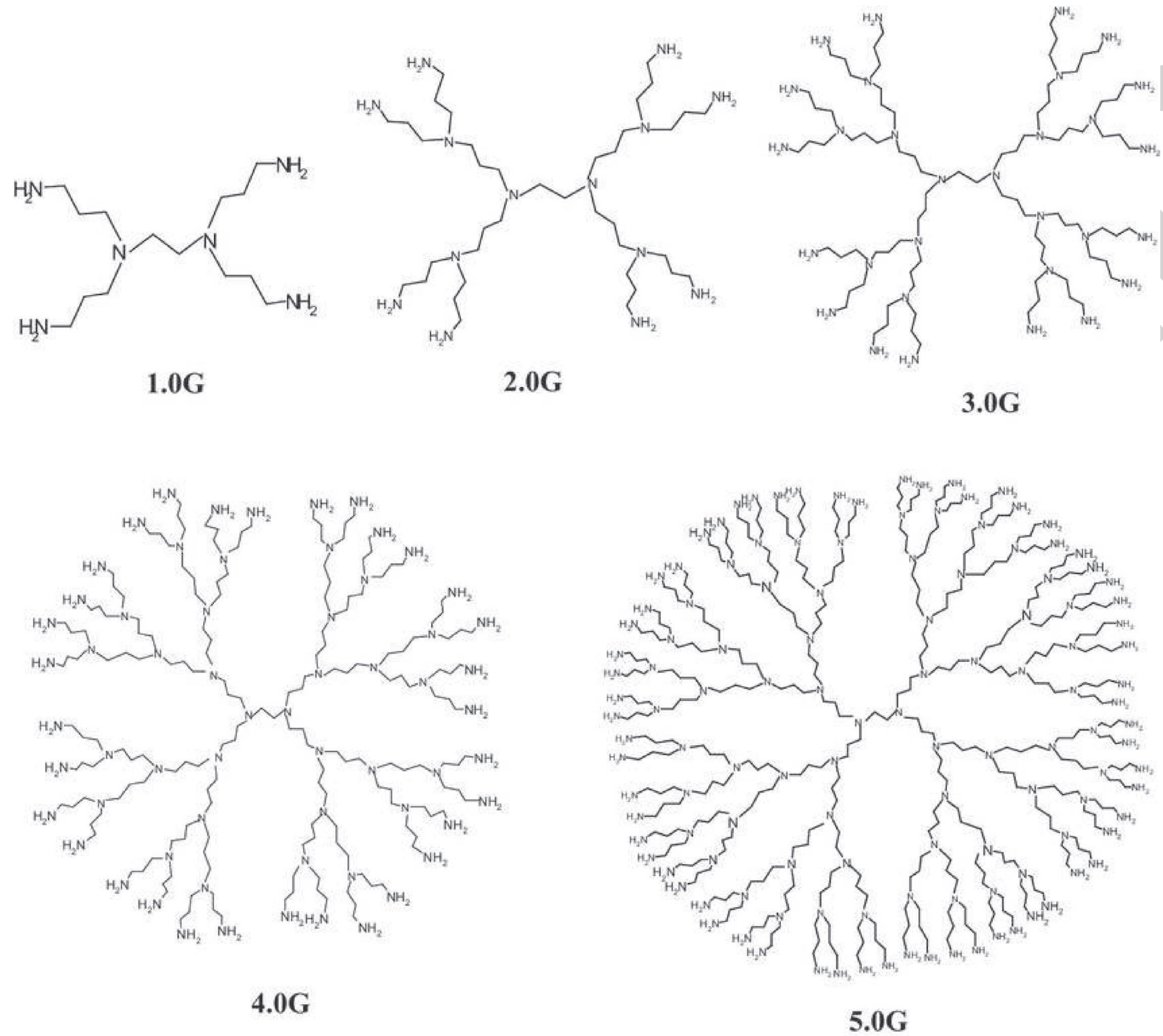

Figure 3: Chemical structural formula of PPIO dendrimer.

