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Exploring the Topological Aspects of Connection-Based Nanostar Dendrimers

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Abstract

Topological indices (TIs) have been found to be extensively useful in describing and simulating the chemical structure of diverse molecular compounds, including dendrimers, nanotubes, and neural networks. Dendrimers represent a distinct class of well-defined, highly branched macromolecules characterized by their symmetrical, tree-like architecture. This review provides a comprehensive overview of dendrimer synthesis, structure, properties, and diverse applications in nanoscience. Currently, the field of chemistry is actively exploring a mathematical approach that involves using topological techniques and numerical graph invariants to characterize molecular structures. Out of all the established descriptors, connection-based Zagreb indices are generally regarded as more efficient than the traditional indices. This manuscript presents the overarching outcome for calculating the Zagreb connection indices, specifically, harmonic connection index (HCI), augmented connection index (ACI), symmetric division connection index ($SDCI$), geometric arithmetic connection index ($GACI$), hyper Zagreb connection index ($HZCI$), inverse sum connection index ($ISCI$), and atom bond connectivity connection index ($ABCCI$). Furthermore, we compare the numerical and graphical values with each other to assess their relative superiority.

Keywords

Topological Index, Zagreb Index, Zagreb Connection Index, Nanostar Dendrimers

1. Introduction

Dendrimers are highly branched, three-dimensional macromolecules with well-defined structures. They were first introduced by Donald A. Tomalia in the early 1980s. The term "dendrimer" is derived from the Greek word "dendron," which means tree. They belong to a special family of nanoscale materials that have several uses in industries, including catalysis, drug delivery, imaging, and nanotechnology.

Dendrimers can be synthesized using two methods, the divergent approach and the convergent approach. In contemporary times, dendrimers stand out as prominently engineered macromolecules with wide-ranging applications in the field of biomedical science. These include gene transfection, drug delivery, tissue engineering, contrast enhancement for magnetic resonance imaging, and immunology. For further information [1]-[3].

Using numerical graphs descriptors, Researchers are attempting to define the chemical attributes of molecular structures. The popular method in computational and mathematical chemistry for characterizing the molecular structures is through numerical graph descriptors (topological indices).

Topological indices are numerical values derived from the molecular structure of chemical compounds, representing their connectivity and shape. These indices are crucial in cheminformatics and QSAR (quantitative structure-activity relationship) modeling to predict molecules' physicochemical properties and biological activities. Topological indices reflect molecules' size, volume, and surface area, which influence properties like boiling point and solubility. Higher branching in a molecule often increases the value of certain indices, correlating with reduced boiling points and densities. Some indices, like the Wiener and Zagreb indices, relate to molecular polarity and hydrophobicity, affecting solubility and partition coefficients. Indices can predict the stability of molecular structures by quantifying electron delocalization and resonance effects, influencing reactivity and chemical stability. Topological indices help model drug-likeness, permeability, and bioavailability by correlating with biological activity.

The current field of study uses TIs to mathematically characterize chemical structures. TI is a numerical measure that helps to correlate the topology of chemical compounds and is associated with graphs. TIs are useful in establishing correlations between many physiochemical characteristics of molecular structures, such as density, strain energy, melting point, volatility, stability, and flammability. Numerous TI that are potential candidates for measuring the physical and chemical properties of chemical compounds may be found in the literature.

The innovative idea of distance-based TI was first proposed by Wiener [4]. The first degree-based Zagreb index (ZI) was established by Gutman and Trinajstic [5]. After this invention, researchers used a variety of degree and distance based TIs to predict the topological characteristics of various substances.

In 1998, Estrada *et al.* [6] conducted a study on a noteworthy topological index known as the atom bond connectivity (ABC) index. Following this, Ghorbani *et al.* [7] introduced an updated version of the ABC index. Additionally, in 2009, Vukicevic and Furtula [8] introduced another significant index known as the geometric arithmetic (*GA*) index.

Additionally, Garaovoc *et al.* [9] provided the fifth iteration of the *GA* index, which he used to verify the chemical characteristics of dendrimers. In 2010, Vukicevic [8] introduced the novel idea of the symmetric division degree (*SDD*) index. The augmented Zagreb index (*AZI*) was first presented by Furtula *et al.* [10]. Furthermore, Fajtlowicz [11] proposed the concept of harmonic index (*HI*). The idea of the inverse sum (*IS*) index was introduced by Vukicevic and Gasperov [12]. Shirdel *et al.* provided the definition of hyper *ZI* (*HZI*) [13].

Ali and Trinajstic [14] have introduced a novel approach to investigate the psycho-chemical characteristics of compounds. They achieved this by introducing a concept known as the connection number (*CN*) of a vertex and initiating the Zagreb connection indices (*ZCIs*). The connection number of a vertex is defined as the count of vertices that are exactly two edges away from that specific vertex.

They found that the recently suggested connection-based *ZIs* as compared to the traditional *ZIs*, are more applicable for predicting the physiochemical features of different molecular structures. Numerous researchers began investigating novel connection-based indices following the development of *CN*. Haoer *et al.* [15] studied multiplicative leap *ZIs*. Recently Arshad *et al.* [16] [17] calculated connection base Zagreb indices of path, cycle and complete graphs.

