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Connection-Based Topological Aspect of PPIO and PPEI Dendrimers

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Abstract

Dendrimers are man-made polymeric macromolecules created from branching chains known as monomers. Topological indices (TIs) are molecular descriptors that define the structure and aid in establishing relationships with various physicochemical properties such as volatility, density, melting point, and more. TIs are categorized according to their distance, spectrum, and degree. Within these TIs, topological descriptors based on connection numbers (CN) hold significant importance. In this article, we calculate the overall outcomes of Zagreb connection indices, including the inverse sum connection index (ISCI), geometric arithmetic connection index (GACI), harmonic connection index (HCI), atom bond connectivity connection index (ABCCI), hyper Zagreb connection index (HZCI), and symmetric division connection index (SDCI) for the polypropyleneimine anoctamin (PPIO) dendrimer and Poly(Propyl) Ether Imine (PPEI) dendrimers. PPIO dendrimers and PPEI dendrimers are a new class of versatile nanostructured materials capable of exhibiting extraordinary physicochemical properties, which are closely related to their intricate tree-like architecture. PPIO dendrimers (synthesized using polypropylene imine) are relatively biocompatible and show promise as drug carriers, mainly because their core is hydrophobic with a hydrophilic surface. The PPEI dendrimers are highly soluble in alcohols and water and offer the ability to introduce a versatile range of functionalities. Their controlled structure, stability and tunable surface functionalities make these dendrimers attract much attention in several fields like biomedical applications, catalysis and nanotechnology. Additionally, a comparative analysis is performed to validate the excellence of our generated graphical and numerical outcomes.

Keywords

Topological Index (TI), Zagreb Index (ZI), Zagreb Connection Index (ZCIs),

Polypropyleneimine Anoctamin (PPIO) Dendrimer, Poly(Propyl) Ether Imine (PPEI) Dendrimers

1. Introduction

Dendrimers are highly branched, synthetic macromolecules with well-defined structures. Resembling miniature trees, they consist of a central core, branching units, and terminal function groups. Their precise architecture offers unique properties, making dendrimers versatile in drug delivery, nanotechnology and other fields due to their controlled size shape, and surface functionalities ref. [1]-[3]. Currently, scientists are focused on characterizing molecular structures using topological perspectives, specifically employing numerical graph descriptors. These graph invariants are widely employed to investigate the quantitative relationships between structure and activity (QSAR) as well as structure and property (QSPR) ref. [4].

A series of number represented by a matrix, polynomial or other number can be conceptualized as a graph. A number that describes the topology of molecules and facilitates the correlation of many of their physiochemical characteristics, including volatility, density, stability, flammability, and strain energy, is called topological index (TI). TIs have many applications in chemistry, pharmacology (D-Index), materials science (Wang-type) and molecular biology as shown in numerous research papers. These indices which are structural properties of molecular graphs serve as quantitative descriptors and help to interpret the structural property relationship at some level between a molecule and its characteristics. TIs have been utilized extensively in studying boiling point, melting point, density, solubility and many other properties of chemical compounds. They have applications in drug design field to predict biological activity and potential pharmacokinetics of new drugs candidate. TIs also have many usability in new nanomaterials and polymers design and characterization within materials science. Reaction mechanisms can also be studied using topological indices related to structural features of reactants and products. This is useful in organic chemistry, since the reaction pathways can be highly complicated and indices can serve as an aid for predicting possible products and intermediates. TIs can be classified into degree, distance, and polynomial categories. A distance-based TI focuses on the length between two nodes or vertices within a graph. Wiener ref. [5] introduced the concept of distance-based topological indices, notably the Wiener index, which stands as the pioneering and extensively researched index in the field. Wiener ref. [5] investigated the concept

of the first Zagreb index (ZI), which marked the inception of TIs theory. Following this breakthrough, various researchers investigated several TIs, employing these indices to delve into the molecular compound's physical and chemical Properties ref. [6] [7].

The atom bond connectivity (ABC) index was proposed by Estrada *et al.* ref. [8] in 1998. Ghorbani *et al.* ref. [9] then investigated the ABC index's fourth iteration. Geometric Arithmetic (GA) index was another noteworthy index introduction by Vukicevic and Furtula ref. [10] in 2009. Garaovoc *et al.* ref. [11] introduced the fifth version of the GA index, employing these indices to assess the chemical characteristics of dendrimers. In 2010, Vukicevic ref. [10] explored the innovative concept of a symmetric division degree (SSD) index. Fajtlowicz proposed the novel idea of the harmonic index (HI) ref. [12]. Gasperove and Vukicevc ref. [13] introduced the concept of the inverse sum (IS) index. Shirdel *et al.* ref. [14] innovatively proposed the notion of hyper (ZI). A recent development in graph theory is the invention of the connection number (CN) or leep degree of a vertex, that has garnered significant attention from researchers.

Ali and Trinnajstic ref. [15] introduced Zagreb Connection Indices (ZCIs) and employed octane isomers to assess their suitability. Additionally, Tang *et al.* ref. [16] applied ZCIs and modified versions to determine the outcomes of T-sum graphs. More recently, in 2020, Ali *et al.* ref. [17] computed modified ZCIs for T-sum graphs. Haoer *et al.* ref. [18] presented the concept of multiplicative leap ZIs, while Javaid *et al.* ref. [19] computed the multiplicative ZIs for various wheel-related graphs. Additionally, Bokhary *et al.* ref. [20] investigated the topological properties of certain nanostars. Bashir *et al.* ref. [21] computed the third Zagreb index (ZI) for a dendrimer nanostar. Additionally, Dorosti *et al.* ref. [22] determined the Cluj index for the first type of dendrimer nanostar. Gharibi *et al.* ref. [23] introduced the concept of Zagreb polynomials for nanotubes and nanocones. Moreover, in 2016, Siddiqui *et al.* ref. [24] proposed the Zagreb polynomial for Dendrimer nanostars.

The highly branching, Poly(propyl) Ether Imine (PPEI) and Polypropylene mine anoctamin (PPIO) dendrimers are two important families of macromolecules that have attracted interest due to their many uses in the domains of biotechnology and nanotechnology. PPEI dendrimers and are high-branched nanoscale polymers. These devices first appeared in the late 20th century within the context of research on dendrimers and other species that resemble them in some properties, such as inducing labile scaffolds. Dendrimers such as PPEI, have a tree-like structure which leads to generations of branching units from the central core. For these reasons, PPEI dendrimers were explored for applications as drug delivery vehicles and genetic vectors. Their tunability on the molecular level also assures their quality as versatile tools for a multitude of applications not least in nanomedicine and other high-tech areas.

In drug delivery systems, PPEI dendrimers are very helpful. They can improve the solubility and bioavailability of hydrophobic pharmaceuticals because of their branching structure and capacity to encapsulate medications. Potential candidates for antibacterial and antiviral coatings, PPIO dendrimers have intrinsic antimicrobial qualities due to their poly(phenyl imine oxide) surfaces. To stop infections and lower the chance of pathogen transmission, they can be applied to surgical

masks, medical equipment, and wound dressings. Because PPEI and PPIO dendrimers may form compounds with nucleic acids, preventing their degradation and promoting cellular absorption, they have demonstrated potential in gene delivery applications. These dendrimers are efficient gene therapy carriers because their positively charged surface groups may attach to negatively charged DNA or RNA.

PPIO dendrimer is a dendritic macromolecule explored in research for its unique properties and potential applications. The term "polypropylene mine" indicates a dendrimer with a polypropylene core, while "octamin" suggests eight amine groups on its periphery. This dendrimer's distinct architecture offers opportunities for diverse functionalities, making it a subject of interest in fields such as materials science. This article presents novel ZCIs specific to a distinctive class of dendrimer nanostars, known as PPIO and PPEI dendrimers. We conduct a numerical and graphical comparison of the outcomes of both dendrimers to assess the advantages of the suggested extension. Javaid and Sattar recently calculated the outcomes of modified (ZCIs) for PPIO and PPEI dendrimers ref. [25].

The structure of this article is as follows: Section 2 addresses the preparatory steps required for an exhaustive understanding of the main concepts presented in this paper. In Section 3, we calculate the ZCIs for the PPIO dendrimer structure and main results. In Section 4, we also calculate the ZCIs for the PPEI dendrimer structure and main results. Section 5 encompasses the computation of numerical and graphical results of PPEI and PPIO dendrimers. Section 6 is dedicated to summarizing the conclusions. Table 1 gives a collection of used acronyms in this paper.

Table 1. List of Acronyms.

Name	Acronyms
Topological index	TI
Zagreb index	ZI
Zagreb connection index	ZCI
Inverse sum connection index	ISCI
Geometric arithmetic connection index	GACI
Harmonic connection index	HCI
Atom bond connectivity connection index	ABCCI
Hyper Zagreb connection index	HZCI
Symmetric division connection index	SDCI
Polypropyleneimine anoctamin	PPIO
Poly(Propyl) Ether Imine	PPEI

2. Preliminaries

Definition 2.1. For a chemical structure $\wp$, then the ISCI is then describe:

$$\mathrm{ISCI}(\wp)=\sum_{c,m\in\mathcal{N}(\wp)}\left[\frac{\varrho(c)\times\varrho(m)}{\varrho(c)+\varrho(m)}\right]$$

$\varrho(c)$ and $\varrho(m)$ represent the CNs of vertices c and m, respectively.

Definition 2.2. In this chemical structure $\wp$, then the GACI is defined as:

$$\mathrm{GACI}(\wp)=\sum_{c,m\in\mathcal{N}(\wp)}\frac{2\sqrt{\varrho(c)\varrho(m)}}{\varrho(c)+\varrho(m)}$$

$\varrho(c)$ and $\varrho(m)$ represent the CNs of vertices c and m, correspondingly.

Definition 2.3. As to a chemical structure $\wp$, then the HCI is stated as:

$$\mathrm{HCI}(\wp)=\sum_{c,m\in\mathcal{N}}\left[\frac{2}{\varrho(c)+\varrho(m)}\right]$$

$\varrho(c)$ and $\varrho(m)$ represent the CNs of vertices c and m, correspondingly.

