On the Studies of Dendrimers via Connection-Based Molecular Descriptors

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Topological indices (TIs) have been utilized widely to characterize and model the chemical structures of various molecular compounds such as dendrimers, neural networks, and nanotubes. Dendrimers are extraordinarily comprehensible, globular, artificially synthesized polymers with a structure of frequently branched units. A mathematical approach to characterize the molecular structures by manipulating the topological techniques, including numerical graphs invariants is the present-day line of research in chemistry. Among all the defined descriptors, the connection-based Zagreb indices are considered to be more effective than the other classical indices. In this manuscript, we find the general results to compute the Zagreb connection indices (ZCIs), namely, first ZCI (1st ZCI), second ZCI (2nd ZCI), modified 1st ZCI, modified 2nd ZCI, and modified 3rd ZCI. Furthermore, we compute the multiplicative ZCI (MZCI), namely, first MZCI (1st MZCI), second MZCI (2nd MZCI), third MZCI (3rd MZCI), fourth MZCI (4th MZCI), modified 1st MZCI, modified 2nd MZCI, and modified 3rd MZCI. In addition, we compare the calculated values with each other in order to check the superiority.

1. Introduction

Dendrimers are compartmentalized, versatile, well-defined, synthetic chemical polymers with numerous attributes which make them advantageous in biological systems. The structure of dendrimers is made up of three components, the multivalent surface, the outer shell, and a core which is protected by the dendritic branches in higher generations of dendrimers. Dendrimers are synthesized by the use of two approaches, divergent, and convergent. Nowadays, dendrimers are considered to be the notably manufactured macromolecules with applicability in the domain of biomedical science including gene transfection, tissue engineering, drug delivery, contrast intensification for magnetic resonance imaging, and immunology, for details see [1–3]. They are extensively employed in the formation of chemical sensors, colored glass, nanolatex, nanotubes, and micro-/macrocapsules. Due to their wide ranging applications in distinct areas, dendrimers are attaining valuable contemplation from the researchers. They are trying to specify these molecular structures by the use of numerical graphs descriptors. The numerical graph descriptors or topological indices are the trending topological approach in computational and mathematical chemistry to characterize or signalize the topology of molecular structures. These graph descriptions or invariants have countless utilizations in quantitative structure-activity relationship (QSAR) and quantitative structure property relationship (QSPR) studies appropriate for hazard analysis of chemicals, the discovery of drugs, and novel molecular designs [4]. Topological index (TI) is a numeric measure which helps to correlate the distinct psychochemical properties of molecular structures like freezing point, melting point, volatility, density, stability, flammability, and strain energy of molecular compounds.

Topological indices (TIs) are classified on the basis of distance, degree, and polynomial. Wiener [5] put forward the innovational conception of distance-based TI which is known by Wiener index. Aslam et al. [6] compute the TIs of some interconnection networks. After the invention of Wiener index, a large number of other distance-based TIs
have been investigated and considered by many analysts in the chemical and mathematico chemical literature, for details see [7–9].

Gutman and Trinajstic [10] initiated the innovational notion of first ZI (1st ZI) in 1972. In 1975, Gutman et al. [11] proposed the conception of second ZI (2nd ZI). These classical ZIs have been utilized broadly in the study of chemical graph theory. Furthermore, the conception of third ZI (3rd ZI), also called forgotten index, was explored by Furtula and Gutman [12]. These degree-based TIs have great significance in the field of cheminformatics, as one can see [13–15]. In 2003, Nikolic et al. [16] explored the new index, called degree-based TI, which have the well-mannered way. Das et al. [18] investigated some MZIs and considered the outcomes concerning these indices in well-mannered way. Das et al. [18] investigated some MZIs of graph operations.

Recently, Ali and Trinajstic [19] explored a new way to study the psychochemical properties of compounds by introducing the connection number (CN) of the vertex and initiated Zagreb connection indices (ZCIs). The number of those vertices which are distance two from a certain vertex is said to be a CN of that vertex. They reported that the newly proposed connection-based ZIs have better applicability to forecast the psychochemical properties of various molecular structures instead of the classical ZIs. After the invention of CN, many researchers started work to explore new connection-based indices. Multiplicative leap ZIs were investigated by Haoer et al. [20]. Du et al. [21] utilized connection-based modified ZFI to find the extremal alkanes. Recently, Sattar et al. [22] computed the general expressions to compute MZCI of dendrimer nanostars. Furthermore, in 2020, Ali et al. [23] worked out to calculate the modified ZCIs for T-sum graphs. Javaid et al. [24] calculated multiplicative ZIs for some wheel graphs. In 2019, Nisar et al. [25] computed ZCIs of two types of dendrimer nanostars. Ye et al. [26] calculated ZCIs of nanotubes and regular hexagonal lattice. Bokhary et al. [27] studied the topological properties of some nanostars. Bashir et al. [28] computed the 3rd ZI of a dendrimer nanostar. Gharibi et al. [29] developed the conception of Zagreb polynomials of nanotubes and nanocones. For the other information, we recommend the readers to study [30,31].

The motivation for this article is as follows:

(1) Topological indices (TIs), the numerical descriptors, are efficient enough to characterize the topology of molecular structures and also assist to correlate their distinct psychochemical properties.

(2) Dendrimers are symmetric, versatile, and well-defined chemical polymers forming a tree-like structure. These nanoparticles are signalized by a number of attributes which make them advantageous for wide-ranging utilizations in various fields of science.

