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Computing Connection-Based Zagreb Indices of Molecular Structures

Aqsa Sattar[1]

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Abstract

Topological indices (TIs), the numerical parameters which link a number with a molecular graph, are broadly utilized in mathematical chemistry and chemical graph theory as molecular descriptors to characterize the topology of chemical structures such as nanotubes, neural networks and dendrimers with respect to their certain chemical properties, namely, low cytotoxicity, chemical stability and solubility. Dendrimers are prolonged artificially manufactured natural macromolecules with a successive layer of branches surrounded by a central core. TIs are classified into three main classes named as polynomial, distance and degree-based TIs. Wiener pioneered the first distance-based TI, which was examined as an essential TI for preserving the psychochemical features of chemical compounds. After that, degree-based TI was explored to calculate the π- electron energy of molecules. Recently, it has been discovered that connection number (CN) based TIs are more effective than a degree and distance-based TIs. In this manuscript, we calculate the ZIs based on CNs for the most significant type of dendrimer, namely, tetrathiafulvalence dendrimer.

Keywords: Zagreb indices; Connection-based Zagreb indices; Topological index; Dendrimer nanostars

1 Introduction

Nanobiotechnology is a newly emerging branch of science that applies the mechanism of nanofabrication to fabricate devices for exploring the biosystem. Dendrimers are considered to be the primary part of this branch. Dendrimers are symmetric, small sized natural macromolecules with monodisperse, well-defined and homogenous structures with tree-like branches (Sampathkumar et al, 2007). They are made up of three main parts, including end groups, branches and the central core. There is a certain amount of functional groups in the exterior shell of each dendrimer that may give a monodispersed platform for nanoparticle tissue and drug interactions. These structures are attaining much more consideration from the scientists due to their vast span of utilizations in distinct fields of science, including vaccine, gene and drug delivery, antimicrobials, development of antivirals and immunology (Kesharwani et al, 2018; Klajnert et al, 2013; Kurczewska et al, 2018).

[1] University of the Punjab, Lahore, Pakistan
e-mail: sattaraqsa47@gmail.com

To characterize these molecular chemical structures with the help of graph theoretic-invariants or TIs is the present-day line of research. A topological index (TI) is a numerical measure of a chemical compound that helps researchers to preserve the psychochemical features of chemical structures in theoretical chemistry by associating a numeric number. TIs help scientists to find the chemical reactivity, physical attributes and biological actions of the molecular compound in a precise and well-defined way. Molecular compounds are handled by molecular graphs. A molecular graph, in terms of graph theory, is the representation of the structural formula of chemical compounds in which the atom are represented by the vertices (nodes) while the bonds are represented by edges between nodes. The applications of TIs in various fields of science are boundless, as one can see in (Afzal et al, 2019; Gao et al, 2018; Imran et al, 2016). There are three main TIs, namely, distance-based TI, degree-based TI and polynomial-based TI. (Wiener et al, 1947) initiated the first distance based TI in 1947, when he was working on the boiling point of paraffin. Gutman and (Trinajstic et al, 1972) invented the idea of first ZI (FZI). The second and third ZIs were investigated by (Gutman et al. 1975) and (Furtula et al, 2015). These introduced classical ZIs have a wide range of applicability in the branch of cheminformatics in which three major branches, namely, chemistry, mathematics and information technology are combined [12–14]. These TIs have been utilized in distinct wide-ranging physicochemical applications, especially to characterize the different chemical structures; for details see (Ali et al, 2018; Borovicanin et al, 2017; Javaid et al, 2021).

Recently, (Ali et al, 2018) invented a new term called connection-number (CN) which is the count of those nodes which are at a distance of two from the certain node. After the invention of CN, they introduced the CN-based ZIs and utilized octane isomers to examine the applicability of these new introduced CN-based ZIs. They found that CN-based ZIs have better ability to preserve the chemical features of molecular structures. (Haoer et al, 2020) computed the multiplicative ZIs of some T-thorny graphs. (Das et al, 2013) and (Dhanalakshmi et al, 2016) found the multiplicative ZIs (MZIs) of some graph operations. (Nikolic et al. 2003) investigated modified ZI in 2003. Moreover, Javaid et al. [24] found the topological aspects of distinct wheel graphs via CN-based multiplicative ZIs (MZCIs). Freshly, For more details about ZIs, see (Bashir et al, 2017; Bokhary et al, 2016; Dorosti et al, 2010). The motivation for this manuscript is as follows;

1. Dendrimers are homogenous, well-defined, nano-sized particles with three basic components, including branches, end groups and cores. These nanoparticles are considered to be the primary part of the field of nanobiotechnology. Dendrimers have a vast span of utilizations in distinct areas of science including drug delivery, gene delivery and energy harvesting.

2. TIs are extensively utilized in mathematical chemistry as molecular descriptors to characterize the topology of chemical structures. TIs help to predict the physical and chemical aspects like, melting point, volume, stability, freezing point and strain energy of different chemical structures by associating a numeric digit with these molecular structures.

3. CN-based ZIs can preserve the chemical properties of molecular structures more precisely and efficiently as compared to other degree and distance based ZIs.

This paper is structured as; In section 1, we state some related basic definitions. In section 2, we compute

CN-based ZIs of tetrathiafulvalence dendrimer, namely first CN-based ZI (FZCI), second CN-based ZI (SZCI), modified FZCI, modified SZCI, modified TZCI. Section 3 involves the general results to compute multiplicative CN-based ZIs, namely, multiplicative first CN-based ZI (MFZCI), multiplicative second CN-based ZI (MSZCI), multiplicative third CN-based ZI (MTZCI), multiplicative fourth CN-based ZI (MFZCI), modified MFZCI, modified MSZCI, modified MTZCI. Section 4 draws the conclusions.

In this section, we define some basic related definitions.

Definition 2.1. [Trinajstic et al, 1972] Consider a graph $\mathcal{G} = (\mathbb{K}(\mathcal{G}), \mathcal{T}(\mathcal{G}))$, where $\mathbb{K}(\mathcal{G})$ and $\mathbb{T}(\mathcal{G})$ be the set of nodes and set of edges, respectively. Then, first and second degree-based ZIs are

$$1.\ \mathbb{Z}_1(\mathcal{G}) = \sum_{k\in\mathbb{K}(\mathcal{G})} \left(d_{\mathcal{G}}(k)\right)^2 = \sum_{kt\in\mathbb{T}(\mathcal{G})} \left(d_{\mathcal{G}}(k) + d_{\mathcal{G}}(t)\right),$$

2 $\mathbb{Z}_2(\mathcal{G}) = \sum_{kt\in\mathbb{T}(\mathcal{G})} \left(d_{\mathcal{G}}(k) \times d_{\mathcal{G}}(t)\right)$

where $d_{\mathcal{G}}(k)$ and $d_{\mathcal{G}}(t)$ are the degrees of the nodes k and t, respectively.

Definition 2.2. [Ali et al, 2018] For a graph $\mathcal{G}$, then first and second CN-based ZIs are given as

$$\mathbb{Z}_1\mathrm{C}(\mathcal{G}) = \sum_{k\in\mathbb{K}(\mathcal{G})} \left[\delta_{\mathcal{G}}(k)\right]^2$$

$$\mathbb{Z}_2\mathrm{C}(\mathcal{G}) = \sum_{kt\in\mathbb{T}(\mathcal{G})} \left[\delta_{\mathcal{G}}(k) \times \delta_{\mathcal{G}}(t)\right]$$

where $\delta_{\mathcal{G}}(k)$ and $\delta_{\mathcal{G}}(t)$ is the CN of the node k and t, respectively.