Nanostar dendrimers are a nanoscale polymer structure with star like architecture, consisting of multiple dendrimer branches radiating from a central core. Their highly branched and symmetric structure gives them unique physicochemical properties, which render them useful in pharmaceutical applications such as drug delivery, nanomedicine, and material science. The relative surface area to volume ratio of nanostar dendrimers allows multiple functional groups for drug conjugation, targeting ligands, or imaging agents. Their nanoscale size (typically 1 - 10 nm) enables efficient penetration of biological membranes. The hydrophilic or hydrophobic nature of dendrimers can be tuned by modifying surface functional groups, enhancing solubility in aqueous or organic solvents. They exhibit high chemical and thermal stability, ensuring longevity in harsh environments. Nanostar dendrimers are synthesized with precise control over size and shape, resulting in monodisperse populations that ensure reproducible behavior in biological systems. The internal pores of nanostar dendrimers enable encapsulation for hydrophobic drugs, and the outer surface can be functionalized for specific targeting such as activation. They modulate drug release to enable sustained drug delivery and targeted drug release to mitigate side effects. Surface modification (e.g., PEGylation) enhances biocompatibility and decreases cytotoxicity, rendering them suitable for biomedical applications. Nanostar dendrimers have low immunogenicity, enabling their safe use in vivo. The star-like architecture offers several attachment points that increase interactions with biological targets and improve binding affinity in both diagnostics and therapeutics.

Recently, Sattar and Javaid [18] derived general expressions for calculating the *MZCI* of dendrimer nanostars. In addition, Ye and Qureshi [19] computed the

ZCIs for nanotubes and a regular hexagonal lattice.

Bokhary and Imran [20] investigated the topological characteristics of certain nanostars, while Gharibi *et al.* [21] introduced the concept of Zagreb polynomials for nanocones and nanotubes.

A few days ago, Aiman and Aqsa [22] recently calculated the *ZCIs* for a PPEI and PPIO dendrimers.

To find additional information, we suggest that readers refer to [23] [24].

This paper introduces a comprehensive expression for calculating various *ZCIs* for significant types of dendrimer nanostar networks, including the Harmonic Connection Index (*HCI*), Augmented Zagreb Connection Index (*AZCI*), Symmetric Division Connection Index (*SDCI*), Geometric Arithmetic Connection Index (*GACI*), Hyper Zagreb Connection Index (*HZCI*), Inverse Sum Connection Index (*ISCI*), and Atom Bond Connectivity Connection Index (*ABCCI*).

Section 2 covers some fundamental definitions. In Section 3, we present the general result for calculating the *ZCIs* of the dendrimer network, including *HCI*, *AZCI*, *SDCI*, *AGCI*, *HZCI*, *ISCI*, and *ABCCI*. Section 4 contains the primary results for *ZCIs* computations in the dendrimer network. Sections 5 and 6 offer a numerical and graphical comparison of the dendrimer network based on the computed results, concluding the article.

Table 1 provides a list of acronyms used in this paper 1.

Table 1. List of acronyms.

Name	Acronyms
Connection numbers	*CN*
Topological index	*TI*
Zagreb connection index	*ZCI*
Harmonic connection index	*HCI*
Augmented Zagreb connection index	*AZCI*
Symmetric division connection index	*SDCI*
Geometric arithmetic connection index	*GACI*
Hyper Zagreb connection index	*HZCI*
Inverse sum connection index	*ISCI*
Atom bond connectivity connection index	*ABCCI*

2. Preliminaries

Consider a network $\varpi = (\mathbf{A}(\varpi), \mathbf{B}(\varpi))$ with $\mathbf{B}(\varpi)$ as a edge set and $\mathbf{A}(\varpi)$ as the set of vertex. The degree of a vertex is defined as the count of vertices at a distance of one from it. The connection number of a specific vertex is the count of vertices at a distance of two from it.

We introduce the connection-based *ZI*, as proposed by Javaid and Sattar [18] [25].

Definition 2.1 *For a network* ϖ, *the HCI is defined as*;

$$HCI(\varpi)=\sum_{d,k\in\mathbf{B}(\varpi)}\frac{2}{\beta(d)+\beta(k)},$$

$\beta(d)$ and $\beta(k)$ represent the *CNs* of vertices d and k, respectively.

Definition 2.2 *For a network* ϖ, *the AZCI is defined as*;

$$AZCI(\varpi)=\sum_{d,k\in\mathbf{B}(\varpi)}\left[\frac{\beta(d)\times\beta(k)}{\beta(h)+\beta(k)-2}\right]^3,$$

$\beta(d)$ and $\beta(k)$ represent the *CNs* of vertices d and k, respectively.

Definition 2.3 *For a network* ϖ, *the SDCI is defined as*;

$$SDCI(\varpi)=\sum_{d,k\in\mathbf{B}(\varpi)}\left[\frac{\min(\beta(d),\beta(k))}{\max(\beta(d),\beta(k))}+\frac{\max(\beta(d),\beta(k))}{\min(\beta(d),\beta(k))}\right],$$

where $\min(\beta(d),\beta(k))$ is the minimum of $\beta(d)$ and $\beta(k)$ and $\max(\beta(d),\beta(k))$ is the maximum of $\beta(d)$ and $\beta(k)$.

Definition 2.4 *For a network* ϖ, *the GACI is defined as*;

$$GACI(\varpi)=\sum_{d,k\in\mathbf{B}(\varpi)}\frac{2\sqrt{\beta(d)\beta(k)}}{\beta(d)+\beta(k)},$$

$\beta(d)$ and $\beta(k)$ represent the *CNs* of vertices d and k, respectively.

Definition 2.5 *For a network* ϖ, *the HZCI is defined as*;

$$HZCI(\varpi)=\sum_{d,k\in\mathbf{B}(\varpi)}\left[\beta(d)+\beta(k)\right]^2,$$

$\beta(d)$ and $\beta(k)$ represent the *CNs* of vertices d and k, respectively.