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

In this paper, we present the general expressions to compute the ZCIs and MZCIs of nanostar. This manuscript is organized as follows: in Section 2, the elementary definitions are discussed which helps the readers to fully understand the main idea of this article. In Section 3, we present the general expressions to compute ZCIs, namely, 1st ZCI, 2nd ZCI, modified 1st ZCI, modified 2nd ZCI, and modified 3rd ZCI. Section 3 involves general expressions to compute the MZCIs, namely, 1st MZCI, 2nd MZCI, 3rd MZCI, 3rd MZCI, modified 1st MZCI, modified 2nd MZCI, and modified 3rd MZCI. Section 4 covers the concluding remarks.

2. Preliminaries

This section involves some useful primary definitions from the literature to understand the main result of this manuscript.

Definition 1. Let \( \Omega = (\mathcal{E}(\Omega), \delta(\Omega)) \) be a graph, where \( \mathcal{E}(\Omega) \) and \( \delta(\Omega) \) be the set of vertices and set of edges, respectively. Then, the degree-based Zagreb indices are defined as follows:

\[
(1) \quad \tilde{Z}_1(\Omega) = \sum_{t \in \mathcal{E}(\Omega)} (d^2_t) = \sum_{x \in \delta(\Omega)} (d_x + d_t)
\]

\[
(2) \quad \tilde{Z}_2(\Omega) = \sum_{t \in \mathcal{E}(\Omega)} (d_t + d_x)
\]

Here, \( d_t(t) \) and \( d_x(x) \) denote the degree of the vertex \( t \) and \( x \), respectively. These degree-based indices, discovered by Gutman and Trinajstic [10], are known as first ZI (1st ZI) and second ZI (2nd ZI), respectively.

Definition 2. For a graph \( \Omega \), connection-based Zagreb indices are given as

\[
(1) \quad \tilde{Z}_C_1(\Omega) = \sum_{t \in \mathcal{E}(\Omega)} (\tilde{\phi}_t(t))^2
\]

\[
(2) \quad \tilde{Z}_C_1(\Omega) = \sum_{t \in \mathcal{E}(\Omega)} (\tilde{\phi}_t(t)\bar{\phi}_t(x))
\]

Here, \( \tilde{\phi}_t(t) \) and \( \bar{\phi}_t(x) \) indicate the connection number (CN) of the vertex \( t \) and \( x \), respectively. These connection-based indices were discovered by Ali and Trinajstic [19] and are known as the first Zagreb connection index (1st ZCI) and second Zagreb connection index (2nd ZCI), respectively.

Definition 3. For a graph \( \Omega \), the modified ZCIs can be given as follows:

\[
(1) \quad \tilde{Z}_C_1^*(\Omega) = \sum_{t \in \mathcal{E}(\Omega)} (\tilde{\phi}_t(t)\bar{\phi}_t(x)) = \sum_{t \in \mathcal{E}(\Omega)} (\tilde{d}_t(t))
\]

\[
(2) \quad \tilde{Z}_C_1^*(\Omega) = \sum_{t \in \mathcal{E}(\Omega)} (\tilde{d}_t(t)\bar{\phi}_t(x) + \tilde{d}_t(x)\bar{\phi}_t(t))
\]

\[
(3) \quad \tilde{Z}_C_1^*(\Omega) = \sum_{t \in \mathcal{E}(\Omega)} (\tilde{d}_t(t)\bar{\phi}_t(x) + \tilde{d}_t(x)\tilde{\phi}_t(t))
\]

These modified ZIs, proposed by Ali [19] and Ali et al. [23], are known as the modified 1st ZCI, modified 2nd ZCI, and modified 3rd ZCI, respectively.

Definition 4. For a graph \( \Omega \), multiplicative ZCIs can be defined as follows:

...
Definition 6. For a graph $\Omega$, first multiplicative ZCI ($1^{st}$ MZCI), modified first multiplicative ZCI ($2^{nd}$ MZCI), and modified third multiplicative ZCI ($3^{rd}$ MZCI) can be defined as follows:

1. $\mathcal{M}\mathcal{Z}C_1(\Omega) = \prod_{t \in \mathcal{R}(\Omega)} (\varphi_\Omega(t))^2$
2. $\mathcal{M}\mathcal{Z}C_2(\Omega) = \prod_{t \in \mathcal{R}(\Omega)} (\varphi_\Omega(t) \times \varphi_\Omega(x))^2$
3. $\mathcal{M}\mathcal{Z}C_3(\Omega) = \prod_{t \in \mathcal{R}(\Omega)} (\varphi_\Omega(t) \times \varphi_\Omega(x))^2$
4. $\mathcal{M}\mathcal{Z}C_4(\Omega) = \prod_{t \in \mathcal{R}(\Omega)} (\varphi_\Omega(t) \times \varphi_\Omega(x))^2$

These multiplicative ZCIs were proposed by Javaid et al. [24] and are known as first multiplicative ZCI ($1^{st}$ MZCI), second multiplicative ZCI ($2^{nd}$ MZCI), third multiplicative ZCI ($3^{rd}$ MZCI), and fourth multiplicative ZCI ($4^{th}$ MZCI), respectively.

