American Journal of Computational Mathematics, 2025, 15(2), 151-164
https://www.scirp.org/journal/ajcm
ISSN Online: 2161-1211
ISSN Print: 2161-1203

On Computing Topological Aspect of TTF Dendrimers

Aiman Arshad[1], Syeda Hina Zainab[2], Aqsa Sattar[1*]

[1]School of Science, University of Management and Technology (UMT), Lahore, Pakistan
[2]Department of Mathematics, Government College University Faisalabad (GCUF), Faisalabad, Pakistan
Email: aimanarshad273@gmail.com, syedafsd@gmail.com, *sattaraqsa47@gmail.com

How to cite this paper: Arshad, A., Zainab, S.H. and Sattar, A. (2025) On Computing Topological Aspect of TTF Dendrimers. *American Journal of Computational Mathematics*, **15**, 151-164.
https://doi.org/10.4236/ajcm.2025.152007

Received: April 12, 2025
Accepted: May 11, 2025
Published: May 14, 2025

Abstract

The theory of networks provides a mathematical basis for building and modeling the chemical structures and complex networks. Topological indices (TIs) are employed in several physicochemical applications, particularly for characterizing and modeling the chemical structures of diverse molecular compounds, including dendrimers. Dendrimers are intentionally synthesized or combined natural macromolecules characterized by a series of branching layers around a central core. In this manuscript, we calculate various connection-based Zagreb indices (ZIs), including the atom-bond connectivity connection index (ABCCI), geometric-arithmetic connection index (GACI), augmented connection index (ACI), symmetric division connection index (SDCI), harmonic connection index (HCI), inverse sum connection index (ISCI), and hyper Zagreb connection index (HZCI). Additionally, we discuss the connection-based ZIs for one of the most significant types of dendrimers, namely Tetrathiafulvalene (TTF) dendrimers. In addition, we provide a detailed numerical and graphical comparative analysis of the calculated results for TTF dendrimers, highlighting their performance and potential advantages in various applications.

Keywords

Topological Index (TI), Zagreb Indices (ZI), Zagreb Connection Indices (ZCI), Tetrathiafulvalene (TTF) Dendrimers

1. Introduction

Dendrimers are the primary objects of nanobiotechnology, rapidly expanding field that utilizes the principles of nanofabrication to construct devices. Dendrimers are star-shaped, heavily branching macromolecules having a distinct, tree-like structure [1]. Dendrimers are described as new generations of macromolecules and appeared in the second half of the twentieth century. The synthesis of these "cascade molecules" was first made by Fritz Vogtle and his colleagues in 1978. After that, in 1981 R.G. Denkewalter at Allied Corporation, Donald Tomalia at Dow Chemical in 1983 & 1985 and George R. Newkome in 1985 have also contributed to the synthesis of dendrimer. In 1990, Craig Hawker and Jean Fréchet initiated a convergent synthetic approach which went further in the process [2]. In recent years, dendrimers have attracted much attention due to their potential in a wide composition of areas specifically in the drug delivery system. They can actively encapsulate therapeutic molecules and the surface properties of these systems can be easily modified for precise tasks.

They are produced via a methodical procedure that produces layers or generations, culminating in a thick, multipurpose surface. The remarkable control that dendrimers provide over molecule size, shape, and functional groups due to their distinct structure makes them useful in a variety of applications, including drug delivery, nanotechnology and biomaterials, immunology, antimicrobials, and antivirals [3]-[5]. For molecular graphs or networks to be properly described mathematically, graph invariants are essential. Several facets of life have benefited greatly from the application of graph theory (GT).

The current research is concerned with the systematic investigation of topological indices of highly branched, symmetric nanostructures, namely the Tetrathiafulvalene (TTF) dendrimers which show great promise in the field of molecular electronics, organic conductors and material science. These dendrimers can have electron donating properties and have emerged as a promising class of materials for developing advanced functional materials. We therefore represent TTF dendrimers as molecular graphs and calculate a number of topological indices, including the Zagreb indices, Randic index, atom-bond connectivity (ABC) index and geometric-arithmetic (GA) index. We propose to obtain the closed-form expressions of these indices at various dendrimer growth stages. The importance of the study is due to the theoretical knowledge of TTF dendrimers and its applicability in QSAR/QSPR model building, which can utilize the topological index for predicting chemical, physical, and biological properties of molecular architectures. This work adds a new dimension to the use of graph theory with novel applications in nanotechnology and computational chemistry.

The research focus is on characterizing this molecular chemical structure using topological indices (TIs) or graph theoretic-invariants. By assigning a numerical value to a chemical substance, a topological index (TI) aids researchers in maintaining the psychochemical aspects of chemical structure in theoretical chemistry. It helps researchers determine the molecular compounds' physical characteristics, biological activities, and chemical reactivity.

Molecular networks are used to simulate molecular substances. Regarding GT analysis, a molecular network can actually be defined as the structural formula of chemical compounds, basically describing what the vertices or the points, as well as the edges in it means. In [5]-[7], it has been highlighted that the application of TIs in various fields of science is infinite. Depending on the type of connection between two nodes, the type of TIs is said to be a distance-based TIs, connection-based TIs, a degree-based TIs, and a polynomial based TI.

