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Computing Topological Indices of Dendrimer Nanostars

Research Article

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Abstract: A dendrimer is an artificially manufactured a synthesized molecule built up from branched units called monomers. In this paper, we compute generalized version of the first Zagreb index, general product connectivity index, general sum connectivity index, general reformulated index and other topological indices of dendrimer nanostars.

MSC: 05C05, 05C12.

Keywords: Zagreb indices, connectivity index, sum connectivity index, reformulated index, K-edge index, dendrimer nanostar.

1. Introduction

We consider only finite, simple and connected graph G with a vertex set $V(G)$ and an edge set $E(G)$. The degree $d_G(v)$ of a vertex v is the number of vertices adjacent to v. The edge connecting vertices u and v will be denoted by uv. Let $d_G(e)$ denote the degree of an edge $e = uv$ in G which is defined by $d_G(e) = d_G(u)+ d_G(v)$-2. For all further notation and terminology, we refer to reader to [1]. A molecular graph is a simple graph related to the structure of a chemical compound. Each vertex of this graph represents an atom of the molecule and its edges to the bonds between atoms. Chemical graph theory is a branch of mathematical chemistry which has an important effect on the development of the chemical sciences. A topological index is a numeric quantity from the structural graph of a molecule. There are several topological descriptors that have some applications in theoretical chemistry, especially in $QSPR/QSAR$ research. In [2], the first and second Zagreb indices were introduced to take account of the contributions of pairs of adjacent vertices. The first and second Zagreb indices of a graph G are defined as

$$M_1(G) = \sum_{u\in V(G)} d_G(u)^2 \quad \text{or} \quad M_1(G) = \sum_{uv\in E(G)} [d_G(u) + d_G(v)]$$
$$M_2(G) = \sum_{uv\in E(G)} d_G(u)\, d_G(v).$$

The modified first and second Zagreb indices [3] are respectively defined as

$${}^{m}M_1(G) = \sum_{u\in V(G)} \frac{1}{d_G(u)^2}, {}^{m}M_2(G) = \sum_{uv\in E(G)} \frac{1}{d_G(u)\, d_G(v)}.$$

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The F-index of a graph G is defined as

$$F(G) = \sum_{u \in V(G)} d_G(u)^3 .$$

The F-index was introduced in [2]. In [4], Furtula and Gutman studied this index and called it forgotten topological index. In [5], Li et al. introduced the generalized version of the first Zagreb index, and it is defined as

$$ZM_1^{a+1}(G) = \sum_{u \in V(G)} d_G(u)^{a+1} = \sum_{uv \in E(G)} \left[d_G(u)^a + d_G(v)^a\right] \tag{1}$$

where a is a real number. The first hyper-Zagreb index [6] of a graph G is defined as

$$HM_1(G) = \sum_{uv \in E(G)} \left[d_G(u) + d_G(v)\right]^2 .$$

The sum connectivity index [7] of a graph G is defined as

$$X(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_G(u) + d_G(v)}}.$$

The product connectivity index [8] of a graph G is defined as

$$\chi(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_G(u)\, d_G(v)}}.$$

The above two topological indices were also studied, for example, in [9, 10]. The general sum connectivity index [11, 12] of a graph G is defined as

$$M_1^a(G) = \sum_{uv \in E(G)} \left[d_G(u) + d_G(v)\right]^a \tag{2}$$

where a is a real number. The general product connectivity index [12, 13] of a graph G is defined as

$$M_2^a(G) = \sum_{uv \in E(G)} \left[d_G(u)\, d_G(v)\right]^a \tag{3}$$

where a is a real number. In [14], Miličević et al. introduced the reformulated first Zagreb index of a graph G and it is defined as

$$EM_1(G) = \sum_{e \in E(G)} d_G(e)^2 .$$

In [15], Kulli introduced the K edge index of a graph G and it is defined as

$$K_e(G) = \sum_{e \in E(G)} d_G(e)^3 .$$

This index was also studied in [16]. In [17], Kulli proposed the general reformulated Zagreb index of a graph and it is defined as

$$EM_1^a(G) = \sum_{e \in E(G)} d_G(e)^a \tag{4}$$

where a is a real number. Recently, some topological indices were studied, for example in [18, 19, 20, 21]. In this paper, we determine generalized version of the first Zagreb index, general product connectivity index, general sum connectivity index and other topological indices of dendrimer nanostars. For dendrimer nanostars, see [22, 23].