Definition 5. For a graph $\Omega$, modified first multiplicative ZCI ($1^{st}$ MZCI), modified second multiplicative ZCI ($2^{nd}$ MZCI), and modified third multiplicative ZCI ($3^{rd}$ MZCI) can be defined as follows:

1. $\mathcal{M}\mathcal{Z}C_1^*(\Omega) = \prod_{t \in \mathcal{R}(\Omega)} (\check{\varphi}_\Omega(t) + \check{\varphi}_\Omega(x))$
2. $\mathcal{M}\mathcal{Z}C_2^*(\Omega) = \prod_{t \in \mathcal{R}(\Omega)} (\check{\varphi}_\Omega(t) \times \check{\varphi}_\Omega(x))$
3. $\mathcal{M}\mathcal{Z}C_3^*(\Omega) = \prod_{t \in \mathcal{R}(\Omega)} (\check{\varphi}_\Omega(t) \times \check{\varphi}_\Omega(x))^2$
4. $\mathcal{M}\mathcal{Z}C_4^*(\Omega) = \prod_{t \in \mathcal{R}(\Omega)} (\check{\varphi}_\Omega(t) \times \check{\varphi}_\Omega(x))^2$

These connection-based modified MZIs were proposed by Javaid et al. [24].

### 3. ZCIs of Nanostar Dendrimer $D[k]$

This section involves the expressions to obtain connection-based ZIs, namely, $1^{st}$ ZCI, $2^{nd}$ ZCI, modified $1^{st}$ ZCI, modified $2^{nd}$ ZCI, and modified $3^{rd}$ ZCI of the nanostar dendrimer. The molecular structure of $D[k]$ for $k = 1, 2, 3$ together with connection number of each vertex is presented in Figure 1, 2 and 3. The molecular structure of $D[k]$ for $k = 1, 2, 3$ together with degree of each vertex is presented in Figures 4, 5, and 6. First, in order to compute all ZCIs, we rewrite the abovementioned ZIs as follows.

**Definition 6.** For a graph $\Omega$, the $1^{st}$ ZCI can be rewritten as

$$\mathcal{Z}C_1^*(\Omega) = \sum_{0 \leq a \leq k-2} |\mathcal{F}_a(\Omega)|\left[\alpha^2\right],$$

where $|\mathcal{F}_a(\Omega)|$ is the total number of vertices in $\Omega$ with CN $a$.

Furthermore, we can rewrite the $2^{nd}$ ZCI as

$$\mathcal{Z}C_2^*(\Omega) = \sum_{0 \leq a \leq k-2} |\mathcal{F}_a(\Omega)|\left[\alpha \times \tau\right].$$

Similarly, the modified $1^{st}$ ZCI can be rewritten as

$$\mathcal{Z}C_1^*(\Omega) = \sum_{0 \leq a \leq k-2} |\mathcal{F}_a(\Omega)|\left[\alpha \times \tau\right].$$

where $|\mathcal{F}_a,\tau(\Omega)|$ is the total number of edges in $\Omega$ with CNs $(a, \tau)$.

The modified $2^{nd}$ ZCI can be rewritten as

$$\mathcal{Z}C_2^*(\Omega) = \sum_{0 \leq a \leq k-2} |\mathcal{F}_a(\Omega)|\left[\alpha \times \tau\right].$$

The modified $3^{rd}$ ZCI can be rewritten as

$$\mathcal{Z}C_3^*(\Omega) = \sum_{0 \leq a \leq k-2} |\mathcal{F}_a(\Omega)|\left[\alpha \times \tau\right].$$

### Theorem 1

Let $\Omega = D[k]$ be a molecular graph for $k = 1, 2, 3$. Then, the general expressions to compute the $1^{st}$ ZCI and $2^{nd}$ ZCI are as follows:

1. $\mathcal{Z}C_1^*(\Omega) = 327(2^3) - 480$
2. $\mathcal{Z}C_2^*(\Omega) = 396(2^3) - 4588$

**Proof.** Initially, we calculate the total vertices and edges of $D[k]$. Simple calculation yields that $57(2^{k-1}) - 38$ and $33(2^{k-1}) - 45$ are the total vertices and edges of $D[k]$, respectively. Now, we do the partitioning of vertices in $\Omega$ on the bases of CNs. It can be easily seen that there are total four connection-based partitions of vertices:

$$\mathcal{F}_2 = \{t \in \mathcal{R}: \varphi_\Omega(t) = 2\},$$
$$\mathcal{F}_3 = \{t \in \mathcal{R}: \varphi_\Omega(t) = 3\},$$
$$\mathcal{F}_4 = \{t \in \mathcal{R}: \varphi_\Omega(t) = 4\},$$
$$\mathcal{F}_6 = \{t \in \mathcal{R}: \varphi_\Omega(t) = 6\}.$$

Now, we find $|\mathcal{F}_2(\Omega)|$. It can be easily seen that only the term-hexagon contain the vertices of CN 2 and there are exactly 3 vertices of CN 2 in each term-hexagon. As we know that the number of term hexagons is $3(2^{k-1})$, the number of vertices with CN 2 must be

$$|\mathcal{F}_2(\Omega)| = 3(3 \times 2^{k-1}) = 9(2^{k-1}).$$
Now, we find $|\mathcal{F}_3(\Omega)|$, i.e., all those vertices whose CN is 3. As every term-hexagon contain exactly two vertices of CN 3, while pivot-hexagon contains exactly four vertices of CN 3. Thus, $|\mathcal{F}_3|$, in term-hexagon and pivot-hexagon must be $2 \times 3(2^{k-1})$ and $4 \times [6(2^{k-1}) - 6]$, respectively. Thus, $|\mathcal{F}_3(\Omega)|$ will be equal to

