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RESEARCH ARTICLE

MULTIPLICATIVE CONNECTIVITY REVERSE INDICES OF TWO FAMILIES OF DENDRIMER NANOSTARS

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ABSTRACT

In Medical Science, the multiplicative connectivity indices are used in the analysis of drug molecular structures which are helpful for medical scientists and pharmaceutical scientists to find out the chemical and biological characteristics of drugs. In this paper, we introduce the multiplicative product connectivity reverse index, multiplicative sum connectivity reverse index, first multiplicative atom bond connectivity reverse index and multiplicative geometric-arithmetic reverse index of a molecular structure. Furthermore, we compute the multiplicative connectivity reverse indices of two types of dendrimer nanostars.

Key words: Molecular structure, Multiplicative connectivity Reverse indices, Dendrimer nanostars.

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INTRODUCTION

In this paper, we consider only a finite, simple connected graph 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. Let $\Delta(G)$($\delta(G)$) denote the maximum (minimum) degree among the vertices of G. The reverse vertex degree of a vertex u in G is defined as $c_u = \Delta(G) - d_G(u) + 1$. The reverse edge connecting the reverse vertices u and v will be denoted by uv. We refer to [1] for undefined term and notation.

A molecular graph is a simple graph related to the structure of a chemical compound. Each vertex of this graph represents an atom to molecule and its edges to the bound between atoms. A topological index is a numerical parameter mathematically derived from the graph structure. Numerous topological indices have been considered in Theoretical Chemistry, see [2].

The Revan vertex degree of a vertex u in G is defined as $r_G(u) = \Delta(G) + \delta(G) - d_G(u)$. The Revan edge connecting the Revan vertices u and v will be denoted by uv. In [3], Kulli introduced the first and second Revan indices of a graph G. Recently some Revan topological indices were studied, for example, in [4, 5, 6].

In [7], Kulli introduced the multiplicative connectivity Revan indices as follows:

The multiplicative product connectivity Revan index of a graph G is defined as

$$PRII(G) = \prod_{uv \in E(G)} \frac{1}{\sqrt{r_G(u) r_G(v)}}$$

The multiplicative sum connectivity Revan index of a graph G is defined as

$$SRII(G) = \prod_{uv \in E(G)} \frac{1}{\sqrt{r_G(u) + r_G(v)}}.$$

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The first multiplicative atom bond connectivity Revan index of a graph G is defined as

$$ABC_1RII(G) = \prod_{uv \in E(G)} \sqrt{\frac{r_G(u) + r_G(v) - 2}{r_G(u) r_G(v)}}.$$

The multiplicative geometric-arithmetic Revan index of a graph G is defined as

$$GARII(G) = \prod_{uv \in E(G)} \frac{2\sqrt{r_G(u) r_G(v)}}{r_G(u) + r_G(v)}.$$

Motivated by the definitions of the multiplicative connectivity Revan indices and their applications, we introduce the multiplicative connectivity reverse indices as follows:

The multiplicative product connectivity reverse index of a graph G is defined as

$$PCII(G) = \prod_{uv \in E(G)} \frac{1}{\sqrt{c_u c_v}}.$$

The multiplicative sum connectivity reverse index of a graph G is defined as

$$SCII(G) = \prod_{uv \in E(G)} \frac{1}{\sqrt{c_u + c_v}}.$$

The first multiplicative atom bond connectivity reverse index of a graph G is defined as

$$ABC_1CII(G) = \prod_{uv \in E(G)} \sqrt{\frac{c_u + c_v - 2}{c_u c_v}}.$$

The multiplicative geometric-arithmetic reverse index of a graph G is defined as

$$GACII(G) = \prod_{uv \in E(G)} \frac{2\sqrt{c_u c_v}}{c_u c_v}.$$

Recently many multiplicative topological indices were studied, for example, [8, 9, 10, 11, 12, 13, 14, 15, 16, 17]. Also some connectivity indices were studied, for example, in [18, 19, 20, 21, 22, 23]. In the this paper, the multiplicative connectivity indices of two families of dendrimer nanostars are computed. For more information about these dendrimer nanostars see [24].

Observation 1. Let G be the graph of a chemical compound. If $\delta(G)=1$, then $c_u = r_G(u)$, where u is vertex of G.

Results for Dendrimer Nanostars $D_1[n]$.

In this section, we consider a family of dendrimer nanostars with n growth stages, denoted by $D_1[n]$, where $n \geq 0$. The molecular graph of $D_1[4]$ with 4 growth stages is depicted in Figure 1.