2. Results for Dendrimer Nanostars

We consider the dendrimer nanostar with n growth stages, denoted by $D_3[n]$, where $n \geq 0$, see Figure 1.

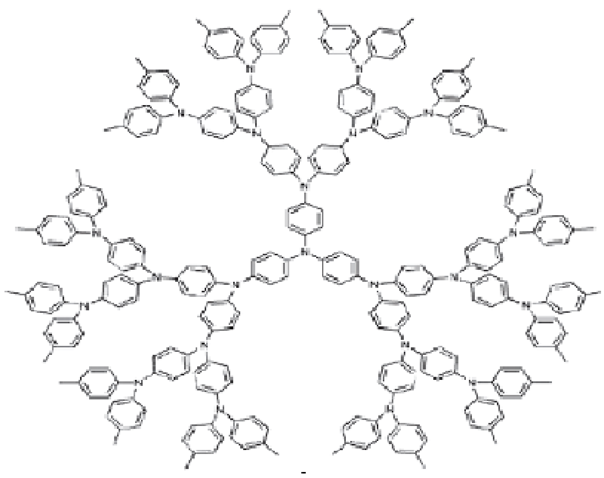

Figure 1. **Dendrimer nanostar with 3-growth stages,** $D_3[3]$

By algebraic method, we obtain $|V(D_3[n])| = 24 \times 2^n - 20$ and $|E(D_3[n])| = 24(2^{n+1} - 1)$. Let $G = D_3[n]$. From Figure 1, it is easy to see that there are three partitions of the vertex set of $D_3[n]$ as follows:

$$V_1 = \{u \in V(G)|d_G(u) = 1\}, \qquad |V_1| = 3 \times 2^n$$
$$V_2 = \{u \in V(G)|d_G(u) = 2\}, \qquad |V_2| = 12\left(2^{n-1} - 1\right)$$
$$V_3 = \{u \in V(G)|d_G(u) = 3\}, \qquad |V_3| = 15 \times 2^n - 8.$$

Also by algebraic method, we obtain three edge partitions of G based on the sum of degrees of the end vertices as follows:

$$E_4 = \{uv \in E(G)|d_G(u) = 1, d_G(v) = 3\} \cup \{uv \in E(G)|d_G(u) = d_G(v) = 2\}, \qquad |E_4| = 15 \times 2^n - 6.$$
$$E_5 = \{uv \in E(G)|d_G(u) = 2, d_G(v) = 3\}, \qquad |E_5| = 12(2^{n+1} - 1).$$
$$E_6 = \{uv \in E(G)|d_G(u) = d_G(v) = 3\}, \qquad |E_6| = 9 \times 2^n - 6.$$

Similarly by algebraic method, we obtain four edge partitions of G based on the product of degrees of the end vertices as follows:

$$E_3^* = \{uv \in E(G)\,|d_G(u) = 1, d_G(v) = 3\}, \qquad |E_3^*| = 3 \times 2^n.$$
$$E_4^* = \{uv \in E(G)\,|d_G(u) = d_G(v) = 2\}, \qquad |E_4^*| = 6\left(2^{n+1} - 1\right).$$
$$E_6^* = \{uv \in E(G)\,|d_G(u) = 2, d_G(v) = 3\}, \qquad |E_6^*| = 12\left(2^{n+1} - 1\right).$$
$$E_9^* = \{uv \in E(G)\,|d_G(u) = d_G(v) = 3\}, \qquad |E_9^*| = 9 \times 2^n - 6.$$

The edge degree partitions of $D_3[n]$ is given in Table 1.

$d_G(u), d_G(v)ne = uv \in E(G)$	$E_4 = (1,3) \cup (2,2)$	$E_5 = (2,3)$	$E_6 = (3,3)$
$d_G(e)$	2	3	4
Number of edges	$15 \times 2^n - 6$	$12(2^{n+1} - 1)$	$9 \times 2^n - 6$

Table 1. **Edge degree partition of** $D_3[n]$

We determine the generalized version of the first Zagreb index of a dentrimer nanostar $D_3[n]$.