Definition 2.4. As to a chemical structure $\wp$, then the ABCCI is stated as:

$$\mathrm{ABCCI}(\wp)=\sum_{c,m\in\mathcal{N}}\sqrt{\frac{\varrho(c)+\varrho(m)-2}{\varrho(c)\times\varrho(m)}}$$

where $\varrho(c)$ and $\varrho(m)$ represent the CN s of vertices c and m, correspondingly.

Definition 2.5. As to a chemical structure $\wp$, then the HZCI is satated as:

$$\mathrm{HZCI}(\wp)=\sum_{c,m\in\mathcal{N}}\left[\varrho(c)+\varrho(m)\right]^2$$

where $\varrho(c)$ and $\varrho(m)$ represent the CNs of vertices c and m, correspondingly.

Definition 2.6. For a chemical structure $\wp$, then the SDCI defined as follows:

$$\mathrm{SDCI}(\wp)=\sum_{c,m\in\mathcal{N}}\left[\frac{\min(\varrho(c),\varrho(m))}{\max(\varrho(c),\varrho(m))}+\frac{\max(\varrho(c),\varrho(m))}{\min(\varrho(c),\varrho(m))}\right]$$

where $\min(\varrho(c),\varrho(m))$ is the minimum of $\varrho(c)$ and $\varrho(m)$ and $\max(\varrho(c),\varrho(m))$ is the maximum of $\varrho(c)$ and $\varrho(m)$.

3. Express the ZCIs for PPIO Dendrimers

In this section, we calculated ZCIs for the PPIO dendrimer, including ISCI, GACI, HCI, ABCCI, HZCI, and SDCI. The PPIO dendrimer exhibits three-dimensional growth, featuring five bonds in the core, as illustrated in Figure 1. Figure 2 shows the molecular shape of PPIO, represented as D[a] for a = 01, 02, 03 along with the connection number (CN) of each vertex.

Theorem 3.1: If $\wp$ represent a chemical structure, then the ISCI, is expressed as follows

$$\mathrm{ISCI}=2^a(18.5334)-15.2$$

Proof: From equation 2.1 and Table 2.

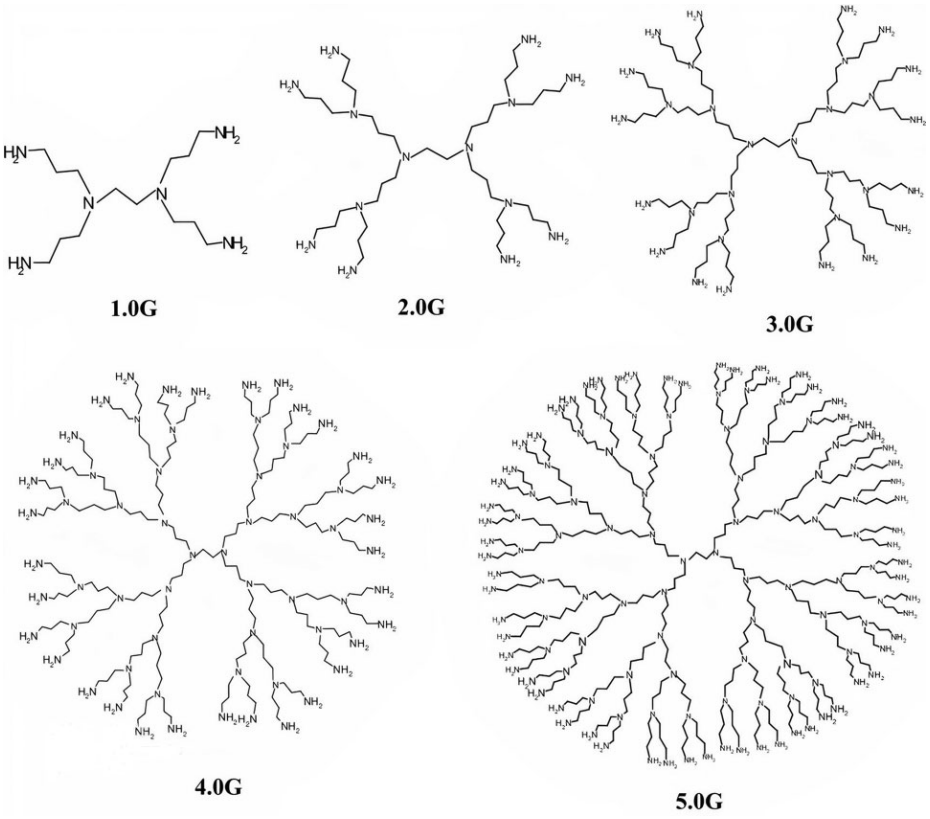

Figure 1. Chemical structural of PPIO dendrimer.

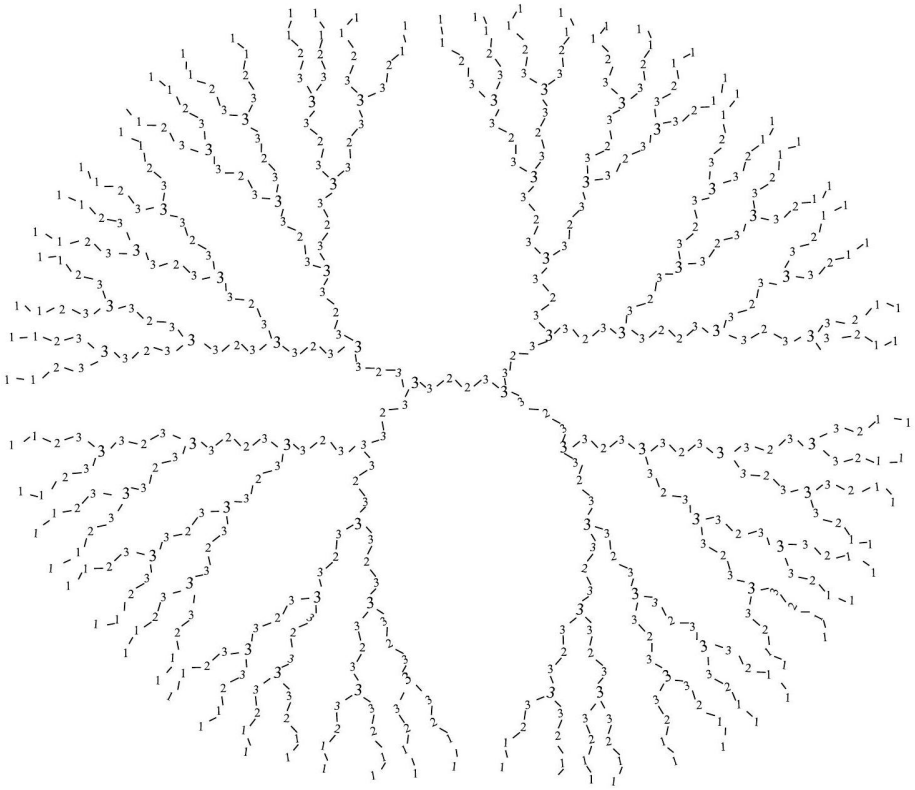

Figure 2. Chemical structure of (PPIO Dendrimer) D[a] together with CN is 1, 2, 3.

Table 2. The total number of edges in connection-based.

S.R	$\left\lvert \aleph_{(n_1,n_2)}(\wp) \right\rvert$	Number of Connection
1	$\left\lvert \aleph_{(1,1)}(\wp) \right\rvert$	$2\left(2^a\right)$
2	$\left\lvert \aleph_{(1,1)}(\wp) \right\rvert$	$2\left(2^a\right)$
3	$\left\lvert \aleph_{(1,1)}(\wp) \right\rvert$	(1)
4	$\left\lvert \aleph_{(1,1)}(\wp) \right\rvert$	$6\left(2^a-1\right)$
5	$\left\lvert \aleph_{(1,1)}(\wp) \right\rvert$	$6\left(2^a-1\right)$

$$\begin{aligned}
\mathrm{ISCI}(\wp) &= \sum_{\mathrm{c,m}\in\aleph(\wp)}\left[\frac{\varrho(\mathrm{c})\times\varrho(\mathrm{m})}{\varrho(\mathrm{c})+\varrho(\mathrm{m})}\right] \\
&= \left\lvert \aleph_{(1,1)}(\wp)\right\rvert\left[\frac{\varrho(\mathrm{c})\times\varrho(\mathrm{m})}{\varrho(\mathrm{c})+\varrho(\mathrm{m})}\right]+\left\lvert \aleph_{(1,2)}(\wp)\right\rvert\left[\frac{\varrho(\mathrm{c})\times\varrho(\mathrm{m})}{\varrho(\mathrm{c})+\varrho(\mathrm{m})}\right] \\
&\quad +\left\lvert \aleph_{(2,2)}(\wp)\right\rvert\left[\frac{\varrho(\mathrm{c})\times\varrho(\mathrm{m})}{\varrho(\mathrm{c})+\varrho(\mathrm{m})}\right]+\left\lvert \aleph_{(2,3)}(\wp)\right\rvert\left[\frac{\varrho(\mathrm{c})\times\varrho(\mathrm{m})}{\varrho(\mathrm{c})+\varrho(\mathrm{m})}\right] \\
&\quad +\left\lvert \aleph_{(3,3)}(\wp)\right\rvert\left[\frac{\varrho(\mathrm{c})\times\varrho(\mathrm{m})}{\varrho(\mathrm{c})+\varrho(\mathrm{m})}\right] \\
&= 2\left(2^a\right)\left(\frac{1\times1}{1+1}\right)+2\left(2^a\right)\left(\frac{1\times2}{1+2}\right)+(1)\left(\frac{2\times2}{2+2}\right) \\
&\quad +6\left(2^a-1\right)\left(\frac{2\times3}{2+3}\right)+6\left(2^a-1\right)\left(\frac{3\times3}{3+3}\right) \\
&= 2^a\left(1+1.3334+7.2+9\right)+\left(1-9-7.2\right) \\
&= 2^a\left(18.5334\right)-15.2
\end{aligned}$$

Theorem 3.2: If $\wp$ represent a chemical structure, then the GACI is expressed as follows

$$\mathrm{GACI} = 2^a\left(15.7644-10.8788\right)$$

Proof: From equation 2.2 and Table 2.

