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ARTICLE

Topological Aspects of Dendrimers via Connection-Based Descriptors

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ABSTRACT

Topological indices (TIs) have been practiced for distinct wide-ranging physicochemical applications, especially used to characterize and model the chemical structures of various molecular compounds such as dendrimers, nanotubes and neural networks with respect to their certain properties such as solubility, chemical stability and low cytotoxicity. Dendrimers are prolonged artificially synthesized or amalgamated natural macromolecules with a sequential layer of branches enclosing a central core. A present-day trend in mathematical and computational chemistry is the characterization of molecular structure by applying topological approaches, including numerical graph invariants. Among topological descriptors, Zagreb connection indices (ZCIs) have much importance. This manuscript involves the establishment of general results to calculate ZCIs, namely first ZCI (FZCI), second ZCI (SZCI), third ZCI (TZCI), modified FZCI, modified SZCI and modified TZCI of two special types of dendrimers nanostars, namely, poly propylene imine octamin (PPIO) dendrimer and poly (propyl) ether imine (PPEtIm) dendrimer. Furthermore, we provide the numerical and graphical comparative analysis of our calculated results for both types of dendrimers with each other.

KEYWORDS

Zagreb indices; zagreb connection indices; topological index; dendrimer nanostars

1 Introduction

Nanobiotechnology is a swiftly growing field of technological and analytical opportunity that applies the mechanism of nanofabrication to fabricate devices for exploring biosystems. One of the main elements of this field is a dendrimer. Dendrimers are prolonged artificially synthesized or amalgamated natural macromolecules with a sequential layer of branches enclosing a central core. Dendrimers are considered to be a primary element of nanobiotechnology. The cores, end groups and branches are the main three parts of dendrimers. Nowadays, dendrimers are getting much more consideration from the researchers due to their exceptional attributes and a large span of utilization in various areas of bioscience, involving immunology, drug delivery and the development of vaccines and antivirals, for more details see [1–3].

At present, in computational and mathematical chemistry, researchers and scientists are taking heed to characterize the molecular structures by utilizing different topological perspectives incorporating graph invariants. These topological descriptors are broadly utilized in the study of quantitative structure-activity relationships (QSAR) and quantitative structure-property relationships (QSPR) [4]. Graph invariants are essential to achieve the mathematical characterization of molecular structures successfully. The field of network theory (NT) has played an indispensable role in distinct areas of life. During the last decade, NT has found a remarkable use in the field of nanobiotechnology. Topological indices (TIs), the numerical parameters which link a number with a molecular network, are widely used in chemical network theory and mathematical chemistry to characterize the topology of a molecular network. TIs can predict many psychochemical properties of molecular structures in theocratical chemistry. TIs enable researchers to find the chemical reactivity, physical attributes and biological actions of molecular compounds. A molecular network in terms of a graph is a portrayal of structural information of a chemical compound in which the atoms are displayed by vertices while the bonds are represented by edges between the vertices. The applications of TIs in various fields of science are boundless, as one can see in [5–7]. According to the reported literature, TIs have great importance in nanotechnology and theoretical chemistry. Some important categories of TIs are degree-based, distance-based and connection-based TIs. In 1972, Wiener [8] introduced the concept of a distance-based TI, which is known as the Wiener index. By theoretical and conceptual framework, the Wiener index was the most studied TI. Moreover, in 2019, Gao et al. [9] utilized distance-based indices to study the topological aspects of dendrimers.

The idea of the first ZI (FZI) was invented by Gutman et al. [10]. The second and third ZIs were discovered by Gutman et al. [11] and Furtula et al. [12]. All of these degree-based TIs have a variety of applications in the field of cheminformatics which is a combination of three major fields, namely, chemistry, mathematics and information technology [13–15]. These TIs have been utilized to distinct wide-ranging physicochemical applications, especially to characterize the different chemical structures such as dendrimers nanostars, for details see [16–18]. Among these defined TIs, the connection-based TIs have much importance because of their utilizations in characterizing the molecular chemical compounds and their ability to predict various physical and chemical properties in a comprehensive and logical way. A number of those vertices at a distance of two from a vertex v is called CN of a vertex v. According to researchers, connection-based TIs as compared to the other classical TIs provide a better absolute value of the correlation coefficient. Ali et al. [19] initiated Zagreb connection indices (ZCIs) and used octane isomers to examine their applicability. For a detailed review of some connection-based TIs, the readers are referred to [20–22]. Haoer et al. [23] computed multiplicative ZIs of some T-thorny graphs. Moreover, Javaid et al. [24] found the topological aspects of distinct wheel graphs. Further, Liu et al. [25] found the topological properties of neural networks. Recently, Sattar et al. [26–28] worked on computing the general expression of ZIs for two types of dendrimers. For the other terminologies not discussed in this paper, the readers are referred to [29–31]. The motivation for this article is as follows:

1. TIs, the numerical descriptors, are efficient enough to characterize the topology of molecular structures and assist in correlating their distinct psychochemical properties.
2. Dendrimers are symmetric, versatile and well defined chemical polymers forming a tree like structure. These nanoparticles are signalized by a numerous attributes which make them advantageous for wide ranging utilizations in various fields of science.

3. The connection-based ZIs have better applicability to predict the various psychochemical properties of distinct molecular structures in chemistry rather than the other classical ZIs present in the literature.

In this paper, first, we define the third Zagreb connection index. Further, we calculate ZCIs of two special types of dendrimer nanostars, namely, PPEtIm dendrimer and PPIO dendrimer. Moreover, we compare the results of both types of dendrimers.

This research article is structured as: in Section 1, we stated preliminaries which help the readers to understand the idea of this article. In Section 2, we computed ZCIs for PPEtIm dendrimer. In Section 3, we calculated ZCIs for the other type of dendrimer, namely, PPIO dendrimer in a comprehensive way. In Section 4, we compared the computed values of both types of dendrimers with each other. Section 5 holds the conclusions. The acronyms used in this paper are given in Table 1.

Table 1: List of acronyms

Acronyms	Description
Topological index	TI
Zagreb index	ZI
Zagreb connection index	ZCI
First Zagreb index	FZI
Second Zagreb index	SZI
First Zagreb connection index	FZCI
Second Zagreb connection index	SZCI
Third Zagreb connection index	TZCI
Poly propylene imine octamin dendrimer	PPIO
Poly (propyl) ether imine dendrimer	PPEtIm

2 Preliminaries

This section gives some primary definitions which are helpful for the good understanding of this manuscript.

Definition 2.1. In [10] let $\xi = (\mathbb{P}(\xi), \mathbb{Q}(\xi))$ be a network, where $\mathbb{P}(\xi)$ be the vertex set and $\mathbb{Q}(\xi)$ be the edge set. Then, the FZI can be defined as

$$\hat{\mathcal{Z}}_1(\xi) = \sum_{m \in \mathbb{P}(\xi)} \left(\breve{\mathrm{d}}_\xi(m)\right)^2.$$

which can also be rewritten in the given form

$$\hat{\mathcal{Z}}_1(\xi) = \sum_{mn \in \mathbb{Q}(\xi)} \left(\breve{\mathrm{d}}_\xi(m) + \breve{\mathrm{d}}_\xi(n)\right),$$

where $\breve{\mathrm{d}}_\xi(m)$ and $\breve{\mathrm{d}}_\xi(n)$ represent the degree of the vertex m and n, respectively.

Definition 2.2. In [11] for network ξ, the SZI can be defined as

$$\hat{\mathcal{Z}}_2(\xi) = \sum_{mn \in \mathbb{Q}(\xi)} \left(\breve{\mathrm{d}}_\xi(m) \times \breve{\mathrm{d}}_\xi(n) \right),$$

where $\breve{\mathrm{d}}_\xi(m)$ and $\breve{\mathrm{d}}_\xi(n)$ represent the degree of the vertex m and n, respectively.