Theorem 2.1. *The generalized version of the first Zagreb index of $D_3[n]$ is given by*

$$ZM_1^{a+1}\left(D_3\left[n\right]\right) = \left(3 + 6 \times 2^{a+1} + 15 \times 3^{a+1}\right) 2^n - \left(12 \times 2^{a+1} + 8 \times 3^{a+1}\right). \tag{5}$$

Proof. Let $G = D_3[n]$, From Equation (1) and cardinalities of the vertex partition of $D_3[n]$, we have

$$\begin{aligned} ZM_1^{a+1}\left(D_3\left[n\right]\right) &= \sum_{u \in V(G)} d_G\left(u\right)^{a+1} = \sum_{u \in V_1} d_G\left(u\right)^{a+1} + \sum_{u \in V_2} d_G\left(u\right)^{a+1} + \sum_{u \in V_3} d_G\left(u\right)^{a+1} \\ &= 3 \times 2^n + 12\left(2^{n-1} - 1\right) \times 2^{a+1} + \left(15 \times 2^n - 8\right) \times 3^{a+1} \\ &= \left(3 + 6 \times 2^{a+1} + 15 \times 3^{a+1}\right) 2^n - \left(12 \times 2^{a+1} + 8 \times 3^{a+1}\right). \end{aligned}$$

□

We obtain the following results by using Theorem 2.1.

Corollary 2.2. *The first Zagreb index of $D_3[n]$ is given by $M_1\left(D_3\left[n\right]\right) = 162 \times 2^n - 120$.*

Proof. Put $a = 1$ in Equation (5), we get the desired result. □

Corollary 2.3. *The F-index of $D_3[n]$ is given by $F(D_3[n]) = 456 \times 2^n - 312$.*

Proof. Put $a = 2$ in Equation (5), we get the desired result. □

Corollary 2.4. *The modified first Zagreb index of $D_3[n]$ is given by*

$${}^mM_1\left(D_3\left[n\right]\right) = \frac{37}{6} \times 2^n - \frac{35}{9}.$$

Proof. Put $a = -3$ in Equation (5), we get the desired result. □

We compute the general sum connectivity index of $D_3[n]$.

Theorem 2.5. *The general sum connectivity index of $D_3[n]$ is given by*

$$M_1^a\left(D_3\left[n\right]\right) = \left(15 \times 4^a + 24 \times 5^a + 9 \times 6^a\right) 2^n - \left(6 \times 4^a + 12 \times 5^a + 6 \times 6^a\right). \tag{6}$$

Proof. Let $G = D_3[n]$. From Equation (2) and cardinalities of the edge partitions of $D_3[n]$, we have

$$\begin{aligned} M_1^a\left(D_3\left[n\right]\right) &= \sum_{uv \in E(D_3[n])} \left[d_{D_3[n]}\left(u\right) + d_{D_3[n]}\left(v\right)\right]^a \\ &= \sum_{uv \in E_4} \left[d_{D_3[n]}\left(u\right) + d_{D_3[n]}\left(v\right)\right]^a + \sum_{uv \in E_5} \left[d_{D_3[n]}\left(u\right) + d_{D_3[n]}\left(v\right)\right]^a + \sum_{uv \in E_6} \left[d_{D_3[n]}\left(u\right) + d_{D_3[n]}\left(v\right)\right]^a \\ &= 4^a\left(15 \times 2^n - 6\right) + 5^a \times 12\left(2^{n+1} - 1\right) + 6^a\left(9 \times 2^n - 6\right) \\ &= \left(15 \times 4^a + 24 \times 5^a + 9 \times 6^a\right) 2^n - \left(6 \times 4^a + 12 \times 5^a + 6 \times 6^a\right). \end{aligned}$$

□

We obtain the following results by using Theorem 2.5.

Corollary 2.6. *The first Zagreb index of $D_3[n]$ is given by $M_1(D_3[n]) = 234 \times 2^n - 120$.*

Proof. Put $a = 1$ in Equation (6), we get the desired result. □

Corollary 2.7. *The first hyper-Zagreb index of $D_3[n]$ is given by $HM_1(D_3[n]) = 1164 \times 2^n - 612$.*

Proof. Put $a = 2$ is Equation (6), we get the desired result. □

Corollary 2.8. *The sum connectivity index of $D_3[n]$ is given by*

$$X(D_3[n]) = \left(\frac{15}{2} + \frac{24}{\sqrt{5}} + \frac{9}{\sqrt{6}}\right) 2^n - \left(\frac{3}{2} + \frac{12}{\sqrt{5}} + \frac{6}{\sqrt{6}}\right).$$

Proof. Put $a = -\frac{1}{2}$ in Equation (6), we get the desired result. □

We now compute the general product connectivity index of $D_3[n]$.