$$|\mathcal{F}_3(\Omega)| = 2 \times 3(2^{k-1}) + 4 \times [6(2^{k-1}) - 6],$$

$$= 30(2^{k-1}) - 24. \quad (9)$$

Now, we find $|\mathcal{F}_4(\Omega)|$, i.e., all those vertices whose CN is 4. Every term-hexagon contains exactly one vertex of CN 4, while pivot-hexagon contains exactly two vertices of CN 3. Thus, $|\mathcal{F}_4|$ in term-hexagon and pivot-hexagon must be $3(2^{k-1})$ and $2 \times [6(2^{k-1}) - 6]$, respectively. Then, $|\mathcal{F}_4(\Omega)|$ will be equal to

$$|\mathcal{F}_4(\Omega)| = 3(2^{k-1}) + 2 \times [6(2^{k-1}) - 6]$$

$$= 15(2^{k-1}) - 12. \quad (10)$$

Now, we find $|\mathcal{F}_6(\Omega)|$, i.e., all those vertices whose CN is 6. Only the primary vertices have CN 6 and the number of primary vertices in $\Omega$ are $3(2^{k-1}) - 2$. Thus, we have

$$|\mathcal{F}_6(\Omega)| = 3(2^{k-1}) - 2. \quad (11)$$

By placing all the above computed values of $|\mathcal{F}_\alpha(\Omega)|$ for $\alpha = 1, 2, 3, 4$ in (1), we have

**Figure 1:** $D_{[13]}$ together with CN of each vertex.

**Figure 2:** $D_{[23]}$ together with CN of each vertex.
\[ \mathcal{C}_1(\Omega) = \sum_{0 \leq n \leq k-2} |\mathcal{F}_n(\Omega)| \llbracket \alpha^2 \rrbracket, \]

\[ = |\mathcal{F}_2(\Omega)| \llbracket 2^2 \rrbracket + |\mathcal{F}_3(\Omega)| \llbracket 3^2 \rrbracket + |\mathcal{F}_4(\Omega)| \llbracket 4^2 \rrbracket + |\mathcal{F}_6(\Omega)| \llbracket 6^2 \rrbracket \]

\[ = 9(2^{k-1})[4] + (30(2^{k-1}) - 24)[9] + (15(2^{k-1}) - 12)[16] + (3(2^{k-1}) - 2)[36] \]

\[ = 327(2^k) - 480. \]  

Secondly, we do the partitioning of edges in \( \Omega \) on the bases of CNs. There are total six connection-based partitions of vertices:
Figure 5: $D_{[23]}$ together with degree of each vertex.

Figure 6: $D_{[23]}$ together with degree of each vertex.
\[ F_{(2,2)} = \{ e = tx \in \delta : \phi_1(t) = 2, \phi_1(x) = 2 \}, \]
\[ F_{(2,3)} = \{ e = tx \in \delta : \phi_1(t) = 2, \phi_1(x) = 3 \}, \]
\[ F_{(3,3)} = \{ e = tx \in \delta : \phi_1(t) = 3, \phi_1(x) = 3 \}, \]
\[ F_{(3,4)} = \{ e = tx \in \delta : \phi_1(t) = 3, \phi_1(x) = 4 \}, \]
\[ F_{(4,4)} = \{ e = tx \in \delta : \phi_1(t) = 4, \phi_1(x) = 4 \}, \]
\[ F_{(4,6)} = \{ e = tx \in \delta : \phi_1(t) = 4, \phi_1(x) = 6 \}. \] (13)

To compute the 2nd ZCI \( \tilde{\mathcal{C}}_2(\Omega) \), we find \( |F_{(\alpha,r)}(\Omega)| \).
As we can see that the number of (2, 2) and (2, 3)-type edges only lies in term-hexagons of \( \Omega \), and the number of (2, 2)
and (2, 3)-type edges is exactly two in every term-hexagon of \( \Omega \). Thus, we have,
\[ |F_{(2,2)}| = 2 \times (2^{k-1}), 6(2^{k-1}), \]  \[ |F_{(2,3)}| = 6(2^{k-1}). \] (14)

Now, we find the number of (3) and (4)-edges, i.e., \( |F_{(3,4)}| \). Every term-hexagon contains exactly two (3, 4)-type
edges, while pivot-hexagon contains exactly four (3, 4)-type edges. Thus, the number of (3, 4)-type edges in term-
hexagon and pivot-hexagon must be \( 6(2^{k-1}) \) and \( 4 \times [6(2^{k-1}) - 6] \), respectively. Therefore, we have
\[ |F_{(3,4)}| = 6(2^{k-1}) + 4 \times [6(2^{k-1}) - 6] \]
\[ = 30(2^{k-1}) - 24. \] (15)

Now, we find the number of (3,3)-edges, i.e., \( |F_{(3,3)}| \). The term-hexagon contains (3,3)-type edges, and there are exactly two (3,3)-type edges in every term-hexagon of \( \Omega \). Thus, the number of (3,3)-type edges in \( \Omega \) are
\[ |F_{(3,3)}| = 2 \times [6(2^{k-1}) - 6] \]
\[ = 12(2^{k-1}) - 12. \] (16)

Similarly, we can find the number of (4,4) and (4,6)-type edges. We have
\[ |F_{(4,4)}| = 9(2^{k-1}) - 6, \]  \[ |F_{(4,6)}| = 3(2^{k-1}) - 3. \] (17)