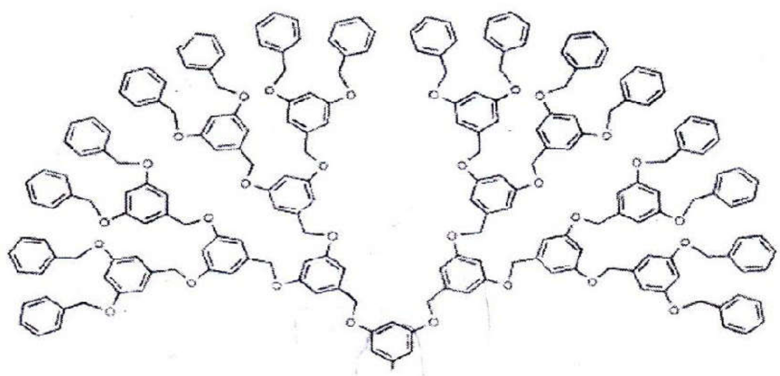

Figure 1. The molecular graph of $D_1[4]$.

Let G be the molecular graph of dendrimer nanostar $D_1[n]$. From Figure 1, it is easy to see that the vertices of dendrimer nanostar $D_1[n]$ are either of degree 1, 2 or 3. Therefore $\Delta(G) = 3$ and $c_u = 4 - d_G(u)$. By calculation, we obtain that G has $2^{n+4} - 9$ vertices and $18 \times 2^n - 11$ edges. Also by calculation, we partition the edge set $E(D_1[n])$ into three sets as follows:

$E_{13} = \{uv \in E(G) \mid d_G(u) = 1, d_G(v) = 3\} |E_{13}| = 1.$

$E_{22} = \{uv \in E(G) \mid d_G(u) = d_G(v) = 2\}|E_{22}| = 6 \times 2^n - 2.$

$E_{23} = \{uv \in E(G) \mid d_G(u) = 2, d_G(v) = 3\}|E_{23}| = 12 \times 2^n - 10.$

The we ensure that there are three types of reverse edges in $D_1[n]$ as follows:

$CE_{31} = \{uv \in E(G) \mid c_u = 3, c_v = 1\},|CE_{31}| = 1.$

$CE_{22} = \{uv \in E(G) \mid c_u = c_v = 2\},|CE_{22}| = 6 \times 2^n - 2.$

$CE_{21} = \{uv \in E(G) \mid c_u = 2, c_v = 1\},|CE_{21}| = 12 \times 2^n - 10.$

In the following theorem, we compute the multiplicative product connectivity reverse index of $D_1[n]$.

Theorem 1. The multiplicative product connectivity reverse index of a dendrimer nanostar $D_1[n]$ is given by

$$PCII(D_1[n]) = \left(\frac{1}{\sqrt{3}}\right)^1 \times \left(\frac{1}{2}\right)^{12\times 2^n - 7}.$$

Proof. By definition, we have $PCII(G) = \prod_{uv\in E(G)} \frac{1}{\sqrt{c_u c_v}}$.

Thus $$PCII(D_1[n]) = \prod_{CE_{31}} \frac{1}{\sqrt{3\times 1}} \times \prod_{CE_{22}} \frac{1}{\sqrt{2\times 2}} \times \prod_{CE_{21}} \frac{1}{\sqrt{2\times 1}} = \left(\frac{1}{\sqrt{3}}\right)^1 \times \left(\frac{1}{2}\right)^{6\times 2^n - 2} \times \left(\frac{1}{\sqrt{2}}\right)^{2\times 2^n - 10}.$$

$$= \left(\frac{1}{\sqrt{3}}\right)^1 \times \left(\frac{1}{2}\right)^{12\times 2^n - 7}.$$

In the following theorem, we compute the multiplicative sum connectivity reverse index of $D_1[n]$.

Theorem 2. The multiplicative sum connectivity reverse index of a dendrimer nanostar $D_1[n]$ is given by

$$SCII(D_1[n]) = \left(\frac{1}{2}\right)^{6\times 2^n - 1} \times \left(\frac{1}{3}\right)^{6\times 2^n - 5}.$$

Proof. By definition, we have $SCII(G) = \prod_{uv\in E(G)} \frac{1}{\sqrt{c_u + c_v}}$.