Definition 2.3. In [12] for network ξ, the TZI can be given as

$$\hat{\mathcal{Z}}_3(\xi) = \sum_{mn \in \mathbb{Q}(\xi)} \left(\breve{\mathrm{d}}^2_\xi(m) + \breve{\mathrm{d}}^2_\xi(n) \right).$$

Third Zagreb index is also called forgotten index.

Definition 2.4. In [19] for a network ξ, the FZCIs and SZCI can be defined as

1. $\hat{\mathcal{Z}}\mathfrak{C}_1(\xi) = \sum_{m \in \mathbb{P}(\xi)} \left(\widetilde{\omega}_\xi(m) \right)^2$,
2. $\hat{\mathcal{Z}}\mathfrak{C}_2(\xi) = \sum_{mn \in \mathbb{Q}(\xi)} \left(\widetilde{\omega}_\xi(m) \times \widetilde{\omega}_\xi(n) \right)$,

where $\widetilde{\omega}_\xi(m)$ and $\widetilde{\omega}_\xi(n)$ indicate the CN of the vertex m and n, respectively.

Definition 2.5. In [19] for a network ξ, the modified FZCI can be defined as

$$\hat{\mathcal{Z}}\mathfrak{C}^*_1(\xi) = \sum_{mn \in \mathbb{Q}(\xi)} \left(\widetilde{\omega}_\xi(m) + \widetilde{\omega}_\xi(n) \right).$$

Definition 2.6. In [20] for a network ξ, the modified SZCI and modified TZCI can be given as

1. $\hat{\mathcal{Z}}\mathfrak{C}^*_2(\xi) = \sum_{mn \in \mathbb{Q}(\xi)} \left[\breve{\mathrm{d}}_\xi(m)\, \widetilde{\omega}_\xi(n) + \breve{\mathrm{d}}_\xi(n)\, \widetilde{\omega}_\xi(m) \right]$,
2. $\hat{\mathcal{Z}}\mathfrak{C}^*_3(\xi) = \sum_{mn \in \mathbb{Q}(\xi)} \left[\breve{\mathrm{d}}_\xi(m)\, \widetilde{\omega}_\xi(m) + \breve{\mathrm{d}}_\xi(n)\, \widetilde{\omega}_\xi(n) \right]$.

Now, we rewrite the above defined ZCIs. Let A be the set of all CNs and B be the set of all degrees of the vertices in ξ. Then the above defines ZCIs can be written as

Definition 2.7. For a network ξ, the FZCI can be rewritten as

$$\hat{\mathcal{Z}}_1\mathfrak{C}(\xi) = \sum_{\phi \in A} \left| \mathcal{A}_\phi(\xi) \right| \left[\phi^2 \right], \tag{1}$$

where $\left| \mathcal{A}_\phi(\xi) \right|$ is the cardinality of those vertices of ξ which have CN ϕ.

The SZCI rewritten as

$$\hat{\mathcal{Z}}_2\mathfrak{C}(\xi) = \sum_{\phi, \psi \in A} \left| \mathcal{A}_{(\phi,\psi)}(\xi) \right| [\phi \times \psi], \tag{2}$$

Similarly, the modified FZCI can be rewritten as

$$\hat{\mathcal{Z}}\mathfrak{C}^*_1(\xi) = \sum_{\phi, \psi \in A} \left| \mathcal{A}_{(\phi,\psi)}(\xi) \right| [\phi + \psi]. \tag{3}$$

where $\left| \mathcal{A}_{(\phi,\psi)}(\xi) \right|$ is the cardinality of those vertices of ξ which have CNs (ϕ, ψ).

Similarly, for the modified SZCI, we have

$$\hat{\mathcal{Z}}\mathfrak{C}_2^*(\xi) = \sum_{\substack{\phi,\psi \in A,\\ \mu,\nu \in B}} \left|\mathcal{A}_{(\mu,\nu)(\phi,\psi)}(\xi)\right| [\mu\psi + \nu\phi]. \tag{4}$$

The modified TZCI can be rewritten as

$$\hat{\mathcal{Z}}\mathfrak{C}_3^*(\xi) = \sum_{\substack{\phi,\psi \in A,\\ \mu,\nu \in B}} \left|\mathcal{A}_{(\mu,\nu)(\phi,\psi)}(\xi)\right| [\mu\phi + \nu\psi]. \tag{5}$$

where $\left|\mathcal{A}_{(\mu,\nu)(\phi,\psi)}(\xi)\right|$ is the cardinality of those edges in ξ which have degrees (μ,ν) and CNs (ϕ,ψ).

3 ZCIs of Poly (propyl) Ether Imine Dendrimer

In this section, we calculate the ZCIs, namely, FZCI, SZCI, TZCI, modified FZCI, modified SZCI and modified TZCI, of PPEtIm dendrimer. PPEtIm dendrimer is a special type of dendrimer constructed by including an ether component as the linker and an imine component as the branching unit. It grows three-dimensionally in which the core is the oxygen element and tertiary nitrogen atoms are at the branches which are separated by eight bonds for each growth of dendrimer. Let ξ be a molecular network of PPEtIm dendrimer of generation Gs, where $s \geq 1$ is the growth of the dendrimer. The construction of PPEtIm dendrimer up to five generations can be depicted in Fig. 1. From Fig. 1, it can be seen that the structure of PPEtIm dendrimer is comprised of one central core having eight edges and four branches. First, we state the third Zagreb connection index in the following.

Definition 3.1. Let $\xi = (\mathbb{P}(\xi), \mathbb{Q}(\xi))$ be a network, where $\mathbb{P}(\xi)$ be the vertex set and $\mathbb{Q}(\xi)$ be the edge set. Then, the third Zagreb connection index (TZCI) can be defined as

$$\hat{\mathcal{Z}}\mathfrak{C}_3(\xi) = \sum_{mn \in \mathbb{Q}(\xi)} \left(\omega_\xi^2(m) + \omega_\xi^2(n)\right),$$

where $\omega_\xi^2(m)$ and $\omega_\xi^2(n)$ indicate the square of the connection number (CN) of the vertex m and n, respectively.

This can also be rewritten as

$$\hat{\mathcal{Z}}\mathfrak{C}_3(\xi) = \sum_{\phi,\psi \in A} \left|\mathcal{A}_{(\phi,\psi)}(\xi)\right| \left[\phi^2 + \psi^2\right], \tag{6}$$

where $\left|\mathcal{A}_{(\phi,\psi)}(\xi)\right|$ is the cardinality of those edges of ξ which have CNs (ϕ,ψ).

Theorem 1. Let ξ be a molecular network of PPEtIm dendrimer. Then FZCI, SZCI and TZCI are given in the following:

1. $\hat{\mathcal{Z}}\mathfrak{C}_1(\xi) = 124 \times 2^s - 132$,
2. $\hat{\mathcal{Z}}\mathfrak{C}_2(\xi) = 128 \times 2^s - 138$,
3. $\hat{\mathcal{Z}}\mathfrak{C}_3(\xi) = 264 \times 2^s - 282$.

Proof.

1. Firstly, we find the cardinality of vertices and edges of ξ. The total number of edges in ξ must be equal to the four times the edges in a each branch plus the number of edges in central core. One can see that central core has eight edges. Therefore,

$$\begin{aligned}\text{Number of edges in each branch} &= (8 + (2 \times 8) + (2^2 \times 8) \\ &\quad + \cdots + (2^{s-2} \times 8) + (2^{s-1} \times 4)), \\ &= 6 \times 2^s - 8. \\ \text{Number of edges in all branches} &= 4 \times (6 \times 2^s - 8), \\ &= 24 \times 2^s - 32. \\ \text{Number of edges in } \zeta &= 8 + (24 \times 2^s - 32), \\ &= 24 \times 2^s - 24.\end{aligned}$$

As ζ is a tree, so the number of vertices must be equals to $24 \times 2^s - 23$.