Imran and Baig introduced the first TI depending on distance [8]. He was researching the boiling point of paraffin in 1947. The concept of the first Zagreb indices (ZI) was developed by Trinajstic and Gunman [9]. In [10] [11], the second and third ZIs were examined. All of these degree-based TIs have successful uses in cheminformatics, which combines three important disciplines: information technology, mathematics, and chemistry [12]-[14]. These TIs have been used in a variety of physicochemical applications, particularly in the characterization of various chemical structures like tetrathiafulvalence (TTF) dendrimers. Tetrathiafulvalene (TTF) dendrimers are a group of dendritic macromolecular compounds that contain TTF fragments, recognized as effective electron donors. The syntheses of TTF dendrimers are based on the aim to use the redox properties of TTF and structural formularity of dendrimers for the apparat of molecular electronics, sensing and drug delivery systems.

From the recent research, Zhang *et al.* [15], have proposed a series of polyamidoamine (PAMAM) dendrimers functionalized with TTF units at the periphery of the dendritic structure (Gn-PAMAM-TTF up to the second generation). These functionalized dendrimers generated nanospheres that were able to incorporate hydrophobic materials. The terminal TTF groups exhibited reversible redox behavior, and upon oxidation, each TTF radical cation formed a 1:1:1 host–guest complex with cucurbit uril (CB [8]). This interaction resulted in structural relaxation of the nanospheres and in the beginning of the process of the release of the encapsulated cargo, which signifies the possibility of a method for the construction of synergistically redox and supramolecular assembly for the drug delivery system. The incorporation of TTF units into dendritic structures is a major development in functional dendrimers that provides a versatile means of developing stimuli-responsive materials for application across a range of fields including electronics and biomedical sciences.

Tetrathiafulvalene (TTF) dendrimers have attracted much interest because of their redox properties and their possible uses in different sectors. For example, TTF-conjugated PAMAM dendrimers have been discussed in the drug delivery systems that could be initiated by redox reactions and supramolecular assemblies [15]. Further, the dendrimer synthesis and the electrochemical characterization of new TTF dendrimers for molecular electronics and materials science have been studied [16]. In addition, the synthesis, structures and redox properties of TTF and related bis (1,3-dithiole) dendrimers have been investigated to find the possible uses in photodynamic therapy and other biomedical developments [17]. These researches demonstrate the possibility to use TTF dendrimers for creating new materials for electronics, sensing and biomedical fields. A few days ago, Aiman and Aqsa [18] recently calculated the ZCIs for a PPEI and PPIO dendrimers.

Among these defined TIs, connection-based TIs have much important and can be brought into play to characterized the chemical compound and forecast their various physiological properties in a wide and numerous ways. In 2018, Ali *et al.* [19] proposed a new term that is called connection number, it refers to the total number of the nodes of the curtain node's neighborhood whose distance is exactly two. Recently Arshad *et al.* [20] [21] calculated connection number-based Zagreb indices of path, cycle and complete graphs. They introduced connection-based TIs once the connection number was invited, and they used octane isomers to test the suitability of these newly presented connection-based ZIs. They discovered that ZIs based on connections are more resilient to the chemical characteristics of molecular structures. In 1998, Estrada *et al.* [22] looked into the atom bond connectivity (ABC) index, a significance degree -based TI. The fourth iteration of the ABC index is presented by Ghorbani *et al.* [23]. Furthermore, in 2009, Vukicevic and Furtula [24] introduced the geometric arithmetic (GA) index, another significant index type. Additionally, Garaovoc *et al.* [25] provided the fifth edition of the (GA) index, which he used to verify the dendrimers' chemical characteristics. Vukicevic's invention [26] in 2010. The augmented Zagreb index (AZI) is introduced by Furtula. In addition, Fajtlowicz [27] proposed the concept of harmonic index (HI). The idea of the inverse sum (IS) index was introduced by VUKicevic and Gasperov [28]. Shirdel *et al.* introduced the idea of hyper ZI (HZI) [29]. Document 27 Recently, refer to [30]-[33] for further information regarding ZCIs. This manuscript was motivated by the following.

Some basic concepts are covered in Section 2. The basic conclusion for determining the TTF dendrimers ZCIs, including HCI, AZCI, SDCI, AGCI, HZCI, ISCI, and ABCCI, is shown in Section 3. The main findings for ZCI calculations in the dendrimer network are presented in Section 4. Section 5 and 6 devote to the numerical and graphical comparisons of the TTF dendrimers depending on the calculated results.

2. Preliminaries

Let ξ be a network, $\xi = (D(\xi), E(\xi))$, where $D(\xi)$ is the set of vertices and $E(\xi)$, is the set of edges. The number of vertices at a distance of one from a vertex is its degree. The number of vertices that are two distances away from a particular vertex is its connection number.

We present the connection-based ZI, which was suggested by Sattar and Javaid [30] [34].

Definition 2.1. [30] [34] If ξ represents a chemical structure then the HCI is defined as;

$$\mathrm{HCI}(\xi) = \sum_{z,v\in\hbar(\xi)} \left[\frac{2}{\S(z)+\S(v)}\right].$$

$\S(z)$ and $\S(v)$ denote the CNs for the vertices z and v, respectively.

Definition 2.2. [30] [34] If ξ represents a chemical structure then the SDCI is defined as;

$$\mathrm{SDCI}(\xi) = \sum_{z,v\in\hbar(\xi)} \left[\frac{\min(\S(z),\S(v))}{\max(\S(z),\S(v))} + \frac{\max(\S(z),\S(v))}{\min(\S(z),\S(v))}\right].$$

where $\min(\S(z),\S(v))$ is the minimum of $\S(z)$ and $\S(v)$ and

$\max(\S(z),\S(v))$ is the maximum of $\S(z)$ and $\S(v)$.

