

Novel Connection Based Zagreb Indices of Dendrimer Nanostars

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Abstract

Dendrimers nanostars are artificially produced radially symmetric macromolecules with monodisperse, homogenous and precise structure. Due to their vast utilizations in distinct medical fields, these structures are getting much more attraction from the scientist day by day. Topological indices (TI) are the graph descriptors which connect a numeric digit with a graph that help to predict the topological aspects of chemical structures. There are numerous TIs investigated by distinct researchers including degree-based, distance-based, and polynomial based TIs. These TIs are helpful to relate the topology of distinct chemical structures. Recently, Zagreb connection indices are introduced which are considered to be more potent to measure the chemical and physical properties of chemical structures than that of other introduced TIs of literature. In this paper, we define some new Zagreb connection indices such as atom bond connectivity connection index, geometric arithmetic connection index, augmented connection index, symmetric division connection index, harmonic connection index, inverse sum connection index, hyper Zagreb connection index. Further, we find the general values to compute our defined zagreb connection indices of a dendrimer nanostar.

Keywords: Zagreb indices, Zagreb connection indices, dendrimer nanostars,

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1. Introduction

Dendrimer nanostars are artificially produced radially symmetric macromolecules with monodisperse, homogenous and precise structure. Dendrimers have vast span of utilizations in supramolecular science, especially in energy harvesting, gene transfection, drug delivery, development of vaccine, catalysis, photo activity and rheology modification, for more details see [1, 2, 3]. Due to their vast utilizations in distinct medical fields, these structures are getting much more attraction from the researchers.

In mathematical chemistry, mathematical tools are employed to resolve the arising problems of chemistry. One of them is the graphical depiction of molecular chemical structures. A molecular graph of compound is graph in which the atoms are taken as the vertices and the bond between the atoms are depicted by the edges. Topological indices (TI) are the graph descriptors which connect a numeric digit with a graph that help to predict the topological aspects of chemical structures in a precise manner. TIs have vast span of applicability in various fields of science. They are helpful in predicting the chemical properties of molecular chemical structures such as, freezing point, boiling point, volume, density, stability and

strain energy. They are extensively utilized in the study of quantitative structure-activity and property relationships [4].

The concept of first Zagreb index (ZI) was investigated by Wiener [5]. This development leads to the beginning of theory of TIs. After this discovery, a number of TIs were investigated by different researchers and they utilized these indices in exploring the physical and chemical properties of molecular compounds [6, 7]. In 1998, Estrada et al. [8] introduced atom bond connectivity (ABC) index. Further, Ghorbani et al. [9] investigated fourth version of ABC index. In 2009, Vukicevic and Furtula [10] introduced another significant type of index named as geometric arithmetic (GA) index. Fifth version of GA index was initiated by Garaovoc et al. [11] and he utilized these indices to check the chemical properties of dendrimers. Vukicevic [10] investigated the novel idea of symmetric division deg (SDD) index in 2010. Furtula et al. [12] initiated augmented Zagreb index (AZI). The novel conception of harmonic index (HI) was given by Fajtlowicz [13]. The idea of inverse sum (IS) index was introduced by Vukicevic and Gasperov [14]. The innovative concept of hyper ZI (HZI) was given by Shirdel et al. [15].

Recently, a new term called connection number or leap degree of vertex is invented which took the serious consideration of researchers. A number of those vertices which are at distance two from a certain vertex is referred to as CN. Ali and Trinajstić [16] initiated Zagreb connection indices (ZCIs) and used octane isomers to examine their applicability. According to their research, ZIs on connection basis as compared to the classical ZIs provide a better absolute value of the correlation coefficient. Recently, Ali et al. [17] calculated the modified ZCIs for T-sum graphs in 2020. Haoer et al. [19] introduced the multiplicative leap ZIs. Javaid et al. [18] calculated multiplicative ZIs of different wheel related graphs. Recently, Sattar et al. [20, 21, 22] computed the ZCIs of a dendrimer nanostar.

In this article, we introduce some new ZCIs, namely, atom bond connectivity connection index, geometric arithmetic connection index, augmented connection index, symmetric division connection index, harmonic connection index, inverse sum connection index, hyper Zagreb connection index. Further we find the general expression to calculate our proposed ZCIs of dendrimer nanostars.