$$\begin{aligned}
\mathrm{GACI}(\wp) &= \sum_{\mathrm{c,m}\in\aleph(\wp)}\frac{2\sqrt{\varrho(\mathrm{c})\varrho(\mathrm{m})}}{\varrho(\mathrm{c})+\varrho(\mathrm{m})} \\
&= \left\lvert \aleph_{(1,1)}(\wp)\right\rvert\frac{2\sqrt{\varrho(\mathrm{c})\varrho(\mathrm{m})}}{\varrho(\mathrm{c})+\varrho(\mathrm{m})}+\left\lvert \aleph_{(1,2)}(\wp)\right\rvert\frac{2\sqrt{\varrho(\mathrm{c})\varrho(\mathrm{m})}}{\varrho(\mathrm{c})+\varrho(\mathrm{m})} \\
&\quad +\left\lvert \aleph_{(2,2)}(\wp)\right\rvert\frac{2\sqrt{\varrho(\mathrm{c})\varrho(\mathrm{m})}}{\varrho(\mathrm{c})+\varrho(\mathrm{m})}+\left\lvert \aleph_{(2,3)}(\wp)\right\rvert\frac{2\sqrt{\varrho(\mathrm{c})\varrho(\mathrm{m})}}{\varrho(\mathrm{c})+\varrho(\mathrm{m})} \\
&\quad +\left\lvert \aleph_{(3,3)}(\wp)\right\rvert\frac{2\sqrt{\varrho(\mathrm{c})\varrho(\mathrm{m})}}{\varrho(\mathrm{c})+\varrho(\mathrm{m})}
\end{aligned}$$

$$
\begin{aligned}
&= 2\left(2^{a}\right)\frac{2\sqrt{1\times 1}}{1+1} + 2\left(2^{a}\right)\frac{2\sqrt{1\times 2}}{1+2} + (1)\frac{2\sqrt{2\times 2}}{2+2} \\
&\quad + 6\left(2^{a}-1\right)\frac{2\sqrt{2\times 3}}{2+3} + 6\left(2^{a}-1\right)\frac{2\sqrt{3\times 3}}{3+3} \\
&= 2^{a}\left(2+1.8856+6+295.8788\right)+\left(1-5.8788-6\right) \\
&= 2^{a}\left(15.7644\right)-10.8788
\end{aligned}
$$

Theorem 3.3: If $\wp$ represent a chemical structure, then the HCI is expressed as follows

$$\mathrm{HCI} = 2^{a}\left(6.7334\right)-3.9$$

Proof: From equation 2.3 and Table 2.

$$
\begin{aligned}
\mathrm{HCI}(\wp) &= \sum\nolimits_{\mathrm{c,m}\in\aleph(\wp)}\left[\frac{2}{\varrho(\mathrm{c})+\varrho(\mathrm{m})}\right] \\
&= \left|\aleph_{(1,1)}(\wp)\right|\left[\frac{2}{\varrho(\mathrm{c})+\varrho(\mathrm{m})}\right] + \left|\aleph_{(1,2)}(\wp)\right|\left[\frac{2}{\varrho(\mathrm{c})+\varrho(\mathrm{m})}\right] \\
&\quad + \left|\aleph_{(2,2)}(\wp)\right|\left[\frac{2}{\varrho(\mathrm{c})+\varrho(\mathrm{m})}\right] + \left|\aleph_{(2,3)}(\wp)\right|\left[\frac{2}{\varrho(\mathrm{c})+\varrho(\mathrm{m})}\right] \\
&\quad + \left|\aleph_{(3,3)}(\wp)\right|\left[\frac{2}{\varrho(\mathrm{c})+\varrho(\mathrm{m})}\right] \\
&= 2\left(2^{a}\right)\left(\frac{2}{1+1}\right) + 2\left(2^{a}\right)\left(\frac{2}{1+2}\right) + (1)\left(\frac{2}{2+2}\right) \\
&\quad + 6\left(2^{a}-1\right)\left(\frac{2}{2+3}\right) + 6\left(2^{a}-1\right)\left(\frac{2}{3+3}\right) \\
&= 2^{a}\left(1+1.3334+2.4+2\right)+\left(0.5-2.4-2\right) \\
&= 2^{a}\left(6.7334\right)-3.9
\end{aligned}
$$

Theorem 3.4: If $\wp$ represent a chemical structure, then the ABCCI is expressed as follows

$$\mathrm{ABCCI} = 2^{a}\left(9.657\right)-7.5357\,.$$

Proof: From equation 2.4 and referencing Table 2.

$$
\begin{aligned}
\mathrm{ABCCI}(\wp) &= \sum\nolimits_{\mathrm{c,m}\in\aleph(\wp)}\sqrt{\frac{\varrho(\mathrm{c})+\varrho(\mathrm{m})-2}{\varrho(\mathrm{c})\times\varrho(\mathrm{m})}} \\
&= \left|\aleph_{(1,1)}(\wp)\right|\sqrt{\frac{\varrho(\mathrm{c})+\varrho(\mathrm{m})-2}{\varrho(\mathrm{c})\times\varrho(\mathrm{m})}} + \left|\aleph_{(1,2)}(\wp)\right|\sqrt{\frac{\varrho(\mathrm{c})+\varrho(\mathrm{m})-2}{\varrho(\mathrm{c})\times\varrho(\mathrm{m})}} \\
&\quad + \left|\aleph_{(2,2)}(\wp)\right|\sqrt{\frac{\varrho(\mathrm{c})+\varrho(\mathrm{m})-2}{\varrho(\mathrm{c})\times\varrho(\mathrm{m})}} + \left|\aleph_{(2,3)}(\wp)\right|\sqrt{\frac{\varrho(\mathrm{c})+\varrho(\mathrm{m})-2}{\varrho(\mathrm{c})\times\varrho(\mathrm{m})}} \\
&\quad + \left|\aleph_{(3,3)}(\wp)\right|\sqrt{\frac{\varrho(\mathrm{c})+\varrho(\mathrm{m})-2}{\varrho(\mathrm{c})\times\varrho(\mathrm{m})}} \\
&= 2\left(2^{a}\right)\sqrt{\frac{1+1-2}{1\times 1}} + 2\left(2^{a}\right)\sqrt{\frac{1+2-2}{1\times 2}} + (1)\sqrt{\frac{2+2-2}{2\times 2}}
\end{aligned}
$$

$$+6\left(2^{a}-1\right)\sqrt{\frac{2+3-2}{2\times 3}}+6\left(2^{a}-1\right)\sqrt{\frac{3+3-2}{3\times 3}}$$
$$=2^{a}\left(1.4142+4.2426+4.0002\right)+\left(0.7071-4.2426-4.0002\right)$$
$$=2^{a}\left(9.657\right)-7.5357$$

Theorem 3.5. If $\wp$ represent a chemical structure, then the HZCI is expressed as follows

$$\mathrm{HZCI}=2^{a}\left(662\right)-620$$

Proof: From equation 2.5 and Table 2.

$$\mathrm{HZCI}\left(\wp\right)=\sum_{\mathrm{c,m}\in\aleph\left(\wp\right)}\left[\varrho\left(\mathrm{c}\right)+\varrho\left(\mathrm{m}\right)\right]^{2}$$
$$=\left|\aleph_{(1,1)}\left(\wp\right)\right|\left[\varrho\left(\mathrm{c}\right)+\varrho\left(\mathrm{m}\right)\right]^{2}+\left|\aleph_{(1,2)}\left(\wp\right)\right|\left[\varrho\left(\mathrm{c}\right)+\varrho\left(\mathrm{m}\right)\right]^{2}$$
$$+\left|\aleph_{(2,2)}\left(\wp\right)\right|\left[\varrho\left(\mathrm{c}\right)+\varrho\left(\mathrm{m}\right)\right]^{2}+\left|\aleph_{(2,3)}\left(\wp\right)\right|\left[\varrho\left(\mathrm{c}\right)+\varrho\left(\mathrm{m}\right)\right]^{2}$$
$$+\left|\aleph_{(3,3)}\left(\wp\right)\right|\left[\varrho\left(\mathrm{c}\right)+\varrho\left(\mathrm{m}\right)\right]^{2}$$
$$=2\left(2^{a}\right)\left(1+1\right)^{2}+2\left(2^{a}\right)\left(1+2\right)^{2}+\left(1\right)\left(2+2\right)^{2}$$
$$+6\left(2^{a}-1\right)\left(2+3\right)^{2}+6\left(2^{a}-1\right)\left(3+3\right)^{2}$$
$$=2^{a}\left(8+18+150+486\right)+\left(16-150-486\right)$$
$$=2^{a}\left(662\right)-620$$

Theorem 3.6. If $\wp$ represent a chemical structure, then the SDCI is expressed as follows

$$\mathrm{SDCI}=2^{a}\left(34\right)-23$$

Proof: From equation 2.6 and Table 2.