By placing all the above computed values of \( |F_{(\alpha,r)}(\Omega)| \) for \( \alpha = 1, 2, 3, 4 \) in (2), we have

\[ \tilde{\mathcal{C}}_2(\Omega) = \sum_{0 \leq a \leq k-2} |F_{(\alpha,r)}(\Omega)|[\alpha + r] \]
\[ = |F_{(2,2)}(\Omega)|[2 \times 2] + |F_{(2,3)}(\Omega)|[2 \times 3] + |F_{(3,3)}(\Omega)|[3 \times 3] + |F_{(3,4)}(\Omega)|[3 \times 4] + |F_{(4,4)}(\Omega)|[4 \times 4] \]
\[ + |F_{(4,6)}(\Omega)|[4 \times 6] \]
\[ = 6(2^{k-1})[4] + 6(2^{k-1})[6] + (12(2^{k-1}) - 12)[9] + (30(2^{k-1}) - 24)[12] + (3(2^{k-1}) - 3)[16] + (9(2^{k-1}) - 6)[24], \]
\[ = 396(2^k) - 588. \] (18)

**Theorem 2.** Let \( \Omega = D[k] \) be a molecular graph for \( k = 1, 2, 3 \). Then, the general expressions to compute the modified 1st ZCI, modified 2nd ZCI and modified 3rd ZCI are

1. \( \tilde{\mathcal{C}}_1^*(\Omega) = 225(2^k) - 324 \)
2. \( \tilde{\mathcal{C}}_2^*(\Omega) = 552(2^k) - 756 \)
3. \( \tilde{\mathcal{C}}_3^*(\Omega) = 792(2^k) - 828 \)

\[ \tilde{\mathcal{C}}_1(\Omega) = \sum_{0 \leq a \leq k-2} |F_{(\alpha,r)}(\Omega)|[\alpha + r] \]
\[ = |F_{(2,2)}(\Omega)|[2 \times 2] + |F_{(2,3)}(\Omega)|[2 \times 3] + |F_{(3,3)}(\Omega)|[3 \times 3] + |F_{(3,4)}(\Omega)|[3 \times 4] + |F_{(4,4)}(\Omega)|[4 \times 4] \]
\[ + |F_{(4,6)}(\Omega)|[4 \times 6] \]
\[ = 6(2^{k-1})[4] + 6(2^{k-1})[5] + (12(2^{k-1}) - 12)[6] + (30(2^{k-1}) - 24)[7] + (3(2^{k-1}) - 3)[8] + (9(2^{k-1}) - 6)[10], \]
\[ = 255(2^k) - 324. \] (19)
(2) Now, we do the partitioning of edges with respect to their degrees of incident vertices. After simple calculation, \(|\varphi_{(2,2)}(\Omega)| = 24(2^{k-1}) - 12\), \(|\varphi_{(2,2)}(\Omega)| = 30(2^{k-1}) - 24\), and \(|\varphi_{(3,3)}(\Omega)| = 12(2^{k-1}) - 9\) are the total number of edges on degree bases. Now, to calculate the general expressions for the modified 1st ZCI, modified 2nd ZCI, and modified 3rd ZCI, we break the partitioned degree-basis edges with respect to the number of edges on connection bases.

\[
\tilde{\mathcal{C}}^*_2(\Omega) = \sum_{0 \leq s \leq t-2, 0 \leq \mu \leq \kappa-2} \big| \varphi_{(\mu,v)}(\Omega) \big| \left[ \mu \tau + \nu \right],
\]

\[
\tilde{\mathcal{C}}^*_3(\Omega) = \sum_{0 \leq s \leq t-2, 0 \leq \mu \leq \kappa-2} \big| \varphi_{(\mu,v)}(\Omega) \big| \left[ \mu \tau + \nu \right],
\]

(3) By placing the values of \(|\varphi_{(\mu,v)}(\Omega)|\) in (5), we get

From row 1 and column 3 of Table 1, we have \(|\varphi_{(2,2)}(\Omega)| = 6(2^{k-1})\), which shows that there are 6 \((2^{k-1})\) number of edges with one end vertex having degree 2 and CN 2 is adjacent to the vertex having degree 2 and CN 2. Similarly, \(|\varphi_{(2,2)}(\Omega)| = 6(2^{k-1})\) represents that the number of those edges with one end vertex having degree 2 and CN 2 adjacent to the vertex having degree 2 and CN 3 are 6 \((2^{k-1})\). By placing the values of \(|\varphi_{(\mu,v)}(\Omega)|\) in (4), we get

\[
\mathcal{M} \mathcal{C}_2(\Omega) = \prod_{0 \leq s \leq t-2} [\alpha \times \tau]^{\varphi_{(\alpha)}(\Omega)},
\]

where \(|\varphi_{(\alpha)}(\Omega)|\) are the total edges with CNs \(\alpha\) and \(\tau\).

The 3rd MZCI can be rewritten as

\[
\mathcal{M} \mathcal{C}_3(\Omega) = \prod_{0 \leq y \leq s \leq t-2} [\gamma \times \alpha]^{\varphi_{(\gamma,\alpha)}(\Omega)},
\]

where \(|\varphi_{(\gamma,\alpha)}(\Omega)|\) are the total vertices with degree \(\gamma\) and CN \(\alpha\).

Similarly, the 4th MZCI can be rewritten as

\[
\mathcal{M} \mathcal{C}_4(\Omega) = \prod_{0 \leq s \leq t-2} [\alpha + \tau]^{\varphi_{(\alpha,\tau)}(\Omega)},
\]

where \(|\varphi_{(\alpha,\tau)}(\Omega)|\) are the total edges in \(\Omega\) with CNs \((\alpha, \tau)\).