Proof

(1) First, we calculate the number of vertices and edges of $\widetilde{C}$, as the graph $\widetilde{C}$ has total four branches and one central core which has five edges. Then, the total amount of edges in $\widetilde{C}$ will be equal to number of edges in central core plus the quadruple of number of edges in each branch. Therefore,

$$\begin{aligned}
\text{Number of edges in each branch} &= \left(4 + (2\times 4) + \left(2^2\times 4\right) + \cdots + \left(2^{t-1}\times 4\right)\right)\\
&= 4\left(2^t - 1\right),\\
\text{Number of edges in all branches} &= 4\times 4\left(s2^t - 1\right)\\
&= 16\left(2^t - 1\right),\\
\text{Number of edges in } \widetilde{C} &= 5 + \left(16\left(2^s - 1\right)\right)\\
&= 16\left(2^t\right) - 11.
\end{aligned} \tag{22}$$

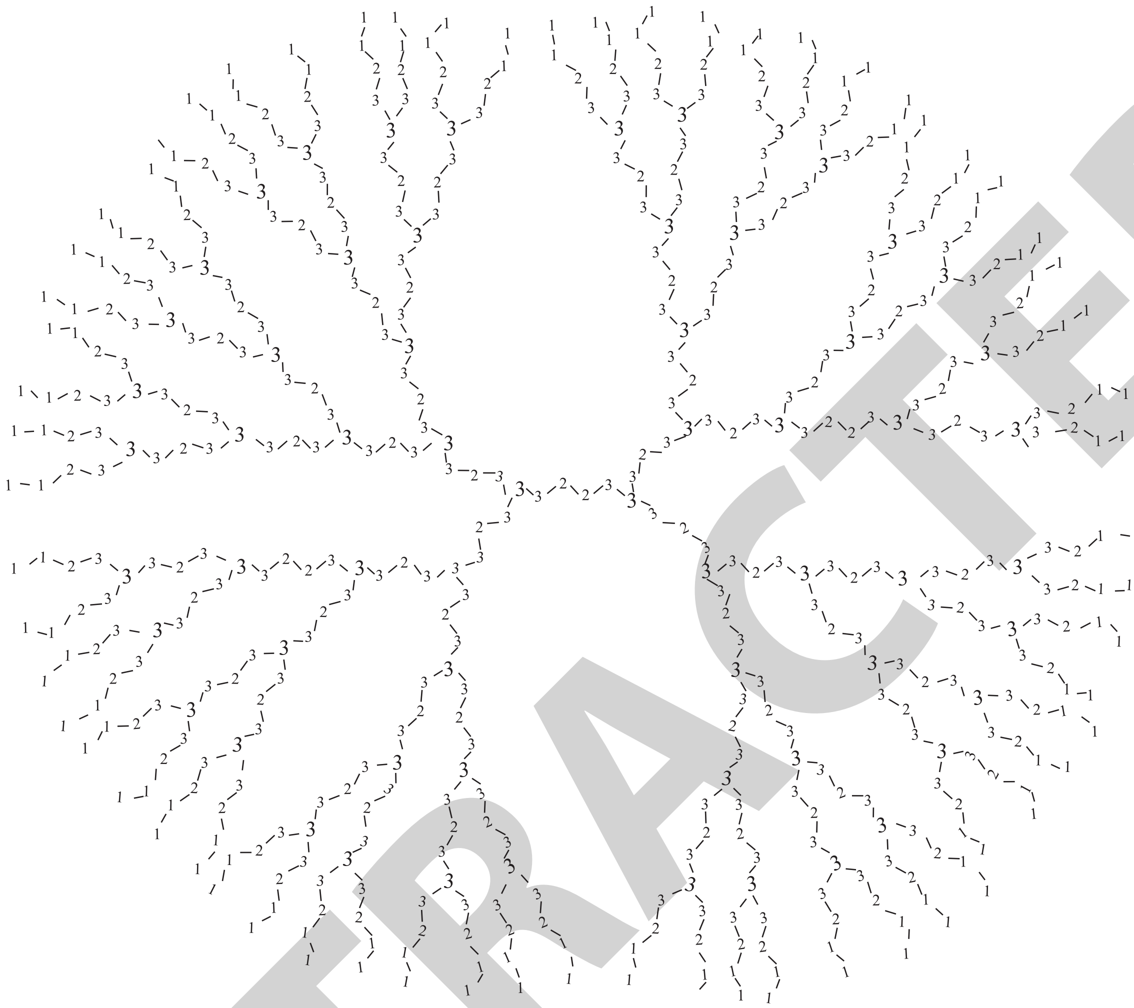

Figure 4: Structural formula of PPIO dendrimer for $t = 5$ along with CNs.

Total amount of vertices in $\widetilde{C}$ is $16\left(2^t\right) - 10$ as $\widetilde{C}$ is a tree.