2. Preliminaries

Let $G = (V(G), E(G))$ be a graph, where $V(G)$ is the vertex set and $E(G)$ is the edges set. The degree of any arbitrary vertex is the number of edges that are incident to that vertex, i.e., the number of vertices which are distance one. The connection number of a particular vertex is the number of vertices which are distance two from that vertex. Let $p = ce$, where $c, e \in V(G)$ be an edge, the degree of the edges is given by $\deg(p) = \deg(c) + \deg(e) - 2$. The important degree based indices introduced in literature are given in Table 1. Now, we define some new Zagreb indices based on connection numbers below.

Table 1: Degree based ZIs of literature

Formulas	Name of indices	Acronyms
$\sum_{c,e \in E(G)} \sqrt{\frac{\deg(c) + \deg(e) - 2}{\deg(c) \times \deg(e)}}$	Atom-bond connectivity index [8]	ABCI
$\sum_{c,e \in E(G)} \frac{2\sqrt{\deg(c)\deg(e)}}{\deg(c) + \deg(e)}$	Geometric arithmetic index [10]	GAI
$\sum_{c,e \in E(G)} \left[\frac{\deg(c) \times \deg(e)}{\deg(c) + \deg(e) - 2} \right]^3$	Augmented Zagreb index [12]	AZI
$\sum_{c,e \in E(G)} \left[\frac{\min(\deg(c), \deg(e))}{\max(\deg(c), \deg(e))} + \frac{\max(\deg(c), \deg(e))}{\min(\deg(c), \deg(e))} \right]$	Symmetry division deg index [10]	SDDI
$\sum_{c,e \in E(G)} \frac{2}{(\deg(c) + \deg(e))}$	Harmonic index [13]	HI
$\sum_{c,e \in E(G)} \frac{\deg(c) \times \deg(e)}{(\deg(c) + \deg(e))}$	Inverse sum index [14]	ISI
$\sum_{c,e \in E(G)} [\deg(c) + \deg(e)]^2$	Hyper Zagreb index [15]	HZI

Definition 2.1. Let $G = (V(G), E(G))$ be a graph. Then, the atom bond connectivity connection index (ABCCI) is defined as;

$$ABCCI(G) = \sum_{c,e \in E(G)} \sqrt{\frac{\tau(c) + \tau(e) - 2}{\tau(c) \times \tau(e)}}, \quad (2.1)$$

where $\tau(c)$ and $\tau(e)$ are the CNs of the vertices c and e , respectively.

Definition 2.2. For a graph G , the geometric arithmetic connection index (GACI) is defined as;

$$GACI(G) = \sum_{c,e \in E(G)} \frac{2\sqrt{\tau(c)\tau(e)}}{\tau(c) + \tau(e)}, \quad (2.2)$$

where $\tau(c)$ and $\tau(e)$ are the CNs of the vertices c and e , respectively.

Definition 2.3. For a graph G , the augmented Zagreb connection index (AZCI) is defined as;

$$AZCI(G) = \sum_{c,e \in E(G)} \left[\frac{\tau(c) \times \tau(e)}{\tau(c) + \tau(e) - 2} \right]^3, \quad (2.3)$$

where $\tau(c)$ and $\tau(e)$ are the CNs of the vertices c and e , respectively.

Definition 2.4. For a graph G , the symmetric division connection index (SDCI) is defined as;

$$SDCI(G) = \sum_{c,e \in E(G)} \left[\frac{\min(\tau(c), \tau(e))}{\max(\tau(c), \tau(e))} + \frac{\max(\tau(c), \tau(e))}{\min(\tau(c), \tau(e))} \right], \quad (2.4)$$

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

Definition 2.5. For a graph G , the harmonic connection index (HCI) is defined as;

$$HCI(G) = \sum_{c,e \in E(G)} \frac{2}{(\tau(c) + \tau(e))}, \quad (2.5)$$

where $\tau(c)$ and $\tau(e)$ are the CNs of the vertices c and e , respectively.

Definition 2.6. For a graph G , the inverse sum connection index (ISCI) is defined as;

$$ISCI(G) = \sum_{c,e \in E(G)} \frac{\tau(c) \times \tau(e)}{(\tau(c) + \tau(e))}, \quad (2.6)$$

where $\tau(c)$ and $\tau(e)$ are the CNs of the vertices c and e , respectively.

Definition 2.7. For a graph G , the hyper Zagreb connection index (HZCI) is defined as;

$$HZCI(G) = \sum_{c,e \in E(G)} [\tau(c) + \tau(e)]^2, \quad (2.7)$$

where $\tau(c)$ and $\tau(e)$ are the CNs of the vertices c and e , respectively.

