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Multiplicative Atom-Bond Connectivity and Multiplicative Geometric-Arithmetic Indices of Dendrimer Nanostars

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Abstract: A chemical graph or a molecular graph is a simple graph related to the structure of a chemical compound. The connectivity indices are applied to measure the chemical characteristics of compounds in Chemical Graph Theory. In this paper, we determine the multiplicative atom bond connectivity index and geometric arithmetic index of three families of dendrimer nanostars.

Keywords: multiplicative atom bond connectivity index, multiplicative geometric-arithmetic index, dendrimer nanostar.

AMS Mathematics Subject Classification (2010): 05*C*05, 05*C*12, 05*C*90

1. Introduction

Let $G = (V(G), E(G))$ be a finite, simple connected graph. The degree $d_G(v)$ of a vertex v is the number of vertices adjacent to v. For other undefined notations and terminology, the readers are referred to [1].

A molecular graph is a finite simple graph such that its vertices correspond to the atoms and the edges to the bonds. Chemical graph theory is a branch of Mathematical chemistry which has an important effect on the development of the chemical sciences. Several topological indices have been found to be useful in chemical documentation isomer discrimination, structure property relationships, structure activity relationships and pharmaceutical drug design in organic chemistry, see [2].

In [3], Kulli introduced the multiplicative atom bond connectivity index and multiplicative geometric arithmetic index of a molecular graph as follows:

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

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

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

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

Recently, several multiplicative indices were studied, for example, in [4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17]. Also some connectivity indices were studied, for example in [18, 19, 20, 21, 22].

We consider three infinite classes of dendrimer nanostars $NS_1[n]$, $NS_2[n]$ and $NS_3[n]$. For more information about these dendrimer nanostars see [23, 24]. In this paper, we compute the multiplicative atom bond connectivity index and multiplicative geometric- arithmetic index for dendrimer nanostars $NS_1[n]$ $NS_2[n]$ and $NS_3[n]$.

2. Results for $NS_1[n]$ dendrimer nanostars

In this section, we focus on the molecular graph structure of the first class of dendrimer nanostars. This family of dendrimer nanostars is denoted by $NS_1[n]$, where n is the steps of growth in this type of dendrimer nanostars. The molecular graph structure of $NS_1[3]$ dendrimer nanostar is depicted in Figure 1.

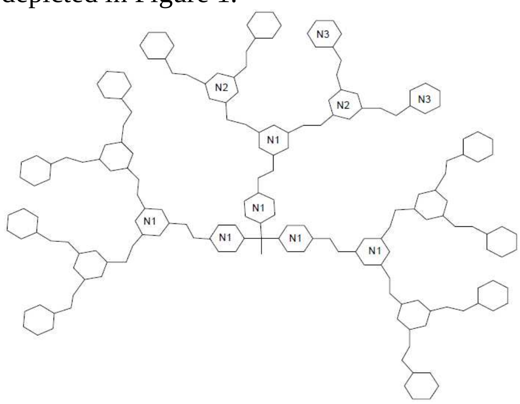

Figure 1: The molecular graph of $NS_1[3]$

Let G be the molecular graph of $NS_1[n]$ dendrimer nanostar. By algebraic method, we obtain that G has $27 \times 2^n - 5$ edges. It is easy to see that the vertices of $NS_1[n]$ are of degree 1, 2, 3 or 4, see Figure 1. Also by algebraic method, we obtain that the edge set $E(NS_1[n])$ can be divided into four partitions based on the degree of end vertices of each edge as follows:

$E_{14} = \{uv \in E(G) \mid d_G(u) = 1, d_G(v) = 4\}$, $|E_{14}| = 1$.

$E_{22} = \{uv \in E(G) \mid d_G(u) = d_G(v) = 2\}$, $|E_{22}| = 9 \times 2^n + 3$.

$E_{23} = \{uv \in E(G) \mid d_G(u) = 2, d_G(v) = 3\}$, $|E_{23}| = 18 \times 2^n - 12$.

$E_{34} = \{uv \in E(G) \mid d_G(u) = 3, d_G(v) = 4\}$, $|E_{34}| = 3$.

In the following theorem, we compute the multiplicative atom bond connectivity index of $NS_1[n]$ dendrimer nanostars.