Thus $$SCII(D_1[n]) = \prod_{CE_{31}} \frac{1}{\sqrt{3+1}} \times \prod_{CE_{22}} \frac{1}{\sqrt{2+2}} \times \prod_{CE_{21}} \frac{1}{\sqrt{2+1}} = \left(\frac{1}{2}\right)^1 \times \left(\frac{1}{2}\right)^{6\times 2^n - 2} \times \left(\frac{1}{\sqrt{3}}\right)^{12\times 2^n - 10}.$$

$$= \left(\frac{1}{2}\right)^{6\times 2^n - 1} \times \left(\frac{1}{3}\right)^{6\times 2^n - 5}.$$

In the following theorem, we compute the first multiplicative atom bond connectivity reverse index of $D_1[n]$.

Theorem 3. The first multiplicative atom bond connectivity reverse index of a dendrimer nanostar $D_1[n]$ is given by

$$ABC_1CII(D_1[n]) = \left(\sqrt{\frac{2}{3}}\right)^1 \times \left(\frac{1}{2}\right)^{9\times 2^n - 6}.$$

Proof. By definition, we have $ABC_1CII(G) = \prod_{uv\in E(G)} \sqrt{\frac{c_u + c_v - 2}{c_u \times c_v}}$.

Thus $$ABC_1CII(D_1[n]) = \prod_{CE_{31}} \sqrt{\frac{3+1-2}{3\times 1}} \times \prod_{CE_{22}} \sqrt{\frac{2+2-2}{2\times 2}} \times \prod_{CE_{21}} \sqrt{\frac{2+1-2}{2\times 1}}$$

$$=\left(\sqrt{\frac{2}{3}}\right)^{1}\times\left(\frac{1}{\sqrt{2}}\right)^{6\times2^{n}-2}\times\left(\frac{1}{\sqrt{2}}\right)^{12\times2^{n}-10}=\left(\sqrt{\frac{2}{3}}\right)^{1}\times\left(\frac{1}{2}\right)^{9\times2^{n}-6}.$$

In the following theorem, we compute the multiplicative geometric-arithmetic index of $D_1[n]$.

Theorem 4. The first multiplicative geometric-arithmetic index of a dendrimer nanostar $D_1[n]$ is given by

$$GACII\left(D_1[n]\right)=\left(\frac{\sqrt{3}}{2}\right)^{1}\times\left(\frac{2\sqrt{2}}{3}\right)^{12\times2^{n}-10}.$$

Proof. By definition, we have $GACII(G)=\prod_{uv\in E(G)}\frac{2\sqrt{c_u\times c_v}}{c_u+c_v}$.

Thus $$GACII\left(D_1[n]\right)=\prod_{CE_{31}}\frac{2\sqrt{3\times1}}{3+1}\times\prod_{CE_{22}}\frac{2\sqrt{2\times2}}{2+2}\times\prod_{CE_{21}}\frac{2\sqrt{2\times1}}{2+1}$$

$$=\left(\frac{\sqrt{3}}{2}\right)^{1}\times(1)^{6\times2^{n}-2}\times\left(\frac{2\sqrt{2}}{3}\right)^{12\times2^{n}-10}=\left(\frac{\sqrt{3}}{2}\right)^{1}\times\left(\frac{2\sqrt{2}}{3}\right)^{12\times2^{n}-10}.$$

Theorem 5. Let G be the graph of a dendrimer nanostar $D_1[n]$. Then

1) $PCII(D_1[n]) = PRII(D_1[n])$.
2) $SCII(D_1[n]) = SRII(D_1[n])$.
3) $ABC_1CII(D_1[n]) = ABC_1RII(D_1[n])$.
4) $GACII(D_1[n]) = GARII(D_1[n])$.

Proof: Since $\delta(G) = 1$, the results follow from Observation 1.

2. Results for dendrimer nanostars $D_3[n]$.

In this section, we consider of dendrimer nanostars with n growth stages, denoted by $D_3[n]$, where n□0. The molecular structure of $D_3[n]$ with 3 growth stages is shown in Figure 2.