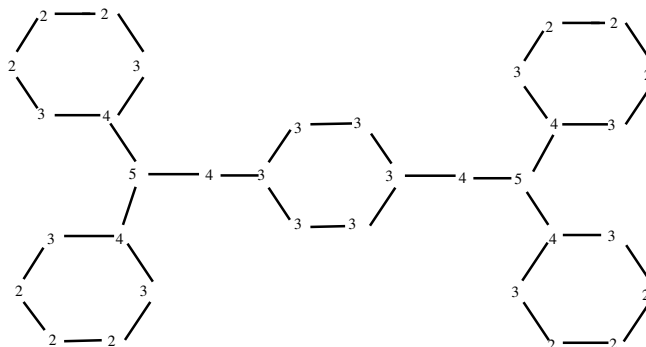


Figure 3.1: $D[1]$ with the CN each vertex.

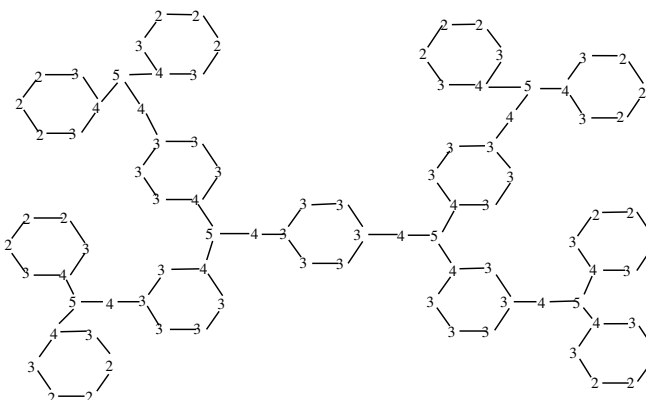


Figure 3.2: $D[2]$ with the CN each vertex.

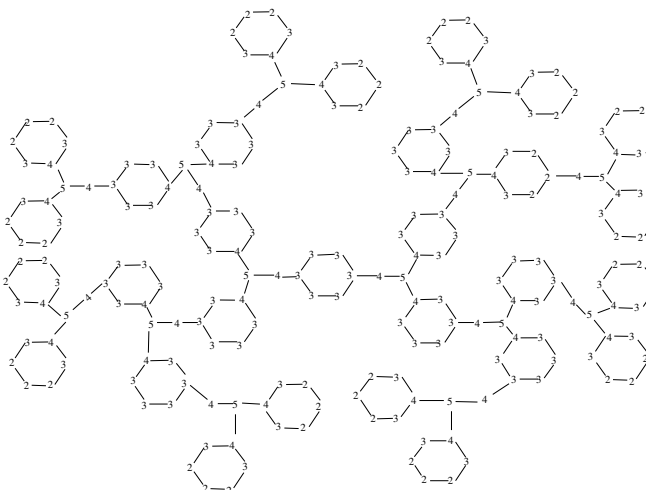


Figure 3.3: $D[3]$ with the CN of each vertex

3. Main Results

In this section, we compute the above defined ZIs for an important type of dendrimer nanostar $D[\hat{n}]$, where $\hat{n}$ is the level of the dendrimer nanostar. Let $G = D[\hat{n}]$ be a molecular graph of $D[\hat{n}]$. The structural formulas of $D_1[\hat{n}]$ with their CNs $\hat{n} = 1, 2, 3$ are displayed in Figure 3.1, Figure 3.2 and Figure 3.3.

First, we divide the hexagons of $D[\hat{n}]$ into $\mathbb{A}$ -hexagon, $\mathbb{B}$ -hexagon and $\mathbb{C}$ -hexagon. Before presenting the main results our paper, we first classify the hexagons of $D[\hat{n}]$ with the help of degrees of the vertices, into terminal hexagon, initial hexagon and λ -hexagon.

- $\mathbb{A}$ -Hexagon: If the degree of five vertices is two in any hexagon, then we call it $\mathbb{A}$ -hexagon.
- $\mathbb{B}$ -Hexagon: The initial hexagon is called $\mathbb{B}$ -hexagon.

- **C-Hexagon**:: A hexagon which is neither $\mathbb{A}$ -hexagon nor $\mathbb{B}$ -hexagon is considered to be C-Hexagon.