Next, we find cardinality of those vertices which have CN 1, 2 and 3 in ξ. Now, we make the partition of the number of vertices on the basis of CNs. From Fig. 2, we can see that there are three partitions of vertices given below.

$$\mathcal{A}_1 = \left\{m \in \mathbb{P} \ : \ \widetilde{\omega}_\xi (m) = 1\right\},$$

$$\mathcal{A}_2 = \left\{m \in \mathbb{P} \ : \ \widetilde{\omega}_\xi (m) = 2\right\},$$

$$\mathcal{A}_3 = \left\{m \in \mathbb{P} \ : \ \widetilde{\omega}_\xi (m) = 3\right\}.$$

Thus, number of vertices with connection numbers 1, 2 and 3 are given as;

$$\begin{aligned}|\mathcal{A}_1| &= 4(2 \times 2^{s-1}), \\ &= 4 \times 2^s. \\ |\mathcal{A}_2| &= 4[5 + (2 \times 5) + (2^2 \times 5) + (2^3 \times 5) + \cdots + (2^{s-1} \times 1)] + 5, \\ &= 12 \times 2^s - 15. \\ |\mathcal{A}_3| &= (24 \times 2s - 23) - (12 \times 2^s - 15) - 4 \times 2^s, \\ &= 8 \times 2^s - 8.\end{aligned}$$

Now, after placing the values of $\left|\mathcal{A}_\phi(\xi)\right|$ in Eq. (1), we have

$$\begin{aligned}\hat{\mathcal{Z}}\mathfrak{C}_1 (\xi) &= \sum_{\phi \in A} \left|\mathcal{A}_\phi (\xi)\right| \left[\phi^2\right] \\ &= |\mathcal{A}_1(\xi)| [1^2] + |\mathcal{A}_2(\xi)| [2^2] + |\mathcal{A}_3(\xi)| [3^2], \\ &= (4 \times 2^s)[1] + (12 \times 2^s - 15)[2^2] + (8 \times 2^s - 8)[3^2], \\ &= 124 \times 2^s - 132.\end{aligned}$$

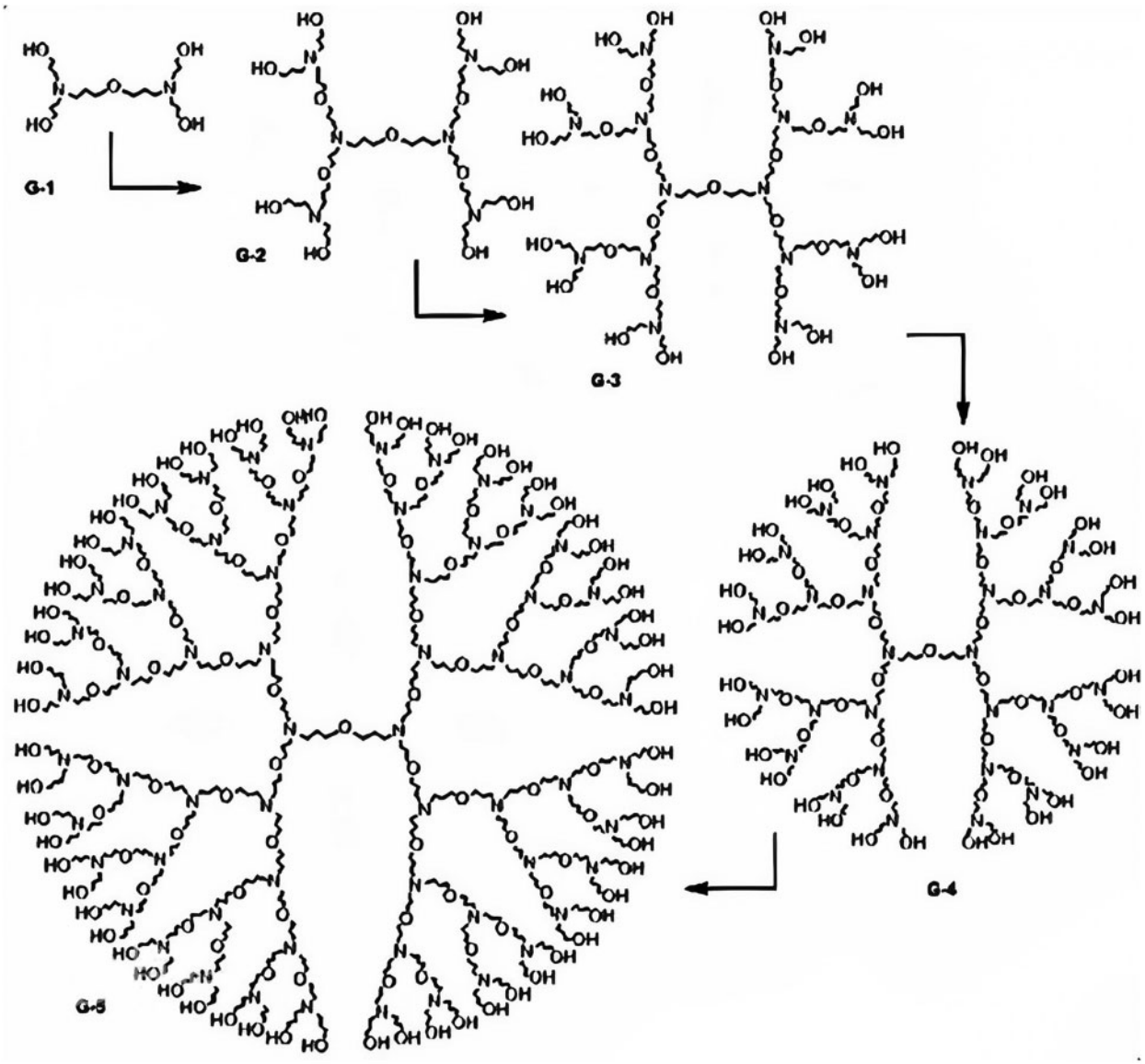

Figure 1: Chemical structural formula of PPEtIm dendrimer

2. Now, we classify the edge set of ξ. From Fig. 2, we can see that there are five classes of edge set as given below

$$\mathcal{A}_{(1,1)} = \left\{e = mn \in \mathbb{Q} \ : \ \widetilde{\omega}_{\xi}(m) = 1, \ \widetilde{\omega}_{\xi}(n) = 1\right\},$$

$$\mathcal{A}_{(1,2)} = \left\{e = mn \in \mathbb{Q} \ : \ \widetilde{\omega}_{\xi}(m) = 1, \ \widetilde{\omega}_{\xi}(n) = 2\right\},$$

$$\mathcal{A}_{(2,2)} = \left\{e = mn \in \mathbb{Q} \ : \ \widetilde{\omega}_{\xi}(m) = 2, \ \widetilde{\omega}_{\xi}(n) = 2\right\},$$

$$\mathcal{A}_{(2,3)} = \left\{e = mn \in \mathbb{Q} \ : \ \widetilde{\omega}_{\xi}(m) = 2, \ \widetilde{\omega}_{\xi}(n) = 3\right\},$$

$$\mathcal{A}_{(3,3)} = \left\{e = mn \in \mathbb{Q} \ : \ \widetilde{\omega}_{\xi}(m) = 3, \ \widetilde{\omega}_{\xi}(n) = 3\right\}.$$