Definition 2.3. [30] [34] If ξ represents a chemical structure then the ABCCI is defined as;

$$\mathrm{ABCCI}(\xi)=\sum_{z,v\in\hbar(\xi)}\sqrt{\frac{\S(z)+\S(v)-2}{\S(z)\times\S(v)}}.$$

Definition 2.4. [30] [34] If ξ represent a chemical structure then the ISCI is define as;

$$\mathrm{ISCI}(\xi)=\sum_{z,v\in\hbar(\xi)}\left[\frac{\S(z)\times\S(v)}{\S(z)+\S(v)}\right].$$

Definition 2.5. [30] [34] If ξ represent a chemical structure then the GACI is defined as;

$$\mathrm{GACI}(\xi)=\sum_{z,v\in\hbar(\xi)}\frac{2\sqrt{\S(z)\S(v)}}{\S(z)+\S(v)}.$$

Definition 2.6. [30] [34] If ξ represent a chemical structure, then the HZCI is define as;

$$\mathrm{HZCI}(\xi)=\sum_{z,v\in\hbar(\xi)}\left[\S(v)+\S(v)\right]^2.$$

Definition 2.7. [30] [34] If ξ represent a chemical structure, then the expression for AZCI is define as:

$$\mathrm{AZCI}(\xi)=\sum_{z,v\in\hbar(\xi)}\left[\frac{\S(z)+\S(v)}{\S(z)+\S(v)-2}\right].$$

3. Connection-Based ZIs for Tetrathiafulvalene (TTF) Dendrimer

We calculated the connection-based ZIs, such as HCI, AZCI, SDCI, GACI, HZCI, ISCI, and ABCCI, of topological features of a significant type of dendrimer known as a TTF dendrimer in this section. TTF dendrimer, denoted as TD[m] with m stages, when $m=1,2,\cdots,n$ is made up of end groups, additional branches, and the basic unit with **Figures 1-3** which include the connection number of every vertex.

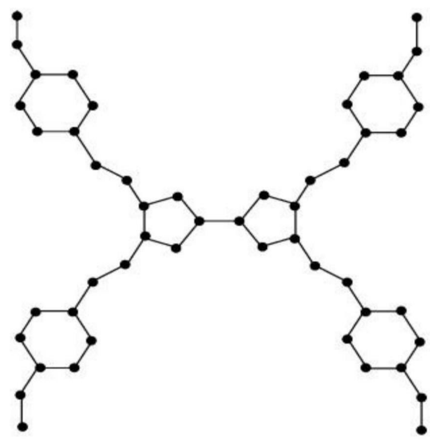

Figure 1. The center of the TTF dendrimer TD [0].

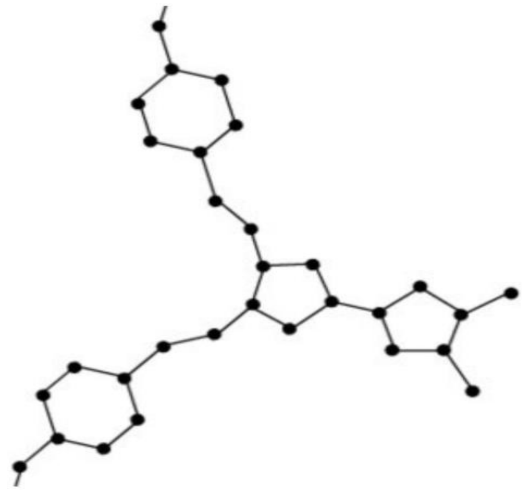

Figure 2. The graph included in every branch of TD [n].

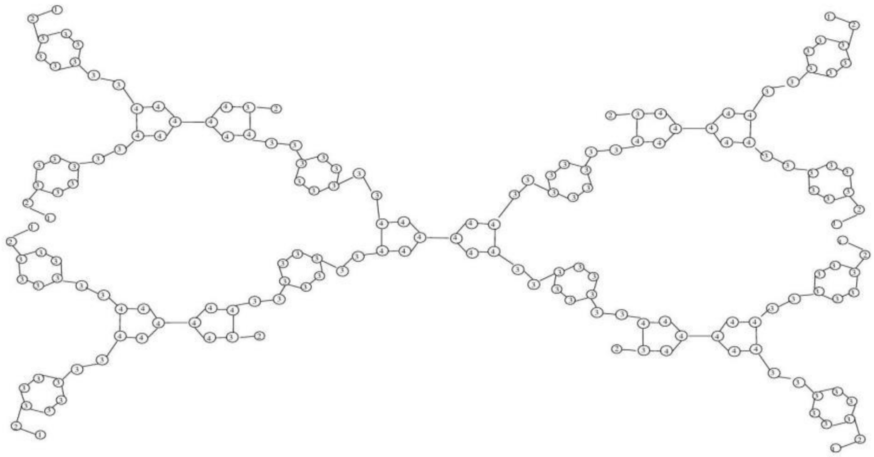

Figure 3. TD [1] with Connection number of each vertex.

4. Main Results

Proposition 4.1: Let ξ be a chemical graph, then the expression for HCI is denoted as:

$$\text{HCI} = 2^k(44.5809) - 25.7548.$$

Proof: by using equation 2.1 and Table 1.

Table 1. Total number of edge on connection number base $\hbar_{(\S(z),\S(v))}(\xi)$.