The count of $\mathbb{A}$, $\mathbb{B}$ and $\mathbb{C}$ hexagons are

$$\text{Number of } \mathbb{A}\text{-hexagons} = 2 \times 2^{\hat{n}},$$

$$\text{Number of } \mathbb{B}\text{-hexagons} = 1,$$

$$\text{Number of } \mathbb{C}\text{-hexagons} = 2 \times 2^{\hat{n}} - 4.$$

All the remaining vertices which does not exist in any hexagon are $4 \times 2^{\hat{n}} - 4$ in number. Now, we compute the above defined CN-based ZIs for the dendrimer $D[\hat{n}]$.

Theorem 3.1. Let $G = D[\hat{n}]$ be a molecular graph. Then, the atom-bond connectivity connection index is given in the following

$$ABCCI(G) = (8 \times 2^{\hat{n}}) \sqrt{\frac{1}{2}} + (8 \times 2^{\hat{n}} - 16) \sqrt{\frac{4}{9}} + (10 \times 2^{\hat{n}} - 10) \sqrt{\frac{5}{12}} + (6 \times 2^{\hat{n}} - 6) \sqrt{\frac{9}{10}}.$$

Proof. To compute the atom bond connectivity index, we make the classes of edges with respect to CNs. We have

$$C_{(2,2)} = \{ce \in \mathbb{E}(G) : \tau(c) = 2, \tau(e) = 2\},$$

$$C_{(2,3)} = \{ce \in \mathbb{E}(G) : \tau(c) = 2, \tau(e) = 3\},$$

$$C_{(3,3)} = \{ce \in \mathbb{E}(G) : \tau(c) = 3, \tau(e) = 3\},$$

$$C_{(3,4)} = \{ce \in \mathbb{E}(G) : \tau(c) = 3, \tau(e) = 4\},$$

$$C_{(4,5)} = \{ce \in \mathbb{E}(G) : \tau(c) = 4, \tau(e) = 5\}.$$

Now, we count these partitioned edges. It can be seen that all (2,2)-type edges lies only in $\mathbb{A}$ hexagon and are in number 2. The total count of $\mathbb{A}$ -hexagons are $2 \times 2^{\hat{n}}$. Thus, the count of (2,2)-types edges must be

$$|C_{(2,2)}(G)| = 2(2 \times 2^{\hat{n}}) = 4 \times 2^{\hat{n}}.$$

Similarly,

$$|C_{(2,3)}(G)| = 2(2 \times 2^{\hat{n}}) = 4 \times 2^{\hat{n}}.$$

Table 2 represent the count of (3,3)-type edges in G . Thus, count of $C_{(3,3)}(G)$ is equal to

Table 2: Number of (3,3)-type edges in hexagons of G

Hexagons	Number of (3,3)-type edges in hexagon (a)	Number of hexagons (b)	Total count of (3,3)-type edges ($a \times b$)
$\mathbb{A}$ -hexagon	0	$2 \times 2^{\hat{n}}$	0
$\mathbb{B}$ -hexagon	6	1	6
$\mathbb{C}$ -hexagon	4	$2 \times 2^{\hat{n}} - 4$	$4(2 \times 2^{\hat{n}} - 4)$

$$|C_{(3,3)}(G)| = 8 \times 2^{\hat{n}} - 16.$$

In Table 3, we calculate the count of (3,4)-type edges in all type of hexagons.

Table 3: Number of (3,4)-type edges in all hexagons of G

hexagons	Number of (3,4)-type edges in hexagon (a)	Number of hexagons (b)	Number of (3,4)-type edges in hexagons ($a \times b$)
$\mathbb{A}$ -hexagon	2	$2 \times 2^{\hat{n}}$	$2 \times 2^{\hat{n}+1}$
$\mathbb{B}$ -hexagon	0	1	0
$\mathbb{C}$ -hexagon	2	$2 \times 2^{\hat{n}} - 4$	$2(2 \times 2^{\hat{n}} - 4)$