Definition 2.3. [Ali et al. 2020] For a graph $\mathcal{G}$, the CN-based modified ZIs are given as

$$\mathbb{Z}_1\mathrm{C}^*(\mathcal{G}) = \sum_{kt\in\mathbb{T}(\mathcal{G})} \left[\delta_{\mathcal{G}}(k) + \delta_{\mathcal{G}}(t)\right],$$

$$\mathbb{Z}_2\mathrm{C}^*(\mathcal{G}) = \sum_{kt\in\mathbb{T}(\mathcal{G})} \left[d_{\mathcal{G}}(k)\delta_{\mathcal{G}}(t) + d_{\mathcal{G}}(t)\delta_{\mathcal{G}}(k)\right],$$

$$\mathbb{Z}_3\mathrm{C}^*(\mathcal{G}) = \sum_{kt\in\mathbb{T}(\mathcal{G})} \left[d_{\mathcal{G}}(k)\delta_{\mathcal{G}}(k) + d_{\mathcal{G}}(t)\delta_{\mathcal{G}}(t)\right].$$

Definition 2.4. [Javaid et al. 2021] For a graph $\mathcal{G}$, CN-based MZIs are given as

$$\mathbb{Z}_1^M\mathrm{C}(\mathcal{G}) = \prod_{k\in\mathbb{K}(\mathcal{G})} \left[\delta_{\mathcal{G}}(k)\right]^2$$

$$\mathbb{Z}_2^M\mathrm{C}(\mathcal{G}) = \prod_{kt\in\mathbb{T}(\mathcal{G})} \left[\delta_{\mathcal{G}}(k) \times \delta_{\mathcal{G}}(t)\right]$$

$$\mathbb{Z}_3^M\mathrm{C}(\mathcal{G}) = \prod_{k\in\mathbb{K}(\mathcal{G})} \left[d(k) \times \delta(k)\right]$$

$$\mathbb{Z}_4^M\mathrm{C}(\mathcal{G}) = \prod_{kt\in\mathbb{T}(\mathcal{G})} \left[\delta_{\mathcal{G}}(k) + \delta_{\mathcal{G}}(t)\right]$$

Definition 2.5. [Javaid et al. 2021] For a graph $\mathcal{G}$, modified MZCIs are given as

$$\mathbb{Z}_1^M C^*(\mathcal{G}) = \prod_{kt\in\mathbb{T}(\mathcal{G})} \left[d_{\mathcal{G}}(k)\delta_{\mathcal{G}}(t) + d_{\mathcal{G}}(t)\delta_{\mathcal{G}}(k)\right],$$
$$\mathbb{Z}_2^M C^*(\mathcal{G}) = \prod_{kt\in\mathbb{T}(\mathcal{G})} \left[d_{\mathcal{G}}(k)\delta_{\mathcal{G}}(k) + d_{\mathcal{G}}(t)\delta_{\mathcal{G}}(t)\right],$$
$$\mathbb{Z}_3^M C^*(\mathcal{G}) = \prod_{kt\in\mathbb{T}(\mathcal{G})} \left[d_{\mathcal{G}}(k)\delta_{\mathcal{G}}(k) \times d_{\mathcal{G}}(t)\delta_{\mathcal{G}}(t)\right].$$

3. CN-based ZIs of Tetrathiafulvalence dendrimer

In this section, we worked on calculating the topological aspects of an important kind of dendrimer named as tetrathiafulvalence dendrimer. Tetrathiafulvalence dendrimer, represented by $\mathcal{TD}[s]$ with s stages, is comprised of basic unit, added branches and end groups. At each stage, it consists of $2^{s+3} - 6$ and $2^{s+3} - 4$ pentagons and hexagons, respectively. At each stage of the graph of $\mathcal{TD}[s]$,$4(2)^{s-1}$ branches are added and thus, their stepwise growth follows a structure of $\mathcal{TD}[s]$. Let $\mathcal{G} = \mathcal{TD}[s]$ be a molecular graph of $\mathcal{TD}[s]$, for $s \geq 1$. The basic graph (core graph) $\mathcal{TD}[0]$ is shown in Figure 1. The graph A which is added in each branch of $\mathcal{TD}[s]$ to get the next level is displayed in Figure 2. In Figure 3 and Figure 4 , for $s = 1$, we have labeled the nodes with respect to their CNs and degrees, respectively. Now, we will compute the CN-based TIs of $\mathcal{TD}[s]$ for $s \geq 1$. The total count of nodes and edges of $\mathcal{G}$ are $124 \times 2^s - 74$ and $140 \times 2^s - 85$, respectively.

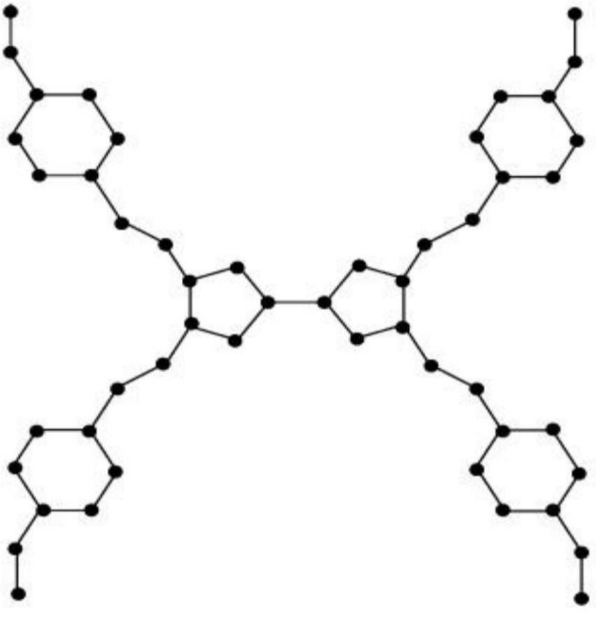

Figure 1: The core of Tetrathiafulvalence dendrimer $\mathcal{TD}[0]$

Theorem 3.1. The FZCI of $\mathcal{G} = \mathcal{TD}[s]$, for $s \geq 1$ is given by

$$\mathbb{Z}_1 C(\mathcal{G}) = 1266 \times 2^s - 828$$

Proof. It can be seen clearly from the Figure 3 that there are total four partitions of nodes with respect to their CNs. The CN-based nodes partitions are given in the following

$$\begin{aligned}
\mathcal{P}_1 &= \{k \in \mathbb{K}(\mathcal{G}): \delta_{\mathcal{G}}(k) = 1\},\\
\mathcal{P}_2 &= \{k \in \mathbb{K}(\mathcal{G}): \delta_{\mathcal{G}}(k) = 2\},\\
\mathcal{P}_3 &= \{k \in \mathbb{K}(\mathcal{G}): \delta_{\mathcal{G}}(k) = 3\},\\
\mathcal{P}_4 &= \{k \in \mathbb{K}(\mathcal{G}): \delta_{\mathcal{G}}(k) = 4\}.
\end{aligned}$$

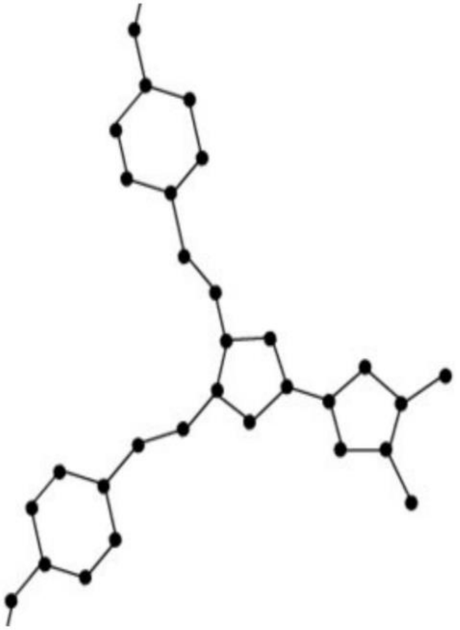

Figure 2: The graph which is added in each branch of $\mathcal{TD}[n]$

Now, we compute the total count of these partitioned nodes, i.e., the number of nodes in every partition. Initially, we find those nodes which have CN 2. From Figure 3, one can easily notice that those nodes which have CN2 does not exist in any pentagons or hexagons. It is clear that only the end nodes have CN2. Thus,

$$\begin{aligned}
\text{Count of nodes with CN 2 in each branch} &= [1 + 2 \times 1 + 2^2 \times 1 + \cdots 2^s \times 1],\\
&= [2^0 + 2^1 + 2^2 + \cdots 2^s],\\
&= 2^{s+1} - 1,\\
\text{Total count of braches} &= 4,\\
|\mathcal{P}_1(\mathcal{G})| &= 8 \times 2^s - 4.
\end{aligned}$$