Now,

$$\left|\mathcal{A}_{(1,1)}\right| = 4 \times 2^{s-1} = 2 \times 2^{s}.$$

$$\left|\mathcal{A}_{(1,2)}\right| = 4 \times 2^{s-1} = 2 \times 2^{s}.$$

$$\begin{aligned}\left|\mathcal{A}_{(2,2)}\right| &= 4(4 + (2 \times 4) + (2^2 \times 4) + (2^3 \times 4) + \cdots + 2^{s-2} \times 4) + 4,\\ &= 4(1 + 2 + 2^2 + 2^3 + \cdots + 2^{s-2}),\\ &= 8 \times 2^{s} - 12.\end{aligned}$$

$$\begin{aligned}\left|\mathcal{A}_{(2,3)}\right| &= 4(2 + (2 \times 2) + (2^2 \times 2) + (2^3 \times 2) + \cdots + 2^{s-2} \times 2) + (2^{s-1} \times 1)) + 2,\\ &= 4 \times 2(1 + 2 + 2^2 + 2^3 + \cdots + 2^{s-2}) + 2^{s-1} + 2,\\ &= 6 \times 2^{s} - 6.\end{aligned}$$

$$\left|\mathcal{A}_{(3,3)}\right| = 6 \times 2^{s} - 6.$$

Here, we have used the following formula to find the sum of the series [32].

$$S = \frac{a(1 - r^{s})}{1 - r},$$

where a is the first term and r is the common difference between two terms of the series. By placing the above calculated values in Eq. (2), we have

$$\begin{aligned}\hat{\mathcal{Z}}\mathfrak{C}_2(\xi) &= \sum_{\phi,\psi \in A} \left|\mathcal{A}_{(\phi,\psi)}(\xi)\right| [\phi \times \psi],\\ &= \left|\mathcal{A}_{(1,1)}(\xi)\right| [1 \times 1] + \left|\mathcal{A}_{(1,2)}(\xi)\right| [1 \times 2]\\ &+ \left|\mathcal{A}_{(2,2)}(\xi)\right| [2 \times 2] + \left|\mathcal{A}_{(2,3)}(\xi)\right| [2 \times 3] + \left|\mathcal{A}_{(3,3)}(\xi)\right| [3 \times 3],\\ &= (2 \times 2^{s})[1] + (2 \times 2^{s})[2] + (8 \times 2^{s} - 12)[4] + (6 \times 2^{s} - 6)[6] + (6 \times 2^{s} - 6)[9],\\ &= 128 \times 2^{s} - 138.\end{aligned}$$

3. By placing the values of $\left|\mathcal{A}_{(\phi,\psi)}(\xi)\right|$ in the above Eq. (1), we have

$$\begin{aligned}\hat{\mathcal{Z}}\mathfrak{C}_3(\xi) &= \sum_{\phi,\psi \in A} \left|\mathcal{A}_{(\phi,\psi)}(\xi)\right| \left[\phi^2 + \psi^2\right],\\ &= \left|\mathcal{A}_{(1,1)}(\xi)\right| [1^2 + 1^2] + \left|\mathcal{A}_{(1,2)}(\xi)\right| [1^2 + 2^2] + \left|\mathcal{A}_{(2,2)}(\xi)\right| [2^2 + 2^2] + \left|\mathcal{A}_{(2,3)}(\xi)\right| [2^2 + 3^2]\\ &+ \left|\mathcal{A}_{(3,3)}(\xi)\right| [3^2 + 3^2],\\ &= (2 \times 2^{s})[2] + (2 \times 2^{s})[5] + 8(\times 2^{s} - 12)[8] + (6 \times 2^{s} - 6)[13] + (6 \times 2^{s} - 6)[18],\\ &= 264 \times 2^{s} - 282.\end{aligned}$$

This proves the theorem.

Theorem 2. Let ξ be a molecular network of PPEtIm dendrimer. Then modified FZCI, modified SZCI and modified TZCI are given in the following

(1) $\hat{\mathcal{Z}}\mathfrak{C}_1^{*}(\xi) = 108 \times 2^{s} - 114,$

(2) $\hat{\mathcal{Z}}\mathfrak{C}_2^*(\xi) = 232 \times 2^s - 246$,

(3) $\hat{\mathcal{Z}}\mathfrak{C}_3^*(\xi) = 232 \times 2^s - 246$.

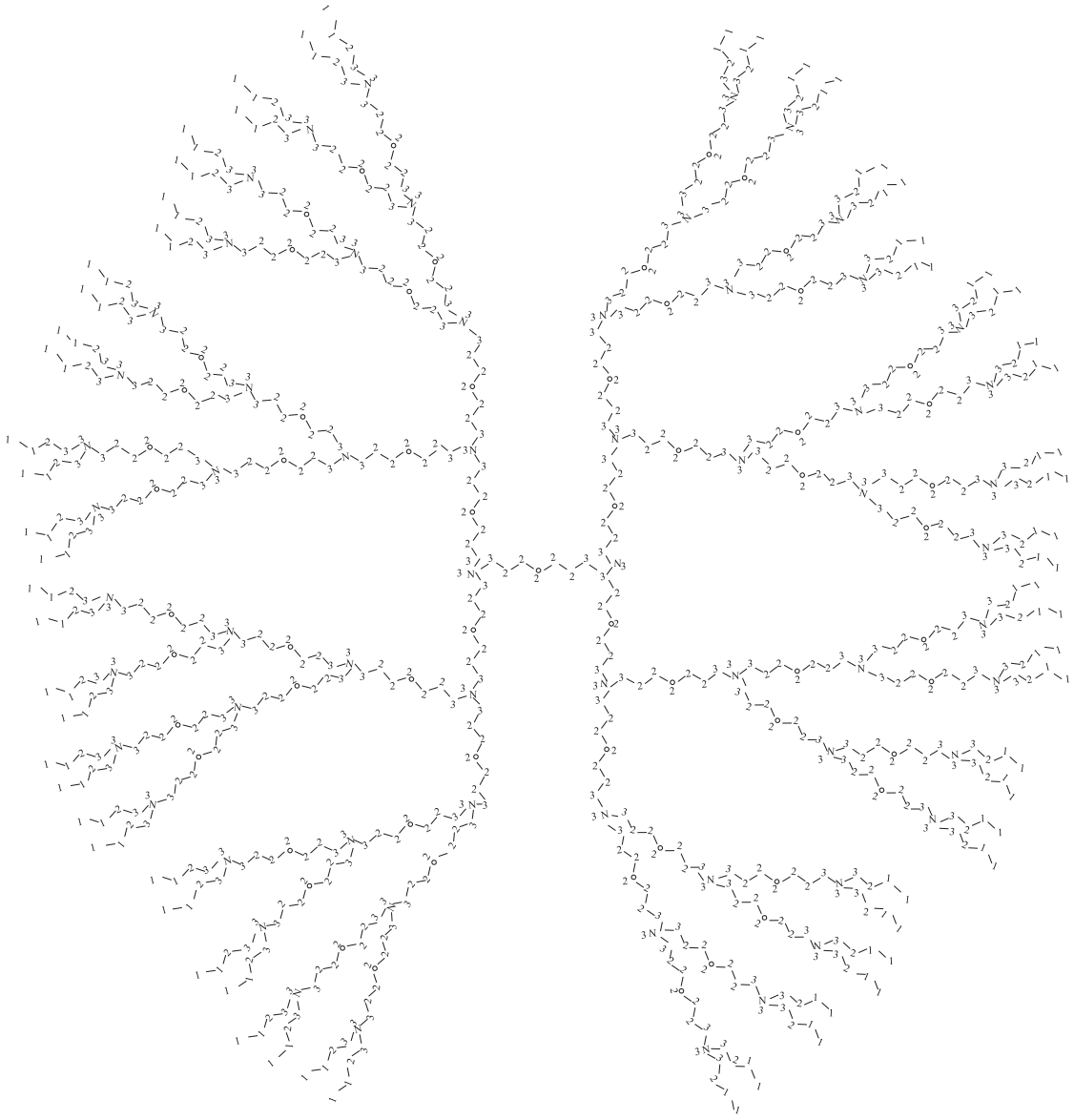

Figure 2: Structural formula of PPEtIm dendrimer for $s = 5$ along with CNs

Proof.