In order to find the general expressions to compute the MZCIs in $\widetilde{C}$, we make the partition of the number of vertices on connection basis. It is clear that there are three partitions of vertices:

$$\begin{aligned}
\mathfrak{N}_1 &= \left\{z \in \mathcal{J}\colon \chi_{\widetilde{C}}(z) = 1\right\},\\
\mathfrak{N}_2 &= \left\{z \in \mathcal{J}\colon \chi_{\widetilde{C}}(z) = 2\right\},\\
\mathfrak{N}_3 &= \left\{z \in \mathcal{J}\colon \chi_{\widetilde{C}}(z) = 3\right\},\\
\left|\mathfrak{N}_1\right| &= 4\left(2 \times 2^{t-1}\right)\\
&= 4\left(2^t\right),\\
\left|\mathfrak{N}_2\right| &= 4\left[1 + (2 \times 1) + \left(2^2 \times\right) + \left(2^3 \times 1\right) + \cdots \left(2^{t-1} \times 1\right)\right] + 2\\
&= 4\left(2^t\right) - 2,\\
\left|\mathfrak{N}_3\right| &= (16\,(2t) - 10) - \left(4\left(2^t\right)\right) - \left(4\left(2^t\right) + 2\right)\\
&= 8\left(2^t - 1\right),
\end{aligned} \tag{23}$$

From equation (1), we have

$$\begin{aligned} M\hat{\mathfrak{Z}}\mathfrak{C}_1(\widetilde{C}) &= \prod_{0\le\theta\le 3}\left[\theta^2\right]^{\left|\mathfrak{N}_\theta(\widetilde{C})\right|},\\ &= \left[1^2\right]^{\left|\mathfrak{N}_1(\widetilde{C})\right|}\times\left[2^2\right]^{\left|\mathfrak{N}_2(\widetilde{C})\right|}\times\left[3^2\right]^{\left|\mathfrak{N}_3(\widetilde{C})\right|}\\ &= [1]^{4\left(2^t\right)}\times\left[2^2\right]^{\left(4\left(2^t\right)-2\right)}\times\left[3^2\right]^{\left(8\left(2^t-1\right)\right)}\\ &= [16]^{2r-1}\times[9]^{8(r-1)}. \end{aligned}\tag{24}$$

(2) Now, we calculate $|\mathfrak{N}_{(\theta,\kappa)}(\widetilde{C})|$:

$$\begin{aligned} \left|\mathfrak{N}_{(1,1)}\right| &= 4\left(2^{t-1}\right) = 2\left(2^t\right),\\ \left|\mathfrak{N}_{(1,2)}\right| &= 4\left(2^{t-1}\right) = 2\left(2^t\right),\\ \left|\mathfrak{N}_{(2,2)}\right| &= 1,\\ \left|\mathfrak{N}_{(2,3)}\right| &= 2+4\Big[2+(2\times 2)+\left(2^2\times 2\right)\\ &\quad +\left(2^3\times 2\right)+\cdots+\left(2^{t-1}\times 2\right)\Big]+2\\ &= 2+8\left[1+2+2^2+2^3+\cdots+2^{t-1}\right]\\ &= 6\left(2^t-1\right),\\ \left|\mathfrak{N}_{(3,3)}\right| &= 6\left(2^t-1\right). \end{aligned}\tag{25}$$

From equation (2), we have

$$\begin{aligned} M\hat{\mathfrak{Z}}\mathfrak{C}_2(\widetilde{C}) &= \prod_{0\le\theta\le\kappa\le 3}\left|\mathfrak{N}_{(\theta,\kappa)}(\widetilde{C})\right|[\theta\times\kappa]\\ &= [1\times 1]^{\left|\mathfrak{N}_{(1,1)}(\widetilde{C})\right|}\times[1\times 2]^{\left|\mathfrak{N}_{(1,2)}(\widetilde{C})\right|}\times[2\times 2]^{\left|\mathfrak{N}_{(2,2)}(\widetilde{C})\right|}\times[2\times 3]^{\left|\mathfrak{N}_{(2,3)}(\widetilde{C})\right|}\times[3\times 3]^{\left|\mathfrak{N}_{(3,3)}(\widetilde{C})\right|}\\ &= [1]^{2\left(2^t\right)}\times[2]^{2\left(2^t\right)}\times[4]\times[6]^{6\left(2^t-1\right)}\times[9]^{6\left(2^t-1\right)}\\ &= 4[2]^{2r}\times[54]^{6(r-1)}. \end{aligned}\tag{26}$$