Next, we count the nodes with CN1 in $\mathcal{G}$. Simple Observation yields that there are 4×2^s nodes having CN 1. Further, we count the nodes having CN3. We have,

$$\begin{aligned}
\text{Count of nodes with CN 3 in each branch} &= [1 \times 11 + 2 \times 11 + 2^2 \times 11 + \cdots 2^{s-1} \times 11] + 2^s \times 8,\\
&= 11[2^0 + 2^1 + 2^2 + \cdots 2^{s-1}] + 2^s \times 8,\\
&= 19 \times 2^s - 11,
\end{aligned}$$

{ Total count of braches }=4

$$|\mathcal{P}_3(\mathcal{G})| = 76 \times 2^s - 44$$

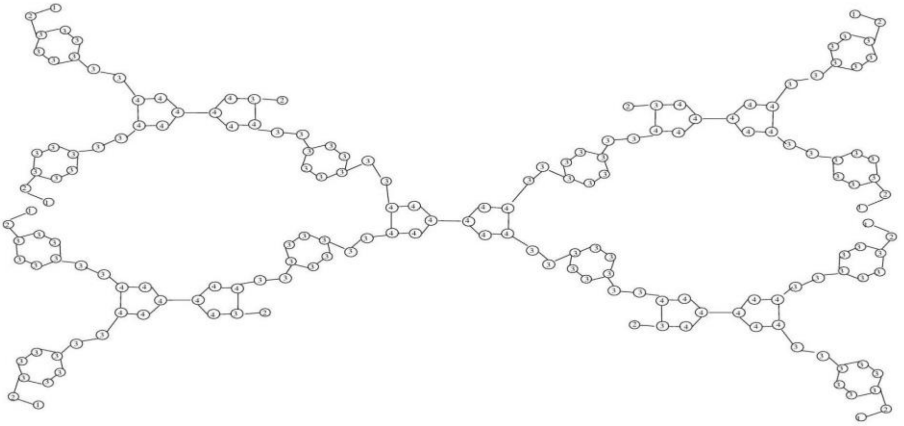

Figure 3: $\mathcal{TD}[1]$ along with CN of each node

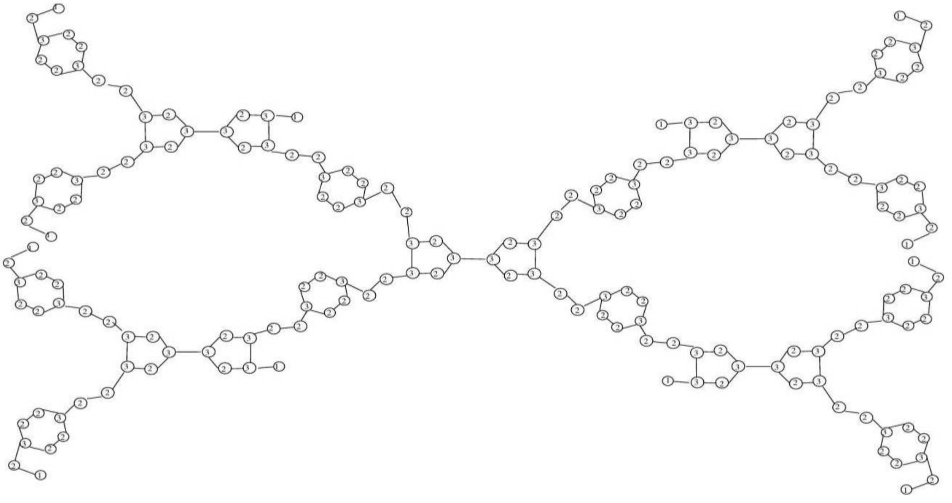

Figure 4: $\mathcal{TD}[1]$ along with degree of each node

For the count of nodes with CN4, we have

Count of nodes with CN 4 in each branch $= [1 \times 9 + 2 \times 9 + 2^2 \times 9 + \cdots 2^{s-1} \times 9]$,

$$= 9[2^0 + 2^1 + 2^2 + \cdots 2^{s-1}]$$

$$= 9 \times 2^s - 9,$$

Total count of braches $= 4$,

$|\mathcal{P}_4(\text{ in all branches })| = 36 \times 2^s - 36$

$|\mathcal{P}_4(\text{ in central core})| = 10,$

$$|\mathcal{P}_4(\mathcal{G})|_6 = 36 \times 2^s - 26$$

By using Equation 1, we have

$$\begin{aligned}
\mathbb{Z}_1\mathrm{C}(\mathcal{G}) &= \sum_{k\in\mathbb{K}} [\delta_{\mathcal{G}}(k)]^2 \\
&= |\mathcal{P}_1(\mathcal{G})|[1^2] + |\mathcal{P}_2(\mathcal{G})|[2^2] + |\mathcal{P}_3(\mathcal{G})|[3^2] + |\mathcal{P}_4(\mathcal{G})|[4^2] \\
&= (4 \times 2^s)[1] + (8 \times 2^s - 4)[4] + (76 \times 2^s - 44)[9] + (36 \times 2^s - 26)[16] \\
&= 4 \times 2^s + 32 \times 2^s - 16 + 684 \times 2^s - 396 + 576 \times 2^s - 416, \\
&= 1266 \times 2^s - 828
\end{aligned}$$

Theorem 3.2. The SZCI of $\mathcal{G} = \mathcal{TD}[s]$, for $s \geq 1$ is given by

$$\mathbb{Z}_2\mathrm{C}(\mathcal{G}) = 1520 \times 2^s - 976.$$

Proof. It is clear from the Figure 3 that there are total five partitions of edges with respect to their CNs. We have

$$\begin{aligned}
\mathcal{E}_{(1,2)} &= \{kt \in \mathbb{T}(\mathcal{G}): \delta_{\mathcal{G}}(k) = 1, \delta_{\mathcal{G}}(k) = 2\}, \\
\mathcal{E}_{(2,3)} &= \{kt \in \mathbb{T}(\mathcal{G}): \delta_{\mathcal{G}}(k) = 2, \delta_{\mathcal{G}}(k) = 3\}, \\
\mathcal{E}_{(3,3)} &= \{kt \in \mathbb{T}(\mathcal{G}): \delta_{\mathcal{G}}(k) = 3, \delta_{\mathcal{G}}(k) = 3\}, \\
\mathcal{E}_{(3,4)} &= \{kt \in \mathbb{T}(\mathcal{G}): \delta_{\mathcal{G}}(k) = 3, \delta_{\mathcal{G}}(k) = 4\}, \\
\mathcal{E}_{(4,4)} &= \{kt \in \mathbb{T}(\mathcal{G}): \delta_{\mathcal{G}}(k) = 4, \delta_{\mathcal{G}}(k) = 4\}.
\end{aligned}$$

Now, we compute the total count of these partitioned edges, i.e., the cardinality of edges in every partition. From Figure 3, one can easily notice that count of (1,2)-type edges are 4×2^s. Next, we find the cardinality of (3,3)-type edges. We have,

$$\begin{aligned}
\text{Count of (3,3)} - \text{ type edges in each branch} &= [1 \times 10 + 2 \times 10 + 2^2 \times 10 + \cdots 2^{s-1} \times 10] + 2^s \times 8, \\
&= 10[2^0 + 2^1 + 2^2 + \cdots 2^{s-1}] + 2^s \times 8, \\
&= 18 \times 2^s - 10, \\
\text{Total count of braches} &= 4, \\
|\mathcal{E}_{(3,3)}(\mathcal{G})| &= 72 \times 2^s - 40.
\end{aligned}$$

Further, for (3,4)-type edges, we have

$$\begin{aligned}
\text{Count of (3,4)} - \text{ type edges in each branch} &= [1 \times 4 + 2 \times 4 + 2^2 \times 4 + \cdots 2^{s-1} \times 4] + 2^s \times 1, \\
&= 4[2^0 + 2^1 + 2^2 + \cdots 2^{s-1}] + 2^s, \\
&= 5 \times 2^s - 4, \\
|\mathcal{E}_{(3,4)}(\mathcal{G})| &= 20 \times 2^s - 16.
\end{aligned}$$