Thus, count of $C_{(3,4)}(G)$ is equal to

$$|C_{(3,4)}(G)| = 10 \times 2^{\hat{n}} - 10.$$

Similarly, we have

$$|C_{(4,5)}(G)| = 6 \times 2^{\hat{n}} - 6.$$

After placing the values in Equation 2.1, we get

$$\begin{aligned}
 ABCCI(G) &= \sum_{c,e \in E(G)} \sqrt{\frac{\tau(c) + \tau(e) - 2}{\tau(c) \times \tau(e)}}, \\
 &= (4 \times 2^{\hat{n}}) \sqrt{\frac{2+2-2}{2 \times 2}} + (4 \times 2^{\hat{n}}) \sqrt{\frac{2+3-2}{2 \times 3}} + (8 \times 2^{\hat{n}} - 16) \sqrt{\frac{3+3-2}{3 \times 3}} \\
 &\quad + (10 \times 2^{\hat{n}} - 10) \sqrt{\frac{3+4-2}{3 \times 4}} + (6 \times 2^{\hat{n}} - 6) \sqrt{\frac{4+5-2}{4 \times 5}}, \\
 &= (4 \times 2^{\hat{n}}) \sqrt{\frac{2}{4}} + (4 \times 2^{\hat{n}}) \sqrt{\frac{3}{6}} + (8 \times 2^{\hat{n}} - 16) \sqrt{\frac{4}{9}} \\
 &\quad + (10 \times 2^{\hat{n}} - 10) \sqrt{\frac{5}{12}} + (6 \times 2^{\hat{n}} - 6) \sqrt{\frac{18}{20}}, \\
 &= (4 \times 2^{\hat{n}}) \sqrt{\frac{1}{2}} + (4 \times 2^{\hat{n}}) \sqrt{\frac{1}{2}} + (8 \times 2^{\hat{n}} - 16) \sqrt{\frac{4}{9}} \\
 &\quad + (10 \times 2^{\hat{n}} - 10) \sqrt{\frac{5}{12}} + (6 \times 2^{\hat{n}} - 6) \sqrt{\frac{9}{10}}, \\
 &= (8 \times 2^{\hat{n}}) \sqrt{\frac{1}{2}} + (8 \times 2^{\hat{n}} - 16) \sqrt{\frac{4}{9}} + (10 \times 2^{\hat{n}} - 10) \sqrt{\frac{5}{12}} + (6 \times 2^{\hat{n}} - 6) \sqrt{\frac{9}{10}}.
 \end{aligned}$$

□

Theorem 3.2. Let $G = D[\hat{n}]$ be a molecular graph. Then, the GACI is given in the following

$$GACI(G) = (12 \times 2^{\hat{n}}) - 16 + (4 \times 2^{\hat{n}}) \frac{2\sqrt{6}}{5} + (10 \times 2^{\hat{n}} - 10) \frac{2\sqrt{12}}{7} + (6 \times 2^{\hat{n}} - 6) \frac{2\sqrt{20}}{9}.$$

Proof. After placing the values in Equation 2.2, we get

$$\begin{aligned}
 GACI(G) &= \sum_{c,e \in E(G)} \frac{2\sqrt{\tau(c)\tau(e)}}{\tau(c) + \tau(e)}, \\
 &= |C_{(2,2)}(G)| \frac{2\sqrt{2 \times 2}}{2+2} + |C_{(2,3)}(G)| \frac{2\sqrt{2 \times 3}}{2+3} + |C_{(3,3)}(G)| \frac{2\sqrt{3 \times 3}}{3+3} \\
 &\quad + |C_{(3,4)}(G)| \frac{2\sqrt{3 \times 4}}{3+4} + |C_{(4,5)}(G)| \frac{2\sqrt{4 \times 5}}{4+5}, \\
 &= (4 \times 2^{\hat{n}}) \frac{2\sqrt{2 \times 2}}{2+2} + (4 \times 2^{\hat{n}}) \frac{2\sqrt{2 \times 3}}{2+3} + (8 \times 2^{\hat{n}} - 16) \frac{2\sqrt{3 \times 3}}{3+3} \\
 &\quad + (10 \times 2^{\hat{n}} - 10) \frac{2\sqrt{3 \times 4}}{3+4} + (6 \times 2^{\hat{n}} - 6) \frac{2\sqrt{4 \times 5}}{4+5}, \\
 &= (4 \times 2^{\hat{n}}) \frac{2\sqrt{4}}{4} + (4 \times 2^{\hat{n}}) \frac{2\sqrt{6}}{5} + (8 \times 2^{\hat{n}} - 16) \frac{2\sqrt{9}}{6} + (10 \times 2^{\hat{n}} - 10) \frac{2\sqrt{12}}{7} \\
 &\quad + (6 \times 2^{\hat{n}} - 6) \frac{2\sqrt{20}}{9}, \\
 &= (4 \times 2^{\hat{n}}) + (4 \times 2^{\hat{n}}) \frac{2\sqrt{6}}{5} + (8 \times 2^{\hat{n}} - 16) + (10 \times 2^{\hat{n}} - 10) \frac{2\sqrt{12}}{7} \\
 &\quad + (6 \times 2^{\hat{n}} - 6) \frac{2\sqrt{20}}{9}, \\
 &= 12 \times 2^{\hat{n}} - 16 + (4 \times 2^{\hat{n}}) \frac{2\sqrt{6}}{5} + (10 \times 2^{\hat{n}} - 10) \frac{2\sqrt{12}}{7} + (6 \times 2^{\hat{n}} - 6) \frac{2\sqrt{20}}{9}.
 \end{aligned}$$