Theorem 2.9. *The general product connectivity index of $D_3[n]$ is given by*

$$M_2^a(D_3[n]) = \left(3^{a+1} + 3 \times 4^{a+1} + 4 \times 6^{a+1} + 9^{a+1}\right) 2^n - \left(6 \times 4^a + 12 \times 6^a + 6 \times 9^a\right). \tag{7}$$

Proof. From Equation (3) and by cardinalities of the edge partition of $D_3[n]$ based on the product degrees of the end vertices, we have

$$\begin{aligned}
M_2^a(D_3[n]) &= \sum_{uv \in E(D_3[n])} \left[d_{D_3[n]}(u)\, d_{D_3[n]}(v)\right]^a \\
&= \sum_{uv \in E_3^*} \left[d_{D_3[n]}(u)\, d_{D_3[n]}(v)\right]^a + \sum_{uv \in E_4^*} \left[d_{D_3[n]}(u)\, d_{D_3[n]}(v)\right]^a + \sum_{uv \in E_6^*} \left[d_{D_3[n]}(u)\, d_{D_3[n]}(v)\right]^a \\
&\quad + \sum_{uv \in E_9^*} \left[d_{D_3[n]}(u)\, d_{D_3[n]}(v)\right]^a \\
&= 3^a (3 \times 2^n) + 4^a \times 6\left(2^{n+1} - 1\right) + 6^a \times 12\left(2^{n+1} - 1\right) + 9^a (9 \times 2^n - 6) \\
&= \left(3^{a+1} + 3 \times 4^{a+1} + 4 \times 6^{a+1} + 9^{a+1}\right) 2^n - \left(6 \times 4^a + 12 \times 6^a + 6 \times 9^a\right).
\end{aligned}$$

□

We obtain the following corollaries by Theorem 2.9.

Corollary 2.10. *The second Zagreb index of $D_3[n]$ is given by $M_2(D_3[n]) = 282 \times 2^n - 150$.*

Proof. Put $a = 1$ in Equation (7), we get the desired result. □

Corollary 2.11. *The modified second Zagreb index of $D_3[n]$ is given by ${}^mM_2(D_3[n]) = 9 \times 2^n - \frac{25}{6}$.*

Proof. Put $a = -1$ in Equation (7), we get the desired result. □

Corollary 2.12. *The product connectivity index of $D_3[n]$ is given by*

$$\chi(D_3[n]) = \left(9 + \sqrt{3} + 4\sqrt{6}\right) 2^n - \left(5 + 6\sqrt{6}\right).$$

Proof. Put $a = -\frac{1}{2}$ in Equation (7), we get the desired result. □

In the following theorem, we compute the general first reformulated Zagreb index of $D_3[n]$.

Theorem 2.13. *The general first reformulated Zagreb index of $D_3[n]$ is given by*

$$EM_1^a(D_3[n]) = \left(15 \times 2^a + 24 \times 3^a + 9 \times 4^a\right) 2^n - \left(6 \times 2^a + 12 \times 3^a + 6 \times 4^a\right). \tag{8}$$

Proof. From equation (4) and by the edge degree partition of $D_3[n]$, we have

$$\begin{aligned} EM_1^a\left(D_3\left[n\right]\right) &= \sum_{e\in E(D_3[n])} d_{D_3[n]}\left(e\right)^a \\ &= \sum_{e\in E_4} d_{D_3[n]}\left(e\right)^a + \sum_{e\in E_5} d_{D_3[n]}\left(e\right)^a + \sum_{e\in E_6} d_{D_3[n]}\left(e\right)^a \\ &= 2^a\left(15\times 2^n-6\right)+3^a\times 12\left(2^{n+1}-1\right)+4^a\left(9\times 2^n-6\right) \\ &= \left(15\times 2^a+24\times 3^a+9\times 4^a\right)2^n-\left(6\times 2^a+12\times 3^a+6\times 4^a\right). \end{aligned}$$

□

Corollary 2.14. *The first reformulated Zagreb index of $D_3[n]$ is given by $EM_1(D_3[n]) = 420\times 2^n - 228$.*

Proof. Put $a = 2$ in Equation (8), we get the desired result. □

Corollary 2.15. *The K-edge index of $D_3[n]$ is given by $K_e(D_3[n]) = 1344\times 2^n - 756$.*

Proof. Put $a = 3$ in Equation (8), we get the desired result. □

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