1. For the proof, the readers are referred to see [33].

2. Now, we classify the edges on the basis of their degrees of incident vertices. It can be seen that $\left|\mathcal{A}_{(1,2)}(\xi)\right| = 2 \times 2^s$, $\left|\mathcal{A}_{(2,2)}(\xi)\right| = 16 \times 2^s - 18$ and $\left|\mathcal{A}_{(2,3)}(\xi)\right| = 6 \times 2^s - 6$. In order to compute the modified SZCI and modified TZCI, we split the partitioned number of edges on degree basis with respect to the number of edges on connection bases.

Row 1 of Table 2 shows that there are total 2×2^s number of edges $mn \in \xi$ in which the vertex m with degree 1 and CN 1 is adjacent to the vertex n with degree 2 and CN 1, i.e., $\left|\mathcal{A}_{(1,2)(1,1)}(\xi)\right| = 2 \times 2^s$. Similarly, the row 2 shows that there are total 2×2^s number of edges mn in which the vertex m with degree 2 and CN 1 is adjacent to the vertex n with degree 2 and CN 2, i.e., $\left|\mathcal{A}_{(2,2)(1,2)}(\xi)\right| = 2 \times 2^s$. Similarly for the others, we have

$$\begin{aligned}
\left|\mathcal{A}_{(2,2)(2,2)}(\xi)\right| &= 8 \times 2^s - 12,\\
\left|\mathcal{A}_{(2,2)(2,3)}(\xi)\right| &= 6 \times 2^s - 6,\\
\left|\mathcal{A}_{(2,3)(3,3)}(\xi)\right| &= 6 \times 2^s - 6.
\end{aligned}$$

Table 2: Total number edges on degree and connection bases

Degree wise	Connection wise
$\left\|\mathcal{A}_{(1,2)}(\xi)\right\| = 2 \times 2^s$	$\left\|\mathcal{A}_{(1,1)}(\xi)\right\| = 2 \times 2^s$
$\left\|\mathcal{A}_{(2,2)}(\xi)\right\| = 2 \times 2^s$	$\left\|\mathcal{A}_{(1,2)}(\xi)\right\| = 2 \times 2^s$
$\left\|\mathcal{A}_{(2,2)}(\xi)\right\| = 8 \times 2^s - 12$	$\left\|\mathcal{A}_{(2,2)}(\xi)\right\| = 8 \times 2^s - 12$
$\left\|\mathcal{A}_{(2,2)}(\xi)\right\| = 6 \times 2^s - 6$	$\left\|\mathcal{A}_{(2,3)}(\xi)\right\| = 6 \times 2^s - 6$
$\left\|\mathcal{A}_{(2,3)}(\xi)\right\| = 6 \times 2^s - 6$	$\left\|\mathcal{A}_{(3,3)}(\xi)\right\| = 6 \times 2^s - 6$

After placing the calculated values of $\left|\mathcal{A}_{(\mu,\nu)(\phi,\psi)}(\xi)\right|$ in Eq. (4), we get

$$\begin{aligned}
\hat{\mathcal{Z}}\mathfrak{C}_2^*(\xi) &= \sum_{\substack{\phi\ \psi \in A,\\ \mu,\nu \in B}} \left|\mathcal{A}_{(\mu,\nu)(\phi,\psi)}(\xi)\right| [\mu\psi + \nu\phi]\\
&= \left|\mathcal{A}_{(1,2)(1,1)}(\xi)\right| [(1)(1) + (2)(1)] + \left|\mathcal{A}_{(2,2)(1,2)}(\xi)\right| [(2)(2) + (2)(1)] + \left|\mathcal{A}_{(2,2)(2,2)}(\xi)\right| [(2)(2) + (2)(2)]\\
&\quad + \left|\mathcal{A}_{(2,2)(2,3)}(\xi)\right| [(2)(3) + (2)(2)] + \left|\mathcal{A}_{(2,3)(3,3)}(\xi)\right| [(2)(3) + (3)(3)],\\
&= (2 \times 2^s)[3] + (2 \times 2^s)[6] + (8 \times 2^s - 12)[8] + (6 \times 2^s - 6)[10] + (6 \times 2^s - 6)[15],\\
&= 232 \times 2^s - 246.
\end{aligned}$$

3. By placing the $\left|\mathcal{A}_{(\mu,\nu)(\phi,\psi)}(\xi)\right|$ in Eq. (5), we get

$$\begin{aligned}
\hat{\mathcal{Z}}\mathfrak{C}_3^*(\xi) &= \sum_{\substack{\phi\ \psi \in A,\\ \mu,\nu \in B}} \left|\mathcal{A}_{(\mu,\nu)(\phi,\psi)}(\xi)\right| [\mu\psi + \nu\phi]\\
&= \left|\mathcal{A}_{(1,2)(1,1)}(\xi)\right| [(1)(1) + (2)(1)] + \left|\mathcal{A}_{(2,2)(1,2)}(\xi)\right| [(2)(1) + (2)(2)]\\
&\quad + \left|\mathcal{A}_{(2,2)(2,2)}(\xi)\right| [(2)(2) + (2)(2)] + \left|\mathcal{A}_{(2,2)(2,3)}(\xi)\right| [(2)(2) + (2)(3)]\\
&\quad + \left|\mathcal{A}_{(2,3)(3,3)}(\xi)\right| [(2)(3) + (3)(3)],\\
&= (2 \times 2^s)[3] + (2 \times 2^s)[6] + (8 \times 2^s - 12)[8] + (6 \times 2^s - 6)[10] + (6 \times 2^s - 6)[15],
\end{aligned}$$

$$= 232 \times 2^s - 246.$$

This proves the theorem.

4 ZCIs of Poly Propylene Imine Octamin Dendrimer

In this section, we find the general expressions to compute the connection-based Zagreb indices, namely, FZCI, SZCI, TZCI, modified FZCI, modified SZCI and modified TZCI of another special type of dendrimer nanostar named as, PPIO dendrimer. PPIO dendrimer grows in three dimensions and it has five bonds in the core. The structural formula of PPIO dendrimer is shown in Fig. 3 for five generations.