$$\mathrm{SDCI}\left(\wp\right)=\sum_{\mathrm{c,m}\in\aleph\left(\wp\right)}\left[\frac{\min\left(\varrho\left(\mathrm{c}\right),\varrho\left(\mathrm{m}\right)\right)}{\max\left(\varrho\left(\mathrm{c}\right),\varrho\left(\mathrm{m}\right)\right)}+\frac{\max\left(\varrho\left(\mathrm{c}\right),\varrho\left(\mathrm{m}\right)\right)}{\min\left(\varrho\left(\mathrm{c}\right),\varrho\left(\mathrm{m}\right)\right)}\right]$$
$$=\left|\aleph_{(1,1)}\left(\wp\right)\right|\left[\frac{\min\left(\varrho\left(\mathrm{c}\right),\varrho\left(\mathrm{m}\right)\right)}{\max\left(\varrho\left(\mathrm{c}\right),\varrho\left(\mathrm{m}\right)\right)}+\frac{\max\left(\varrho\left(\mathrm{c}\right),\varrho\left(\mathrm{m}\right)\right)}{\min\left(\varrho\left(\mathrm{c}\right),\varrho\left(\mathrm{m}\right)\right)}\right]$$
$$+\left|\aleph_{(1,2)}\left(\wp\right)\right|\left[\frac{\min\left(\varrho\left(\mathrm{c}\right),\varrho\left(\mathrm{m}\right)\right)}{\max\left(\varrho\left(\mathrm{c}\right),\varrho\left(\mathrm{m}\right)\right)}+\frac{\max\left(\varrho\left(\mathrm{c}\right),\varrho\left(\mathrm{m}\right)\right)}{\min\left(\varrho\left(\mathrm{c}\right),\varrho\left(\mathrm{m}\right)\right)}\right]$$
$$+\left|\aleph_{(2,2)}\left(\wp\right)\right|\left[\frac{\min\left(\varrho\left(\mathrm{c}\right),\varrho\left(\mathrm{m}\right)\right)}{\max\left(\varrho\left(\mathrm{c}\right),\varrho\left(\mathrm{m}\right)\right)}+\frac{\max\left(\varrho\left(\mathrm{c}\right),\varrho\left(\mathrm{m}\right)\right)}{\min\left(\varrho\left(\mathrm{c}\right),\varrho\left(\mathrm{m}\right)\right)}\right]$$
$$+\left|\aleph_{(2,3)}\left(\wp\right)\right|\left[\frac{\min\left(\varrho\left(\mathrm{c}\right),\varrho\left(\mathrm{m}\right)\right)}{\max\left(\varrho\left(\mathrm{c}\right),\varrho\left(\mathrm{m}\right)\right)}+\frac{\max\left(\varrho\left(\mathrm{c}\right),\varrho\left(\mathrm{m}\right)\right)}{\min\left(\varrho\left(\mathrm{c}\right),\varrho\left(\mathrm{m}\right)\right)}\right]$$
$$+\left|\aleph_{(3,3)}\left(\wp\right)\right|\left[\frac{\min\left(\varrho\left(\mathrm{c}\right),\varrho\left(\mathrm{m}\right)\right)}{\max\left(\varrho\left(\mathrm{c}\right),\varrho\left(\mathrm{m}\right)\right)}+\frac{\max\left(\varrho\left(\mathrm{c}\right),\varrho\left(\mathrm{m}\right)\right)}{\min\left(\varrho\left(\mathrm{c}\right),\varrho\left(\mathrm{m}\right)\right)}\right]$$
$$=2\left(2^{a}\right)\left(\frac{\min\left(1,1\right)}{\max\left(1,1\right)}+\frac{\max\left(1,1\right)}{\min\left(1,1\right)}\right)+2\left(2^{a}\right)\left(\frac{\min\left(1,2\right)}{\max\left(1,2\right)}+\frac{\max\left(1,2\right)}{\min\left(1,2\right)}\right)$$

$$+(1)\left(\frac{\min(2,2)}{\max(2,2)}+\frac{\max(2,2)}{\min(2,2)}\right)+6\left(2^a-1\right)\left(\frac{\min(2,3)}{\max(2,3)}+\frac{\max(2,3)}{\min(2,3)}\right)$$

$$+6\left(2^a-1\right)\left(\frac{\min(3,3)}{\max(3,3)}+\frac{\max(3,3)}{\min(3,3)}\right)$$

$$=2\left(2^a\right)(2)+2\left(2^a\right)\left(\frac{5}{2}\right)+(1)(2)+6\left(2^a-1\right)\left(\frac{13}{6}\right)+6\left(2^a-1\right)(2)$$

$$=2^a\left(4+5+13+12\right)+\left(2-13-12\right)$$

$$=2^a\left(34\right)-23$$

4. Express the ZCIs for PPEI Dendrimers

In this segment, we calculated ZCIs for the PPEI dendrimer, including ISCI, GACI, HCI, ABCCI, HZCI, and SDCI. The PPIO dendrimer exhibits three-dimensional growth, featuring five bonds in the core, as illustrated in Figure 3. Figure 4 show the molecular shape of PPEI, represented as D[a] for a = 01, 02, 03 along with the connection number (CN) of each vertex.

Theorem 4.1: If ϖ represent a chemical structure, then the ISCI, is expressed as follows

$$\mathrm{ISCI}=2^a\left(26.5334\right)-28.2$$

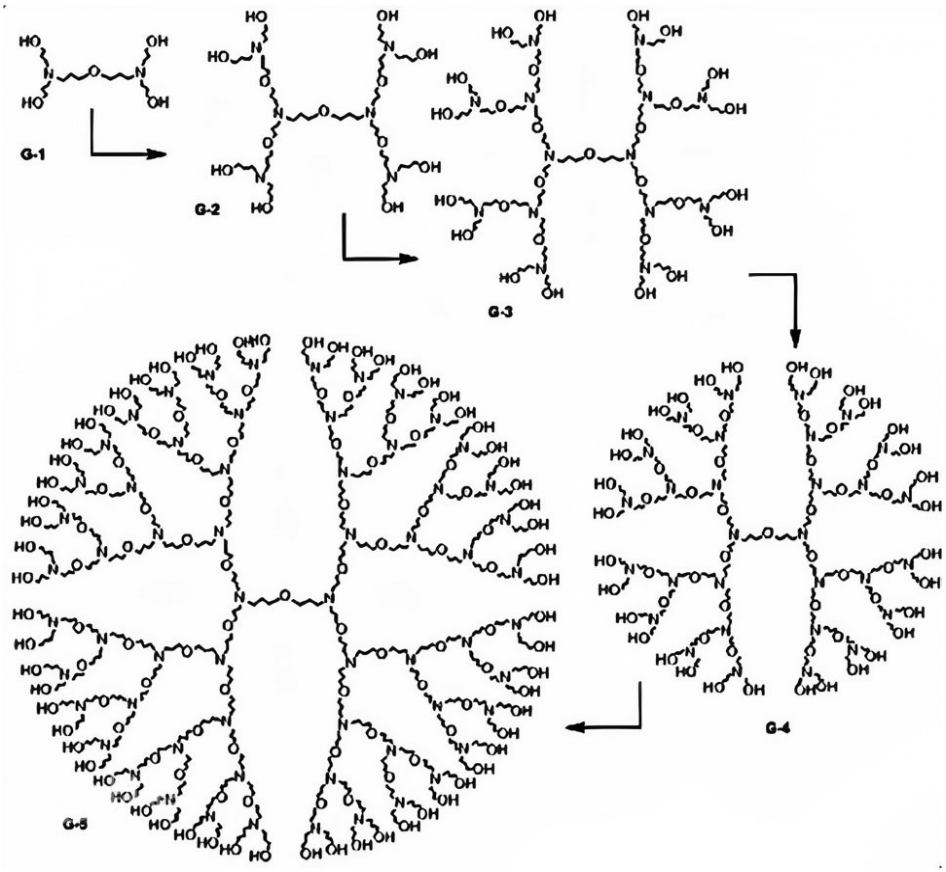

Figure 3. Chemical structural of PPEI Dendrimer.

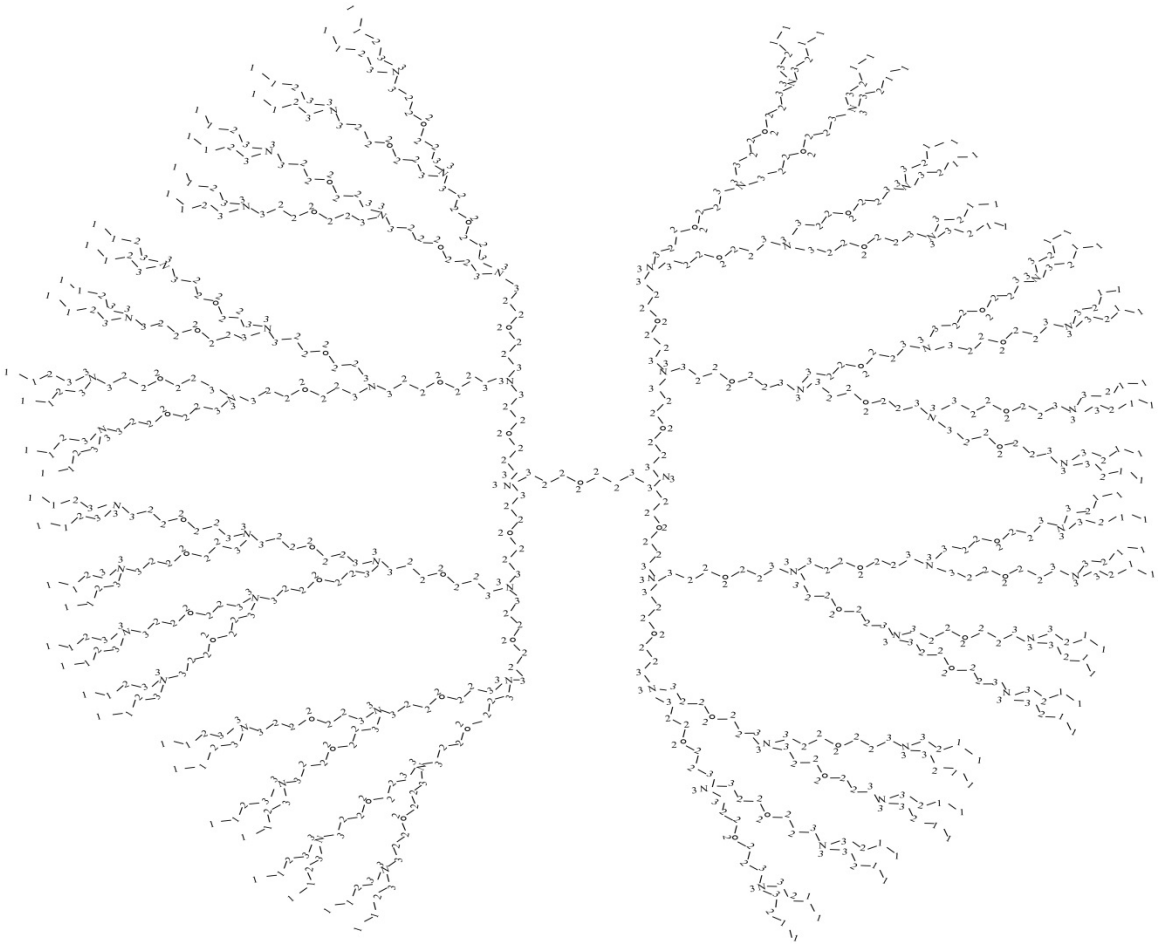

Figure 4. Chemical structure of (PPEI Dendrimer) D[a] together with CN is 1, 2, 3.