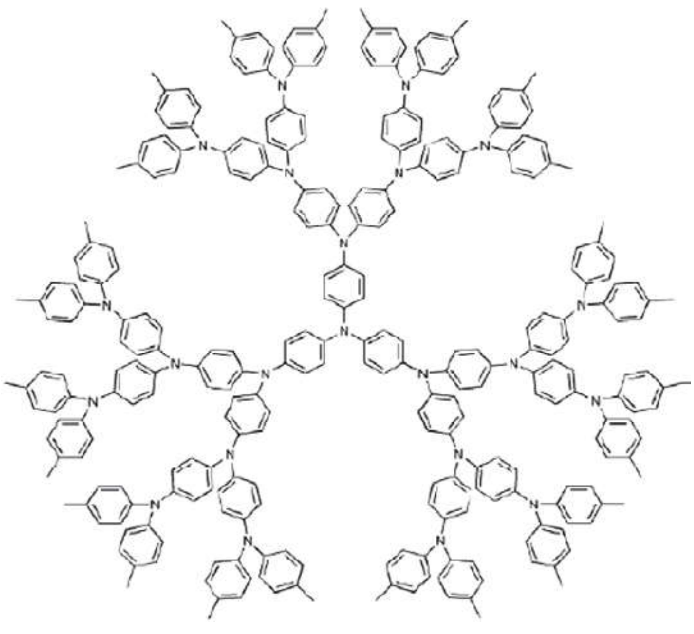

Figure 2. The molecular structure of $D_3[3]$

Let G be the graph of a dendrimer nanostar $D_3[n]$. From Figure 2, it is easy to see that the vertices of dendrimter nanostar $D_3[n]$ are either of degree 1, 2 or 3. Therefore $\Delta(G) = 3$ and $c_u = 4 - d_G(u)$. By algebraic method, we obtain that G has $24 \times 2^n - 20$ vertices and $24 \times 2^{n+1} - 24$ edges. Also by algebraic method, we obtain that the edge set $E(D_3[n])$ can be divided into four partitions:

$E_{13} = \{uv \in E(G) \mid d_G(u) = 1, d_G(v) = 3\}|E_{13}| = 3\times2^n$.
$E_{22} = \{uv \in E(G) \mid d_G(u) = d_G(v) = 2\}|E_{22}| = 12\times2^n - 6$.
$E_{23} = \{uv \in E(G) \mid d_G(u) = 2, d_G(v) = 3\}|E_{23}| = 24\times2^n - 12$.
$E_{33} = \{uv \in E(G) \mid d_G(u) = d_G(v) = 3\}|E_{33}| = 9\times2^n - 6$.

Thus there are four types of reverse edges in $D_3[n]$ as follows:

$CE_{31} = \{uv \in E(G) \mid c_u = 3, c_v = 1\},|CE_{31}| = 3\times2^n$.
$CE_{22} = \{uv \in E(G) \mid c_u = c_v = 2\},|CE_{22}| = 12 \times 2^n - 6$.
$CE_{21} = \{uv \in E(G) \mid c_u = 2, c_v = 1\},|CE_{21}| = 24 \times 2^n - 12$.
$CE_{11} = \{uv \in E(G) \mid c_u = c_v = 1\},|CE_{11}| = 9 \times 2^n - 6$.

In the following theorem, we determine the multiplicative product connectivity reverse index of $D_3[n]$.

Theorem 6. The multiplicative product connectivity reverse index of a dendrimer nanostar $D_3[n]$ is given by

$$PCII\left(D_3[n]\right) = \left(\frac{1}{\sqrt{3}}\right)^{3\times2^n} \times \left(\frac{1}{2}\right)^{12\times2^n-6} \times \left(\frac{1}{\sqrt{2}}\right)^{24\times2^n-12}.$$

Proof. By definition, we have $PCII(G) = \prod_{uv\in E(G)} \frac{1}{\sqrt{c_u c_v}}$.

Thus $$PCII\left(D_3[n]\right) = \prod_{CE_{31}} \frac{1}{\sqrt{3\times1}} \times \prod_{CE_{22}} \frac{1}{\sqrt{2\times2}} \times \prod_{CE_{21}} \frac{1}{\sqrt{2\times1}} \times \prod_{CE_{11}} \frac{1}{\sqrt{1\times1}}$$

$$= \left(\frac{1}{\sqrt{3}}\right)^{3\times2^n} \times \left(\frac{1}{2}\right)^{12\times2^n-6} \times \left(\frac{1}{\sqrt{2}}\right)^{24\times2^n-12} \times (1)^{9\times2^n-6}.$$

$$= \left(\frac{1}{\sqrt{3}}\right)^{3\times2^n} \times \left(\frac{1}{2}\right)^{12\times2^n-6} \times \left(\frac{1}{\sqrt{2}}\right)^{24\times2^n-12}.$$

In the following theorem, we determine the multiplicative sum connectivity reverse index of $D_3[n]$.