(3) In order to find $M\hat{\mathfrak{Z}}\mathfrak{C}_3(\widetilde{C})$, we have to calculate and find the number of vertices which have degree γ and CN θ, i.e., $|\mathfrak{N}'_{(\gamma,\theta)}(\widetilde{C})|$:

$$\begin{aligned} \left|\mathfrak{N}'_{((1,1))}(\widetilde{C})\right| &= \left(41\times 2^{t-1}\right) = 2\left(2^t\right),\\ \left|\mathfrak{N}'_{((2,1))}(\widetilde{C})\right| &= 4\left(1\times 2^{t-1}\right) = 2\left(2^t\right),\\ \left|\mathfrak{N}'_{((2,2))}(\widetilde{C})\right| &= 2+4\left(1+(1\times 2)+\left(1\times 2^2\right)+\cdots+\left(1\times 2^{t-2}\right)\times\left(1\times 2^{t-1}\right)\right)\\ &= 2+4\left(1+2+2^2+2^3+\cdots+2^{t-1}\right) = 4\left(2^t\right)-2,\\ \left|\mathfrak{N}'_{((2,3))}(\widetilde{C})\right| &= 2+4\left(2+(2\times 2)+\left(2\times 2^2\right)+\cdots+\left(2\times 2^{t-2}\right)\times\left(1\times 2^{t-1}\right)\right)\\ &= 2+8\left(1+2+2^2+2^3+\cdots+2^{t-2}\right)+4\left(2^{t-1}\right) = 6\left(2^t-1\right),\\ \left|\mathfrak{N}'_{((3,3))}(\widetilde{C})\right| &= 2+4\left(1+(1\times 2)+\left(1\times 2^2\right)+\cdots+\left(1\times 2^{t-2}\right)\right)\\ &= 2+4\left(1+2+2^2+2^3+\cdots+2^{t-2}\right) = 2\left(2^t-1\right),\\ M\hat{\mathfrak{Z}}\mathfrak{C}_3(\widetilde{C}) &= \prod_{0\le\gamma\le\theta\le\hat{t}-2}[\gamma\times\theta]^{\left|\mathfrak{N}'_{(\gamma,\theta)}(\widetilde{C})\right|}\\ &= [1]^{\left|\mathfrak{N}'_{((1,1))}(\widetilde{C})\right|}\times[2\times 1]^{\left|\mathfrak{N}'_{((2,1))}(\widetilde{C})\right|}\times[2\times 2]^{\left|\mathfrak{N}'_{((2,2))}(\widetilde{C})\right|}\times[2\times 3]^{\left|\mathfrak{N}'_{((2,3))}(\widetilde{C})\right|}\times[3\times 3]^{\left|\mathfrak{N}'_{((3,3))}(\widetilde{C})\right|}\\ &= [1]^{2\left(2^t\right)}\times[2]^{2\left(2^t\right)}\times[4]^{4\left(2^t\right)-2}\times[6]^{6\left(2^t-1\right)}\times[9]^{2\left(2^t-1\right)}\\ &= [2]^{2r}\times[4]^{4r-2}\times[6]^{6(r-1)}\times[9]^{2(r-1)}. \end{aligned}\tag{27}$$

Table 2: Total amount of edges on degree and connection basis.

Degree wise	Connection wise
$\lvert\mathfrak{N}_{(1,2)}(\widetilde{C})\rvert = 2(2^t)$	$\lvert\mathfrak{N}_{(1,1)}(\widetilde{C})\rvert = 2(2^t)$
$\lvert\mathfrak{N}_{(2,2)}(\widetilde{C})\rvert = 2(2^t)$	$\lvert\mathfrak{N}_{(1,2)}(\widetilde{C})\rvert = 2(2^t)$
$\lvert\mathfrak{N}_{(2,2)}(\widetilde{C})\rvert = 1$	$\lvert\mathfrak{N}_{(2,2)}(\widetilde{C})\rvert = 1$
$\lvert\mathfrak{N}_{(2,2)}(\widetilde{C})\rvert = 6(2^t-1)$	$\lvert\mathfrak{N}_{(2,3)}(\widetilde{C})\rvert = 6(2^t-1)$
$\lvert\mathfrak{N}_{(2,3)}(\widetilde{C})\rvert = 6(2^t-1)$	$\lvert\mathfrak{N}_{(3,3)}(\widetilde{C})\rvert = 6(2^t-1)$