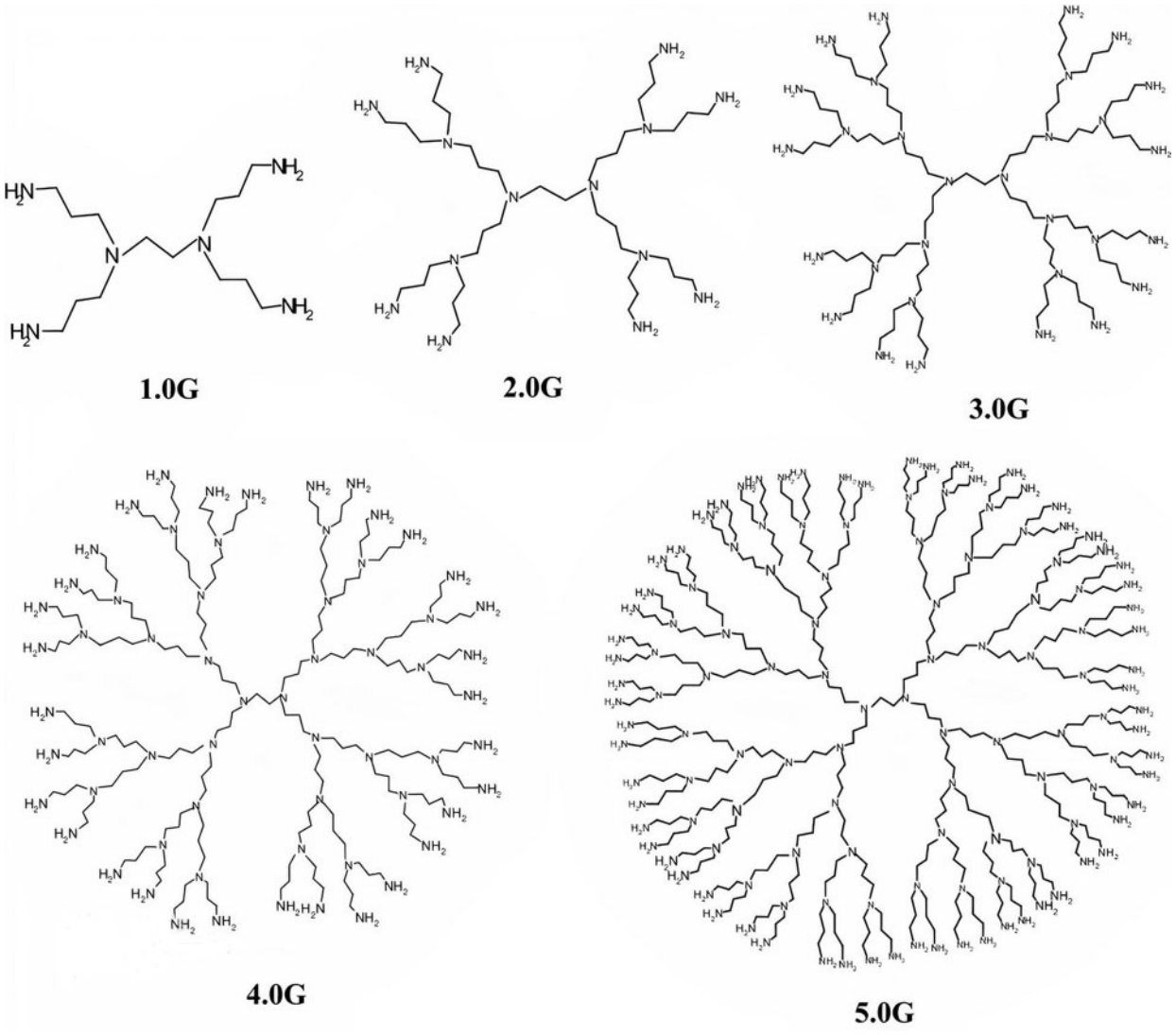

Figure 3: Structural formula of PPIO dendrimer

Theorem 3. Let ξ be a molecular network of PPIO dendrimer. Then, FZCI, SZCI and TZCI are given in the following

1. $\hat{\mathcal{Z}}\mathfrak{C}_1(\xi) = 92 \times 2^s - 80$,
2. $\hat{\mathcal{Z}}\mathfrak{C}_2(\xi) = 96 \times 2^s - 86$,
3. $\hat{\mathcal{Z}}\mathfrak{C}_3(\xi) = 200 \times 2^s - 178$.

Proof.

1. Initially, we find cardinality of edges of ξ. The total number of edges in ξ must be equal to the four times of number of edges in each branch plus the number of edges in central core. It can be easily seen that central core has 5 edges. Therefore,

$$\begin{aligned}\text{Number of edges in each branch} &= (4 + (2 \times 4) + (2^2 \times 4) + \cdots + (2^{s-1} \times 4)),\\ &= 4 \times 2^s - 4.\\ \text{Number of edges in all branches} &= 4 \times (4 \times 2^s - 4),\\ &= 16 \times 2^s - 16.\\ \text{Number of edges in } \zeta &= 5 + (16 \times 2^s - 16),\\ &= 16 \times 2^s - 11.\end{aligned}$$

As ζ is a tree, so the number of vertices must be equals to $16 \times 2^s - 10$.

Furthermore, we find the cardinality of those vertices which have CN 1, 2 and 3 in ξ.

$$\begin{aligned}|\mathcal{A}_1| &= 4(2 \times 2^{s-1}),\\ &= 4 \times 2^s.\\ |\mathcal{A}_2| &= 4\left[1 + (2 \times 1) + (2^2\times) + (2^3 \times 1) + \cdots (2^{s-1} \times 1)\right] + 2,\\ &= 4 \times 2^s - 2.\\ |\mathcal{A}_3| &= (16 \times 2s - 10) - (4 \times 2^s) - (4 \times 2^s + 2),\\ &= 8 \times 2^s - 8.\end{aligned}$$

In Fig. 4, we have labeled the vertices of PPIO dendrimer for $s = 5$ with respect to their CNs. Now, by placing the values of $\left|\mathcal{A}_\phi(\xi)\right|$ in Eq. (1), we get

$$\begin{aligned}\hat{\mathcal{Z}}_1\mathfrak{C}(\xi) &= \sum_{\phi \in A} \left|\mathcal{A}_\phi(\xi)\right| \left[\phi^2\right]\\ &= |\mathcal{A}_1(\xi)|\,[1^2] + |\mathcal{A}_2(\xi)|\,[2^2] + |\mathcal{A}_3(\xi)|\,[3^2],\\ &= (4 \times 2^s)[1] + (4 \times 2^s - 2)[2^2] + (8 \times 2^s - 8)[3^2],\\ &= 92 \times 2^s - 80.\end{aligned}$$

2. Now, we calculate $\left|\mathcal{A}_{(\phi,\psi)}(\xi)\right|$.

$$\left|\mathcal{A}_{(1,1)}\right| = 4 \times 2^{s-1} = 2 \times 2^s.$$

$$\left|\mathcal{A}_{(1,2)}\right| = 4 \times 2^{s-1} = 2 \times 2^s.$$

$$\left|\mathcal{A}_{(2,2)}\right| = 1.$$

$$\begin{aligned}\left|\mathcal{A}_{(2,3)}\right| &= 4[2 + (2 \times 2) + (2^2 \times 2) + (2^3 \times 2) + \cdots + (2^{s-1} \times 2)] + 2 \\ &= 4 \times 2[1 + 2 + 2^2 + 2^3 + \cdots + 2^{s-1}] + 2 \\ &= 6 \times 2^s - 6.\end{aligned}$$

$$\begin{aligned}\left|\mathcal{A}_{(3,3)}\right| &= 4(2 + (2 \times 2) + (2^2 \times 2) + (2^3 \times 2) + \cdots + (2^{s-2} \times 2) + (2^{s-1} \times 1)) + 2, \\ &= 4 \times 2(1 + 2 + 2^2 + 2^3 + \cdots + 2^{s-2}) + 2^{s-1} + 2, \\ &= 6 \times 2^s - 6.\end{aligned}$$