The modified 1st MZCI can be rewritten as

\[
\mathcal{M} \tilde{\mathcal{C}}^*_2(\Omega) = \prod_{0 \leq s \leq t-2} [\mu \tau + \nu]^{\varphi_{(\mu,v)}(\Omega)},
\]

\[
\mathcal{M} \tilde{\mathcal{C}}^*_3(\Omega) = \prod_{0 \leq s \leq t-2} [\mu \tau + \nu]^{\varphi_{(\mu,v)}(\Omega)},
\]

\[
\mathcal{M} \mathcal{C}_2(\Omega) = \prod_{0 \leq s \leq t-2} [\alpha \times \tau]^{\varphi_{(\alpha)}(\Omega)},
\]

\[
\mathcal{M} \mathcal{C}_3(\Omega) = \prod_{0 \leq y \leq s \leq t-2} [\gamma \times \alpha]^{\varphi_{(\gamma,\alpha)}(\Omega)},
\]

\[
\mathcal{M} \mathcal{C}_4(\Omega) = \prod_{0 \leq s \leq t-2} [\alpha + \tau]^{\varphi_{(\alpha,\tau)}(\Omega)},
\]
Table 1: Total number of edges on degree and connection bases.

| $|\mathcal{F}_{(\mu,r)}(\Omega)|$ | $|\mathcal{F}_{(\alpha,t)}(\Omega)|$ | $|\mathcal{F}_{(\mu,r)(\alpha,t)}(\Omega)|$ |
|---|---|---|
| On degree bases | On connection bases |  

| $|\mathcal{F}_{(2,2)}(\Omega)| = 6(2k-1)$ | $|\mathcal{F}_{(2,2)}(\Omega)| = 6(2k-1)$ | $|\mathcal{F}_{(2,2)(2,2)}(\Omega)| = 6(2k-1) - 24$ |
| $|\mathcal{F}_{(2,3)}(\Omega)| = 6(2k-1)$ | $|\mathcal{F}_{(2,3)}(\Omega)| = 12(2k-1) - 12$ | $|\mathcal{F}_{(2,2)(2,3)}(\Omega)| = 12(2k-1) - 12$ |
| $|\mathcal{F}_{(3,3)}(\Omega)| = 3(2k-1)$ | $|\mathcal{F}_{(4,4)}(\Omega)| = 3(2k-1) - 3$ | $|\mathcal{F}_{(2,3)(3,3)}(\Omega)| = 3(2k-1) - 3$ |
| $|\mathcal{F}_{(3,3)}(\Omega)| = 9(2k-1) - 6$ | $|\mathcal{F}_{(4,6)}(\Omega)| = 9(2k-1) - 6$ | $|\mathcal{F}_{(3,3)(4,6)}(\Omega)| = 9(2k-1) - 6$ |

\[ \mathcal{M}\mathcal{C}_1(\Omega) = \prod_{0 \leq a \leq k-2} [\mu a + \nu r]|\mathcal{F}_{(\mu,\nu,\alpha,\tau)}(\Omega)|. \]  

(26)

The modified 2nd MZCI can be rewritten as

\[ \mathcal{M}\mathcal{C}_2(\Omega) = \prod_{0 \leq a \leq k-2} [\mu a + \nu r]|\mathcal{F}_{(\mu,\nu,\alpha,\tau)}(\Omega)|. \]  

(27)

The modified 3rd MZCI can be rewritten as

\[ \mathcal{M}\mathcal{C}_3(\Omega) = \prod_{0 \leq a \leq k-2} [\mu a + \nu r]|\mathcal{F}_{(\alpha,\tau)}(\Omega)|. \]  

(28)

where $\mathcal{F}_{(\mu,\nu,\alpha,\tau)}(\Omega)$ is the total number of edges in $\Omega$ with degrees ($\mu, \nu$) and CNs ($\alpha, \tau$).

Theorem 3. Let $\Omega = D[k]$ be a molecular graph for $k = 1, 2, 3$. Then, the general expressions to compute the 1st MZCI, 2nd MZCI, 3rd MZCI and 4th MZCI are as follows:

1. By placing all the computed values of $|\mathcal{F}_\alpha(\Omega)|$ for $\alpha = 1, 2, 3, 4$ in equation (6), we have

\[ \mathcal{M}\mathcal{C}_1(\Omega) = \prod_{0 \leq a \leq k-2} [\alpha^2]|\mathcal{F}_\alpha(\Omega)| \]

\[ = [2^2]|\mathcal{F}_1(\Omega)| \times [3^2]|\mathcal{F}_3(\Omega)| \times [4^2]|\mathcal{F}_4(\Omega)| \times [6^2]|\mathcal{F}_6(\Omega)| \]

\[ = [4]^9(2^k-1) \times [9](30(2^k-24) \times [16](15(2^k-12)) \times [36](3(2^k)-2) \]

\[ = [4]^9(2^k-1) \times [9](30(2^k-24) \times [16](15(2^k)-12)) \times [36](3(2^k)-2) \]

(29)

(2) By placing all the computed values of $|\mathcal{F}_{(\alpha,\tau)}(\Omega)|$ for $\alpha = 1, 2, 3, 4$ in (23), we have

\[ \mathcal{M}\mathcal{C}_2(\Omega) = \prod_{0 \leq a \leq k-2} [\alpha \times \tau]|\mathcal{F}_{(\alpha,\tau)}(\Omega)| \]

\[ = [2 \times 2]|\mathcal{F}_{(1,2)}(\Omega)| \times [2 \times 3]|\mathcal{F}_{(1,3)}(\Omega)| \times [3 \times 3]|\mathcal{F}_{(3,3)}(\Omega)| \times [3 \times 4]|\mathcal{F}_{(3,4)}(\Omega)| \]

\[ = [4]^6(2^k-1) \times [6]^6(2^k) \times [9] \times [12](2^k-12) \times [12](30(2^k-24) \times [16](3(2^k-12)) \times [24](9(2^k)-6) \]

\[ = [24]^6 \times [9](12(2^k-12)) \times [12](30(2^k-24) \times [16](3(2^k)+12) \times [24](9(2^k)-6) \]