Theorem 1. The multiplicative atom bond connectivity index of $NS_1[n]$ dendrimer nanostar is

$$ABCII\left(NS_1[n]\right)=\left(\frac{3}{4}\right)^{\frac{1}{2}}\times\left(\frac{5}{12}\right)^{\frac{1}{2}}\times\left(\frac{1}{\sqrt{2}}\right)^{27\times 2^n-9}$$

Proof: By definition, we have

$$ABCII\left(NS_1[n]\right)=\prod_{uv\in E(G)}\sqrt{\frac{d_G(u)+d_G(v)-2}{d_G(u)d_G(v)}}$$

Thus $ABCII\left(NS_1[n]\right)=\left(\sqrt{\frac{1+4-2}{1\times 4}}\right)^{1}\times\left(\sqrt{\frac{2+2-2}{2\times 2}}\right)^{9\times 2^n+3}\times\left(\sqrt{\frac{2+3-2}{2\times 3}}\right)^{18\times 2^n-12}\times\left(\sqrt{\frac{3+4-2}{3\times 4}}\right)^{3}$

$$=\left(\frac{3}{4}\right)^{\frac{1}{2}}\times\left(\frac{5}{12}\right)^{\frac{3}{2}}\times\left(\frac{1}{\sqrt{2}}\right)^{27\times 2^n-9}$$

In the following theorem, we compute the multiplicative geometric arithmetic index of $NS_1[n]$ dendrimer nanostars.

Theorem 2. The multiplicative geometric arithmetic index of $NS_1[n]$ dendrimer nanostar is

$$GAII\left(NS_1[n]\right)=\left(\frac{4}{5}\right)\times\left(\frac{4\sqrt{3}}{7}\right)^{3}\times\left(\frac{2\sqrt{6}}{5}\right)^{18\times 2^n-12}.$$

Proof: By definition, we have

$$GAII(G)=\prod_{uv\in E(G)}\frac{2\sqrt{d_G(u)d_G(v)}}{d_G(u)+d_G(v)}$$

Thus $GAII\left(NS_1[n]\right)=\left(\frac{2\sqrt{1\times 4}}{1+4}\right)^{1}\times\left(\frac{2\sqrt{2\times 2}}{2+2}\right)^{9\times 2^n+3}\times\left(\frac{2\sqrt{2\times 3}}{2+3}\right)^{18\times 2^n-12}\times\left(\frac{2\sqrt{3\times 4}}{3+4}\right)^{3}$

$$=\left(\frac{4}{5}\right)\times\left(\frac{4\sqrt{3}}{7}\right)^{3}\times\left(\frac{2\sqrt{6}}{5}\right)^{18\times 2^n-12}.$$

3. Results for $NS_2[n]$ dendrimer nanostars

In this section, we focus on the molecular graph structure of the second class of dendrimer nanostars. This family of dendrimer nanostars is symbolized by $NS_2[n]$, where n is the steps of growth in this type of dendrimer nanostars. The molecular graph structure of $NS_2[2]$ dendrimer nanostar is presented in Figure 2.

Let G be the molecular graph of $NS_2[n]$ dendrimer nanostar. By algebraic method, we obtain that G has $36 \times 2^n - 5$ edges. It is easy to see that the vertices of $NS_2[n]$ are of degree 2 or 3, see Figure 2. Also by algebraic method, we obtain that G has three types of edges based on the degree of end vertices of each edge as follows:

$$E_{22} = \{uv \in E(G) \mid d_G(u) = d_G(v) = 2\}, \qquad |E_{22}| = 12\times 2^n + 2.$$

$$E_{23} = \{uv \in E(G) \mid d_G(u) = 2, d_G(v) = 3\}, \qquad |E_{23}| = 24\times 2^n - 8.$$

$$E_{33} = \{uv \in E(G) \mid d_G(u) = d_G(v) = 3\}, \qquad |E_{33}| = 1.$$

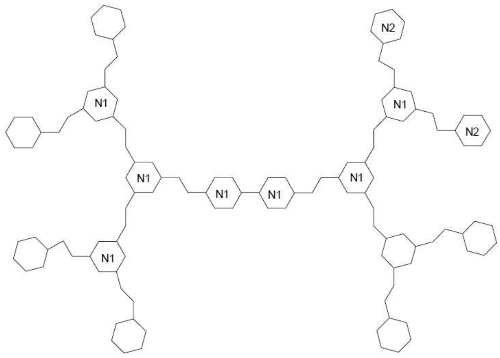

Figure 2: The molecular graph of $NS_2[2]$

In the following theorem, we compute the multiplicative atom bond connectivity index of $NS_2[n]$ dendrimer nanostars.