S.R	$\hbar_{(\S(z),\S(v))}(\xi)$	Number of edges
1	$\hbar_{(1,2)}(\xi)$	$4(2^k)$
2	$\hbar_{(2,3)}(\xi)$	$8(2^k)-4$
3	$\hbar_{(3,3)}(\xi)$	$72(2^k)-40$
4	$\hbar_{(3,4)}(\xi)$	$20(2^k)-16$
5	$\hbar_{(4,4)}(\xi)$	$36(2^k)-25$

$$
\begin{aligned}
\mathrm{HCI}(\xi) &= \sum_{z,v\in\hbar(\xi)}\left[\frac{2}{\S(z)+\S(v)}\right] \\
&= \left|\hbar_{(1,2)}(\xi)\right|\left[\frac{2}{\S(z)+\S(v)}\right]+\left|\hbar_{(2,3)}(\xi)\right|\left[\frac{2}{\S(z)+\S(v)}\right] \\
&\quad +\left|\hbar_{(3,3)}(\xi)\right|\left[\frac{2}{\S(z)+\S(v)}\right]+\left|\hbar_{(3,4)}(\xi)\right|\left[\frac{2}{\S(z)+\S(v)}\right] \\
&\quad +\left|\hbar_{(4,4)}(\xi)\right|\left[\frac{2}{\S(z)+\S(v)}\right] \\
&= \left[4\left(2^k\right)\left(\frac{2}{1+2}\right)\right]+\left[\left(8\left(2^k\right)-4\right)\left(\frac{2}{2+3}\right)\right]+\left[\left(72\left(2^k\right)-40\right)\left(\frac{2}{3+3}\right)\right] \\
&\quad +\left[\left(20\left(2^k\right)-16\right)\left(\frac{2}{3+4}\right)\right]+\left[\left(36\left(2^k\right)-25\right)\left(\frac{2}{4+4}\right)\right] \\
&= 2^k\left(2.6667+3.2+24+5.71420+9\right) \\
&\quad +\left(-1.6-13.3334-4.5714-6.25\right) \\
&= 2^k\left(44.5809\right)-25.7548.
\end{aligned}
$$

Proposition 4.2: Let ξ be a chemical graph, then the expression for SDCI is denoted as:

$$
\mathrm{SDCI} = 2^k\left(285.0001\right)-172.0001
$$

Proof: By using equation 2.2 and Table 1.

$$
\begin{aligned}
\mathrm{SDCI}(\xi) &= \sum_{z,v\in\hbar(\xi)}\left[\frac{\min(\S(z),\S(v))}{\max(\S(z),\S(v))}+\frac{\max(\S(z),\S(v))}{\min(\S(z),\S(v))}\right] \\
&= \left|\hbar_{(1,2)}(\xi)\right|\left[\frac{\min(\S(z),\S(v))}{\max(\S(z),\S(v))}+\frac{\max(\S(z),\S(v))}{\min(\S(z),\S(v))}\right] \\
&\quad +\left|\hbar_{(2,3)}(\xi)\right|\left[\frac{\min(\S(z),\S(v))}{\max(\S(z),\S(v))}+\frac{\max(\S(z),\S(v))}{\min(\S(z),\S(v))}\right] \\
&\quad +\left|\hbar_{(3,3)}(\xi)\right|\left[\frac{\min(\S(z),\S(v))}{\max(\S(z),\S(v))}+\frac{\max(\S(z),\S(v))}{\min(\S(z),\S(v))}\right] \\
&\quad +\left|\hbar_{(3,4)}(\xi)\right|\left[\frac{\min(\S(z),\S(v))}{\max(\S(z),\S(v))}+\frac{\max(\S(z),\S(v))}{\min(\S(z),\S(v))}\right] \\
&\quad +\left|\hbar_{(4,4)}(\xi)\right|\left[\frac{\min(\S(z),\S(v))}{\max(\S(z),\S(v))}+\frac{\max(\S(z),\S(v))}{\min(\S(z),\S(v))}\right] \\
&= \left[4\left(2^k\right)\left(\frac{\min(1,2)}{\max(1,2)}+\frac{\max(1,2)}{\min(1,2)}\right)\right] \\
&\quad +\left[\left(8\left(2^k\right)-4\right)\left(\frac{\min(2,3)}{\max(2,3)}+\frac{\max(2,3)}{\min(2,3)}\right)\right] \\
&\quad +\left[\left(72\left(2^k\right)-40\right)\left(\frac{\min(3,3)}{\max(3,3)}+\frac{\max(3,3)}{\min(3,3)}\right)\right]
\end{aligned}
$$

$$+\left[\left(20\left(2^k-16\right)\right)\left(\frac{\min(3,4)}{\max(3,4)}+\frac{\max(2,3)}{\min(2,3)}\right)\right]$$
$$+\left[\left(36\left(2^k-25\right)\right)\left(\frac{\min(3,3)}{\max(4,4)}+\frac{\max(4,4)}{\min(3,3)}\right)\right]$$
$$=\left[\left(4\left(2^k\right)\right)\left(\frac{5}{2}\right)\right]+\left[\left(8\left(2^k\right)-4\right)\left(\frac{13}{6}\right)\right]+\left[\left(72\left(2^k\right)-40\right)(2)\right]$$
$$+\left[\left(20\left(2^k\right)-16\right)\left(\frac{25}{12}\right)\right]+\left[\left(36\left(2^k\right)-25\right)(2)\right]$$
$$=2^k\left(10+17.3334+144+41.6667+72\right)$$
$$+\left(-8.6667-80-33.3334-50\right)$$
$$=2^k\left(285.0001\right)-172.0001.$$

Proposition 4.3: Let ξ be a chemical graph, then the expression for ABBCI is denoted as:

$$\text{ABCCI}=2^k\left(90.4025\right)-54.6129$$

Proof: By using equation 2.3 and Table 1.