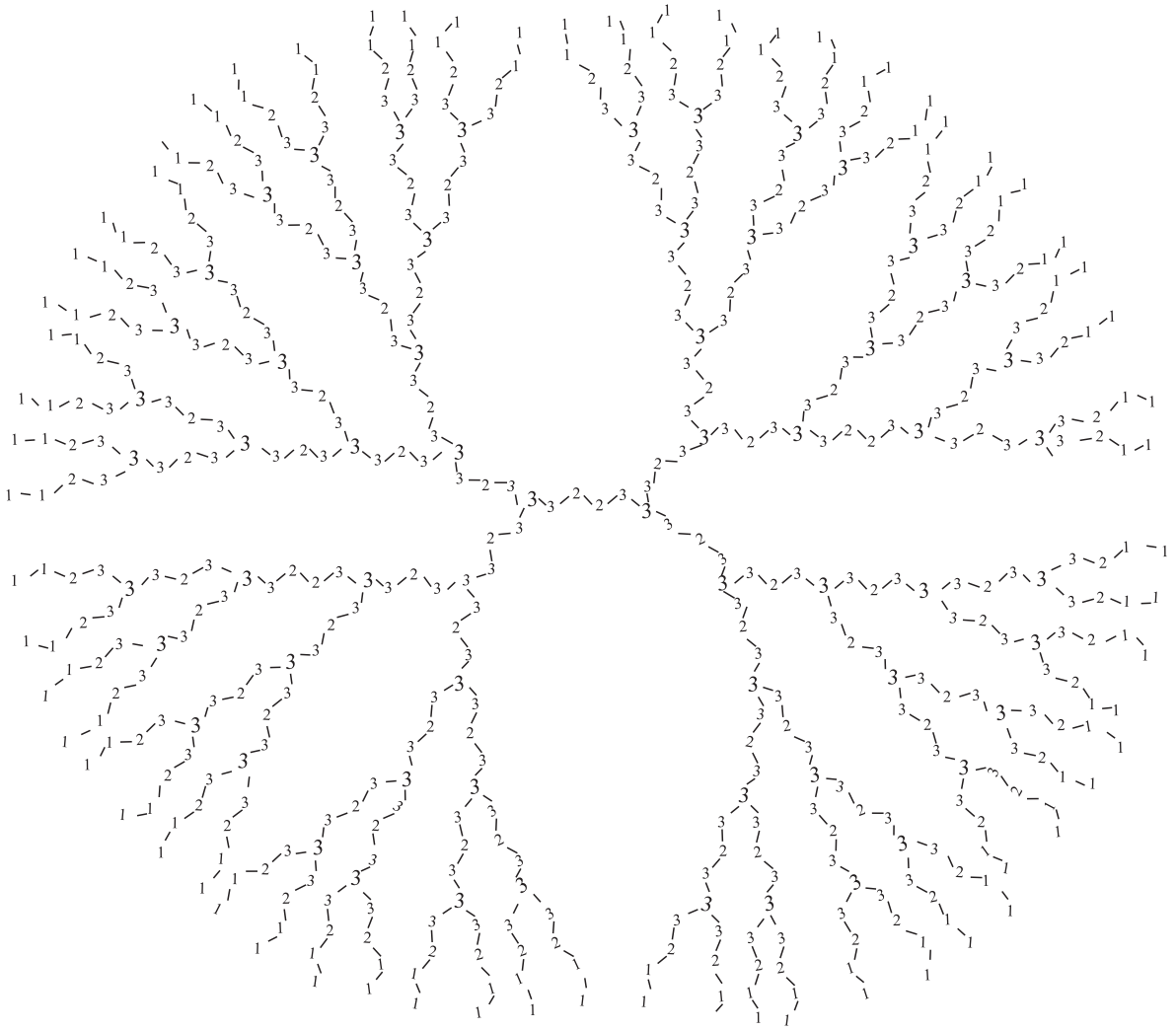

Figure 4: Structural formula of PPIO dendrimer for $s = 5$ along with CNs

After placing the above calculated values in Eq. (2), we have

$$\begin{aligned}\hat{\mathcal{Z}}\mathfrak{C}_2(\xi) &= \sum_{\phi,\psi\in A}\left|\mathcal{A}_{(\phi,\psi)}(\xi)\right|[\phi\times\psi],\\ &= \left|\mathcal{A}_{(1,1)}(\xi)\right|[1\times 1]+\left|\mathcal{A}_{(1,2)}(\xi)\right|[1\times 2]+\left|\mathcal{A}_{(2,2)}(\xi)\right|[2\times 2]+\left|\mathcal{A}_{(2,3)}(\xi)\right|[2\times 3]\\ &\quad+\left|\mathcal{A}_{(3,3)}(\xi)\right|[3\times 3],\\ &= (2\times 2^s)[1]+(2\times 2^s)[2]+[4](1)+(6\times 2^s-6)[6]+(6\times 2^s-6)[9],\\ &= 96\times 2^s-86.\end{aligned}$$

3. After placing the values of $\left|\mathcal{A}_{(\phi,\psi)}(\xi)\right|$ in Eq. (6), we get

$$\begin{aligned}\hat{\mathcal{Z}}\mathfrak{C}_3(\xi) &= \sum_{0\le\phi\le\psi\le 3}\left|\mathcal{A}_{(\phi,\psi)}(\xi)\right|\left[\phi^2+\psi^2\right],\\ &= \left|\mathcal{A}_{(1,1)}(\xi)\right|[1^2+1^2]+\left|\mathcal{A}_{(1,2)}(\xi)\right|[1^2+2^2]+\left|\mathcal{A}_{(2,2)}(\xi)\right|[2^2+2^2]\\ &\quad+\left|\mathcal{A}_{(2,3)}(\xi)\right|[2^2+3^2]+\left|\mathcal{A}_{(3,3)}(\xi)\right|[3^2+3^2],\\ &= (2\times 2^s)[2]+(2\times 2^s)[5]+(1)[8]+(6\times 2^s-6)[13]+(6\times 2^s-6)[18],\\ &= 200\times 2^s-178.\end{aligned}$$

This proves the theorem.

Theorem 4. Let ξ be a molecular network of PPIO dendrimer. Then modified FZCI, modified SZCI and modified TZCI are given in the following

1. $\hat{\mathcal{Z}}\mathfrak{C}_1^*(\xi)=76\times 2^s-62$,
2. $\hat{\mathcal{Z}}\mathfrak{C}_2^*(\xi)=168\times 2^s-142$,
3. $\hat{\mathcal{Z}}\mathfrak{C}_3^*(\xi)=168\times 2^s-142$.

Proof.

1. For the proof, the readers are referred to see [32].

2. Now we make the partition of the edges based on their degrees of incident vertices. It can be easily seen that $\left|\mathcal{A}_{(1,2)}(\xi)\right|=2\times 2^s$, $\left|\mathcal{A}_{(2,2)}(\xi)\right|=8\times 2^s-5$ and $\left|\mathcal{A}_{(2,3)}(\xi)\right|=6\times 2^s-6$. In order to compute the modified SZCI and modified TZCI, we split the number edges on degree basis with respect to the number of edges on connection bases as shown in Table 3.

Table 3: Total number edges on degree and connection bases

Degree wise	Connection wise
$\left\|\mathcal{A}_{(1,2)}(\xi)\right\|=2\times 2^s$	$\left\|\mathcal{A}_{(1,1)}(\xi)\right\|=2\times 2^s$
$\left\|\mathcal{A}_{(2,2)}(\xi)\right\|=2\times 2^s$	$\left\|\mathcal{A}_{(1,2)}(\xi)\right\|=2\times 2^s$
$\left\|\mathcal{A}_{(2,2)}(\xi)\right\|=1$	$\left\|\mathcal{A}_{(2,2)}(\xi)\right\|=1$
$\left\|\mathcal{A}_{(2,2)}(\xi)\right\|=6\times 2^s-6$	$\left\|\mathcal{A}_{(2,3)}(\xi)\right\|=6\times 2^s-6$
$\left\|\mathcal{A}_{(2,3)}(\xi)\right\|=6\times 2^s-6$	$\left\|\mathcal{A}_{(3,3)}(\xi)\right\|=6\times 2^s-6$

Thus, we have

$$\left|\mathcal{A}_{(1,2)(1,1)}(\xi)\right| = 2 \times 2^s,$$
$$\left|\mathcal{A}_{(2,2)(1,2)}(\xi)\right| = 2 \times 2^s,$$
$$\left|\mathcal{A}_{(2,2)(2,2)}(\xi)\right| = 1,$$
$$\left|\mathcal{A}_{(2,2)(2,3)}(\xi)\right| = 6 \times 2^s - 6,$$
$$\left|\mathcal{A}_{(2,3)(3,3)}(\xi)\right| = 6 \times 2^s - 6.$$