□

Theorem 3.3. Let $G = D[\hat{n}]$ be a molecular graph. Then, the AZCI is given in the following

$$AZCI(G) = 16(4 \times 2^{\hat{n}}) + (8 \times 2^{\hat{n}} - 16) \left[\frac{729}{64} \right]^3 + (10 \times 2^{\hat{n}} - 10) \left[\frac{1728}{125} \right]^3 + (6 \times 2^{\hat{n}} - 6) \left[\frac{8000}{343} \right]^3.$$

Proof. After placing the values in Equation 2.3, we get

$$\begin{aligned}
 AZCI(G) &= \sum_{c,e \in E(G)} \left[\frac{\tau(c) \times \tau(e)}{\tau(c) + \tau(e) - 2} \right]^3, \\
 &= |C_{(2,2)}(G)| \left[\frac{2 \times 2}{(2+2)-2} \right]^3 + |C_{(2,3)}(G)| \left[\frac{2 \times 3}{(2+3)-2} \right]^3 + |C_{(3,3)}(G)| \left[\frac{3 \times 3}{(3+3)-2} \right]^3 \\
 &\quad + |C_{(3,4)}(G)| \left[\frac{3 \times 4}{(3+4)-2} \right]^3 + |C_{(4,5)}(G)| \left[\frac{4 \times 5}{(4+5)-2} \right]^3, \\
 &= (4 \times 2^{\hat{n}}) \left[\frac{4}{2} \right]^3 + (4 \times 2^{\hat{n}}) \left[\frac{6}{3} \right]^3 + (8 \times 2^{\hat{n}} - 16) \left[\frac{9}{4} \right]^3 + (10 \times 2^{\hat{n}} - 10) \left[\frac{12}{5} \right]^3 \\
 &\quad + (6 \times 2^{\hat{n}} - 6) \left[\frac{20}{7} \right]^3, \\
 &= 16(4 \times 2^{\hat{n}}) + (8 \times 2^{\hat{n}} - 16) \left[\frac{729}{64} \right] + (10 \times 2^{\hat{n}} - 10) \left[\frac{1728}{125} \right] + (6 \times 2^{\hat{n}} - 6) \left[\frac{8000}{343} \right].
 \end{aligned}$$

□

Theorem 3.4. Let $G = D[\hat{n}]$ be a molecular graph. Then, the SDCI is given in the following

$$SDCI(G) = (24 \times 2^{\hat{n}} - 32) + (4 \times 2^{\hat{n}}) \left[\frac{13}{6} \right] + (10 \times 2^{\hat{n}} - 10) \left[\frac{25}{12} \right] + (6 \times 2^{\hat{n}} - 6) \left[\frac{41}{20} \right].$$