$$\text{ABCCI}(\xi)=\sum_{z,v\in\hbar(\xi)}\sqrt{\frac{\S(z)+\S(v)-2}{\S(z)\times\S(v)}}$$
$$=\left|\hbar_{(1,2)}(\varpi)\right|\sqrt{\frac{\S(z)+\S(v)-2}{\S(z)\times\S(v)}}+\left|\hbar_{(2,3)}(\varpi)\right|\sqrt{\frac{\S(z)+\S(v)-2}{\S(z)\times\S(v)}}$$
$$+\left|\hbar_{(3,3)}(\varpi)\right|\sqrt{\frac{\S(z)+\S(v)-2}{\S(z)\times\S(v)}}+\left|\hbar_{(3,4)}(\varpi)\right|\sqrt{\frac{\S(z)+\S(v)-2}{\S(z)\times\S(v)}}$$
$$+\left|\hbar_{(4,4)}(\varpi)\right|\sqrt{\frac{\S(z)+\S(v)-2}{\S(z)\times\S(v)}}$$
$$=\left[4\left(2^k\right)\sqrt{\frac{1+2-2}{1\times2}}\right]+\left[\left\{8\left(2^k\right)-4\right\}\sqrt{\frac{2+3-2}{2\times3}}\right]$$
$$+\left[\left\{72\left(2^k\right)-40\right\}\sqrt{\frac{3+3-2}{3\times3}}\right]$$
$$+\left[\left\{20\left(2^k-16\right)\right\}\sqrt{\frac{3+4-2}{3\times4}}\right]$$
$$+\left[\left\{36\left(2^k-25\right)\right\}\sqrt{\frac{4+4-2}{4\times4}}\right]$$
$$=2^k\left(2.8284+4.6188+48+12.9099+22.0454\right)$$
$$+\left(-2.3092-26.6667-10.3279-15.3093\right)$$
$$=2^k\left(90.4025\right)-54.6129.$$

Proposition 4.4: Let ξ be a chemical graph, then the expression for ISCI is denoted as:

$$\text{ISCI}=2^k\left(226.5524\right)-142.2285$$

Proof: By using equation 2.4 and Table 1.

$$\mathrm{ISCI}(\xi)=\sum_{z,v\in\hbar(\xi)}\left[\frac{\S(z)\times\S(v)}{\S(z)+\S(v)}\right]$$

$$=\left|\hbar_{(1,2)}(\xi)\right|\left[\frac{\S(z)\times\S(v)}{\S(z)+\S(v)}\right]+\left|\hbar_{(2,3)}(\xi)\right|\left[\frac{\S(z)\times\S(v)}{\S(z)+\S(v)}\right]$$

$$+\left|\hbar_{(3,3)}(\xi)\right|\left[\frac{\S(z)\times\S(v)}{\S(z)+\S(v)}\right]+\left|\hbar_{(3,4)}(\xi)\right|\left[\frac{\S(z)\times\S(v)}{\S(z)+\S(v)}\right]$$

$$+\left|\hbar_{(4,4)}(\xi)\right|\left[\frac{\S(z)\times\S(v)}{\S(z)+\S(v)}\right]$$

$$=\left[4\left(2^k\right)\left(\frac{1\times 2}{1+2}\right)\right]+\left[\left(8\left(2^k\right)-4\right)\left(\frac{2\times 3}{2+3}\right)\right]+\left[\left(72\left(2^k\right)-40\right)\left(\frac{3\times 3}{3+3}\right)\right]$$

$$+\left[\left(20\left(2^k\right)-16\right)\left(\frac{3\times 4}{3+4}\right)\right]+\left[\left(36\left(2^k\right)-25\right)\left(\frac{4\times 4}{4+4}\right)\right]$$

$$=2^k\left(2.6667+9.6+108+34.2857+72\right)+\left(-4.8-60-27.4285-50\right)$$

$$=2^k\left(226.5524\right)-142.2285.$$

Proposition 4.5: Let ξ be a chemical graph, then the expression for GACI is denoted as:

$$\mathrm{GACI}=2^k\left(103.4036\right)-\left(84.7544\right)$$

Proof: By using equation 2.5 and Table 1.

$$\mathrm{GACI}(\xi)=\sum_{z,v\in\hbar(\xi)}\frac{2\sqrt{\S(z)\S(v)}}{\S(z)+\S(v)}$$

$$=\left|\hbar_{(1,2)}(\xi)\right|\frac{2\sqrt{\S(z)\S(v)}}{\S(z)+\S(v)}+\left|\hbar_{(2,3)}(\xi)\right|\frac{2\sqrt{\S(z)\S(v)}}{\S(z)+\S(v)}$$

$$+\left|\hbar_{(3,3)}(\xi)\right|\frac{2\sqrt{\S(z)\S(v)}}{\S(z)+\S(v)}+\left|\hbar_{(3,4)}(\xi)\right|\frac{2\sqrt{\S(z)\S(v)}}{\S(z)+\S(v)}$$

$$+\left|\hbar_{(4,4)}(\xi)\right|\frac{2\sqrt{\S(z)\S(v)}}{\S(z)+\S(v)}$$

$$=\left[4\left(2^k\right)\frac{2\sqrt{1\times 2}}{1+2}\right]+\left[\left(8\left(2^k\right)-4\right)\frac{2\sqrt{2\times 3}}{2+3}\right]$$

$$+\left[\left(72\left(2^k\right)-40\right)\frac{2\sqrt{3\times 3}}{3+3}\right]+\left[\left(20\left(2^k\right)-16\right)\frac{2\sqrt{3\times 4}}{3+4}\right]$$

$$+\left[\left(36\left(2^k\right)-25\right)\frac{2\sqrt{3\times 4}}{3+4}\right]$$

$$=2^k\left(3.7712+7.8384+72+19.794+36\right)$$
$$+\left(-3.9192-40-25-15.8352\right)$$
$$=2^k\left(103.4036\right)-84.7544.$$