(4) By putting all the calculated values of $|\mathfrak{N}_{(\theta,\kappa)}(\widetilde{C})|$ in equation (4), we have

$$\begin{aligned}
M\widehat{\mathfrak{Z}}\mathfrak{C}_4(\widetilde{C}) &= \prod_{0\le\theta\le\kappa\le 3} \left|\mathfrak{N}_{(\theta,\kappa)}(\widetilde{C})\right|[\theta+\kappa] \\
&= [1+1]^{\left|\mathfrak{N}_{(1,1)}(\widetilde{C})\right|} \times [1+2]^{\left|\mathfrak{N}_{(1,2)}(\widetilde{C})\right|} \times [2+2]^{\left|\mathfrak{N}_{(2,2)}(\widetilde{C})\right|} \times [2+3]^{\left|\mathfrak{N}_{(2,3)}(\widetilde{C})\right|} \times [3+3]^{\left|\mathfrak{N}_{(3,3)}(\widetilde{C})\right|} \\
&= [2]^{2(2^t)} \times [3]^{2(2^t)} \times [4] \times [5]^{6(2^t-1)} \times [6]^{6(2^t-1)} \\
&= 4[6]^{2r} \times [30]^{6(r-1)}.
\end{aligned} \tag{28}$$

This proves the theorem. □

Theorem 4. *Let $\widetilde{C}$ be a molecular graph of PPIO dendrimer, as given in Figure 4. Then, modified FMZCI, modified SMZCI, and modified TMZCI are given in the following:*

(1) $M\widehat{\mathfrak{Z}}\mathfrak{C}_1^*(\widetilde{C}) = 8[18]^{2r} \times [150]^{6(r-1)}$

(2) $M\widehat{\mathfrak{Z}}\mathfrak{C}_2^*(\widetilde{C}) = 8[18]^{2r} \times [150]^{6(r-1)}$

(3) $M\widehat{\mathfrak{Z}}\mathfrak{C}_3^*(\widetilde{C}) = 16[18]^{2r} \times [1296]^{6(r-1)}$

where $r = 2^t$.

Proof

(1) First, we do the partitioning of edges on the basis of their degrees of incident vertices. Clearly, $|\mathfrak{N}_{(1,2)}(\widetilde{C})| = 2(2^t)$, $|\mathfrak{N}_{(2,2)}(\widetilde{C})| = 8(2^s) - 5$, and $|\mathfrak{N}_{(2,3)}(\widetilde{C})| = 6(2^t-1)$. In order to compute the modified FMZCI, modified SMZCI, and modified TMZCI, we split the partitioned number of edges on degree basis with respect to the number of edges on connection basis.

From row 1 of Table 2, it can be seen that the number of edges $zp \in \widetilde{C}$, where vertex z has degree 1 and CN 1 is adjacent to the vertex p having degree 2 and CN 1 is $2(2^t)$, i.e., $|\mathfrak{N}_{(1,2)(1,1)}(\widetilde{C})| = 2(2^t)$. Similarly, for the others, we have

$$\begin{aligned}
&\left|\mathfrak{N}_{(2,2)(1,2)}(\widetilde{C})\right| = 2\left(2^t\right), \left|\mathfrak{N}_{(2,2)(2,2)}(\widetilde{C})\right| = 1, \\
&\left|\mathfrak{N}_{(2,2)(2,3)}(\widetilde{C})\right| = 6\left(2^t-1\right), \left|\mathfrak{N}_{(2,3)(3,3)}(\widetilde{C})\right| = 6\left(2^t-1\right).
\end{aligned} \tag{29}$$

By putting the values of value of $|\mathfrak{N}_{(\mu,\nu)(\theta,\kappa)}(\widetilde{C})|$ in equation (5), we have

$$\begin{aligned}
M\widehat{\mathfrak{Z}}\mathfrak{C}_1^*(\widetilde{C}) &= \prod_{\substack{0\le\theta\le\kappa\le\widehat{t}-2 \\ 0\le\mu\le\nu\le\widehat{t}-2}} [\mu\kappa+\nu\theta]^{\left|\mathfrak{N}_{(\mu,\nu)(\theta,\kappa)}(\widetilde{C})\right|} \\
&= [(1)(1)+(2)(1)]^{\left|\mathfrak{N}_{(1,2)(1,1)}(\widetilde{C})\right|} \times [(2)(2)+(2)(1)]^{\left|\mathfrak{N}_{(2,2)(1,2)}(\widetilde{C})\right|} + [(2)(2)+(2)(2)]^{\left|\mathfrak{N}_{(2,2)(2,2)}(\widetilde{C})\right|} \\
&\quad \times [(2)(3)+(2)(2)]^{\left|\mathfrak{N}_{(2,2)(2,3)}(\widetilde{C})\right|} \times [(2)(3)+(3)(3)]^{\left|\mathfrak{N}_{(2,3)(3,3)}(\widetilde{C})\right|} \\
&= [3]^{2(2^t)} \times [6]^{2(2^t)} \times [8] \times [10]^{6(2^t)-1} \times [15]^{6(2^t-1)} \\
&= 8[18]^{2r} \times [150]^{6(r-1)}.
\end{aligned} \tag{30}$$

Table 3: Comparison between the value of PPEI and PPIO dendrimer.