(30)

(3) In order to compute the 3rd MZCI $\mathcal{M}\mathcal{C}_3(\Omega)$, we find the $|\mathcal{F}_{(\mu,\nu)}(\Omega)|$. From Figures 3 and 6, only the term-hexagon of $\Omega$ involves the vertices with degree 2 and CN 2. Thus, the total amount of such vertices is
equal to two times of number of term-hexagons of \( \Omega \). So,
\[
|F_{(2,2)}'(\Omega)| = 9(2^{k-1}).
\] (31)

Furthermore, we find \( |F_{(2,3)}'(\Omega)| \). It can be easily seen that the every term-hexagon of \( \Omega \) contains two vertices having degree 2 and CN 3 while pivot-hexagon contains 4 vertices. The total amount of such vertices in term-hexagon and pivot-hexagon of \( \Omega \) are 6\( (2^{k-1}) \) and 24\( (2^{k-1}) - 1 \), respectively. Thus,
\[
|F_{(2,3)}'(\Omega)| = 6(2^{k-1}) + 24(2^{k-1}) - 24,
\] (32)
\[
|F_{(3,3)}'(\Omega)| = 30(2^{k-1}) - 24.
\]

(4) By placing all the computed values of \( |F_{(\gamma,\delta)}'(\Omega)| \) for \( \alpha = 1, 2, 3, 4 \) in \( (24) \), we have

\[
M \mathcal{DC}_\alpha (\Omega) = \prod_{0 \leq n \leq k - 2} [\alpha \times \tau]^{\mathcal{MC}_{\alpha, n}(\Omega)}
\]
\[
= [2 \times 2]^{\mathcal{MC}_{(2,2)}(\Omega)} + [2 \times 3]^{\mathcal{MC}_{(2,3)}(\Omega)} + [3 \times 2]^{\mathcal{MC}_{(3,2)}(\Omega)} + [3 \times 3]^{\mathcal{MC}_{(3,3)}(\Omega)}
\]
\[
= [4]^6(2^{k-1}) \times [6]^{30(2^{k-1}) - 24} + [12]^{15(2^{k-1}) - 12} + [18]^3(2^{k-1}) - 3
\]
\[
= [4]^{6h} \times [9]^{12(h-1)} \times [12]^{30h-24} \times [16]^{15h-12} \times [24]^{3h-2}.
\] (34)

Similarly, we have
\[
|F_{(3,4)}'(\Omega)| = 15(2^{k-1}) - 12
\]
\[
|F_{(3,6)}'(\Omega)| = 3(2^{k-1}) - 2.
\] (33)

By placing all the computed values of \( |F_{(\gamma,\delta)}'(\Omega)| \) for \( \alpha = 1, 2, 3, 4 \) in \( (24) \), we have

\[
M \mathcal{DC}_\alpha (\Omega) = \prod_{0 \leq n \leq k - 2} [\alpha \times \tau]^{\mathcal{MC}_{\alpha, n}(\Omega)}
\]
\[
= [2 \times 2]^{\mathcal{MC}_{(2,2)}(\Omega)} \times [2 \times 3]^{\mathcal{MC}_{(2,3)}(\Omega)} \times [3 \times 2]^{\mathcal{MC}_{(3,2)}(\Omega)} \times [3 \times 3]^{\mathcal{MC}_{(3,3)}(\Omega)}
\]
\[
= [4]^4(2^{k-1})^3 \times [6]^{9(2^{k-1}) - 6} \times [7]^{10(2^{k-1}) - 24} \times [8]^{3(2^{k-1}) - 3} \times [10]^{9(2^{k-1}) - 6}
\]
\[
= [20]^{6h} \times [6]^{12(h-1)} \times [7]^{30h-24} \times [8]^{3(h-1)} \times [24]^{9h-6}.
\] (35)

\[
\mathcal{MC}_\alpha (\Omega) = \left[ 80 \right]^{6h} \times \left[ 12 \right]^{12(h-1)} \times \left[ 18 \right]^{30h-24} \times \left[ 24 \right]^{12h-12} \times \left[ 30 \right]^{9h-6}.
\]

\( \) Here, \( h = 2^{k-1} \).

**Theorem 4.** Let \( \Omega = D[k] \) be a molecular graph for \( k = 1, 2, 3 \). Then, the general expressions to compute the modified 1st ZCI, modified 2nd ZCI and modified 3rd ZCI are as follows:

1. \( \mathcal{DC}_\alpha (\Omega) = [80]^{6h} \times [12]^{12h-12} \times [15]^{30h-24} \times [24]^{3h-3} \times [30]^{9h-6} \),
2. \( \mathcal{DC}_\alpha (\Omega) = [80]^{6h} \times [12]^{12h-12} \times [18]^{30h-24} \times [24]^{3h-3} \times [30]^{9h-6} \),
3. \( \mathcal{DC}_\alpha (\Omega) = [80]^{6h} \times [12]^{12h-12} \times [18]^{30h-24} \times [24]^{3h-3} \times [30]^{9h-6} \).