Proposition 4.6: Let ξ be a chemical graph, then the expression for HZCI is denoted as:

$$\mathrm{HZCI} = 2^k(6112) - 3884.$$

Proof: by using equation 2.7 and Table 1.

$$\begin{aligned}
\mathrm{HZCI}(\xi) &= \sum\nolimits_{z,v\in\hbar(\xi)}\left[\S(v)+\S(v)\right]^2 \\
&= \left|\hbar_{(1,2)}(\xi)\right|\left[\S(v)+\S(v)\right]^2 + \left|\hbar_{(2,3)}(\xi)\right|\left[\S(v)+\S(v)\right]^2 \\
&\quad + \left|\hbar_{(3,3)}(\xi)\right|\left[\S(v)+\S(v)\right]^2 + \left|\hbar_{(3,4)}(\xi)\right|\left[\S(v)+\S(v)\right]^2 \\
&\quad + \left|\hbar_{(4,4)}(\xi)\right|\left[\S(v)+\S(v)\right]^2 \\
&= \left[4(2^k)(1+2)^2\right] + \left[\left(8(2^k)-4\right)(2+3)^2\right] + \left[\left(72(2^k)-40\right)(3+3)^2\right] \\
&\quad + \left[\left(20(2^k)-16\right)(3+4)^2\right] + \left[\left(36(2^k)-25\right)(4+4)\right] \\
&= 2^k(36+200+2592+980+2304) + (-100-1440-784-1600) \\
&= 2^k(6112) - 3884.
\end{aligned}$$

Proposition 4.7: Let ξ be a chemical graph, then the expression for AZCI is denoted as:

$$\mathrm{AZCI} = 2^k(330) - 548.6667\,.$$

Proof: By using equation 2.6 and Table 1.

$$\begin{aligned}
\mathrm{AZCI}(\xi) &= \sum\nolimits_{z,v\in\hbar(\xi)}\left[\frac{\S(z)+\S(v)}{\S(z)+\S(v)-2}\right] \\
&= \left|\hbar_{(1,2)}(\xi)\right|\left[\frac{\S(z)+\S(v)}{\S(z)+\S(v)-2}\right] + \left|\hbar_{(2,3)}(\xi)\right|\left[\frac{\S(z)+\S(v)}{\S(z)+\S(v)-2}\right] \\
&\quad + \left|\hbar_{(3,3)}(\xi)\right|\left[\frac{\S(z)+\S(v)}{\S(z)+\S(v)-2}\right] + \left|\hbar_{(3,4)}(\xi)\right|\left[\frac{\S(z)+\S(v)}{\S(z)+\S(v)-2}\right] \\
&\quad + \left|\hbar_{(4,4)}(\xi)\right|\left[\frac{\S(z)+\S(v)}{\S(z)+\S(v)-2}\right] \\
&= \left[4(2^k)\left(\frac{1+2}{1+2-2}\right)\right] + \left[\left(8(2^k)-4\right)\left(\frac{2+3}{2+3-2}\right)\right] \\
&\quad + \left[\left(72(2^k)-40\right)\left(\frac{3+3}{3+3-2}\right)\right] + \left[\left(20(2^k)-16\right)\left(\frac{3+4}{3+4-2}\right)\right] \\
&\quad + \left[\left(36(2^k)-25\right)\left(\frac{4+4}{4+4-2}\right)\right] \\
&= 2^k(8+16+162+48+96) + (-8-90-38.4-66.6667) \\
&= 2^k(330) - 548.6667.
\end{aligned}$$

5. Comparative Analysis

In this subsection, we compare those aforementioned connection-based ZIs to each other to figure out which connection-based ZIs is superior to all others. For the present calculations, we have presented the necessary parameters with which the ZCI values of TTF dendrimers have been estimated.

$k = 1, 2, 3, \cdots, 7$, and have incorporated them in the following Table 2. In Table 2, we have given the ZCI values of TTF dendrimers for $k = 1, 2, 3, \cdots, 7$. The ZCIs of the TTF dendrimer (Figure 4) are graphically compared.

Table 2. ZCI values of graph ξ for $a = 1, 2, 3, \cdots, 8$ are calculated in Table 2.

ZCIs	$k=1$	$k=2$	$k=3$	$k=4$	$k=5$	$k=6$	$k=7$
$\mathrm{HCI}(\xi)$	63.41	152.57	330.89	687.53	1400.81	2827.37	5680.49
$\mathrm{SDCI}(\xi)$	398	968	2108	4388	8948	18068	36308
$\mathrm{ABCCI}(\xi)$	126.19	306.99	668.59	1391.79	2838.19	5730.99	11516.59
$\mathrm{ISCI}(\xi)$	310.88	763.98	1670.18	3482.58	7107.38	41356.90	28856.18
$\mathrm{GACI}(\xi)$	122.05	328.85	742.45	1569.65	3234.05	6532.85	13150.45
$\mathrm{HZCI}(\xi)$	8340	20564	45012	93908	191700	387284	778452
$\mathrm{AZCI}(\xi)$	111.33	771.33	2091.33	4731.33	10011.33	20571.33	41691.33