Table 3. The total number of edges in connection based.

S.R	$\lvert\aleph_{(n_1,n_2)}(\varpi)\rvert$	Number of Connection
1	$\lvert\aleph_{(1,1)}(\varpi)\rvert$	$2(2^a)$
2	$\lvert\aleph_{(1,1)}(\varpi)\rvert$	$2(2^a)$
3	$\lvert\aleph_{(1,1)}(\varpi)\rvert$	$8(2^a)-12$
4	$\lvert\aleph_{(1,1)}(\varpi)\rvert$	$6(2^a-1)$
5	$\lvert\aleph_{(1,1)}(\varpi)\rvert$	$6(2^a-1)$

Proof: From equation 2.1 and Table 3.

$$\mathrm{ISCI}(\varpi)=\sum_{c,m\in\aleph(\varpi)}\left[\frac{\varrho(c)\times\varrho(m)}{\varrho(c)+\varrho(m)}\right]$$

$$=\left|\aleph_{(1,1)}(\varpi)\right|\left[\frac{\varrho(c)\times\varrho(m)}{\varrho(c)+\varrho(m)}\right]+\left|\aleph_{(1,2)}(\varpi)\right|\left[\frac{\varrho(c)\times\varrho(m)}{\varrho(c)+\varrho(m)}\right]$$

$$+\left|\aleph_{(2,2)}(\varpi)\right|\left[\frac{\varrho(c)\times\varrho(m)}{\varrho(c)+\varrho(m)}\right]+\left|\aleph_{(2,3)}(\varpi)\right|\left[\frac{\varrho(c)\times\varrho(m)}{\varrho(c)+\varrho(m)}\right]$$
$$+\left|\aleph_{(3,3)}(\varpi)\right|\left[\frac{\varrho(c)\times\varrho(m)}{\varrho(c)+\varrho(m)}\right]$$
$$=2\left(2^{a}\right)\left(\frac{1\times1}{1+1}\right)+2\left(2^{a}\right)\left(\frac{1\times2}{1+2}\right)+\left(8\left(2^{a}\right)-12\right)\left(\frac{2\times2}{2+2}\right)$$
$$+6\left(2^{a}-1\right)\left(\frac{2\times3}{2+3}\right)+6\left(2^{a}-1\right)\left(\frac{3\times3}{3+3}\right)$$
$$=2^{a}\left(1+1.3334+7.2+9+8\right)+\left(-9-7.2-12\right)$$
$$=2^{a}\left(26.5334\right)-28.2$$

Theorem 4.2: If ϖ represent a chemical structure, then the GACI is expressed as follows

$$\mathrm{GACI}=2^{a}\left(23.7644\right)-17.8788$$

Proof: From equation 2.2 and Table 3.

$$\mathrm{ISCI}(\varpi)=\sum_{c,m\in\aleph(\varpi)}\frac{2\sqrt{\varrho(c)\varrho(m)}}{\varrho(c)+\varrho(m)}$$
$$=\left|\aleph_{(1,1)}(\varpi)\right|\frac{2\sqrt{\varrho(c)\varrho(m)}}{\varrho(c)+\varrho(m)}+\left|\aleph_{(1,2)}(\varpi)\right|\frac{2\sqrt{\varrho(c)\varrho(m)}}{\varrho(c)+\varrho(m)}$$
$$+\left|\aleph_{(2,2)}(\varpi)\right|\frac{2\sqrt{\varrho(c)\varrho(m)}}{\varrho(c)+\varrho(m)}+\left|\aleph_{(2,3)}(\varpi)\right|\frac{2\sqrt{\varrho(c)\varrho(m)}}{\varrho(c)+\varrho(m)}$$
$$+\left|\aleph_{(3,3)}(\varpi)\right|\frac{2\sqrt{\varrho(c)\varrho(m)}}{\varrho(c)+\varrho(m)}=$$
$$=2\left(2^{a}\right)\frac{2\sqrt{1\times1}}{1+1}+2\left(2^{a}\right)\frac{2\sqrt{1\times2}}{1+2}+\left(8\left(2^{a}\right)-12\right)\frac{2\sqrt{2\times2}}{2+2}$$
$$=6\left(2^{a}-1\right)\frac{2\sqrt{2\times3}}{2+3}+6\left(2^{a}-1\right)\frac{2\sqrt{3\times3}}{3+3}$$
$$=2^{a}\left(2+1.8856+6+5.8788+8\right)+\left(-6-5.8788-6\right)$$
$$=2^{a}\left(23.7644\right)-17.8788$$

Theorem 4.3: If ϖ represent a chemical structure, then the HCI is expressed as follows

$$\mathrm{HCI}=2^{a}\left(10.7334\right)-10.4$$

Proof: From equation 2.3 and Table 3

$$\mathrm{ISCI}(\varpi)=\sum_{c,m\in\aleph(\varpi)}\left[\frac{2}{\varrho(c)+\varrho(m)}\right]$$
$$=\left|\aleph_{(1,1)}(\varpi)\right|\left[\frac{2}{\varrho(c)+\varrho(m)}\right]+\left|\aleph_{(1,2)}(\varpi)\right|\left[\frac{2}{\varrho(c)+\varrho(m)}\right]$$
$$+\left|\aleph_{(2,2)}(\varpi)\right|\left[\frac{2}{\varrho(c)+\varrho(m)}\right]+\left|\aleph_{(2,3)}(\varpi)\right|\left[\frac{2}{\varrho(c)+\varrho(m)}\right]$$

$$
\begin{aligned}
&+\left|\aleph_{(3,3)}(\varpi)\right|\left[\frac{2}{\varrho(\mathrm{c})+\varrho(\mathrm{m})}\right]\\
&=2\left(2^{a}\right)\left(\frac{2}{1+1}\right)+2\left(2^{a}\right)\left(\frac{2}{1+2}\right)+\left(8\left(2^{a}\right)-12\right)\left(\frac{2}{2+2}\right)\\
&+6\left(2^{a}-1\right)\left(\frac{2}{2+3}\right)+6\left(2^{a}-1\right)\left(\frac{2}{3+3}\right)\\
&=2^{a}\left(2+1.334+2.4+2+3\right)+\left(-2.4-2-6\right)\\
&=2^{a}\left(10.7334\right)-10.4
\end{aligned}
$$

Theorem 4.4: If ϖ represent a chemical structure, then the ABCCI is expressed as follows

$$\mathrm{ABCCI}=2^{a}\left(15.312\right)-8.7294\,.$$

Proof: From equation 2.4 and Table 3

$$
\begin{aligned}
\mathrm{ABCCI}(\varpi)&=\sum_{\mathrm{c,m}\in\aleph(\varpi)}\sqrt{\frac{\varrho(\mathrm{c})+\varrho(\mathrm{m})-2}{\varrho(\mathrm{c})\times\varrho(\mathrm{m})}}\\
&=\left|\aleph_{(1,1)}(\varpi)\right|\sqrt{\frac{\varrho(\mathrm{c})+\varrho(\mathrm{m})-2}{\varrho(\mathrm{c})\times\varrho(\mathrm{m})}}+\left|\aleph_{(1,2)}(\varpi)\right|\sqrt{\frac{\varrho(\mathrm{c})+\varrho(\mathrm{m})-2}{\varrho(\mathrm{c})\times\varrho(\mathrm{m})}}\\
&+\left|\aleph_{(2,2)}(\varpi)\right|\sqrt{\frac{\varrho(\mathrm{c})+\varrho(\mathrm{m})-2}{\varrho(\mathrm{c})\times\varrho(\mathrm{m})}}+\left|\aleph_{(2,3)}(\varpi)\right|\sqrt{\frac{\varrho(\mathrm{c})+\varrho(\mathrm{m})-2}{\varrho(\mathrm{c})\times\varrho(\mathrm{m})}}\\
&+\left|\aleph_{(3,3)}(\varpi)\right|\sqrt{\frac{\varrho(\mathrm{c})+\varrho(\mathrm{m})-2}{\varrho(\mathrm{c})\times\varrho(\mathrm{m})}}\\
&=2\left(2^{a}\right)\sqrt{\frac{1+1-2}{1\times1}}+2\left(2^{a}\right)\sqrt{\frac{1+2-2}{1\times2}}+\left(8\left(2^{a}\right)-12\right)\sqrt{\frac{2+2-2}{2\times2}}\\
&+6\left(2^{a}-1\right)\sqrt{\frac{2+3-2}{2\times3}}+6\left(2^{a}-1\right)\sqrt{\frac{3+3-2}{3\times3}}\\
&=2^{a}\left(1.4142+4.2426+4.2226+3.9984\right)\\
&+\left(-4.2426-3.9984-8.4852\right)\\
&=2^{a}\left(15.312\right)-8.7294
\end{aligned}
$$

Theorem 4.5: If ϖ represent a chemical structure, then the HZCI is expressed as follows

$$\mathrm{HZCI}=2^{a}\left(790\right)-828$$

Proof: From equation 2.5 and Table 3

$$
\begin{aligned}
\mathrm{HZCI}(\varpi)&=\sum_{\mathrm{c,m}\in\aleph(\varpi)}\left[\varrho(\mathrm{c})+\varrho(\mathrm{m})\right]^{2}\\
&=\left|\aleph_{(1,1)}(\varpi)\right|\left[\varrho(\mathrm{c})+\varrho(\mathrm{m})\right]^{2}+\left|\aleph_{(1,2)}(\varpi)\right|\left[\varrho(\mathrm{c})+\varrho(\mathrm{m})\right]^{2}\\
&+\left|\aleph_{(2,2)}(\varpi)\right|\left[\varrho(\mathrm{c})+\varrho(\mathrm{m})\right]^{2}+\left|\aleph_{(2,3)}(\varpi)\right|\left[\varrho(\mathrm{c})+\varrho(\mathrm{m})\right]^{2}\\
&+\left|\aleph_{(3,3)}(\varpi)\right|\left[\varrho(\mathrm{c})+\varrho(\mathrm{m})\right]^{2}\\
&=2\left(2^{a}\right)(1+1)^{2}+2\left(2^{a}\right)(1+2)^{2}+\left(8\left(2^{a}\right)-12\right)(2+2)^{2}
\end{aligned}
$$

$$
\begin{aligned}
&+6\left(2^{a}-1\right)(2+3)^{2}+6\left(2^{a}-1\right)(3+3)^{2}\\
&=2^{a}(8+18+150+486+128)+(-150-486-192)\\
&=2^{a}(790)-828
\end{aligned}
$$