For (4,4)-type edges, we have

$$
\begin{aligned}
\text{Count of } (4,4) - \text{ type edges in each branch} &= [1\times 9 + 2\times 9 + 2^2\times 9 + \cdots 2^{s-1}\times 9],\\
&= 9[2^0 + 2^1 + 2^2 + \cdots 2^{s-1}],\\
&= 9\times 2^s - 9,\\
\text{Total count of braches} &= 4,\\
|\,\mathcal{E}_{(4,4)}(\text{ in all branches })\,| &= 36\times 2^s - 36,\\
|\,\mathcal{E}_{(4,4)}(\text{ in central core })\,| &= 11,\\
\left|\mathcal{E}_{(4,4)}(\mathcal{G})\right| &= 36\times 2^s - 25.
\end{aligned}
$$

Similarly, the count of $(2,3) -$ type edges are $8\times 2^s - 4$. By using Equation 2, we get

$$
\begin{aligned}
\mathbb{Z}_2\mathrm{C}(\mathcal{G}) &= \sum_{kt\in\mathbb{T}} \left[\delta_{\mathcal{G}}(k)\times\delta_{\mathcal{G}}(t)\right]\\
&= \left|\mathcal{E}_{(1,2)}(\mathcal{G})\right|[1\times 2] + \left|\mathcal{E}_{(2,3)}(\mathcal{G})\right|[2\times 3] + \left|\mathcal{E}_{(3,3)}(\mathcal{G})\right|[3\times 3]\\
&+\left|\mathcal{E}_{(3,4)}(\mathcal{G})\right|[3\times 4] + |\,\mathcal{E}_{(4,4)}(\mathcal{G})[|\,4\times 4],\\
&= (4\times 2^s)[1\times 2] + (8\times 2^s - 4)[2\times 3] + (72\times 2^s - 40)[3\times 3]\\
&+(20\times 2^s - 16)[3\times 4] + (36\times 2^s - 25)[4\times 4]\\
&= (4\times 2^s)[2] + (8\times 2^s - 4)[6] + (72\times 2^s - 40)[9]\\
&+(20\times 2^s - 16)[12] + (36\times 2^s - 25)[16],\\
&= 8\times 2^s + 48\times 2^s - 24 + 648\times 2^s - 360\\
&+240\times 2^s - 192 + 576\times 2^s - 400,\\
&= 1520\times 2^s - 976.
\end{aligned}
$$

Theorem 3.3. The modified FZCI of $\mathcal{G} = \mathcal{TD}[s]$, for $s \geq 1$ is given by

$$\mathbb{Z}_1\mathrm{C}^*(\mathcal{G}) = 916\times 2^s - 572$$

Proof. By using Equation 3, we get

$$
\begin{aligned}
\mathbb{Z}_1\mathrm{C}^*(\mathcal{G}) &= \sum_{kt\in\mathbb{T}} \left[\delta_{\mathcal{G}}(k)+\delta_{\mathcal{G}}(t)\right]\\
&= \left|\mathcal{E}_{(1,2)}(\mathcal{G})\right|[1+2] + \left|\mathcal{E}_{(2,3)}(\mathcal{G})\right|[2+3] + \left|\mathcal{E}_{(3,3)}(\mathcal{G})\right|[3+3]\\
&+\left|\mathcal{E}_{(3,4)}(\mathcal{G})\right|[3+4] + \left|\mathcal{E}_{(4,4)}(\mathcal{G})\right|4+4]\\
&= (4\times 2^s)[1+2] + (8\times 2^s - 4)[2+3] + (72\times 2^s - 40)[3+3]\\
&+(20\times 2^s - 16)[3+4] + (36\times 2^s - 25)[4+4]\\
&= (4\times 2^s)[3] + (8\times 2^s - 4)[5] + (72\times 2^s - 40)[6]\\
&+(20\times 2^s - 16)[7] + (36\times 2^s - 25)[8]\\
&= 12\times 2^s + 40\times 2^s - 20 + 436\times 2^s - 240\\
&+ \quad 140\times 2^s - 112 + 288\times 2^s - 200\\
&= 916\times 2^s - 572
\end{aligned}
$$

Theorem 3.4. The modified SZCI of $\mathcal{G} = \mathcal{TD}[s]$, for $s \geq 1$ is given by

$$\mathbb{Z}_2\mathrm{C}^*(\mathcal{G}) = 2336\times 2^s - 1392$$

Proof. To calculate the modified SZCI, we do the partitioning of edges of $\mathcal{G}$ on degree bases. It is clear from the Figure 4 that there are total five partitions of edges with respect to their CNs. We have

$$\mathcal{E}^{d}_{(1,2)} = \{kt \in \mathbb{T}(\mathcal{G}): \delta_{\mathcal{G}}(k) = 1, \delta_{\mathcal{G}}(k) = 2\},$$
$$\mathcal{E}^{d}_{(1,3)} = \{kt \in \mathbb{T}(\mathcal{G}): \delta_{\mathcal{G}}(k) = 1, \delta_{\mathcal{G}}(k) = 3\},$$
$$\mathcal{E}^{d}_{(2,2)} = \{kt \in \mathbb{T}(\mathcal{G}): \delta_{\mathcal{G}}(k) = 2, \delta_{\mathcal{G}}(k) = 2\},$$
$$\mathcal{E}^{d}_{(2,3)} = \{kt \in \mathbb{T}(\mathcal{G}): \delta_{\mathcal{G}}(k) = 2, \delta_{\mathcal{G}}(k) = 3\},$$
$$\mathcal{E}^{d}_{(3,3)} = \{kt \in \mathbb{T}(\mathcal{G}): \delta_{\mathcal{G}}(k) = 3, \delta_{\mathcal{G}}(k) = 3\},$$

The cardinalities of these partitioned nodes are given in Table 1.

Table 1: Edge partition on degree bases

$kt \in \mathbb{T}$	Cardinalities
$\lvert\mathcal{E}^{d}_{(1,2)}\rvert$	4×2^{s}
$\lvert\mathcal{E}^{d}_{(1,3)}\rvert$	$4 \times 2^{s} - 1$
$\lvert\mathcal{E}^{d}_{(2,2)}\rvert$	$28 \times 2^{s} - 16$
$\lvert\mathcal{E}^{d}_{(2,3)}\rvert$	$92 \times 2^{s} - 56$
$\lvert\mathcal{E}^{d}_{(3,3)}\rvert$	$12 \times 2^{s} - 9$

The further classification of edges on the bases of CNs and degrees is displayed in Table 2.

Table 2: Edge partitioning depending on degrees and CNs

$\lvert\mathcal{E}^{d}_{(d(k),d(t))}\rvert$	$\lvert\mathcal{E}_{(\delta(k),\delta(t))}\rvert$	$\lvert\mathcal{E}_{(d(k),d(t))(\delta(k),\delta(t))}\rvert$
$\lvert\mathcal{E}^{d}_{(1,2)}\rvert = 4 \times 2^{s}$	$\lvert\mathcal{E}_{(1,2)}\rvert = 4 \times 2^{s}$	$\lvert\mathcal{E}_{(1,2),(1,2)}\rvert = 4 \times 2^{s}$
$\lvert\mathcal{E}^{d}_{(1,3)}\rvert = 4 \times 2^{s} - 4$	$\lvert\mathcal{E}_{(2,3)}\rvert = 4 \times 2^{s} - 4$	$\lvert\mathcal{E}_{(1,3),(2,3)}\rvert = 4 \times 2^{s} - 4$
$\lvert\mathcal{E}^{d}_{(2,2)}\rvert = 28 \times 2^{s} - 16$	$\lvert\mathcal{E}_{(3,3)}\rvert = 28 \times 2^{s} - 16$	$\lvert\mathcal{E}_{(2,2),(3,3)}\rvert = 28 \times 2^{s} - 16$
$\lvert\mathcal{E}^{d}_{(2,3)}\rvert = 4 \times 2^{s}$	$\lvert\mathcal{E}_{(2,3)}\rvert = 4 \times 2^{s}$	$\lvert\mathcal{E}_{(2,3),(2,3)}\rvert = 4 \times 2^{s}$
$\lvert\mathcal{E}^{d}_{(2,3)}\rvert = 44 \times 2^{s} - 24$	$\lvert\mathcal{E}_{(3,3)}\rvert = 44 \times 2^{s} - 24$	$\lvert\mathcal{E}_{(2,3),(3,3)}\rvert = 44 \times 2^{s} - 24$