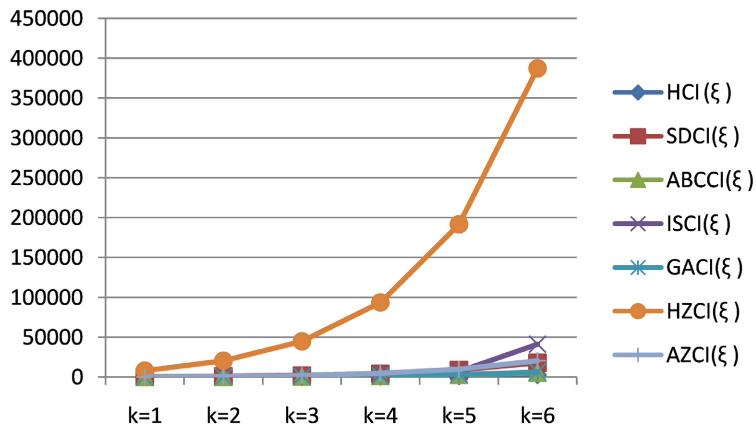

Figure 4. Comparing the connection-based ZIs of the graph ξ graphically for $k = 1, 2, 3, \cdots, 7$.

6. Conclusions

The following observations mark the end of our talk.

The developed general equation for calculating TTF dendrimers utilizing ZCIs specifically, HCI, AZCI, SDCI, GACI, HZCI, ISCI, and ABCCI is presented in this paper. Additionally, we have performed both numerical and graphical comparisons of the previously described ZCIs of TTF dendrimer.

It is clear from looking at Table 2 and Figure 4 that the HZCI and TTF dendrimers regularly obtain the highest values in this network. Figure 4's graphical depiction shows that the HZCI has a higher line than any other ZCI in the TTF dendrimer.

Future Direction: Tetrathiafulvalene (TTF) dendrimers are dendritic macromolecules containing TTF units and are popular for their specific electrochemical behavior. More future work for TTF dendrimers involves the application of TTF dendrimers in molecular electronics as a potential candidate as well as the synthesis of highly conductive and rich components for molecular devices at the nanoscale. Further, research efforts are directed towards optimizing their electrochemical stability and precise control of redox characteristics for application in organic photovoltaics and sensors. Developments in synthetic techniques continue to focus on generating further elaborate TTF dendrimer structures since the compounds, with their broader functionalities, may easily be incorporated into additional technological systems.

Data Availability

The information used to support the study's findings is included in this article. For further information on the data, the reader can get in touch with the corresponding authors.

Financial Statement

This proposal has no financial sources.

Conflicts of Interest

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

References

[1] Sampathkumar, S.G. and Yarema, K.J. (2007) Dendrimers in Cancer Treatment and Diagnosis. In: Kumar, C.S.S.R., Ed., *Nanotechnologies for the Life Sciences*, Wiley, 105-134.

[2] Bacha, K., Chemotti, C., Mbakidi, J., Deleu, M. and Bouquillon, S. (2023) Dendrimers: Synthesis, Encapsulation Applications and Specific Interaction with the Stratum Corneum—A Review. *Macromol*, **3**, 343-370. https://doi.org/10.3390/macromol3020022

[3] Kesharwani, P., Gothwal, A., Iyer, A.K., Jain, K., Chourasia, M.K. and Gupta, U. (2018) Dendrimer Nanohybrid Carrier Systems: An Expanding Horizon for Targeted Drug and Gene Delivery. *Drug Discovery Today*, **23**, 300-314. https://doi.org/10.1016/j.drudis.2017.06.009

[4] Klajnert, B., Peng, L. and Ceoa, V. (2013) Dendrimers in Biomedical Applications. Royal Society of Chemistry.

[5] Kurczewska, J., Cegłowski, M., Messyasz, B. and Schroeder, G. (2018) Dendrimer-functionalized Halloysite Nanotubes for Effective Drug Delivery. *Applied Clay Science*, **153**, 134-143. https://doi.org/10.1016/j.clay.2017.12.019

[6] Afzal, H.U. and Fatima, T. (2019) On Topological Indices of OT [M, N] Octagonal Tillings and TiO_2 Nanotubes. *Acta Chimica Slovenica*, **66**, 435-442. https://doi.org/10.17344/acsi.2018.4897

[7] Gao, W., Younas, M., Farooq, A., Mahboob, A. and Nazeer, W. (2018) M-Polynomials and Degree-Based Topological Indices of the Crystallographic Structure of Molecules. *Biomolecules*, **8**, Article 107. https://doi.org/10.3390/biom8040107

[8] Imran, M., Baig, A.Q. and Ali, H. (2016) On Molecular Topological Properties of Hex-Derived Networks. *Journal of Chemometrics*, **30**, 121-129.

https://doi.org/10.1002/cem.2785

[9] Wiener, H. (1947) Structural Determination of Paraffin Boiling Points. *Journal of the American Chemical Society*, **69**, 17-20. https://doi.org/10.1021/ja01193a005

[10] Gutman, I. and Trinajstić, N. (1972) Graph Theory and Molecular Orbitals. Total φ-Electron Energy of Alternant Hydrocarbons. *Chemical Physics Letters*, **17**, 535-538. https://doi.org/10.1016/0009-2614(72)85099-1

[11] Gutman, I., Ruscić, B., Trinajstić, N. and Wilcox, C.F. (1975) Graph Theory and Molecular Orbitals. XII. Acyclic Polyenes. *The Journal of Chemical Physics*, **62**, 3399-3405. https://doi.org/10.1063/1.430994

[12] Ali, A., Gutman, I., Milovanovic, E. and Milovanovic, I. (2018) Sum of Powers of the Degrees of Graphs Extremal Results and Bounds. *MATCH Communications in Mathematical and in Computer Chemistry*, **80**, 5-84.