Proof. After placing the values in Equation 2.4, we get

$$\begin{aligned} SDCI(G) &= \sum_{c,e \in E(G)} \left[\frac{\min(\tau(c), \tau(e))}{\max(\tau(c), \tau(e))} + \frac{\max(\tau(c), \tau(e))}{\min(\tau(c), \tau(e))} \right], \\ &= |C_{(2,2)}(G)| \left[\frac{\min(2,2)}{\max(2,2)} + \frac{\max(2,2)}{\min(2,2)} \right] + |C_{(2,3)}(G)| \left[\frac{\min(2,3)}{\max(2,3)} + \frac{\max(2,3)}{\min(2,3)} \right] \\ &+ |C_{(3,3)}(G)| \left[\frac{\min(3,3)}{\max(3,3)} + \frac{\max(3,3)}{\min(3,3)} \right] + |C_{(3,4)}(G)| \left[\frac{\min(3,4)}{\max(3,4)} + \frac{\max(3,4)}{\min(3,4)} \right] \\ &+ |C_{(4,5)}(G)| \left[\frac{\min(4,5)}{\max(4,5)} + \frac{\max(4,5)}{\min(4,5)} \right], \\ &= (4 \times 2^{\hat{n}}) \left[\frac{2}{2} + \frac{2}{2} \right] + (4 \times 2^{\hat{n}}) \left[\frac{2}{3} + \frac{3}{2} \right] + (8 \times 2^{\hat{n}} - 16) \left[\frac{3}{3} + \frac{3}{3} \right] \\ &+ (10 \times 2^{\hat{n}} - 10) \left[\frac{3}{4} + \frac{4}{3} \right] + (6 \times 2^{\hat{n}} - 6) \left[\frac{4}{5} + \frac{5}{4} \right], \\ &= (4 \times 2^{\hat{n}}) [2] + (4 \times 2^{\hat{n}}) \left[\frac{13}{6} \right] + (8 \times 2^{\hat{n}} - 16) [2] + (10 \times 2^{\hat{n}} - 10) \left[\frac{25}{12} \right] + (6 \times 2^{\hat{n}} - 6) \left[\frac{41}{20} \right], \\ &= (8 \times 2^{\hat{n}}) + (4 \times 2^{\hat{n}}) \left[\frac{13}{6} \right] + (16 \times 2^{\hat{n}} - 32) + (10 \times 2^{\hat{n}} - 10) \left[\frac{25}{12} \right] + (6 \times 2^{\hat{n}} - 6) \left[\frac{41}{20} \right], \\ &= (24 \times 2^{\hat{n}} - 32) + (4 \times 2^{\hat{n}}) \left[\frac{13}{6} \right] + (10 \times 2^{\hat{n}} - 10) \left[\frac{25}{12} \right] + (6 \times 2^{\hat{n}} - 6) \left[\frac{41}{20} \right]. \end{aligned}$$

□

Theorem 3.5. Let $G = D[\hat{n}]$ be a molecular graph. Then, the HCI is given in the following

$$HCI(G) = (4 \times 2^{\hat{n}}) \left[\frac{9}{10} \right] + (8 \times 2^{\hat{n}} - 16) \left[\frac{2}{6} \right] + (10 \times 2^{\hat{n}} - 10) \left[\frac{2}{7} \right] + (6 \times 2^{\hat{n}} - 6) \left[\frac{2}{9} \right].$$

Proof. After placing the values in Equation 2.5, we get

$$\begin{aligned} HCI(G) &= \sum_{c,e \in E(G)} \frac{2}{(\tau(c) + \tau(e))}, \\ &= |C_{(2,2)}(G)| \left[\frac{2}{(2+2)} \right] + |C_{(2,3)}(G)| \left[\frac{2}{(2+3)} \right] + |C_{(3,3)}(G)| \left[\frac{2}{(3+3)} \right] + |C_{(3,4)}(G)| \left[\frac{2}{(3+4)} \right] \\ &+ |C_{(4,5)}(G)| \left[\frac{2}{(4+5)} \right], \\ &= (4 \times 2^{\hat{n}}) \left[\frac{2}{(2+2)} \right] + (4 \times 2^{\hat{n}}) \left[\frac{2}{(2+3)} \right] + (8 \times 2^{\hat{n}} - 16) \left[\frac{2}{(3+3)} \right] + (10 \times 2^{\hat{n}} - 10) \left[\frac{2}{(3+4)} \right] \\ &+ (6 \times 2^{\hat{n}} - 6) \left[\frac{2}{(4+5)} \right], \\ &= (4 \times 2^{\hat{n}}) \left[\frac{9}{10} \right] + (8 \times 2^{\hat{n}} - 16) \left[\frac{2}{6} \right] + (10 \times 2^{\hat{n}} - 10) \left[\frac{2}{7} \right] + (6 \times 2^{\hat{n}} - 6) \left[\frac{2}{9} \right]. \end{aligned}$$

□

Theorem 3.6. Let $G = D[\hat{n}]$ be a molecular graph. Then, the ISCI is given in the following

$$ISCI(G) = (4 \times 2^{\hat{n}}) + (4 \times 2^{\hat{n}}) \left[\frac{6}{5} \right] + (8 \times 2^{\hat{n}} - 16) \left[\frac{3}{2} \right] + (10 \times 2^{\hat{n}} - 10) \left[\frac{12}{7} \right] + (6 \times 2^{\hat{n}} - 6) \left[\frac{20}{9} \right].$$