**Proof**

1. By placing the values of \( |F_{(\mu,\nu)}(\Omega)| \) in equation (10), we get
(2) By placing the values of \(|\mathcal{F}(\mu,\gamma)(\alpha,\tau)\) in (27), we get

\[
\tilde{Z}C_1^+ (\Omega) = \prod_{0 \leq \alpha \leq k, 2 \leq \mu, \gamma \leq k-2} \left[ \mathcal{F}(\mu,\gamma)(\alpha,\tau) \right] [\mu\tau + \nu\alpha] \\
= [(2)(2) + (2)(2)]^{|\mathcal{F}(\mu(2),\gamma(2))|} + [(2)(3) + (2)(2)]^{|\mathcal{F}(\mu(2),\gamma(3))|} + [(2)(2) + (2)(3)]^{|\mathcal{F}(\mu(2),\gamma(3))|} \\
+ [(2)(4) + (3)(3)]^{|\mathcal{F}(\mu(3),\gamma(3))|} + [(3)(4) + (3)(4)]^{|\mathcal{F}(\mu(4),\gamma(4))|} + [(3)(6) + (3)(4)]^{|\mathcal{F}(\mu(6),\gamma(4))|} \\
= [8]^6(2^{k-1}) + [10]^6(2^{k-1}) + [12]^{12}(2^{k-1}) - 12 + [15]^{30}(2^{k-1}) - 24 + [24]^{3}(2^{k-1}) - 3 + [30]^{9}(2^{k-1}) - 6 ,
\]

(26)

(3) By placing the values of \(|\mathcal{F}(\mu,\gamma)(\alpha,\tau)\) in (28), we get

\[
\tilde{Z}C_2^+ (\Omega) = \prod_{0 \leq \alpha \leq k, 2 \leq \mu, \gamma \leq k-2} \left[ \mathcal{F}(\mu,\gamma)(\alpha,\tau) \right] [\mu\tau + \nu\alpha] \\
= [(2)(2) + (2)(2)]^{|\mathcal{F}(\mu(2),\gamma(2))|} + [(2)(2) + (2)(3)]^{|\mathcal{F}(\mu(2),\gamma(3))|} + [(2)(3) + (2)(3)]^{|\mathcal{F}(\mu(2),\gamma(3))|} \\
+ [(2)(3) + (3)(4)]^{|\mathcal{F}(\mu(3),\gamma(4))|} + [(3)(4) + (3)(4)]^{|\mathcal{F}(\mu(4),\gamma(4))|} + [(3)(6) + (3)(4)]^{|\mathcal{F}(\mu(6),\gamma(4))|} \\
= [8]^6(2^{k-1}) + [10]^6(2^{k-1}) + [12]^{12}(2^{k-1}) - 12 + [18]^{30}(2^{k-1}) - 24 + [24]^{3}(2^{k-1}) - 3 + [30]^{9}(2^{k-1}) - 6 ,
\]

(27)

(3) By placing the values of \(|\mathcal{F}(\mu,\gamma)(\alpha,\tau)\) in (29), we get

\[
\tilde{Z}C_3^+ (\Omega) = \prod_{0 \leq \alpha \leq k, 2 \leq \mu, \gamma \leq k-2} \left[ \mathcal{F}(\mu,\gamma)(\alpha,\tau) \right] [\mu\tau + \nu\alpha] \\
= [(2)(2) + (2)(2)]^{|\mathcal{F}(\mu(2),\gamma(2))|} + [(2)(2) + (2)(3)]^{|\mathcal{F}(\mu(2),\gamma(3))|} + [(2)(3) + (2)(3)]^{|\mathcal{F}(\mu(2),\gamma(3))|} \\
+ [(2)(3) + (3)(4)]^{|\mathcal{F}(\mu(3),\gamma(4))|} + [(3)(4) + (3)(4)]^{|\mathcal{F}(\mu(4),\gamma(4))|} + [(3)(6) + (3)(4)]^{|\mathcal{F}(\mu(6),\gamma(4))|} \\
= [8]^6(2^{k-1}) + [10]^6(2^{k-1}) + [12]^{12}(2^{k-1}) - 12 + [18]^{30}(2^{k-1}) - 24 + [24]^{3}(2^{k-1}) - 3 + [30]^{9}(2^{k-1}) - 6 ,
\]

(28)

5. Concluding remarks

The concluding remarks are as follows:

(1) TIs, the numerical descriptors, are efficient enough to characterize the topology of molecular structures and also assist to correlate their distinct psychochemical properties.

(2) Dendrimers are symmetric, versatile, and well-defined chemical polymers forming a tree-like structure. Dendrimers are signalized by a numerous attributes which make them advantageous for wide ranging utilizations in various fields of science.

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

(4) In this manuscript, we have calculated the general expression to compute the Zagreb connection indices (ZCIs), namely, first ZCI (1st ZCI), second ZCI (2nd ZCI), modified 1st ZCI, modified 2nd ZCI, and modified 3rd ZCI. Furthermore, we have computed the multiplicative ZCI (MZCI), namely, first MZCI (1st MZCI), second MZCI (2nd MZCI), third MZCI (3rd ZCI), fourth MZCI (4th MZCI), modified
1st ZCI, modified (2nd ZCI), and modified 3rd ZCI. The computed results are general and depends only upon the value of k.

Future directions: in future, we are interested to compute the connection-based Zagreb indices for the other type of dendrimers.

Data Availability

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

Conflicts of Interest

The authors have no conflicts of interest regarding this article.

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