Theorem 4.6. If ϖ represent a Chemical structure, then the SDCI is expressed as follows

$$\mathrm{SDCI}=2^{a}(50)-47$$

Proof: From equation 2.6 and Table 3

$$
\begin{aligned}
\mathrm{SDCI}(\varpi)&=\sum_{\mathrm{c,m}\in\aleph(\varpi)}\left[\frac{\min(\varrho(\mathrm{c}),\varrho(\mathrm{m}))}{\max(\varrho(\mathrm{c}),\varrho(\mathrm{m}))}+\frac{\max(\varrho(\mathrm{c}),\varrho(\mathrm{m}))}{\min(\varrho(\mathrm{c}),\varrho(\mathrm{m}))}\right]\\
&=\left|\aleph_{(1,1)}(\varpi)\right|\left[\frac{\min(\varrho(\mathrm{c}),\varrho(\mathrm{m}))}{\max(\varrho(\mathrm{c}),\varrho(\mathrm{m}))}+\frac{\max(\varrho(\mathrm{c}),\varrho(\mathrm{m}))}{\min(\varrho(\mathrm{c}),\varrho(\mathrm{m}))}\right]\\
&\quad+\left|\aleph_{(1,2)}(\varpi)\right|\left[\frac{\min(\varrho(\mathrm{c}),\varrho(\mathrm{m}))}{\max(\varrho(\mathrm{c}),\varrho(\mathrm{m}))}+\frac{\max(\varrho(\mathrm{c}),\varrho(\mathrm{m}))}{\min(\varrho(\mathrm{c}),\varrho(\mathrm{m}))}\right]\\
&\quad+\left|\aleph_{(2,2)}(\varpi)\right|\left[\frac{\min(\varrho(\mathrm{c}),\varrho(\mathrm{m}))}{\max(\varrho(\mathrm{c}),\varrho(\mathrm{m}))}+\frac{\max(\varrho(\mathrm{c}),\varrho(\mathrm{m}))}{\min(\varrho(\mathrm{c}),\varrho(\mathrm{m}))}\right]\\
&\quad+\left|\aleph_{(2,3)}(\varpi)\right|\left[\frac{\min(\varrho(\mathrm{c}),\varrho(\mathrm{m}))}{\max(\varrho(\mathrm{c}),\varrho(\mathrm{m}))}+\frac{\max(\varrho(\mathrm{c}),\varrho(\mathrm{m}))}{\min(\varrho(\mathrm{c}),\varrho(\mathrm{m}))}\right]\\
&\quad+\left|\aleph_{(3,3)}(\varpi)\right|\left[\frac{\min(\varrho(\mathrm{c}),\varrho(\mathrm{m}))}{\max(\varrho(\mathrm{c}),\varrho(\mathrm{m}))}+\frac{\max(\varrho(\mathrm{c}),\varrho(\mathrm{m}))}{\min(\varrho(\mathrm{c}),\varrho(\mathrm{m}))}\right]\\
&=2\left(2^{a}\right)\left(\frac{\min(1,1)}{\max(1,1)}+\frac{\max(1,1)}{\min(1,1)}\right)+2\left(2^{a}\right)\left(\frac{\min(1,2)}{\max(1,2)}+\frac{\max(1,2)}{\min(1,2)}\right)\\
&\quad+\left(8\left(2^{a}\right)-12\right)\left(\frac{\min(2,2)}{\max(2,2)}+\frac{\max(2,2)}{\min(2,2)}\right)\\
&\quad+6\left(2^{a}-1\right)\left(\frac{\min(2,3)}{\max(2,3)}+\frac{\max(2,3)}{\min(2,3)}\right)\\
&\quad+6\left(2^{a}-1\right)\left(\frac{\min(3,3)}{\max(3,3)}+\frac{\max(3,3)}{\min(3,3)}\right)\\
&=2\left(2^{a}\right)(2)+2\left(2^{a}\right)\left(\frac{5}{2}\right)+\left(8\left(2^{a}\right)-12\right)(2)\\
&\quad+6\left(2^{a}-1\right)\left(\frac{13}{6}\right)+6\left(2^{a}-1\right)(2)\\
&=2^{a}(4+5+13+12+16)+(-13-12-24)\\
&=2^{a}(50)-47
\end{aligned}
$$

5. Comparative Analysis

This section examines the dendrimers' improved chemical applicability. Based on calculated ZCIs, we compare the PPEI and PPIO dendrimers. In addition, we

contrast the previously stated ZCIs to see whether one is better than the others in maintaining the chemical structure's characteristics.

5.1. Comparison among ZCIs

PPIO and PPEI dendrimers are compared numerically and graphically in this section using Tables 4-11 to compare them based on connection-based ZIs such ISCI, HCI, ABCCI, HZCI, and SDCI. Figures 5-12 show the graphical representation of these indices.

Table 4. Calculated ISCI values for the graph $\wp$ and ϖ for $a=1,2,3,\cdots,8$.

ZCIs	$a=1$	$a=2$	$a=3$	$a=4$	$a=5$	$a=6$	$a=7$	$a=8$
$\mathrm{ISCI}(\wp)$	21.86	58.93	133.06	281.33	577.86	1170.93	2357.07	4729.35
$\mathrm{ISCI}(\varpi)$	24.86	77.93	184.06	396.33	820.86	1669.93	3368.07	6764.35

Table 5. Calculated GACI values for the graph $\wp$ and ϖ for $a=1,2,3,\cdots,8$.

ZCIs	$a=1$	$a=2$	$a=3$	$a=4$	$a=5$	$a=6$	$a=7$	$a=8$
$\mathrm{GACI}(\wp)$	20.65	52.17	115.23	252.23	493.58	998.04	2006.96	4024.80
$\mathrm{GACI}(\varpi)$	31.29	80.45	178.79	375.47	768.82	155.52	3128.93	6275.75

Table 6. Calculated HCI values for the graph $\wp$ and ϖ for $a=1,2,3,\cdots,8$.

ZCIs	$a=1$	$a=2$	$a=3$	$a=4$	$a=5$	$a=6$	$a=7$	$a=8$
$\mathrm{HCI}(\wp)$	9.5668	23.03	49.96	103.83	211.56	427.03	857.97	1919.85
$\mathrm{HCI}(\varpi)$	11.06	32.53	75.46	161.33	333.06	6.76.53	1363.47	2737.35

Table 7. Calculated ABCCI values for the graph $\wp$ and ϖ for $a=1,2,3,\cdots,8$.

ZCIs	$a=1$	$a=2$	$a=3$	$a=4$	$a=5$	$a=6$	$a=7$	$a=8$
$\mathrm{ABCCI}(\wp)$	11.77	31.09	69.72	146.97	31.48	610.51	1228.56	2464.65
$\mathrm{ABCCI}(\varpi)$	21.83	52.51	113.76	236.26	481.25	971.23	1951.20	3911.14

Table 8. Calculated SDCI values for the graph $\wp$ and ϖ for $a=1,2,3,\cdots,8$.

ZCIs	$a=1$	$a=2$	$a=3$	$a=4$	$a=5$	$a=6$	$a=7$	$a=8$
$\mathrm{SDCI}(\wp)$	45	113	249	521	1065	2153	4329	8681
$\mathrm{SDCI}(\varpi)$	53	153	353	753	1553	3153	6353	8681

Table 9. Calculated HZCI values for the graph $\wp$ and ϖ for $a=1,2,3,\cdots,8$.

ZCIs	$a=1$	$a=2$	$a=3$	$a=4$	$a=5$	$a=6$	$a=7$	$a=8$
$\mathrm{HZCI}(\wp)$	704	2028	4676	9972	20564	41748	84116	168852
$\mathrm{HZCI}(\varpi)$	752	2332	5492	11812	24452	49732	100292	201412

From Table 4-9, we can see that PPEI structure (ϖ) has maximum all these ZCIs values than all other ZCIs value of PPIO structure ($\wp$).

From Figure 5-10, we can say that PPEI structure (ϖ) is higher curve for all these ZCIs values and than all other ZCIs value of PPIO structure ($\wp$).

5.2. Comparison between PPIO Dendrimer and PPEI Dendrimer

We compare the aforementioned ZCIs with one another in this subsection to determine which ZCI is better than all the others. We have calculated the ZCI

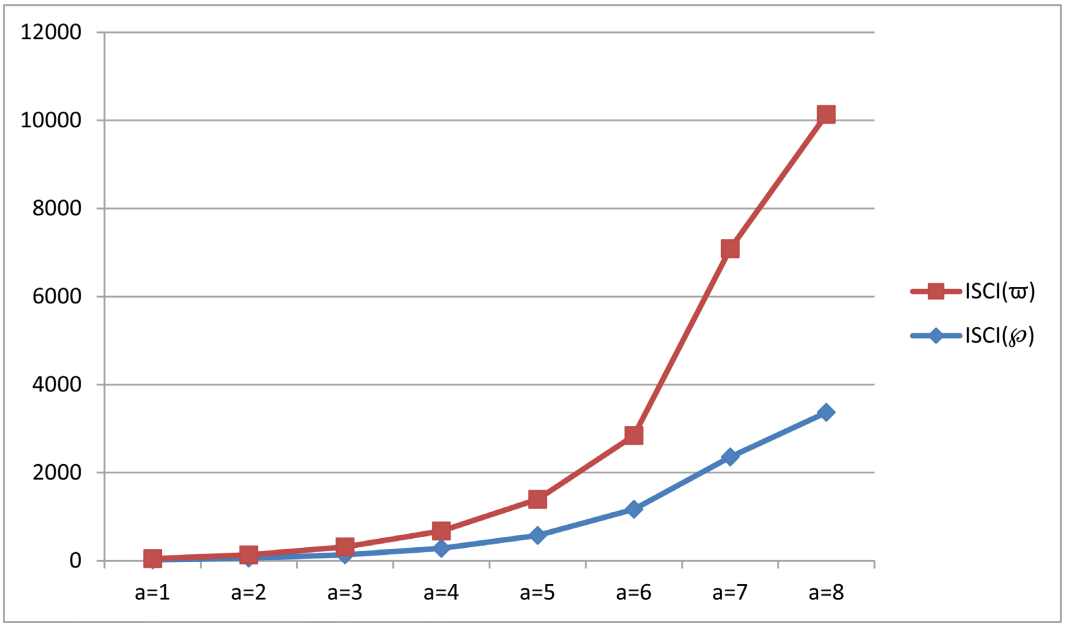

Figure 5. Graphical comparison ISCI for $\wp$ and ϖ graphs.