Definition 2.6 *For a network* ϖ, *the ISCI is defined as*;

$$ISCI(\varpi)=\sum_{d,k\in\mathbf{B}(\varpi)}\left[\frac{\beta(d)\times\beta(k)}{\beta(h)+\beta(k)}\right],$$

$\beta(d)$ and $\beta(k)$ represent the *CNs* of vertices d and k, respectively.

Definition 2.7 *For a network* ϖ, *the ABCCI is defined as*;

$$ABCCI(\varpi)=\sum_{d,k\in\mathbf{B}(\varpi)}\sqrt{\frac{\beta(d)+\beta(k)-2}{\beta(d)\times\beta(k)}},$$

$\beta(d)$ and $\beta(k)$ represent the *CNs* of vertices d and k, respectively.

3. Connection-Based ZIs of Nanostar Dendrimers

In this portion, we calculate the connection-based *ZIs*, such as *HCI*, *AZCI*, *SDCI*, *GACI*, *HZCI*, *ISCI*, and *ABCCI* for Nanostar dendrimers with molecular structures $D[m]$ for $m = 1, 2$, and 3, you need to use the information provided in Figure 1, Figure 2, and Figure 3, which includes the connection numbers of each vertex.

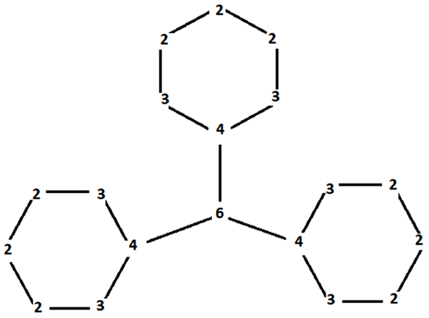

Figure 1. $D[m]$ together with CN is 2, 3, 4.

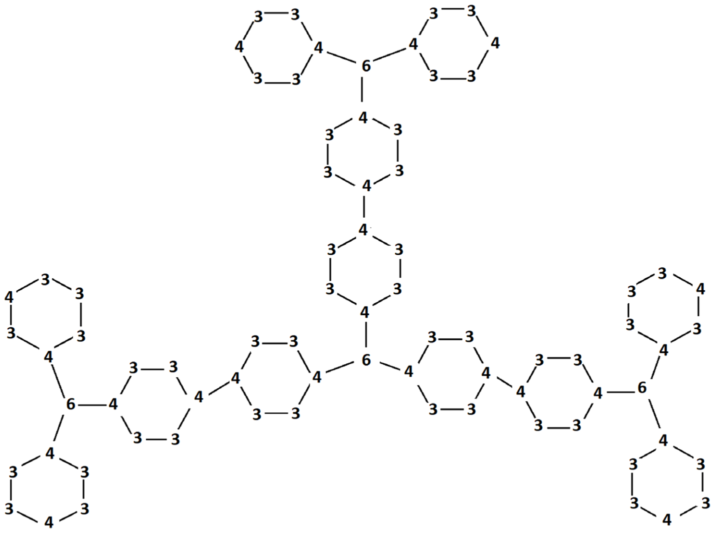

Figure 2. $D[m]$ together with CN is 2, 3, 4, 6.

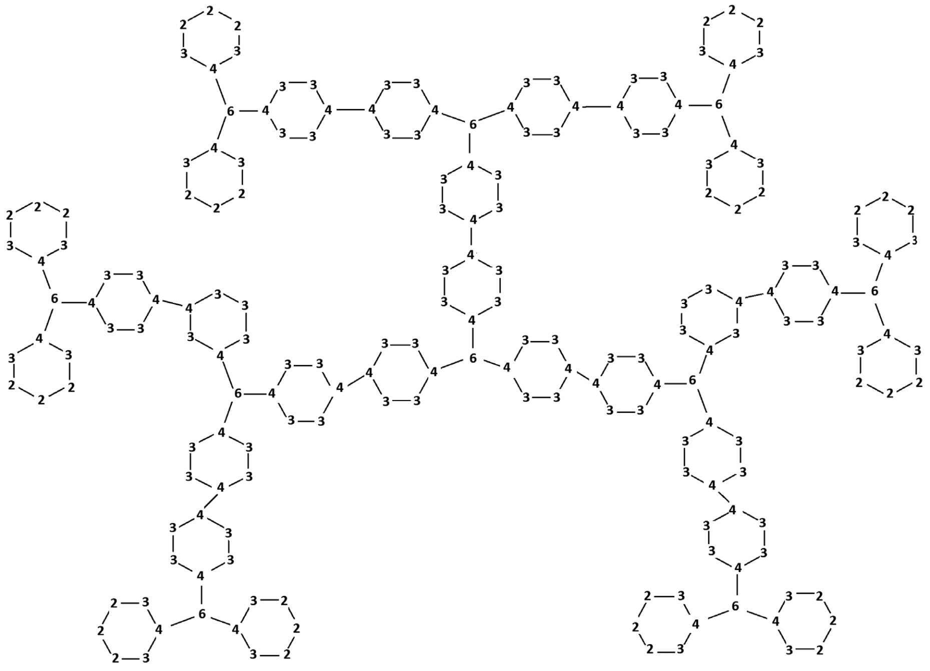

Figure 3. $D[m]$ together with CN is 2, 3, 4, 6.

Now, let's discuss the total number of edges across all hexagons.

Table 2. Total number of edge on CN base.