$\lvert\mathcal{E}^{d}_{(2,3)}\rvert = 20 \times 2^{s} - 16$	$\lvert\mathcal{E}_{(3,4)}\rvert = 20 \times 2^{s} - 16$	$\lvert\mathcal{E}_{(2,3),(3,4)}\rvert = 28 \times 2^{s} - 16$
$\lvert\mathcal{E}^{d}_{(2,3)}\rvert = 24 \times 2^{s} - 16$	$\lvert\mathcal{E}_{(4,4)}\rvert = 24 \times 2^{s} - 16$	$\lvert\mathcal{E}_{(2,3),(4,4)}\rvert = 24 \times 2^{s} - 16$
$\lvert\mathcal{E}^{d}_{(3,3)}\rvert = 12 \times 2^{s} - 9$	$\lvert\mathcal{E}_{(4,4)}\rvert = 12 \times 2^{s} - 9$	$\lvert\mathcal{E}_{(3,3),(4,4)}\rvert = 12 \times 2^{s} - 9$

By using Table 2 and Equation 4, we get

$$
\begin{aligned}
\mathbb{Z}_2\mathrm{C}^*(\mathcal{G}) &= \sum_{kt\in\mathbb{T}(\mathcal{G})} \left[d_{\mathcal{G}}(k)\delta_{\mathcal{G}}(t) + d_{\mathcal{G}}(t)\delta_{\mathcal{G}}(k)\right] \\
&= \lvert\mathcal{E}_{(1,2),(1,2)}\rvert[(1)(2) + (2)(1)] + \lvert\mathcal{E}_{(1,3),(2,3)}\rvert[(1)(3) + (3)(2)] \\
&+\lvert\mathcal{E}_{(2,2),(3,3)}\rvert[(2)(3) + (2)(3)] + \lvert\mathcal{E}_{(2,3),(2,3)}\rvert[(2)(3) + (3)(2)] \\
&+\lvert\mathcal{E}_{(2,3),(3,3)}\rvert[(2)(3) + (3)(3)] + \lvert\mathcal{E}_{(2,3),(3,4)}\rvert[(2)(4) + (3)(3)] \\
&+\lvert\mathcal{E}_{(2,3),(4,4)}\rvert[(2)(4) + (3)(4)] + \lvert\mathcal{E}_{(3,3),(4,4)}\rvert[(3)(4) + (3)(4)] \\
&= (4 \times 2^{s})[2 + 2] + (4 \times 2^{s} - 4)[3 + 5] + (28 \times 2^{s} - 16)[6 + 6] \\
&+(4 \times 2^{s})[6 + 6] + (44 \times 2^{s} - 24)[6 + 9] + (28 \times 2^{s} - 16)[8 + 9] \\
&+(24 \times 2^{s} - 16)[8 + 12] + (12 \times 2^{s} - 9)[12 + 12] \\
&= (4 \times 2^{s})[4] + (4 \times 2^{s} - 4)[8] + (28 \times 2^{s} - 16)[12] \\
&+(4 \times 2^{s})[12] + (44 \times 2^{s} - 24)[15] + (28 \times 2^{s} - 16)[17] \\
&+(24 \times 2^{s} - 16)[20] + (12 \times 2^{s} - 9)[24], \\
&= (16 \times 2^{s}) + (32 \times 2^{s} - 32) + (336 \times 2^{s} - 192) + (48 \times 2^{s}) \\
&+(660 \times 2^{s} - 360) + (476 \times 2^{s} - 272) + (480 \times 2^{s} - 320) \\
&+(288 \times 2^{s} - 216), \\
&= 2336 \times 2^{s} - 1392
\end{aligned}
$$

Theorem 3.5. The modified TZCI of $\mathcal{G} = \mathcal{TD}[s]$, for $s \geq 1$ is given by

$$\mathbb{Z}_3\mathrm{C}^*(\mathcal{G}) = 2384 \times 2^{s} - 1420.$$

Proof. By using Table 2 and Equation 5, we get

$$
\begin{aligned}
\mathbb{Z}_3\mathrm{C}^*(\mathcal{G}) &= \sum_{kt\in\mathbb{T}(\mathcal{G})} \left[d_{\mathcal{G}}(k)\delta_{\mathcal{G}}(k) + d_{\mathcal{G}}(t)\delta_{\mathcal{G}}(t)\right] \\
&= \left|\mathcal{E}_{(1,2),(1,2)}\right|[(1)(1)+(2)(2)] + \left|\mathcal{E}_{(1,3),(2,3)}\right|[(1)(2)+(3)(3)] \\
&+\left|\mathcal{E}_{(2,2),(3,3)}\right|[(2)(3)+(2)(3)] + \left|\mathcal{E}_{(2,3),(2,3)}\right|[(2)(2)+(3)(3)] \\
&+\left|\mathcal{E}_{(2,3),(3,3)}\right|[(2)(3)+(3)(3)] + \left|\mathcal{E}_{(2,3),(3,4)}\right|[(2)(3)+(3)(4)] \\
&+\left|\mathcal{E}_{(2,3),(4,4)}\right|[(2)(4)+(3)(4)] + \left|\mathcal{E}_{(3,3),(4,4)}\right|[(3)(4)+(3)(4)] \\
&= (4\times 2^s)[1+4] + (4\times 2^s-4)[3+9] + (28\times 2^s-16)[6+6] \\
&+(4\times 2^s)[4+9] + (44\times 2^s-24)[6+9] + (28\times 2^s-16)[6+12] \\
&+(24\times 2^s-16)[8+12] + (12\times 2^s-9)[12+12] \\
&= (4\times 2^s)[5] + (4\times 2^s-4)[11] + (28\times 2^s-16)[12] \\
&+(4\times 2^s)[13] + (44\times 2^s-24)[15] + (28\times 2^s-16)[18] \\
&+(24\times 2^s-16)[20] + (12\times 2^s-9)[24] \\
&= (20\times 2^s) + (44\times 2^s-44) + (336\times 2^s-192) + (52\times 2^s) \\
&+(660\times 2^s-360) + (504\times 2^s-288) + (480\times 2^s-320) \\
&+(288\times 2^s-216), \\
&= 2384\times 2^s-1420
\end{aligned}
$$

4. MZCI of Tetrathiafulvalence Dendrimer

In this section, we find the general results to calculate the multiplicative CN-based ZIs of tetrathiafulvalence dendrimer $\mathcal{TD}[s]$, for $s \geq 1$

Theorem 4.1. The MFZCI of $\mathcal{G} = \mathcal{TD}[s]$, for $s \geq 1$ is given by

$$\mathbb{Z}_1^M\mathrm{C}(\mathcal{G}) = [4]^{(8x-4)} \times [9]^{(76x-44)} \times [16]^{(36x-26)}$$

Proof. By setting all the values computed in proof of Theorem 1 in Equation (6), we have

$$
\begin{aligned}
\mathbb{Z}_1^M\mathrm{C}(\mathcal{G}) &= \prod_{k\in\mathbb{K}} \left[\delta_{\mathcal{G}}(k)\right]^2 \\
&= [1^2]^{|\mathcal{P}_1(\mathcal{G})|} \times [2^2]^{|\mathcal{P}_2(\mathcal{G})|} \times [3^2]^{|\mathcal{P}_3(\mathcal{G})|} \times [4^2]^{|\mathcal{P}_4(\mathcal{G})|} \\
&= [1]^{(4\times 2^s)} \times [4]^{(8\times 2^s-4)} \times [9]^{(76\times 2^s-44)} \times [16]^{(36\times 2^s-26)} \\
&= [4]^{(8x-4)} \times [9]^{(76x-44)} \times [16]^{(36x-26)}.
\end{aligned}
$$

Theorem 4.2. The MSZCI of $\mathcal{G} = \mathcal{TD}[s]$, for $s \geq 1$ is given by

$$\mathbb{Z}_2^M\mathrm{C}(\mathcal{G}) = [2]^{(4x)} \times [6]^{(8x-4)} \times [9]^{(72x-40)} \times [12]^{(20x-16)} \times [16]^{(36x-25)}$$