Theorem 7. The multiplicative sum connectivity reverse index of a dendrimer nanostar $D_3[n]$ is given by

$$SCII\left(D_3[n]\right) = \left(\frac{1}{\sqrt{2}}\right)^{39\times2^n-18} \times \left(\frac{1}{3}\right)^{12\times2^n-6}.$$

Proof. By definition, we have $SCII(G) = \prod_{uv\in E(G)} \frac{1}{\sqrt{c_u + c_v}}$.

Thus $$SCII\left(D_1[n]\right) = \prod_{CE_{31}} \frac{1}{\sqrt{3+1}} \times \prod_{CE_{22}} \frac{1}{\sqrt{2+2}} \times \prod_{CE_{21}} \frac{1}{\sqrt{2+1}} \times \prod_{CE_{11}} \frac{1}{\sqrt{1+1}}.$$

$$= \left(\frac{1}{2}\right)^{3\times2^n} \times \left(\frac{1}{2}\right)^{12\times2^n-6} \times \left(\frac{1}{\sqrt{3}}\right)^{24\times2^n-12} \times \left(\frac{1}{\sqrt{2}}\right)^{9\times2^n-6}$$

$$= \left(\frac{1}{\sqrt{2}}\right)^{39\times2^n-18} \times \left(\frac{1}{3}\right)^{12\times2^n-6}.$$

In the following theorem, we determine the first multiplicative atom bond connectivity reverse index of $D_3[n]$.

Theorem 8. The first multiplicative atom bond connectivity reverse index of a dendrimer nanostar $D_3[n]$ is given by

$$ABC_1CII\left(D_3[n]\right) = 0.$$

Proof. By definition, we have $ABC_1CII(G) = \prod_{uv\in E(G)} \sqrt{\frac{c_u + c_v - 2}{c_u \times c_v}}$.

Thus $$ABC_1CII(D_1[n]) = \prod_{RC_{31}} \sqrt{\frac{3+1-2}{3\times 1}} \times \prod_{RC_{22}} \sqrt{\frac{2+2-2}{2\times 2}} \times \prod_{CE_{21}} \sqrt{\frac{2+1-2}{2\times 1}} \times \prod_{CE_{11}} \sqrt{\frac{1+1-2}{1\times 1}}$$

$$= 0$$

In the following theorem, we determine the multiplicative geometric-arithmetic reverse index of $D_3[n]$.

Theorem 9. The first multiplicative geometric-arithmetic reverse index of a dendrimer nanostar $D_3[n]$ is given by

$$GACII(D_3[n]) = \left(\frac{\sqrt{3}}{2}\right)^{3\times 2^n} \times \left(\frac{2\sqrt{2}}{3}\right)^{24\times 2^n - 12}.$$

Proof. By definition, we have $GACII(G) = \prod_{uv\in E(G)} \frac{2\sqrt{c_u \times c_v}}{c_u + c_v}$.

Thus $$GACII(D_3[n]) = \prod_{CE_{31}} \frac{2\sqrt{3\times 1}}{3+1} \times \prod_{CE_{22}} \frac{2\sqrt{2\times 2}}{2+2} \times \prod_{CE_{21}} \frac{2\sqrt{2\times 1}}{2+1} \times \prod_{CE_{11}} \frac{2\sqrt{1\times 1}}{1+1}$$

$$= \left(\frac{\sqrt{3}}{2}\right)^{3\times 2^n} \times (1)^{12\times 2^n - 6} \times \left(\frac{2\sqrt{2}}{3}\right)^{24\times 2^n - 6} \times (1)^{9\times 2^n - 6} = \left(\frac{\sqrt{3}}{2}\right)^{3\times 2^n} \times \left(\frac{2\sqrt{2}}{3}\right)^{24\times 2^n - 6}.$$

Theorem 10. Let G be the graph of a dendrimer nanostar $D_3[n]$. Then

1) $PCII(D_1[n]) = PRII(D_3[n])$.
2) $SCII(D_1[n]) = SRII(D_3[n])$.
3) $ABC_1CII(D_1[n]) = ABC_1RII(D_3[n])$.
4) $GACII(D_1[n]) = GARII(D_3[n])$.

Proof: Since $\delta(G) = 1$, the results follow from Observation 1.

Definition 1. If the graph of a nanostructure S has a vertex of degree 1, then S is called Vedavin nanostruture.

Observation. 2. For any Vedavin nanostructure S, the Revan index and corresponding reverse index of S coincide.

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