S.R	$\mathbf{B}_{(\beta(d),\beta(k))}(\varpi)$	Number of edges
	$\mathbf{B}_{(2,2)}(\varpi)$	$6(2^{m-1})$
	$\mathbf{B}_{(2,3)}(\varpi)$	$6(2^{m-1})$
	$\mathbf{B}_{(3,3)}(\varpi)$	$12(2^{m-1})-12$
	$\mathbf{B}_{(3,4)}(\varpi)$	$30(2^{m-1})-24$
	$\mathbf{B}_{(4,4)}(\varpi)$	$9(2^{m-1})-6$
	$\mathbf{B}_{(4,6)}(\varpi)$	$3(2^{m-1})-3$

4. Main Results

Theorem 4.1 *HCI of a network* ϖ *is given by*

$$HCI = 2^{m-1}(20.8214)-12.9571.$$

Proof. By using Definition 2.1 and Table 2, we get

$$\begin{aligned}
HCI(\varpi) &= \sum_{d,k\in\mathbf{B}(\varpi)}\left[\frac{2}{\beta(d)+\beta(k)}\right] \\
&= \left|\mathbf{B}_{(2,2)}(\varpi)\right|\left[\frac{2}{\beta(d)+\beta(k)}\right]+\left|\mathbf{B}_{(2,3)}(\varpi)\right|\left[\frac{2}{\beta(d)+\beta(k)}\right] \\
&\quad+\left|\mathbf{B}_{(3,3)}(\varpi)\right|\left[\frac{2}{\beta(d)+\beta(k)}\right]+\left|\mathbf{B}_{(3,4)}(\varpi)\right|\left[\frac{2}{\beta(d)+\beta(k)}\right] \\
&\quad+\left|\mathbf{B}_{(4,4)}(\varpi)\right|\left[\frac{2}{\beta(d)+\beta(k)}\right]+\left|\mathbf{B}_{(4,6)}(\varpi)\right|\left[\frac{2}{\beta(d)+\beta(k)}\right] \\
&= 6(2^{m-1})\left(\frac{2}{2+2}\right)+6(2^{m-1})\left(\frac{2}{2+3}\right) \\
&\quad+\left(12(2^{m-1})-12\right)\left(\frac{2}{3+3}\right)+\left(30(2^{m-1})-24\right)\left(\frac{2}{3+4}\right) \\
&\quad+\left(9(2^{m-1})-6\right)\left(\frac{2}{4+4}\right)+\left(3(2^{m-1})-3\right)\left(\frac{2}{4+6}\right) \\
&= 3(2^{m-1})+2.4(2^{m-1})+\left[4(2^{m-1})-4\right]+\left[8.5714(2^{m-1})-6.8571\right] \\
&\quad+\left[2.25(2^{m-1})-1.5\right]+\left[0.6(2^{m-1})-0.6\right] \\
&= 2^{m-1}(3+2.4+5714+2.25+0.6)+(-4-6.8571-1.5-0.6) \\
&= 2^{m-1}(20.8214)-12.9571.
\end{aligned}$$

Theorem 4.2 *AZCI of a network* ϖ *is given by*

$$AZCI = 2^{m-1}(899.0742)-663.2413.$$

Proof. By using Definition 2.2 and Table 2, we get

$$
\begin{aligned}
AZCI(\varpi) &= \sum_{d,k\in\mathbf{B}(\varpi)}\left[\frac{\beta(d)\times\beta(k)}{\beta(d)+\beta(k)-2}\right]^3\\
&= \left|\mathbf{B}_{(2,2)}(\varpi)\right|\left[\frac{\beta(d)\times\beta(k)}{\beta(d)+\beta(k)-2}\right]^3+\left|\mathbf{B}_{(2,3)}(\varpi)\right|\left[\frac{\beta(d)\times\beta(k)}{\beta(d)+\beta(k)-2}\right]^3\\
&\quad+\left|\mathbf{B}_{(3,3)}(\varpi)\right|\left[\frac{\beta(d)\times\beta(k)}{\beta(d)+\beta(k)-2}\right]^3+\left|\mathbf{B}_{(3,4)}(\varpi)\right|\left[\frac{\beta(d)\times\beta(k)}{\beta(d)+\beta(k)-2}\right]^3\\
&\quad+\left|\mathbf{B}_{(4,4)}(\varpi)\right|\left[\frac{\beta(d)\times\beta(k)}{\beta(d)+\beta(k)-2}\right]^3+\left|\mathbf{B}_{(4,6)}(\varpi)\right|\left[\frac{\beta(d)\times\beta(k)}{\beta(d)+\beta(k)-2}\right]^3\\
&= 6\left(2^{m-1}\right)\left(\frac{2\times2}{2+2-2}\right)^3+6\left(2^{m-1}\right)\left(\frac{2\times3}{2+3-2}\right)^3\\
&\quad+\left(12\left(2^{m-1}\right)-12\right)\left(\frac{3\times3}{3+3-2}\right)^3+\left(30\left(2^{m-1}\right)-24\right)\left(\frac{3\times4}{3+4-2}\right)^3\\
&\quad+\left(9\left(2^{m-1}\right)-6\right)\left(\frac{4\times4}{4+4-2}\right)^3+\left(3\left(2^{m-1}\right)-3\right)\left(\frac{4\times6}{4+6-2}\right)^3\\
&= 6\left(2^{m-1}\right)2^3+6\left(2^{m-1}\right)2^3+\left(12\left(2^{m-1}\right)-12\right)\left(\frac{9}{4}\right)^3\\
&\quad+\left(30\left(2^{m-1}\right)-24\right)\left(\frac{12}{5}\right)^3+\left(9\left(2^{m-1}\right)-6\right)\left(\frac{8}{3}\right)^3+\left(3\left(2^{m-1}\right)-3\right)3^3\\
&= 2^{m-1}\left(48+48+136.6875+414.72+170.667\right)\\
&\quad+\left(-136.6875-331.776-113.7778-81\right),\\
&= 2^{m-1}\left(899.0742\right)-663.2413.
\end{aligned}
$$