MZCIs	PPEI dendrimer	PPIO dendrimer
$\mathfrak{Z}_1\mathfrak{C}(\widetilde{C})$	$[4]^{12r-15} \times [9]^{8(r-1)}$	$4[2]^{2r} \times [54]^{6(r-1)}$
$\mathfrak{Z}_2\mathfrak{C}(\widetilde{C})$	$[2]^{2r} \times [4]^{8r-12} \times [54]^{6(r-1)}$	$[16]^{2r-1} \times [9]^{8(r-1)}$
$\mathfrak{Z}_3\mathfrak{C}(\widetilde{C})$	$[2]^{2r} \times [2]^{12r-15} \times [6]^{6(r-1)} \times [9]^{2(r-1)}$	$[2]^{2r} \times [4]^{4r-2} \times [6]^{6(r-1)} \times [9]^{2(r-1)}$
$\mathfrak{Z}_4\mathfrak{C}(\widetilde{C})$	$[6]^{2r} \times [4]^{8r-12} \times [30]^{6(r-1)}$	$4[6]^{2r} \times [30]^{6(r-1)}$
$\widehat{\mathfrak{Z}\mathfrak{C}}_1^*(\widetilde{C})$	$[18]^{2r} \times [8]^{8r-12} \times [150]^{6(r-1)}$	$8[18]^{2r} \times [150]^{6(r-1)}$
$\widehat{\mathfrak{Z}\mathfrak{C}}_2^*(\widetilde{C})$	$[18]^{2r} \times [8]^{8r-12} \times [150]^{6(r-1)}$	$8[18]^{2r} \times [150]^{6(r-1)}$
$\widehat{\mathfrak{Z}\mathfrak{C}}_3^*(\widetilde{C})$	$[18]^{2r} \times [8]^{8r-12} \times [1296]^{6(r-1)}$	$16[18]^{2r} \times [1296]^{6(r-1)}$

(2) By putting the values of $|\mathfrak{N}_{(\mu,\nu)(\theta,\kappa)}(\widetilde{C})|$ in equation (6), we have

$$\begin{aligned} M\widehat{\mathfrak{Z}\mathfrak{C}}_2^*(\widetilde{C}) &= \prod_{\substack{0\le\theta\le\kappa\le\widehat{t}-2,\\ 0\le\mu\le\nu\le\widehat{t}-2}} [\mu\theta+\nu\kappa]^{|\mathfrak{N}_{(\mu,\nu)(\theta,\kappa)}(\widetilde{C})|} \\ &= [(1)(1)+(2)(1)]^{|\mathfrak{N}_{(1,2)(1,1)}(\widetilde{C})|} \times [(2)(1)+(2)(2)]^{|\mathfrak{N}_{(2,2)(1,2)}(\widetilde{C})|} + [(2)(2)+(2)(2)]^{|\mathfrak{N}_{(2,2)(2,2)}(\widetilde{C})|} \\ &\quad \times [(2)(2)+(2)(3)]^{|\mathfrak{N}_{(2,2)(2,3)}(\widetilde{C})|} \times [(2)(3)+(3)(3)]^{|\mathfrak{N}_{(2,3)(3,3)}(\widetilde{C})|} \\ &= [3]^{2(2^t)} \times [6]^{2(2^t)} \times [8] \times [10]^{6(2^t-1)} \times [15]^{6(2^t-1)} \\ &= 8[18]^{2r} \times [150]^{6(r-1)}. \end{aligned} \tag{31}$$

(3) By putting the values of $|\mathfrak{N}_{(\mu,\nu)(\theta,\kappa)}(\widetilde{C})|$ in equation (7), we have

$$\begin{aligned} M\widehat{\mathfrak{Z}\mathfrak{C}}_3^*(\widetilde{C}) &= \prod_{\substack{0\le\theta\le\kappa\le\widehat{t}-2,\\ 0\le\mu\le\nu\le\widehat{t}-2}} [\mu\theta+\nu\kappa]^{|\mathfrak{N}_{(\mu,\nu)(\theta,\kappa)}(\widetilde{C})|} \\ &= [(1)(1)\times(2)(1)]^{|\mathfrak{N}_{(1,2)(1,1)}(\widetilde{C})|} \times [(2)(1)\times(2)(2)]^{|\mathfrak{N}_{(2,2)(1,2)}(\widetilde{C})|} \times [(2)(2)\times(2)(2)]^{|\mathfrak{N}_{(2,2)(2,2)}(\widetilde{C})|} \\ &\quad \times [(2)(2)\times(2)(3)]^{|\mathfrak{N}_{(2,2)(2,3)}(\widetilde{C})|} \times [(2)(3)\times(3)(3)]^{|\mathfrak{N}_{(2,3)(3,3)}(\widetilde{C})|} \\ &= [2]^{2(2^t)} \times [8]^{2(2^t)} \times [16] \times [24]^{6(2^t-1)} \times [54]^{6(2^t-1)} \\ &= 16[18]^{2r} \times [1296]^{6(r-1)}. \end{aligned} \tag{32}$$