Proof. By setting all the values computed in proof of Theorem 1 in Equation (7), we have

$$
\begin{aligned}
\mathbb{Z}_2^M \mathrm{C}(\mathcal{G}) \quad &= \prod_{kt \in \mathbb{T}} \left[\delta_{\mathcal{G}}(k) \times \delta_{\mathcal{G}}(t)\right], \\
&= [1 \times 2]^{|\mathcal{E}_{(1,2)}(\mathcal{G})|} \times [2 \times 3]^{|\mathcal{E}_{(2,3)}(\mathcal{G})|} \times [3 \times 3]^{|\mathcal{E}_{(3,3)}(\mathcal{G})|} \\
&\times [3 \times 4]^{|\mathcal{E}_{(3,4)}(\mathcal{G})|} \times [4 \times 4]^{|\mathcal{E}_{(4,4)}(\mathcal{G})|}, \\
&= [1 \times 2]^{(4\times 2^s)} \times [2 \times 3]^{(8\times 2^s)-4} \times [3 \times 3]^{(72\times 2^s-40)} \\
&\times [3 \times 4]^{(20\times 2^s-16)} \times [4 \times 4]^{(36\times 2^s-25)}, \\
&= [2]^{(4\times 2^s)} \times [6]^{(8\times 2^s-4)} \times [9]^{(72\times 2^s-40)} \times [12]^{(20\times 2^s-16)} \times [16]^{(36\times 2^s-25)}, \\
&= [2]^{(4x)} \times [6]^{(8x-4)} \times [9]^{(72x-40)} \times [12]^{(20x-16)} \times [16]^{(36x-25)}.
\end{aligned}
$$

Theorem 4.3. The MTZCI of $\mathcal{G} = \mathcal{TD}[s]$, for $s \geq 1$ is given by

$$
\mathbb{Z}_3^M \mathrm{C}(\mathcal{G}) = [2]^{(4x-4)} \times [4]^{(4x)} \times [6]^{(56x-32)|} \times [8]^{(16x-12)} \times [9]^{(20x-12)} \times [12]^{(20x-14)}
$$

Proof. In order to compute MTZCI, we make the classes of CN-based nodes with respect to their degrees. From Figure 3 Figure 4, it is clear that there are total five partitions of such nodes as given below.

$$
\begin{aligned}
\mathcal{E}'_{(1,1)}(\mathcal{G}) &= \{k \in \mathbb{K}(\mathcal{G}) : d_{\mathcal{G}}(k) = 1, \delta_{\mathcal{G}}(k) = 1\}, \\
\mathcal{E}'_{(1,2)}(\mathcal{G}) &= \{k \in \mathbb{K}(\mathcal{G}) : d_{\mathcal{G}}(k) = 1, \delta_{\mathcal{G}}(k) = 2\}, \\
\mathcal{E}'_{(2,2)}(\mathcal{G}) &= \{k \in \mathbb{K}(\mathcal{G}) : d_{\mathcal{G}}(k) = 2, \delta_{\mathcal{G}}(k) = 2\}, \\
\mathcal{E}'_{(2,3)}(\mathcal{G}) &= \{k \in \mathbb{K}(\mathcal{G}) : d_{\mathcal{G}}(k) = 2, \delta_{\mathcal{G}}(k) = 3\}, \\
\mathcal{E}'_{(2,4)}(\mathcal{G}) &= \{k \in \mathbb{K}(\mathcal{G}) : d_{\mathcal{G}}(k) = 2, \delta_{\mathcal{G}}(k) = 4\}, \\
\mathcal{E}'_{(3,3)}(\mathcal{G}) &= \{k \in \mathbb{K}(\mathcal{G}) : d_{\mathcal{G}}(k) = 3, \delta_{\mathcal{G}}(k) = 3\}, \\
\mathcal{E}'_{(3,4)}(\mathcal{G}) &= \{k \in \mathbb{K}(\mathcal{G}) : d_{\mathcal{G}}(k) = 3, \delta_{\mathcal{G}}(k) = 4\}.
\end{aligned}
$$

Table 3 represents the cardinalities of above degree based partitioned nodes.

Table 3: Count of nodes on the bases of their degrees

$(k,t) \in \mathbb{T}$	Count of nodes
$\lvert\mathcal{E}'_{(1,1)}(\mathcal{G})\rvert$	4×2^s
$\lvert\mathcal{E}'_{(1,2)}(\mathcal{G})\rvert$	$4 \times 2^s - 4$
$\lvert\mathcal{E}'_{(2,2)}(\mathcal{G})\rvert$	4×2^s
$\lvert\mathcal{E}'_{(2,3)}(\mathcal{G})\rvert$	$56 \times 2^s - 32$
$\lvert\mathcal{E}'_{(2,4)}(\mathcal{G})\rvert$	$16 \times 2^s - 12$

$\lvert\mathcal{E}'_{(3,3)}(\mathcal{G})\rvert$	$20\times 2^s-12$
$\lvert\mathcal{E}'_{(3,4)}(\mathcal{G})\rvert$	$20\times 2^s-14$

Now, by using Table 3 and Equation (8), we have

$$\begin{aligned}\mathbb{Z}_3^M\mathrm{C}(\mathcal{G}) &= \prod_{k\in\mathbb{K}}[d(k)\times\delta(k)]\\ &= [1\times 1]^{\lvert\mathcal{E}'_{(1,1)}(\mathcal{G})\rvert}\times[1\times 2]^{\lvert\mathcal{E}'_{(1,2)}(\mathcal{G})\rvert}\times[2\times 2]^{\lvert\mathcal{E}'_{(2,2)}(\mathcal{G})\rvert}\times[2\times 3]^{\lvert\mathcal{E}'_{(2,3)}(\mathcal{G})\rvert}\\ &\times[2\times 4]^{\lvert\mathcal{E}'_{(2,4)}(\mathcal{G})\rvert}\times[3\times 3]^{\lvert\mathcal{E}'_{(3,3)}(\mathcal{G})\rvert}\times[3\times 4]^{\lvert\mathcal{E}'_{(3,4)}(\mathcal{G})\rvert}\\ &= [1]^{(4\times 2^S)}\times[2]^{(4\times 2^S-4)}\times[2\times 2]^{(4\times 2^S)}\times[2\times 3]^{(56\times 2^S-32)|}\\ &\times[2\times 4]^{(16\times 2^S-12)}\times[3\times 3]^{(20\times 2^S-12)}\times[3\times 4]^{(20\times 2^S-14)}\\ &= [1]^{(4\times 2^S)}\times[2]^{(4\times 2^S-4)}\times[4]^{(4\times 2^S)}\times[6]^{(56\times 2^S-32)|}\times[8]^{(16\times 2^S-12)}\\ &\times[9]^{(20\times 2^S-12)}\times[12]^{(20\times 2^S-14)}\\ &= [2]^{(4x-4)}\times[4]^{(4x)}\times[6]^{(56x-32)|}\times[8]^{(16x-12)}\\ &\times[9]^{(20x-12)}\times[12]^{(20x-14)}\end{aligned}$$

Theorem 4.4. The MFZCI of $\mathcal{G}=\mathcal{TD}[s]$, for $s\geq 1$ is given by

$$\mathbb{Z}_4^M\mathrm{C}(\mathcal{G})=[2]^{(4x-4)}\times[4]^{(4x)}\times[5]^{(56x-32)|}\times[6]^{(16x-12)}\times[6]^{(20x-12)}\times[7]^{(20x-14)}$$

Proof. By using Table 3 and Equation 9, we have

$$\begin{aligned}\mathbb{Z}_4^M\mathrm{C}(\mathcal{G}) &= \prod_{k\in\mathbb{K}}[d(k)+\delta(k)],\\ &= [1+1]^{\lvert\mathcal{E}_{(1,1)}(\mathcal{G})\rvert}\times[2+2]^{\lvert\mathcal{E}_{(2,2)}(\mathcal{G})\rvert}\times[2+3]^{\lvert\mathcal{E}_{(2,3)}(\mathcal{G})\rvert}\\ &\times[2+4]^{\lvert\mathcal{E}_{(2,4)}(\mathcal{G})\rvert}\times[3+3]^{\lvert\mathcal{E}_{(3,3)}(\mathcal{G})\rvert}\times[3+4]^{\lvert\mathcal{E}_{(3,4)}(\mathcal{G})\rvert},\\ &= [1+1]^{(4\times 2^S-4)}\times[2+2]^{(4\times 2^S)}\times[2+3]^{(56\times 2^S-32)|}\\ &\times[2+4]^{(16\times 2^S-12)}\times[3+3]^{(20\times 2^S-12)}\times[3+4]^{(20\times 2^S-14)},\\ &= [2]^{(4\times 2^S-4)}\times[4]^{(4\times 2^S)}\times[5]^{(56\times 2^S-32)|}\times[6]^{(16\times 2^S-12)}\\ &\times[6]^{(20\times 2^S-12)}\times[7]^{(20\times 2^S-14)},\\ &= [2]^{(4x-4)}\times[4]^{(4x)}\times[5]^{(56x-32)|}\times[6]^{(16x-12)}\times[6]^{(20x-12)}\times[7]^{(20x-14)}.\end{aligned}$$