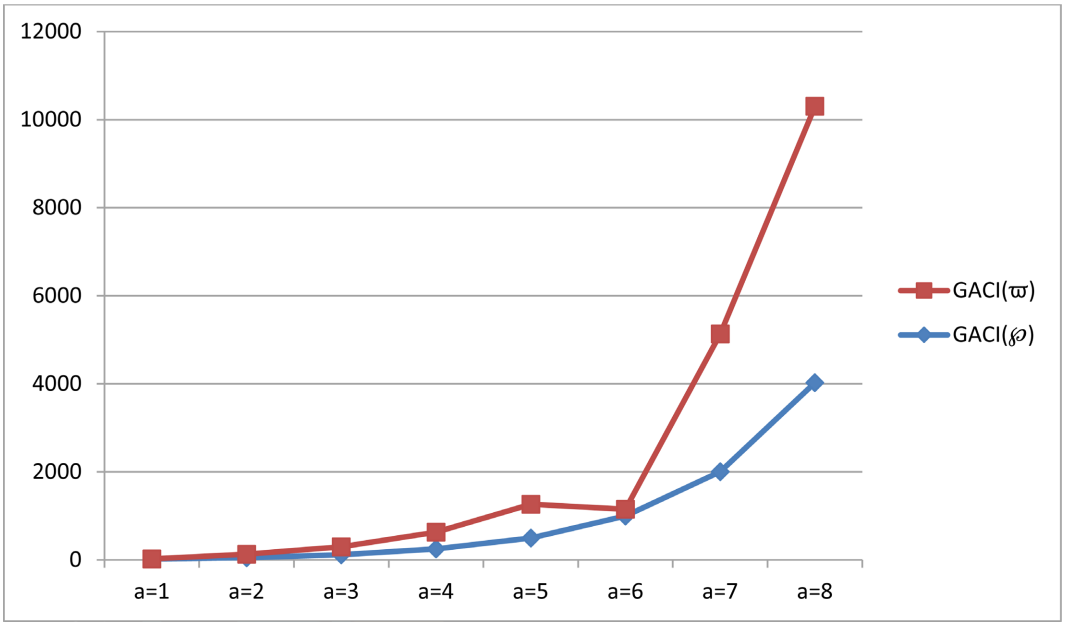

Figure 6. Graphical comparison GACI for $\wp$ and ϖ graphs.

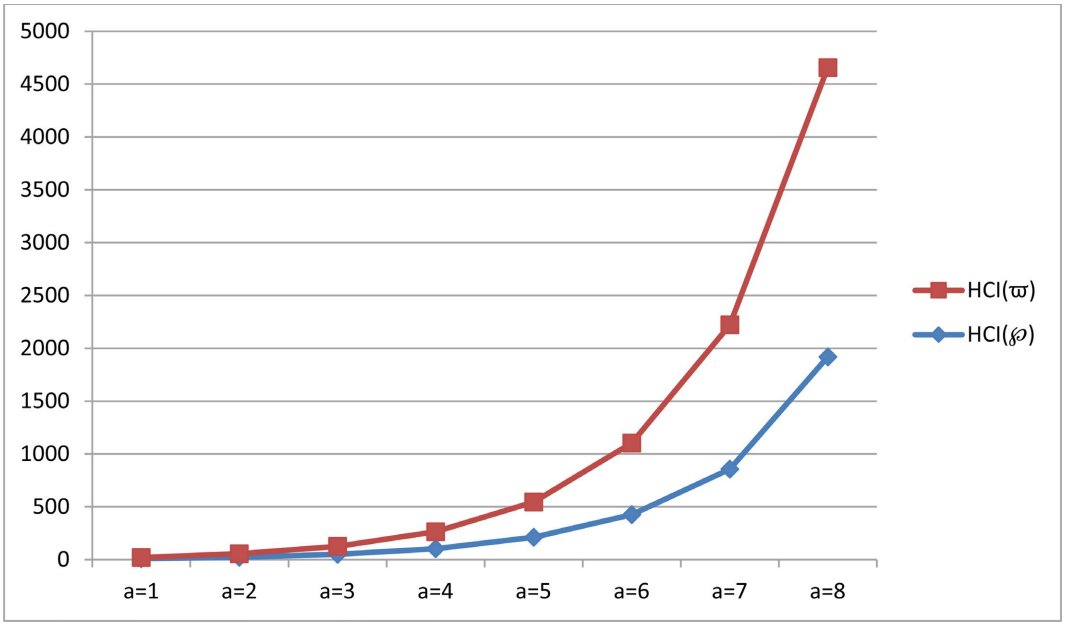

Figure 7. Graphical comparison HCI for $\wp$ and ϖ graphs.

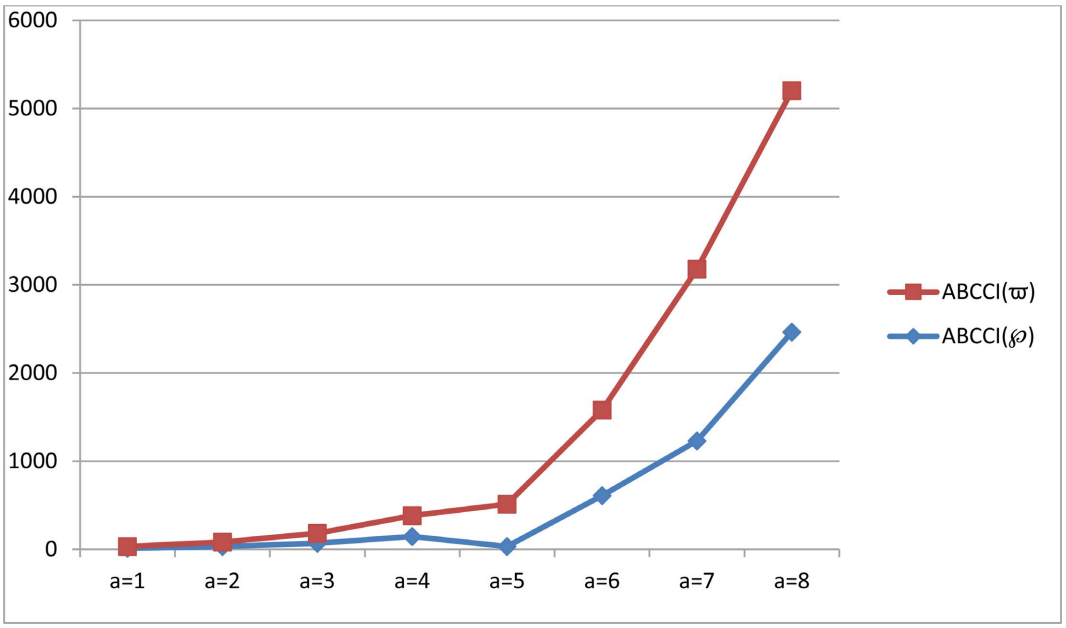

Figure 8. Graphical comparison ABCCI for $\wp$ and ϖ graphs.

values of PPIO dendrimers for

$a = 1, 2, 3, \cdots, 8$ and have included them in **Table 10**. We have calculated the ZCI values of PPEI dendrimers for $a = 1, 2, 3, \cdots, 8$ in **Table 11**. The ZCIs of the PPEI dendrimer (**Figure 12**) and the PPIO dendrimer (**Figure 11**) are graphically compared.

From **Table 10** and **Table 11**, it is clear that HZCI has higher values for both PPIO and PPEI dendrimers than other computed indices. **Figure 11** and **Figure 12** show that the HZCI curve is higher than those of other ZCIs, including PPIO

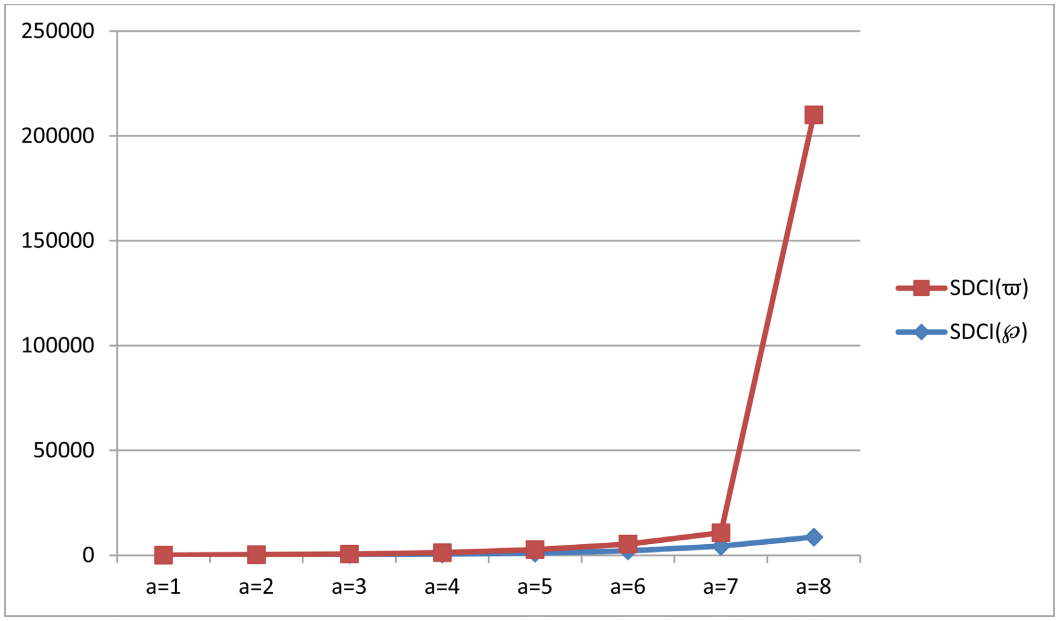

Figure 9. Graphical comparison SDCI for $\wp$ and ϖ graphs.