This proves the theorem. □

5. Comparative Analysis

This section provides the comparison between the calculated results of both the dendrimers with each other. Table 3 shows the comparison between the proposed results of PPEI and PPIO dendrimers.

From Table 3, it can be easily seen that PPEI dendrimer and PPIO dendrimer gets the greatest value of modified TMZCI $\widehat{\mathfrak{Z}\mathfrak{C}}*_3(\widetilde{C})$.

6. Conclusions

The concluding remarks of this article are as follows:

Dendrimers are hyperbranched radially symmetric macromolecules with monodisperse, well-defined, and homogenous tree-like structure. Dendrimers have lots of applications in various domains. TIs are the molecular descriptors which characterize the topology and help to correlate the distinct psychochemical properties of various molecular compounds.

In this study, the general results to calculate MZCIs, namely, first MZCI, second MZCI, third MZCI and fourth MZCI have been developed for two distinct types of dendrimer nanostars, namely, PPEI dendrimer and PPIO dendrimer.

We also have calculated modified first MZCI, modified second MZCI, and modified third MZCI for the abovementioned dendrimers. The calculated expressions just depend upon the value of $t \geq 1$.

Furthermore, we have compared our calculated result for both types of dendrimers in order to check the superiority. It is clear that the modified third MZCI gets the greatest value for both types of dendrimers.

Future directions: in future, we are interested to compute the following [30]:

(1) Connection-based Zagreb indices for the other type of dendrimers

(2) Connection-based Zagreb indices for metal organic networks

Data Availability

The data used to support the findings of this study are included within the article and can be obtained from the corresponding author upon request.

Conflicts of Interest

The authors have no conflicts of interest regarding this article.

References

[1] P. Kesharwani, A. Gothwal, A. K. Iyer, K. Jain, M. K. Chourasia, and U. Gupta, "Dendrimer nanohybrid carrier systems: an expanding horizon for targeted drug and gene delivery," *Drug Discovery Today*, vol. 23, no. 2, pp. 300–314, 2018.

[2] B. Klajnert, L. Peng, and V. Cea, *Dendrimers in Biomedical Applications*, Royal Society of Chemistry, London, UK, 2013.

[3] J. Kurczewska, M. Cegłowski, B. Messyasz, and G. Schroeder, "Dendrimer-functionalized halloysite nanotubes for effective drug delivery," *Applied Clay Science*, vol. 153, pp. 134–143, 2018.

[4] R. Todeschini and V. Consonni, *Molecular Descriptors for Chemoinformatics: Volume I: Alphabetical Listing/volume II: Appendices*, John Wiley and Sons, Hoboken, NJ, USA, 2009.

[5] H. Wiener, "Structural determination of paraffin boiling points," *Journal of the American Chemical Society*, vol. 69, no. 1, pp. 17–20, 1947.

[6] J. P. Mazorodze, S. Mukwembi, and T. Vetrík, "On the Gutman index and minimum degree," *Discrete Applied Mathematics*, vol. 173, pp. 77–82, 2014.

[7] W. Gao, Z. Iqbal, M. Ishaq, A. Aslam, and R. Sarfraz, "Topological aspects of dendrimers via distance based descriptors," *IEEE access*, vol. 7, pp. 35619–35630, 2019.

[8] I. Gutman and N. Trinajstić, "Graph theory and molecular orbitals. Total φ-electron energy of alternant hydrocarbons," *Chemical Physics Letters*, vol. 17, no. 4, pp. 535–538, 1972.

[9] I. Gutman, B. Ruscic, N. Trinajstic, and C. F. Wilcox Jr, "Graph theory and molecular orbitals. XII. Acyclic polyenes," *The Journal of Chemical Physics*, vol. 62, no. 9, pp. 3399–3405, 1975.

[10] K. C. Das and I. Gutman, "Some properties of the second Zagreb index," *MATCH Communications in Mathematical and in Computer Chemistry*, vol. 52, no. 1, pp. 3–1, 2004.

[11] B. Furtula and I. Gutman, "A forgotten topological index," *Journal of Mathematical Chemistry*, vol. 53, no. 4, pp. 1184–1190, 2015.