Theorem 4.5. The modified FZCI of $\mathcal{G}=\mathcal{TD}[s]$, for $s\geq 1$ is given by

$$\begin{aligned}\mathbb{Z}_1^M\mathrm{C}^*(\mathcal{G}) &= [48]^{(4x)}\times[9]^{(4x-4)}\times[12]^{(28x-16)}\times[15]^{(44x-24)}\times[17]^{(28x-16)}\\ &\times[20]^{(24x-16)}\times[24]^{(12x-9)}\end{aligned}$$

Proof. By using Table 2 and Equation (10), we get

$$
\begin{aligned}
\mathbb{Z}_1^M \mathrm{C}^*(\mathcal{G}) &= \prod_{kt\in\mathbb{T}(\mathcal{G})} \left[d_{\mathcal{G}}(k)\delta_{\mathcal{G}}(t) + d_{\mathcal{G}}(t)\delta_{\mathcal{G}}(k)\right],\\
&= [(1)(2)+(1)(2)]^{|\mathcal{E}_{(1,2),(1,2)}|} \times [(1)(3)+(3)(2)]^{|\mathcal{E}_{(1,3),(2,3)}|}\\
&\times [(2)(3)+(2)(3)]^{|\mathcal{E}_{(2,2),(3,3)}|} \times [(2)(3)+(3)(2)]^{|\mathcal{E}_{(2,3),(2,3)}|}\\
&\times [(2)(3)+(3)(3)]^{|\mathcal{E}_{(2,3),(3,3)}|} \times [(2)(4)+(3)(3)]^{|\mathcal{E}_{(2,3),(3,4)}|}\\
&\times [(2)(4)+(3)(4)]^{|\mathcal{E}_{(2,3),(4,4)}|} \times [(3)(4)+(3)(4)]^{|\mathcal{E}_{(3,3),(4,4)}|},\\
&= [2+2]^{(4\times 2^S)} \times [3+6]^{(4\times 2^S-4)} \times [6+6]^{(28\times 2^S-16)}\\
&\times [6+6]^{(4\times 2^S)} \times [6+9]^{(44\times 2^S-24)} \times [8+9]^{(28\times 2^S-16)}\\
&\times [8+12]^{(24\times 2^S-16)} \times [12+12]^{(12\times 2^S-9)},\\
&= [4]^{(4\times 2^S)} \times [9]^{(4\times 2^S-4)} \times [12]^{(28\times 2^S-16)} \times [12]^{(4\times 2^S)}\\
&\times [15]^{(44\times 2^S-24)} \times [17]^{(28\times 2^S-16)} \times [20]^{(24\times 2^S-16)} \times [24]^{(12\times 2^S-9)},\\
&= [48]^{(4x)} \times [9]^{(4x-4)} \times [12]^{(28x-16)} \times [15]^{(44x-24)} \times [17]^{(28x-16)}\\
&\times [20]^{(24x-16)} \times [24]^{(12x-9)}.
\end{aligned}
$$

Theorem 4.6. The modified SZCI of $\mathcal{G} = \mathcal{TD}[s]$, for $s \geq 1$ is given by

$$
\begin{aligned}
\mathbb{Z}_2^M \mathrm{C}^*(\mathcal{G}) &= [65]^{(4x)} \times [11]^{(4x-4)} \times [12]^{(28x-16)} \times [15]^{(44x-24)} \times [18]^{(28x-16)}\\
&\times [20]^{(24x-16)} \times [24]^{(12x-9)}
\end{aligned}
$$

Proof. By using Table 2 and Equation (11), we get

$$
\begin{aligned}
\mathbb{Z}_2^M \mathrm{C}^*(\mathcal{G}) &= \prod_{kt\in\mathbb{T}(\mathcal{G})} \left[d_{\mathcal{G}}(k)\delta_{\mathcal{G}}(k) + d_{\mathcal{G}}(t)\delta_{\mathcal{G}}(t)\right]\\
&= [(1)(1)+(2)(2)]^{|\mathcal{E}_{(1,2),(1,2)}|} \times [(1)(2)+(3)(3)]^{|\mathcal{E}_{(1,3),(2,3)}|}\\
&\times [(2)(3)+(2)(3)]^{|\mathcal{E}_{(2,2),(3,3)}|} \times [(2)(2)+(3)(3)]^{|\mathcal{E}_{(2,3),(2,3)}|}\\
&\times [(2)(3)+(3)(3)]^{|\mathcal{E}_{(2,3),(3,3)}|} + [(2)(3)+(3)(4)]^{|\mathcal{E}_{(2,3),(3,4)}|}\\
&\times [(2)(4)+(3)(4)]^{|\mathcal{E}_{(2,3),(4,4)}|} \times [(3)(4)+(3)(4)]^{|\mathcal{E}_{(3,3),(4,4)}|},\\
&= [1+4]^{(4\times 2^S)} \times [2+9]^{(4\times 2^S-4)} \times [6+6]^{(28\times 2^S-16)}\\
&\times [4+9]^{(4\times 2^S)} \times [6+9]^{(44\times 2^S-24)} \times [6+12]^{(28\times 2^S-16)}\\
&\times [8+12]^{(24\times 2^S-16)} \times [12+12]^{(12\times 2^S-9)},\\
&= [5]^{(4\times 2^S)} \times [10]^{(4\times 2^S-4)} \times [12]^{(28\times 2^S-16)} \times [13]^{(4\times 2^S)}\\
&\times [15]^{(44\times 2^S-24)} \times [18]^{(28\times 2^S-16)} \times [20]^{(24\times 2^S-16)} \times [24]^{(12\times 2^S-9)},\\
&= [65]^{(4x)} \times [11]^{(4x-4)} \times [12]^{(28x-16)} \times [15]^{(44x-24)} \times [18]^{(28x-16)}\\
&\times [20]^{(24x-16)} \times [24]^{(12x-9)}.
\end{aligned}
$$

Theorem 4.7. Th e modified TZCI of $\mathcal{G} = \mathcal{TD}[s]$, for $s \geq 1$ is given by

$$
\begin{aligned}
\mathbb{Z}_3^M \mathrm{C}^*(\mathcal{G}) &= [144]^{(4x)} \times [18]^{(4x-4)} \times [36]^{(28x-16)} \times [54]^{(44x-24)} \times [72]^{(28x-16)}\\
&\times [96]^{(24x-16)} \times [144]^{(12x-9)}
\end{aligned}
$$