Proof. After placing the values in Equation 2.6, we get

$$\begin{aligned} ISCI(G) &= \sum_{c,e \in E(G)} \frac{\tau(c) \times \tau(e)}{(\tau(c) + \tau(e))}, \\ &= |C_{(2,2)}(G)| \frac{2 \times 2}{(2+2)} + |C_{(2,3)}(G)| \frac{2 \times 3}{(2+3)} + |C_{(3,3)}(G)| \frac{3 \times 3}{(3+3)} + |C_{(3,4)}(G)| \frac{3 \times 4}{(3+4)} \\ &\quad + |C_{(4,5)}(G)| \frac{4 \times 5}{(4+5)}, \\ &= (4 \times 2^{\hat{n}}) \frac{2 \times 2}{(2+2)} + (4 \times 2^{\hat{n}}) \frac{2 \times 3}{(2+3)} + (8 \times 2^{\hat{n}} - 16) \frac{3 \times 3}{(3+3)} + (10 \times 2^{\hat{n}} - 10) \frac{3 \times 4}{(3+4)} \\ &\quad + (6 \times 2^{\hat{n}} - 6) \frac{4 \times 5}{(4+5)}, \\ &= (4 \times 2^{\hat{n}}) + (4 \times 2^{\hat{n}}) \left[\frac{6}{5} \right] + (8 \times 2^{\hat{n}} - 16) \left[\frac{3}{2} \right] + (10 \times 2^{\hat{n}} - 10) \left[\frac{12}{7} \right] + (6 \times 2^{\hat{n}} - 6) \left[\frac{20}{9} \right]. \end{aligned}$$

□

Theorem 3.7. Let $G = D[\hat{n}]$ be a molecular graph. Then, the HZCI is given in the following

$$\begin{aligned} HZCI(G) &= 16(4 \times 2^{\hat{n}}) + 25(4 \times 2^{\hat{n}}) + 36(8 \times 2^{\hat{n}} - 16) + 49(10 \times 2^{\hat{n}} - 10) \\ &\quad + 81(6 \times 2^{\hat{n}} - 6). \end{aligned}$$

Proof. After placing the values in Equation 2.7, we get

$$\begin{aligned} HZCI(G) &= \sum_{c,e \in E(G)} [\tau(c) + \tau(e)]^2, \\ &= |C_{(2,2)}(G)| [2+2]^2 + |C_{(2,3)}(G)| [2+3]^2 + |C_{(3,3)}(G)| [3+3]^2 + |C_{(3,4)}(G)| [3+4]^2 \\ &\quad + |C_{(4,5)}(G)| [4+5]^2, \\ &= (4 \times 2^{\hat{n}}) [4]^2 + (4 \times 2^{\hat{n}}) [5]^2 + (8 \times 2^{\hat{n}} - 16) [6]^2 + (10 \times 2^{\hat{n}} - 10) [7]^2 \\ &\quad + (6 \times 2^{\hat{n}} - 6) [9]^2, \\ &= (4 \times 2^{\hat{n}}) [16] + (4 \times 2^{\hat{n}}) [25] + (8 \times 2^{\hat{n}} - 16) [36] + (10 \times 2^{\hat{n}} - 10) [49] \\ &\quad + (6 \times 2^{\hat{n}} - 6) [81], \\ &= 16(4 \times 2^{\hat{n}}) + 25(4 \times 2^{\hat{n}}) + 36(8 \times 2^{\hat{n}} - 16) + 49(10 \times 2^{\hat{n}} - 10) \\ &\quad + 81(6 \times 2^{\hat{n}} - 6). \end{aligned}$$

□

4. Conclusion

Dendrimers nanostars are artificially produced radially symmetric macromolecules with monodisperse, homogenous and precise structure. They have wide span of utilizations in supra molecular science, especially in energy harvesting, gene transfection, drug delivery, catalysis, photo activity and rheology modification. Topological indices are the graph descriptors which are helpful in predicting the topological

aspects of dendrimers. TIs help to relate the topology of distinct chemical structures. Recently, connection number based Zagreb indices are investigated which are considered to be more potent to measure the chemical and physical properties than other TIs of literature. In this paper, we develop some new CN-based Zagreb indices, namely, atom bond connectivity connection index, geometric arithmetic connection index, augmented connection index, symmetric division connection index, harmonic connection index, inverse sum connection index, hyper Zagreb connection index. Further, we find the general values to compute our defined CN-based ZIs of dendrimer nanostar.

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