Theorem 4.3 *SDCI of a network* ϖ *is given by*

$$SDCI = 2^{m-1}\left(135.999\right)-92.5.$$

Proof. By using Definition 2.3 and Table 2, we get

$$
\begin{aligned}
SDCI(\varpi) &= \sum_{d,k\in\mathbf{B}(\varpi)}\left[\frac{\min\left(\beta(d),\beta(k)\right)}{\max\left(\beta(d),\beta(k)\right)}+\frac{\max\left(\beta(d),\beta(k)\right)}{\min\left(\beta(d),\beta(k)\right)}\right]\\
&= \left|\mathbf{B}_{(2,2)}(\varpi)\right|\left[\frac{\min\left(\beta(d),\beta(k)\right)}{\max\left(\beta(d),\beta(k)\right)}+\frac{\max\left(\beta(d),\beta(k)\right)}{\min(\beta(d),\beta(k)}\right]\\
&\quad+\left|\mathbf{B}_{(2,3)}(\varpi)\right|\left[\frac{\min\left(\beta(d),\beta(k)\right)}{\max\left(\beta(d),\beta(k)\right)}+\frac{\max\left(\beta(d),\beta(k)\right)}{\min\left(\beta(d),\beta(k)\right)}\right]\\
&\quad+\left|\mathbf{B}_{(3,3)}(\varpi)\right|\left[\frac{\min\left(\beta(d),\beta(k)\right)}{\max\left(\beta(d),\beta(k)\right)}+\frac{\max\left(\beta(d),\beta(k)\right)}{\min(\beta(d),\beta(k)}\right]\\
&\quad+\left|\mathbf{B}_{(3,4)}(\varpi)\right|\left[\frac{\min\left(\beta(d),\beta(k)\right)}{\max\left(\beta(d),\beta(k)\right)}+\frac{\max\left(\beta(d),\beta(k)\right)}{\min\left(\beta(d),\beta(k)\right)}\right]\\
&\quad+\left|\mathbf{B}_{(4,4)}(\varpi)\right|\left[\frac{\min\left(\beta(d),\beta(k)\right)}{\max\left(\beta(d),\beta(k)\right)}+\frac{\max\left(\beta(d),\beta(k)\right)}{\min\left(\beta(d),\beta(k)\right)}\right]\\
&\quad+\left|\mathbf{B}_{(4,6)}(\varpi)\right|\left[\frac{\min\left(\beta(d),\beta(k)\right)}{\max\left(\beta(d),\beta(k)\right)}+\frac{\max\left(\beta(d),\beta(k)\right)}{\min\left(\beta(d),\beta(k)\right)}\right]
\end{aligned}
$$

$$
\begin{aligned}
&= 6\left(2^{k-1}\right)\left(\frac{\min(2,2)}{\max(2,2)}+\frac{\max(2,2)}{\min(2,2)}\right)\\
&\quad+6\left(2^{k-1}\right)\left(\frac{\min(2,3)}{\max(2,3)}+\frac{\max(2,3)}{\min(2,3)}\right)\\
&\quad+\left(12\left(2^{k-1}\right)-12\right)\left(\frac{\min(3,3)}{\max(3,3)}+\frac{\max(3,3)}{\min(3,3)}\right)\\
&\quad+\left(30\left(2^{k-1}\right)-24\right)\left(\frac{\min(3,4)}{\max(3,4)}+\frac{\max(3,4)}{\min(3,4)}\right)\\
&\quad+\left(9\left(2^{k-1}\right)-6\right)\left(\frac{\min(4,4)}{\max(4,4)}+\frac{\max(4,4)}{\min(4,4)}\right)\\
&\quad+\left(3\left(2^{k-1}\right)-3\right)\left(\frac{\min(4,6)}{\max(4,6)}+\frac{\max(4,6)}{\min(4,6)}\right)\\
&= 6\left(2^{m-1}\right)\left(\frac{2}{2}+\frac{2}{2}\right)+6\left(2^{m-1}\right)\left(\frac{2}{3}+\frac{3}{2}\right)\\
&\quad+\left(12\left(2^{m-1}\right)-12\right)\left(\frac{3}{3}+\frac{3}{3}\right)+\left(30\left(2^{m-1}\right)-24\right)\left(\frac{3}{4}+\frac{4}{3}\right)\\
&\quad+\left(9\left(2^{m-1}\right)-6\right)\left(\frac{4}{4}+\frac{4}{4}\right)+\left(3\left(2^{m-1}\right)-3\right)\left(\frac{4}{6}+\frac{6}{4}\right)\\
&= 6\left(2^{m-1}\right)(2)+6\left(2^{m-1}\right)(13)+\left[24\left(2^{m-1}\right)-24\right]\\
&\quad+\left[62.499\left(2^{m-1}\right)-50\right]+\left[18\left(2^{m-1}\right)-12\right]+\left[6.5\left(2^{m-1}\right)-6.5\right]\\
&= 2^{m-1}(12+13+24+62.499+18+6.5)+(-24-50-12-6.5)\\
&= 2^{m-1}(136)-92.5.
\end{aligned}
$$