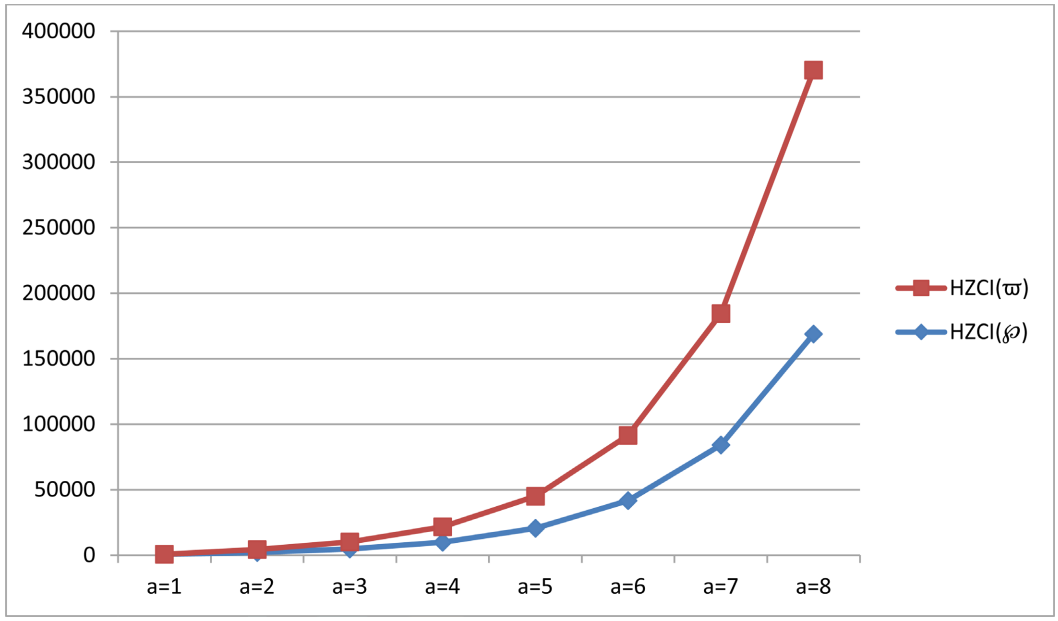

Figure 10. Graphical comparison HZCI for $\wp$ and ϖ graphs.

Table 10. Calculated ZCIs values of graph $\wp$ for $a=1,2,3,\cdots,8$.

ZCIs	$a=1$	$a=2$	$a=3$	$a=4$	$a=5$	$a=6$	$a=7$	$a=8$
$\mathrm{ISCI}(\wp)$	21.86	58.93	133.06	281.33	577.86	1170.93	2357.07	4729.35
$\mathrm{GACI}(\wp)$	20.65	52.17	115.23	252.23	493.58	998.04	2006.96	4024.80
$\mathrm{HCI}(\wp)$	9.56	23.03	49.96	103.83	211.56	427.03	857.97	1919.85
$\mathrm{ABCCI}(\wp)$	11.77	31.09	69.72	146.97	31.48	610.51	1228.56	2464.65

Continued

$\mathrm{SDCI}(\wp)$	45	113	249	521	1065	2153	4329	8681
$\mathrm{HZCI}(\wp)$	704	2028	4676	9972	20564	41748	84116	168852

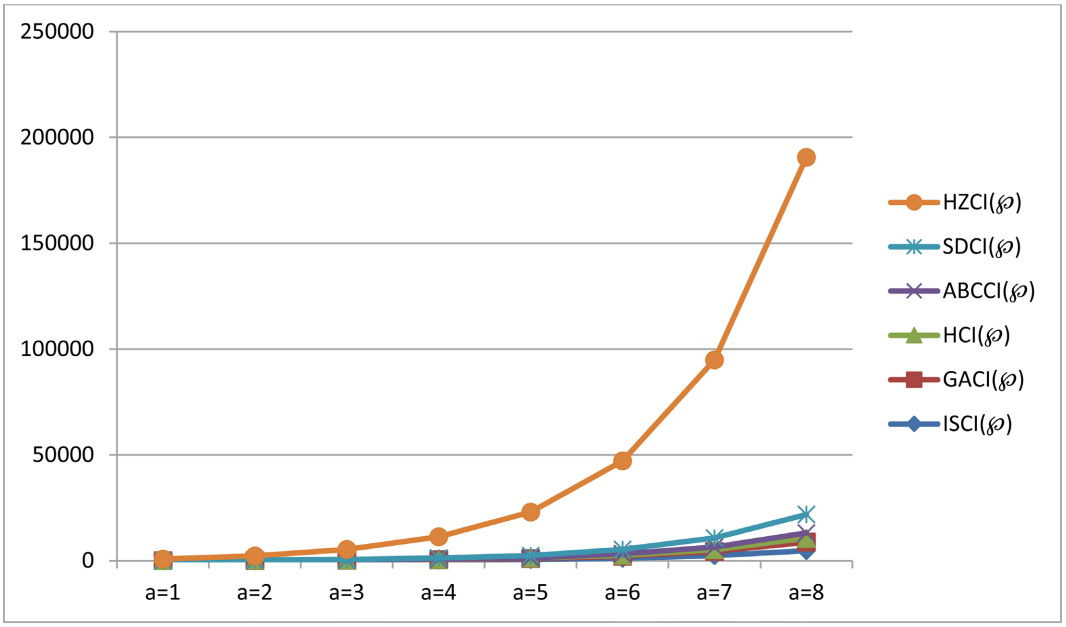

Figure 11. Graphical comparison of ZCIs of the graph $\wp$ for $a = 1, 2, 3, \cdots, 8$.

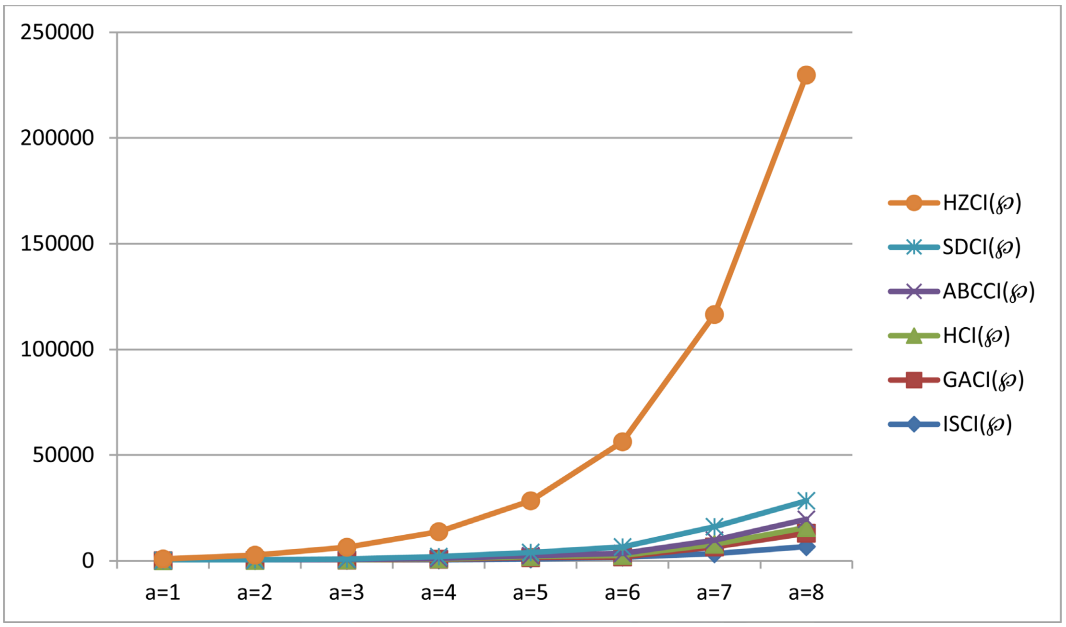

Figure 12. Graphical comparison of ZCIs of the graph ϖ for $a = 1, 2, 3, \cdots, 8$.

and PPEI dendrimers. This suggests that HZCI is a more suitable index for predicting the chemical and physical properties of chemical structures as compared to the others indices of literature. Thus, in conclusion, we found that HZCI is

Table 11. Calculated ZCIs values of graph ϖ for $a=1,2,3,\cdots,8$.

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

superior in preserving the psychochemical properties of these dendrimers and PPEI dendrimer has greater chemical dendrimer has greater chemical applicability than PPIO dendrimer.

6. Conclusions

Dendrimers exhibit hyperbranched, radially symmetric molecular structures with monodisperse, well defined, and uniform tree-like configurations. These molecules find extensive applications across diverse domains. Topological indices (TIs) serve as molecular descriptors, capturing the structural characteristics that enable correlation with the distinct physicochemical properties of different molecular compounds. In this paper, we compared two dendrimers, PPIO and PPEI, based on various ZCIs, including ISCI, GACI, HCI, ABCCI, HZCI, and SDCI. From Figures 5-10 and Tables 4-9, we observed that the PPEI dendrimer consistently showed higher values than the PPIO dendrimer. However, this indicates that the PPIO dendrimer exhibits better chemical applicability compared to the PPEI dendrimer.

Future Directions: The development of more complex and accurate mathematical models that take into account 3D molecule structures and interactions should be the main goal of future research on the topological indices of PPIO and PPEI dendrimers. Predictive accuracy may also be increased by investigating how solvent conditions and functional groups affect dendrimer characteristics. Lastly, combining these indices with computational techniques such as molecular dynamics simulations may offer a more profound understanding of dendrimer behaviour and its uses. The intricate molecular connections and dynamic behaviours of PPIO and PPEI dendrimers may be difficult for the topological indices to adequately represent. Assumptions made in the mathematical models and failure to account for solvent effects or steric hindrance may limit their application.

Data Availability

The study's supporting data are available upon request from the corresponding author and are included in the publication.

Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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