Proof. By using Table 2 and Equation (12), we get

$$\begin{aligned}
\mathbb{Z}_3^M \mathrm{C}^*(\mathcal{G}) &= \prod_{kt \in \mathbb{T}(\mathcal{G})} \left[d_{\mathcal{G}}(k)\delta_{\mathcal{G}}(k) \times d_{\mathcal{G}}(t)\delta_{\mathcal{G}}(t)\right] \\
&= [(1)(1) \times (2)(2)]^{|\mathcal{E}_{(1,2),(1,2)}|} \times [(1)(2) \times (3)(3)]^{|\mathcal{E}_{(1,3),(2,3)}|} \\
&\times [(2)(3) \times (2)(3)]^{|\mathcal{E}_{(2,2),(3,3)}|} \times [(2)(2) \times (3)(3)]^{|\mathcal{E}_{(2,3),(2,3)}|} \\
&\times [(2)(3) \times (3)(3)]^{|\mathcal{E}_{(2,3),(3,3)}|} \times [(2)(3) \times (3)(4)]^{|\mathcal{E}_{(2,3),(3,4)}|} \\
&\times [(2)(4) \times (3)(4)]^{|\mathcal{E}_{(2,3),(4,4)}|} \times [(3)(4) \times (3)(4)]^{|\mathcal{E}_{(3,3),(4,4)}|} \\
&= [1 \times 4]^{(4\times 2^{S})} \times [2 \times 9]^{(4\times 2^{S}-4)} \times [6 \times 6]^{(28\times 2^{S}-16)} \\
&\times [4 \times 9]^{(4\times 2^{S})} \times [6 \times 9]^{(44\times 2^{S}-24)} \times [6 \times 12]^{(28\times 2^{S}-16)} \\
&\times [8 \times 12]^{(24\times 2^{S}-16)} \times [12 \times 12]^{(12\times 2^{S}-9)}, \\
&= [144]^{(4\times 2^{S})} \times [18]^{(4\times 2^{S}-4)} \times [36]^{(28\times 2^{S}-16)} \times [54]^{(44\times 2^{S}-24)} \times [72]^{(28\times 2^{S}-16)} \\
&\times [96]^{(24\times 2^{S}-16)} \times [144]^{(12\times 2^{S}-9)}, \\
&= [144]^{(4x)} \times [18]^{(4x-4)} \times [36]^{(28x-16)} \times [54]^{(44x-24)} \times [72]^{(28x-16)} \\
&\times [96]^{(24x-16)} \times [144]^{(12x-9)}.
\end{aligned}$$

2 Conclusion

Dendrimers are nano-sized, homogeneous particles with three fundamental components: branches, end groups, and cores. These nanoparticles are thought to be the most important component in the field of nanobiotechnology. Dendrimers have a wide range of applications in research, including medication delivery, gene transfer, and energy harvesting. The graph-theoretic invariants help to relate the molecular properties like, melting point, volume, stability, freezing point and strain energy of different chemical structures by associating a numeric digit with these molecular structures. CN-based ZIs can preserve the chemical properties of molecular structures more precisely and efficiently as compared to other degree and distance based ZIs. This manuscript involves the computation of CN-based ZIs, namely, first second, third and fourth ZIs of tetrathiafulvalence dendrimer. Moreover, modified ZIs have also been computed. The TIs calculated in this manuscript help to analyze the defined structure and may assist in preserving many psychochemical properties in a comprehensive way. In the future, our aim is to compute TI for the other molecular structures.

3 References

S.G. Sampathkumar and K.J. Yarema, K. J. Dendrimers in cancer treatment and diagnosis. *Nanotechnologies for the Life Sciences*, (2007).

P. Kesharwani, A. Gothwal, A.K. Iyer, K. Jain, M.K. Chourasia and U. Gupta, Dendrimer nanohybrid carrier systems: *An expanding horizon for targeted drug and gene delivery*. *Drug discovery today*, 23(2) (2018), 300-314. https://doi.org/10.1016/j.drudis.2017.06.009

B. Klajnert, L. Peng and V. Ceoa, (Eds.). Dendrimers in biomedical applications. *Royal Society of Chemistry*, (2013).

J. Kurczewska, M. Ceglowski, B. Messyasz and G. Schroeder, Dendrimer-functionalized halloysite nanotubes for effective drug delivery. *Applied Clay Science*, 153 (2018), 134-143. https://doi.org/10.1016/j.clay.2017.12.019

H.U. Afzal and T. Fatima, On Topological Indices of OT [m, n] Octagonal Tillings and TiO2 Nanotubes. *Acta Chimica Slovenica,* 66(2) (2019), 435-442. http://dx.doi.org/10.17344/acsi.2018.4897

W. Gao, M. Younas, A. Farooq, A. Mahboob and W. Nazeer, M-polynomials and degree-based topological indices of the crystallographic structure of molecules.*Biomolecules*, 8(4) (2018), 107. https://doi.org/10.3390/biom8040107

M. Imran, A.Q. Baig and H. Ali, On molecular topological properties of hex-derived networks.*Journal of Chemometrics,* 30(3), (2016) 121-129.

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

H. Wiener, Structural determination of paraffin boiling points. *Journal of the American Chemical Society*, 69(1) (1947), 17-20. https://doi.org/10.1021/ja01193a005

I. Gutman and N. Trinajstic, Graph theory and molecular orbitals. Total π-electron energy of alternant hydrocarbons. *Chemical Physics Letters*, 17(4) (1972), 535-538. https://doi.org/10.1016/0009-2614(72)85099-1

I. Gutman, B. Ruscic, N. Trinajstic, C.F. Wilcox Jr, Graph theory and molecular orbitals. XII. Acyclic polyenes. *The journal of Chemical Physics*, 62(9) (1975), 3399-3405. https://doi.org/10.1063/1.430994

B. Furtula and I. Gutman, A forgotten topological index. *Journal of Mathematical Chemistry,* 53(4) (2015), 1184-1190. https://doi.org/10.1007/s10910-015-0480-z

A. Ali, I. Gutman, E. Milovanovic, I. Milovanovic, Sum of powers of the degrees of graphs extremal results and bounds. *MATCH Communications in Mathematical and in Computer Chemistry*, 80(1) (2018), 5-84.

B. Borovicanin, K.C. Das, B. Furtula and I. Gutman, Bounds for Zagreb indices. *MATCH Communications in Mathematical and in Computer Chemistry*, 78(1) (2017), 17-100. https://scidar.kg.ac.rs/handle/123456789/17404

M. Javaid, U. Ali and J.B. Liu, Computing analysis for first Zagreb connection index and coindex of resultant graphs. *Mathematical Problems in Engineering*, (2021), 2021. https://doi.org/10.1155/2021/6019517

Y. Bashir, A. Aslam, M. Kamran, M.I. Qureshi, A. Jahangir, M. Rafiq and N. Muhammad, On forgotten topological indices of some dendrimers structure. *Molecules,* 22(6) (2017), 867. https://doi.org/10.3390/molecules22060867

S.A.U.H. Bokhary, M. Imran and S. Manzoor, On molecular topological properties of dendrimers. *Canadian Journal of Chemistry,* 94(2) (2016), 120-125. https://doi.org/10.1139/cjc-2015-046

N. Dorosti, A. Iranmanesh and M.V. Diudea, Computing the Cluj index of the first type dendrimer nanostar. *Optoelectronics and Advanced Materials-Rapid Communications,* 4 (2010), 381-384.

A. Ali and N. Trinajstic, A novel/old modification of the first Zagreb index. *Molecular informatics*, 37(6-7) (2018), 1800008.

https://doi.org/10.1002/minf.201800008

U. Ali, M. Javaid and A. Kashif, Modified Zagreb connection indices of the T-sum graphs. *Main Group Metal Chemistry*, 43(1) (2020), 43-55.

J. Cao, U. Ali, M. Javaid and C. Huang, Zagreb connection indices of molecular graphs based on operations. *Complexity*, (2020), 2020. https://doi.org/10.1155/2020/7385682

Z. Du, A. Ali and N. Trinajstic, Alkanes with the first three maximal/minimal modified first Zagreb connection indices. *Molecular informatics*, 38(4) (2019), 1800116.

https://doi.org/10.1002/minf.201800116

R.S. Haoer, M.A. Mohammed, T. Selvarasan, N. Chidambaram and N. Devadoss, Multiplicative leap Zagreb indices of T-thorny graphs. *Eurasian Chemical Communications*, 2(8) (2020), 841-846. DOI: 10.33945/SAMI/ECC.2020.8.2

S. Nikolic, G. Kovacevic, A. Milicevic and N. Trinajstic, The Zagreb indices 30 years after. *Croatica Chemica Acta*, 76(2) (2003), 113-124. https://hrcak.srce.hr/103086

M. Javaid, U. Ali and K. Siddiqui, Novel connection-based Zagreb indices of several wheel-related graphs. *Computational Journal of Combinatorial Mathematics*, 1 (2021), 1-28.

K.C. Das, A. Yurttas, M. Togan, A.S. Cevik and I.N. Cangul, The multiplicative Zagreb indices of graph operations. *Journal of Inequalities and Applications*, 2013(1) (2013), 1-14. https://doi.org/10.1186/1029-242X-2013-90

K. Dhanalakshmi, J. Amalorpava Jerline and L. Benedict Michaelraj, Modified and Multiplicative Zagreb Indices on Graph Operators. *Journal of Computer and Mathematical Sciences* 7(4) (2016), 225-232.