[13] Borovicanin, B., Das, K.C., Furtula, B. and Gutman, I. (2017) Bounds for Zagreb Indices. *MATCH Communications in Mathematical and in Computer Chemistry*, **78**, 17-100.

[14] Javaid, M., Ali, U. and Liu, J. (2021) Computing Analysis for First Zagreb Connection Index and Coindex of Resultant Graphs. *Mathematical Problems in Engineering*, **2021**, Article ID: 6019517. https://doi.org/10.1155/2021/6019517

[15] Zhang, X., Zeng, Y., Yu, T., Chen, J., Yang, G. and Li, Y. (2014) Tetrathiafulvalene Terminal-Decorated PAMAM Dendrimers for Triggered Release Synergistically Stimulated by Redox and CB[7]. *Langmuir*, **30**, 718-726. https://doi.org/10.1021/la404349w

[16] Wang, C., Bryce, M.R., Batsanov, A.S., Goldenberg, L.M. and Howard, J.A.K. (1997) Synthesis and Electrochemistry of New Tetrathiafulvalene (TTF) Dendrimers: X-Ray Crystal Structure of a Tetrafunctionalised TTF Core Unit. *Journal of Materials Chemistry*, **7**, 1189-1197. https://doi.org/10.1039/a607597e

[17] Bryce, M., Nicholas, G. and Christensen, C. (2002) Synthesis, Structures and Redox Properties of Tetrathiafulvalene and Related Bis(1, 3-Dithiole) Dendrimers. *Abstracts of Papers: American Chemical Society Meetings*, **223**, D64.

[18] Arshad, A., Zainab, S.H., Javed, S., Sattar, A. and Javaid, M. (2024) Connection-Based Topological Aspect of PPIO and PPEI Dendrimers. *Journal of Applied Mathematics and Physics*, **12**, 4128-4149. https://doi.org/10.4236/jamp.2024.1212253

[19] Ali, A. and Trinajstić, N. (2018) A Novel/Old Modification of the First Zagreb Index. *Molecular Informatics*, **37**, Article ID: 1800008. https://doi.org/10.1002/minf.201800008

[20] Arshad, A., Sattar, A., Javaid, M. and Abebe Ashebo, M. (2023) Connection Number-Based Topological Indices of Cartesian Product of Graphs. *Journal of Mathematics*, **2023**, Article ID: 8272936. https://doi.org/10.1155/2023/8272936

[21] Arshad, A. and Afzal, A. (2024) Computing Zagreb Connection Indices for the Cartesian Product of Path and Cycle Graphs. *Scientific Inquiry and Review*, **8**, 102-118. https://doi.org/10.32350/sir.83.05

[22] Estrada, E., Torres, L., Rodriguez, L. and Gutman, I. (1998) An Atom-Bond Connectivity Index: Modelling the Enthalpy of Formation of Alkanes. *Indian Journal of Chemistry*, **37A**, 849-855.

[23] Ghorbani, M. and Hosseinzadeh, M.A. (2010) Computing ABC4 Index of Nanostar Dendrimers. *Optoelectronics and Advanced Materials-Rapid Communications*, **4**, 1419-1422.

[24] Vukičević, D. and Furtula, B. (2009) Topological Index Based on the Ratios of Geo-

metrical and Arithmetical Means of End-Vertex Degrees of Edges. *Journal of Mathematical Chemistry*, **46**, 1369-1376. https://doi.org/10.1007/s10910-009-9520-x

[25] Graovac, A., Ghorbani, M. and Hosseinzadeh, M.A. (2011) Computing Fifth Geometric-Arithmetic Index for Nanostar Dendrimers. *Journal of Discrete Mathematics and Its Applications*, **1**, 33-42.

[26] Vukičević, D. (2010) Bond Additive Modeling 2. Mathematical Properties of Max-Min Rodeg Index. *Croatica Chemica Acta*, **83**, 261-273.

[27] Fajtlowicz, S. (1987) On Conjectures of Graffiti II. *Congressus Numerantium*, **60**, 187-197.

[28] Vukicevic, D. and Gasperov, M. (2010) Bond Additive Modeling 1. Adriatic Indices. *Croatica Chemica Acta*, **83**, 243-260.

[29] Shirdel, G., Rezapour, H. and Sayadi, A. (2013) The Hyper-Zagreb Index of Graph Operations. *Iranian Journal of Mathematical Chemistry*, **4**, 213-220.

[30] Sattar, A., Javaid, M. and Bonyah, E. (2022) Computing Connection-Based Topological Indices of Dendrimers. *Journal of Chemistry*, **2022**, Article ID: 7204641. https://doi.org/10.1155/2022/7204641

[31] Bokhary, S.A.U.H., Imran, M. and Manzoor, S. (2016) On Molecular Topological Properties of Dendrimers. *Canadian Journal of Chemistry*, **94**, 120-125. https://doi.org/10.1139/cjc-2015-0466

[32] Dorosti, N., Iranmanesh, A. and Diudea, M.V. (2010) Computing the Cluj Index of the First Type Dendrimer Nanostar. *Optoelectronics and Advanced Materials-Rapid Communications*, **4**, 381-384.

[33] Sattar, A. (2023) Computing Connection-Based Zagreb Indices of Molecular Structures. *Applications of Mathematical Sciences*, **2**, 71-87.

[34] Javaid, M. and Sattar, A. (2022) Novel Connection Based Zagreb Indices of Dendrimer Nanostars. *Journal of Combinatorial Mathematics and Combinatorial Computing*, **3**, 23-32.