Theorem 4.4 *GACI of a network* ϖ *is given by*

$$GACI = 2^{m-1}(65.5102)-44.6931.$$

Proof. By using Definition 2.4 and Table 2, we get

$$
\begin{aligned}
GACI(\varpi) &= \sum_{d,k\in\mathbf{B}(\varpi)}\frac{2\sqrt{\beta(d)\beta(k)}}{\beta(d)+\beta(k)}\\
&= \left|\mathbf{B}_{(2,2)}(\varpi)\right|\frac{2\sqrt{\beta(d)\beta(k)}}{\beta(d)+\beta(k)}+\left|\mathbf{B}_{(2,3)}(\varpi)\right|\frac{2\sqrt{\beta(d)\beta(k)}}{\beta(d)+\beta(k)}\\
&\quad+\left|\mathbf{B}_{(3,3)}(\varpi)\right|\frac{2\sqrt{\beta(d)\beta(k)}}{beta(d)+beta(k)}+\left|\mathbf{B}_{(3,4)}(\varpi)\right|\frac{2\sqrt{\beta(d)\beta(k)}}{\beta(d)+\beta(k)}\\
&\quad+\left|\mathbf{B}_{(4,4)}(\varpi)\right|\frac{2\sqrt{\beta(d)\beta(k)}}{\beta(d)+\beta(k)}+\left|\mathbf{B}_{(4,6)}(\varpi)\right|\frac{2\sqrt{\beta(d)\beta(k)}}{\beta(d)+\beta(k)}\\
&= 6\left(2^{m-1}\right)\frac{2\sqrt{2\times2}}{2+2}+6\left(2^{m-1}\right)\frac{2\sqrt{2\times3}}{2+3}\\
&\quad+\left(12\left(2^{m-1}\right)-12\right)\frac{2\sqrt{3\times3}}{3+3}+\left(30\left(2^{m-1}\right)-24\right)\frac{2\sqrt{3\times4}}{3+4}\\
&\quad+\left(9\left(2^{m-1}\right)-6\right)\frac{2\sqrt{4\times4}}{4+4}+\left(3\left(2^{m-1}\right)-3\right)\frac{2\sqrt{4\times6}}{4+6}
\end{aligned}
$$

$$
\begin{aligned}
&= 6\left(2^{m-1}\right)\frac{4}{4} + 6\left(2^{m-1}\right)\frac{2\sqrt{6}}{2} + \left(12\left(2^{m-1}\right)-12\right)\frac{6}{6} \\
&\quad + \left(30\left(2^{m-1}\right)-24\right)\frac{4\sqrt{3}}{7} + \left(9\left(2^{m-1}\right)-6\right)\frac{8}{8} + \left(3\left(2^{m-1}\right)-3\right)\frac{4\sqrt{6}}{10} \\
&= 2^{m-1}\left(6+5.8787+12+29.29.6922+9+2.9393\right) \\
&\quad + \left(-12-23.7538-6-2.9393\right), \\
&= 2^{m-1}\left(65.5102\right)-44.6931.
\end{aligned}
$$

Theorem 4.5 *HZCI of a network* ϖ *is given by*

$$HZCI = 2^{m-1}\left(3124\right)-2292.$$

Proof. By using Definition 2.5 and Table 2, we get

$$
\begin{aligned}
HZCI(\varpi) &= \sum_{d,k\in\mathbf{B}(\varpi)} \left[\beta(d)+\beta(k)\right]^2 \\
&= \left|\mathbf{B}_{(2,2)}(\varpi)\right|\left[\beta(d)+\beta(k)\right]^2 + \left|\mathbf{B}_{(2,3)}(\varpi)\right|\left[\beta(d)+\beta(k)\right]^2 \\
&\quad + \left|\mathbf{B}_{(3,3)}(\varpi)\right|\left[\beta(d)+\beta(k)\right]^2 + \left|\mathbf{B}_{(3,4)}(\varpi)\right|\left[\beta(d)+\beta(k)\right]^2 \\
&\quad + \left|\mathbf{B}_{(4,4)}(\varpi)\right|\left[\beta(d)+\beta(k)\right]^2 + \left|\mathbf{B}_{(4,6)}(\varpi)\right|\left[\beta(d)+\beta(k)\right]^2 \\
&= 6\left(2^{m-1}\right)(2+2)^2 + 6\left(2^{m-1}\right)(2+3)^2 \\
&\quad + \left(12\left(2^{m-1}\right)-12\right)(3+3)^2 + \left(30\left(2^{m-1}\right)-24\right)(3+4)^2 \\
&\quad + \left(12\left(2^{m-1}\right)-12\right)(4+4)^2 + \left(3\left(2^{m-1}\right)-3\right)(4+6)^2 \\
&= 2^{m-1}\left(96+150+432+1470+576+300\right) \\
&\quad + \left(-432-1176-384-300\right) \\
&= 2^{m-1}\left(3124\right)-2292.
\end{aligned}
$$

Theorem 4.6 *ISCI of a network* ϖ *is given by*

$$ISCI = 2^{m-1}\left(107.8285\right)-66.3428.$$

Proof. By using Definition 2.6 and Table 2, we get

$$
\begin{aligned}
ISCI(\varpi) &= \sum_{d,k\in\mathbf{B}(\varpi)} \left[\frac{\beta(d)\times\beta(k)}{\left(\beta(d)+\beta(k)\right)}\right] \\
&= \left|\mathbf{B}_{(2,2)}(\varpi)\right|\left[\frac{\beta(d)\times\beta(k)}{\left(\beta(d)+\beta(k)\right)}\right] + \left|\mathbf{B}_{(2,3)}(\varpi)\right|\left[\frac{\beta(d)\times\beta(k)}{\left(\beta(d)+\beta(k)\right)}\right] \\
&\quad + \left|\mathbf{B}_{(3,3)}(\varpi)\right|\left[\frac{\beta(d)\times\beta(k)}{\left(\beta(d)+\beta(k)\right)}\right] + \left|\mathbf{B}_{(3,4)}(\varpi)\right|\left[\frac{\beta(d)\times\beta(k)}{\left(\beta(d)+\beta(k)\right)}\right] \\
&\quad + \left|\mathbf{B}_{(4,4)}(\varpi)\right|\left[\frac{\beta(d)\times\beta(k)}{\left(\beta(d)+\beta(k)\right)}\right] + \left|\mathbf{B}_{(4,6)}(\varpi)\right|\left[\frac{\beta(d)\times\beta(k)}{\left(\beta(d)+\beta(k)\right)}\right] \\
&= 6\left(2^{m-1}\right)\left(\frac{2\times 2}{2+2}\right) + 6\left(2^{m-1}\right)\left(\frac{2\times 3}{2+3}\right) \\
&\quad + \left(12\left(2^{m-1}\right)-12\right)\left(\frac{3\times 3}{3+3}\right) + \left(30\left(2^{m-1}\right)-24\right)\left(\frac{3\times 4}{3+4}\right)
\end{aligned}
$$