[12] A. Ali, I. Gutman, E. Milovanovic, and I. Milovanovic, "Sum of powers of the degrees of graphs extremal results and bounds," *MATCH Communications in Mathematical and in Computer Chemistry*, vol. 80, no. 1, pp. 5–84, 2018.

[13] B. Borovicanin, K. C. Das, B. Furtula, and I. Gutman, "Bounds for Zagreb indices," *MATCH Communications in Mathematical and in Computer Chemistry*, vol. 78, no. 1, pp. 17–100, 2017.

[14] M. Javaid, U. Ali, and J. B. Liu, "Computing analysis for first Zagreb connection index and coindex of resultant graphs," *Mathematical Problems in Engineering*, vol. 2021, Article ID 6019517, 19 pages, 2021.

[15] S. Nikolic, G. Kovacevic, A. Milicevic, and N. Trinajstic, "The Zagreb indices 30 years after," *Croatica Chemica Acta*, vol. 76, no. 2, pp. 113–124, 2003.

[16] J. Hao, "Theorems about Zagreb indices and modified Zagreb indices," *MATCH Communications in Mathematical and in Computer Chemistry*, vol. 65, pp. 659–670, 2011.

[17] K. Dhanalakshmi, J. Amalorpava Jerline, and L. Benedict Michaelraj, "Modified and multiplicative Zagreb indices on graph operators," *Journal of Computer and Mathematical Sciences*, vol. 7, no. 4, pp. 225–232, 2016.

[18] A. Ali and N. Trinajstić, "A novel/old modification of the first Zagreb index," *Molecular informatics*, vol. 37, no. 6-7, Article ID e1800008, 2018.

[19] J. Cao, U. Ali, M. Javaid, and C. Huang, "Zagreb connection indices of molecular graphs based on operations," *Complexity*, vol. 2020, Article ID 7385682, 15 pages, 2020.

[20] Z. Du, A. Ali, and N. Trinajstić, "Alkanes with the first three maximal/minimal modified first Zagreb connection indices," *Molecular informatics*, vol. 38, no. 4, Article ID 1800116, 2019.

[21] J. H. Tang, U. Ali, M. Javaid, and K. Shabbir, "Zagreb connection indices of subdivision and semi-total point operations on graphs," *Journal of Chemistry*, vol. 2019, Article ID 9846913, 14 pages, 2019.

[22] U. Ali, M. Javaid, and A. Kashif, "Modified Zagreb connection indices of the T-sum graphs," *Main Group Metal Chemistry*, vol. 43, no. 1, pp. 43–55, 2020.

[23] R. S. Haoer, M. A. Mohammed, T. Selvarasan, N. Chidambaram, and N. Devadoss, "Multiplicative leap Zagreb indices of T-thorny graphs," *Eurasian Chemical Communications*, vol. 2, no. 8, pp. 841–846, 2020.

[24] M. Javaid, U. Ali, and K. Siddiqui, "Novel connection based Zagreb indices of several wheel-related graphs," *Computational Journal of Combinatorial Mathematics*, vol. 1, pp. 1–28, 2021.

[25] S. A. U. H. Bokhary, M. Imran, and S. Manzoor, "On molecular topological properties of dendrimers," *Canadian Journal of Chemistry*, vol. 94, no. 2, pp. 120–125, 2016.

[26] Y. Bashir, A. Aslam, M. Kamran et al., "On forgotten topological indices of some dendrimers structure," *Molecules*, vol. 22, no. 6, p. 867, 2017.

[27] N. Dorosti, A. Iranmanesh, and M. V. Diudea, "Computing the Cluj index of the first type dendrimer nanostar,"

Optoelectronics and Advanced Materials-Rapid Communications, vol. 4, pp. 381–384, 2010.

[28] W. Gharibi, A. Ahmad, and M. K. Siddiqui, "On Zagreb indices, Zagreb polynomials of nanocone and nanotubes," *Journal of Computational and Theoretical Nanoscience*, vol. 13, no. 8, pp. 5086–5092, 2016.

[29] M. K. Siddiqui, M. Imran, and A. Ahmad, "On Zagreb indices, Zagreb polynomials of some nanostar dendrimers," *Applied Mathematics and Computation*, vol. 280, pp. 132–139, 2016.

[30] K. C. Das, A. Yurttas, M. Togan, A. S. Cevik, and I. N. Cangul, "The multiplicative Zagreb indices of graph operations," *Journal of Inequalities and Applications*, vol. 2013, no. 1, pp. 1–14, Article ID 90, 2013.