By putting the $\left|\mathcal{A}_{(\mu,\nu)(\phi,\psi)}(\xi)\right|$ in Eq. (4), we have

$$\hat{\mathcal{Z}}\mathfrak{C}_2^*(\xi) = \sum_{\substack{\phi\ \ \psi \in A,\\ \mu,\nu \in B}} \left|\mathcal{A}_{(\mu,\nu)(\phi,\psi)}(\xi)\right| [\mu\psi + \nu\phi]$$

$$= \left|\mathcal{A}_{(1,2)(1,1)}(\xi)\right| [(1)(1) + (2)(1)] + \left|\mathcal{A}_{(2,2)(1,2)}(\xi)\right| [(2)(2) + (2)(1)] + \left|\mathcal{A}_{(2,2)(2,2)}(\xi)\right| [(2)(2) + (2)(2)]$$

$$+ \left|\mathcal{A}_{(2,2)(2,3)}(\xi)\right| [(2)(3) + (2)(2)] + \left|\mathcal{A}_{(2,3)(3,3)}(\xi)\right| [(2)(3) + (3)(3)],$$

$$= (2 \times 2^s)[3] + (2 \times 2^s)[6] + (1)[8] + (6 \times 2^s - 6)[10] + (6 \times 2^s - 6)[15],$$

$$= 168 \times 2^s - 142.$$

3. By putting the $\left|\mathcal{A}_{(\mu,\nu)(\phi,\psi)}(\xi)\right|$ in Eq. (5), we have

$$\hat{\mathcal{Z}}\mathfrak{C}_3^*(\xi) = \sum_{\substack{\phi\ \ \psi \in A,\\ \mu,\nu \in B}} \left|\mathcal{A}_{(\mu,\nu)(\phi,\psi)}(\xi)\right| [\mu\phi + \nu\psi]$$

$$= \left|\mathcal{A}_{(1,2)(1,1)}(\xi)\right| [(1)(1) + (2)(1)] + \left|\mathcal{A}_{(2,2)(1,2)}(\xi)\right| [(2)(1) + (2)(2)]$$

$$+ \left|\mathcal{A}_{(2,2)(2,2)}(\xi)\right| [(2)(2) + (2)(2)]$$

$$+ \left|\mathcal{A}_{(2,2)(2,3)}(\xi)\right| [(2)(2) + (2)(3)] + \left|\mathcal{A}_{(2,3)(3,3)}(\xi)\right| [(2)(3) + (3)(3)],$$

$$= (2 \times 2^s)[3] + (2 \times 2^s)[6] + (1)[8] + (6 \times 2^s - 6)[10] + (6 \times 2^s - 6)[15],$$

$$= 168 \times 2^s - 142.$$

This proves the theorem.

5 Comparative Analysis and Concluding Remarks

The analysis of networks plays a remarkable role to conclude their fundamental topologies. TIs specified on chemical structures can assist the researchers to recognize the biological activity, chemical reactivity and physical features. Through TIs, researchers can easily predict the distinct psychochemical properties of the molecular structures. To check the superiority of consequences of this research article, we compare our computed values for two nanostars. Table 4 displays the comparison between the calculated results of PPEtIm and PPIO dendrimers.

From Table 4, it can be easily seen that PPEtIm dendrimer and PPIO dendrimer get the greatest value of TZCI $\hat{\mathcal{Z}}_3\mathfrak{C}(\xi)$. The values of defined ZCIs of PPEtIm dendrimer and PPIO dendrimer for some values of s are given in Tables 5 and 6, respectively.

Table 4: Comparison between the value of PPEtIm and PPIO dendrimer

ZCIs	PPEtIm dendrimer	PPIO dendrimer
$\hat{\mathcal{Z}}_1\mathfrak{C}(\xi)$	$124 \times 2^s - 132$	$92 \times 2^s - 80$
$\hat{\mathcal{Z}}_2\mathfrak{C}(\xi)$	$128 \times 2^s - 138$	$96 \times 2^s - 86$
$\hat{\mathcal{Z}}_3\mathfrak{C}(\xi)$	$\mathbf{264 \times 2^s - 282}$	$\mathbf{200 \times 2^s - 178}$
$\hat{\mathcal{Z}}\mathfrak{C}_1^*(\xi)$	$108 \times 2^s - 114$	$76 \times 2^s - 62$
$\hat{\mathcal{Z}}\mathfrak{C}_2^*(\xi)$	$232 \times 2^s - 246$	$168 \times 2^s - 142$
$\hat{\mathcal{Z}}\mathfrak{C}_3^*(\xi)$	$232 \times 2^s - 246$	$168 \times 2^s - 142.$

Table 5: ZCIs of PPEtIm dendrimer

ZCIs	$s=1$	$s=2$	$s=3$	$s=4$	$s=5$
$\hat{\mathcal{Z}}_1\mathfrak{C}(\xi)$	116	364	860	1852	3836
$\hat{\mathcal{Z}}_2\mathfrak{C}(\xi)$	118	358	854	1846	3830
$\hat{\mathcal{Z}}_3\mathfrak{C}(\xi)$	246	774	1830	3942	8166
$\hat{\mathcal{Z}}\mathfrak{C}_1^*(\xi)$	102	318	750	1614	3342
$\hat{\mathcal{Z}}\mathfrak{C}_2^*(\xi)$	218	626	1610	3466	7178
$\hat{\mathcal{Z}}\mathfrak{C}_3^*(\xi)$	218	626	1610	3466	7178

Table 6: ZCIz of PPIO dendrimer dendrimer

ZCIs	$s=1$	$s=2$	$s=3$	$s=4$	$s=5$
$\hat{\mathcal{Z}}_1\mathfrak{C}(\xi)$	104	288	656	1392	2854
$\hat{\mathcal{Z}}_2\mathfrak{C}(\xi)$	106	298	682	1450	2986
$\hat{\mathcal{Z}}_3\mathfrak{C}(\xi)$	222	622	1422	3022	6222
$\hat{\mathcal{Z}}\mathfrak{C}_1^*(\xi)$	86	234	530	1122	2306
$\hat{\mathcal{Z}}\mathfrak{C}_2^*(\xi)$	194	530	1202	2546	5234
$\hat{\mathcal{Z}}\mathfrak{C}_3^*(\xi)$	194	530	1202	2546	5234

The graphical comparison of $\hat{\mathcal{Z}}_3\mathfrak{C}(\xi)$ for both dendrimers is displayed in Fig. 5.

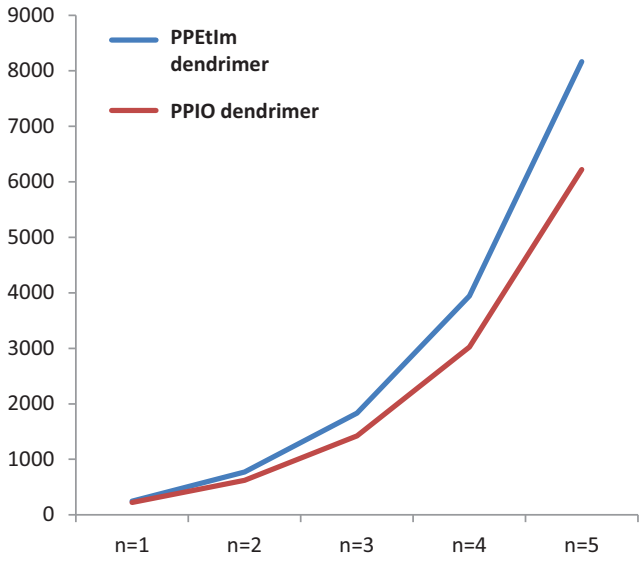

Figure 5: Graphical display of TZCI for PPEtIm and PPIO dendrimers

Now, we conclude our discussion with the following lines. In this manuscript, we have established the general results to compute ZCIs namely, FZCI, SZCI and TZCI of two special types of dendrimer nanostars, namely, PPEtIm dendrimer and PPIO dendrimer which will be helpful in computational chemistry to predict many physical and chemical attributes of the chemical substances. Moreover, we have computed modified FZCI, modified SZCI and modified TZCI for these dendrimers. The computed results just depend upon the value of $s \geq 1$. Further, we have compared the calculated results for both types of dendrimers with each other. We have found that our developed TZCI gets the greatest value for both types of dendrimers. Thus, we found that TZCI is superior in preserving the psychochemical properties of these dendrimers and PPEtIm dendrimer has greater chemical applicability than PPIO dendrimer. Now, the problem is still open to computing the Zagreb connection indices for the other types of dendrimers.

Data Availability: The data used to support the findings of this study are included within this article. However, the reader may contact the corresponding author for more details on the data.

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