$$\begin{aligned}
&+\left(9\left(2^{m-1}\right)-6\right)\left(\frac{4\times 4}{4+4}\right)+\left(3\left(2^{m-1}\right)-3\right)\left(\frac{4\times 6}{4+6}\right)\\
&=2^{m-1}\left(6+7.2+18+51.4285+18+7.2\right)\\
&\quad+\left(-18-41.1428-12-7.2\right)\\
&=2^{m-1}\left(107.8285\right)-66.3428.
\end{aligned}$$

Theorem 4.7 *ABCCI of a network* ϖ *is given by*

$$ABCCI=2^{m-1}\left(41.3614\right)-28.8861.$$

Proof. By using Definition 2.7 and Table 2, we get

$$\begin{aligned}
ABCCI\left(\varpi\right)&=\sum_{d,k\in\mathbf{B}(\varpi)}\sqrt{\frac{\beta(d)+\beta(k)-2}{\beta(d)\times\beta(k)}}\\
&=\left|\mathbf{B}_{(2,2)}\left(\varpi\right)\right|\sqrt{\frac{\beta(d)+\beta(k)-2}{\beta(d)\times\beta(k)}}+\left|\mathbf{B}_{(2,3)}\left(\varpi\right)\right|\sqrt{\frac{\beta(d)+\beta(k)-2}{\beta(d)\times\beta(d)}}\\
&\quad+\left|\mathbf{B}_{(3,3)}\left(\varpi\right)\right|\sqrt{\frac{\beta(d)+\beta(k)-2}{\beta(d)\times\beta(k)}}+\left|\mathbf{B}_{(3,4)}\left(\varpi\right)\right|\sqrt{\frac{\beta(d)+\beta(k)-2}{\beta(d)\times\beta(k)}}\\
&\quad+\left|\mathbf{B}_{(4,4)}\left(\varpi\right)\right|\sqrt{\frac{\beta(d)+\beta(k)-2}{\beta(d)\times\beta(k)}}+\left|\mathbf{B}_{(4,6)}\left(\varpi\right)\right|\sqrt{\frac{\beta(d)+\beta(k)-2}{\beta(d)\times\beta(k)}}\\
&=6\left(2^{m-1}\right)\sqrt{\frac{2+2-2}{2\times 2}}+6\left(2^{m-1}\right)\sqrt{\frac{2+3-2}{2\times 3}}\\
&\quad+\left[12\left(2^{m-1}\right)-12\sqrt{\frac{3+3-2}{3\times 3}}\right]+\left[30\left(2^{m-1}\right)-24\sqrt{\frac{3+4-2}{3\times 4}}\right]\\
&\quad+\left[9\left(2^{m-1}\right)-6\sqrt{\frac{4+4-2}{4\times 4}}\right]+\left[3\left(2^{m-1}\right)-3\sqrt{\frac{4+6-2}{4\times 6}}\right]\\
&=6\left(2^{m-1}\right)\sqrt{\frac{1}{2}}+6\left(2^{m-1}\right)\sqrt{\frac{1}{2}}+\left(12\left(2^{m-1}\right)-12\right)\sqrt{\frac{4}{9}}\\
&\quad+\left(30\left(2^{m-1}\right)-24\right)\sqrt{\frac{5}{12}}+\left(9\left(2^{m-1}\right)-6\right)\sqrt{\frac{6}{16}}+\left(3\left(2^{m-1}\right)-3\right)\sqrt{\frac{1}{3}}\\
&=2^{m-1}\left(4.2426+4.2426+8+19.3649+5.5113+1.7320\right)\\
&\quad+\left(-8-15.4919-3.6742-1.7320\right)\\
&=2^{m-1}\left(41.3614\right)-28.8861.
\end{aligned}$$

5. Comparative Analysis

5.1. Comparison among Nanostar Dendrimer of ZCIs

In this section, we will analyze the graphical and numerical comparisons of Nanostar dendrimers using connection-based *ZIs*, including *HCI*, *AZCI*, *SDCI*, *AGCI*, *HZCI*, *ISCI*, and *ABCCI*. We will refer to Table 3 for the numerical data, and the graphical representation is shown in Figure 4.

By examining both Table 3 and Figure 4, it becomes evident that the nanostar dendrimers and *HZCI* consistently achieve the highest values within this network. The graphical representation in Figure 4 illustrates that *HZCI* has a higher line than all the other *ZCIs* within the dendrimers network.

Table 3. Calculated connection-based *ZIs* values of Graph (ϖ) from $m = 1,2,3,\cdots,8$.

ZCIs	$m=1$	$m=2$	$m=3$	$m=4$	$m=5$	$m=6$	$m=7$	$m=8$
HCI	7.8643	28.6857	70.3285	153.6141	320.1853	653.27	1319.61	2652.18
AZCI	226.83	111.6907	2897.0556	6457.3523	13577.94	27819.13	56301.50	113266.25
SDCI	43.499	179.498	451.496	995.492	2083.48	4259.46	8611.43	17315.37
GACI	20.8171	86.3273	217.3477	479.3885	1003.47	2051.63	4147.95	8340.61
HZCI	832	3956	10204	22700	47692	97676	197644	397580
ISCI	41.4857	149.3142	364.9712	796.2852	1658.91	3384.16	3498.68	3735.70
ABCCI	12.4753	53.8367	136.5595	302.0051	632.89	1294.67	2618.24	5265.37

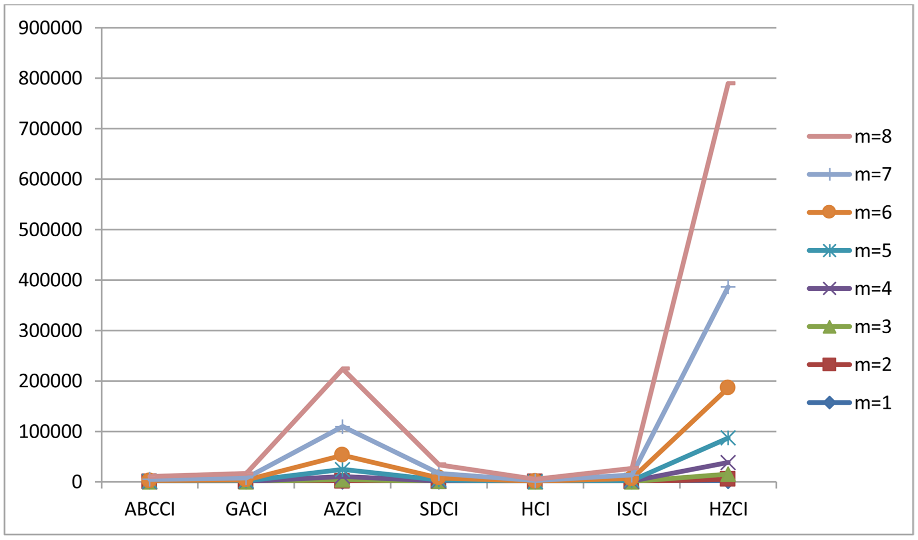

Figure 4. Graph (ϖ) for values of m ranging from $1,2,3,\cdots,8$.

5.2. Comparison between Nanostar Dendrimer and PPEI Dendrimer

In this section, we numerically compare connection-based *ZIs* values of nanostar dendrimer and PPEI dendrimer.

Table 4. Calculated connection-based *ZIs* values of Graph (Ω) from $m = 1,2,3,\cdots,8$ [22].

ZCIs	$m=1$	$m=2$	$m=3$	$m=4$	$m=5$	$m=6$	$m=7$	$m=8$
$ISCI(\Omega)$	24.86	77.93	184.06	396.33	820.86	1669.93	3368.07	6764.35
$GACI(\Omega)$	31.29	80.45	178.79	375.47	768.82	155.52	3128.93	6275.75
$HCI(\Omega)$	11.06	32.53	75.46	161.33	333.06	676.53	1363.47	2737.35
$ABCCI(\Omega)$	21.83	52.51	113.76	236.26	481.25	971.23	1951.20	3911.14
$HZCI(\Omega)$	752	2332	5492	11812	24452	49732	100292	201412
$SDCI(\Omega)$	53	153	353	753	1553	3153	6353	8681

In **Table 3**, we calculated all *ZCI* values of Nanostar dendrimer and in **Table 4** calculated *ZCI* values of PPEI dendrimer. So, we compare *ZCI* values (*ISCI*, *GACI*, *HCI*, *ABCCI*, *HZCI*, and *SDCI* and *AZCI*) of both dendrimers. We finalize the results of these dendrimers. The first *ISCI* has the highest value of PPEI dendrimer, followed by the Nanostar dendrimer. The *GACI* is the highest values of Nanostar dendrimer, HCI is the highest values of PPEI dendrimer, *ABCCI* is the highest value of Nanostar dendrimer, *HZCI* is the highest value of Nanostar dendrimer, *SDCI* is the highest value of Nanostar dendrimer and the last one *AZCI* single dendrimer highest value because PPEI denderimer could not find the indices. So, we observed that the *HZCI* has the highest value of both dendrimers. However, this indicates that the Nanostar dendrimer exhibits better chemical applicability compared to the PPEI dendrimer.

6. Concluding Remarks

We conclude our discussion with the following remarks.

1) This article presents the derived general expression for computing nanostar dendrimers using *ZCIs*, specifically *HCI*, *AZCI*, *SDCI*, *GACI*, *HZCI*, *ISCI*, and *ABCCI*. Furthermore, we have conducted a comparison of the aforementioned *ZCIs* of Nanostar dendrimer, and also numerically comparison of Nanostar dendrimer and PPEI dendrimer.

2) By examining using **Table 3** and **Figure 4**, HZCI is the highest value numerically and the highest line through graphically in Nanostar dendrimer. After numerically comparsion of Nanostar dendrimer and PPEI dendrimer, the Nanostar dendrimer has better chemical applicability compared to the PPEI dendrimer.

Future Directions

Advancement of nanostar dendrimers in targeted drug delivery, cancer therapy and diagnostics is their future. Their architecture increases biocompatibility, regulates drug release, and increases imaging. Other potential uses include antimicrobial agents, gene delivery, and tissue engineering. If the current research works out, nanostar dendrimers could change the course of nanomedicine, catalysis and environmental solutions by overcoming the limitations of scalability, toxicity and cost.

Data Availability

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

Conflicts of Interest

The authors have no conflict of interest regarding this article.

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