Theorem 3. The multiplicative atom bond connectivity index of $NS_2[n]$ dendrimer nanostar is

$$ABCII(NS_2[n]) = \left(\frac{2}{3}\right) \times \left(\frac{1}{2}\right)^{18\times 2^n - 3}.$$

Proof: By definition, we have

$$ABCII(G) = \prod_{uv \in E(G)} \sqrt{\frac{d_G(u) + d_G(v) - 2}{d_G(u) d_G(v)}}$$

Thus $$ABCII(NS_2[n]) = \left(\sqrt{\frac{2+2-2}{2\times 2}}\right)^{12\times 2^n + 2} \times \left(\sqrt{\frac{2+3-2}{2\times 3}}\right)^{24\times 2^n - 8} \left(\sqrt{\frac{3+3-2}{3\times 3}}\right)^{1}$$

$$= \left(\frac{2}{3}\right) \times \left(\frac{1}{2}\right)^{18\times 2^n - 3}.$$

In the following theorem, we compute the multiplicative geometric arithmetic index of $NS_2[n]$ dendrimer nanostars.

Theorem 4. The multiplicative geometric arithmetic index of $NS_2[n]$ demdrimer nanostar is

$$GAII\left(NS_2[n]\right)=\left(\frac{2\sqrt{6}}{5}\right)^{24\times 2^n-8}.$$

Proof: By definition, we have

$$GAII(G)=\prod_{uv\in E(G)}\frac{2\sqrt{d_G(u)d_G(v)}}{d_G(u)+d_G(v)}$$

Thus $$GAII\left(NS_2[n]\right)=\left(\frac{2\sqrt{2\times 2}}{2+2}\right)^{12\times 2^n+2}\times\left(\frac{2\sqrt{2\times 3}}{2+3}\right)^{24\times 2^n-8}\times\left(\frac{2\sqrt{3\times 3}}{3+3}\right)^{1}$$

$$=\left(\frac{2\sqrt{6}}{5}\right)^{24\times 2^n-8}.$$

4. Results for $NS_3[n]$ dendrimer nanostars

In this section, we focus on the molecular graph structure of the third class of dendrimer nanostars. This family of dendrimer nanostars is denoted by $NS_3[n]$, where n is the steps of growth in this type of dendrimer nanostars. The molecular graph structure of $NS_3[n]$ dendrimer nanostars is shown in Figure 3.

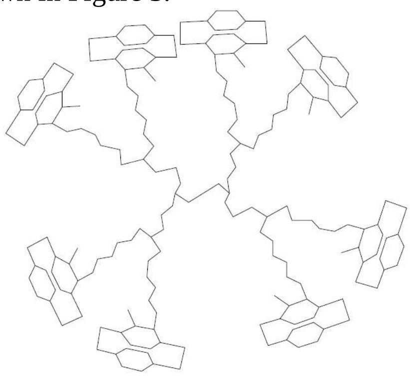

Figure 3: The molecular graph of $NS_3[n]$

Let G be the molecular graph of $NS_3[n]$ dendrimer nanostar. By algebraic method, we obtain that G has $58 \times 2^n - 13$ edges. It is easy to see that the vertices of $NS_3[n]$ are of degree 1, 2 or 3, see Figure 3. Also by algebraic method, we obtain that G has four types of edges based on the degree of the end vertices of each edge as follows:

$E_{13}=\{uv\in E(G)\mid d_G(u)=1, d_G(v)=3\}$, $|E_{13}| = 2^{n+1}$.

$E_{22}=\{uv\in E(G)\mid d_G(u)=d_G(v)=2\}$, $|E_{22}| = 22\times 2^n - 7$.

$E_{23}=\{uv\in E(G)\mid d_G(u)=2, d_G(v)=3\}$, $|E_{23}| = 28\times 2^n - 6$.

$E_{33}=\{uv\in E(G)\mid d_G(u)=d_G(v)=3\}$, $|E_{33}| = 6\times 2^n$.

In the following theorem, we compute the multiplicative atom bond connectivity index of $NS_3[n]$ dendrimer nanostars.

Theorem 5. The multiplicative atom bond connectivity index of $NS_3[n]$ dendrimer nanostar is

$$ABCII\left(NS_3[n]\right)=\left(\frac{2}{3}\right)^{7\times 2^n}\times\left(\frac{1}{\sqrt{2}}\right)^{50\times 2^n-13}.$$

Proof: By definition, we have

$$ABCII(G)=\prod_{uv\in E(G)}\sqrt{\frac{d_G(u)+d_G(v)-2}{d_G(u)d_G(v)}}$$

Thus

$$ABCII\left(NS_3[n]\right)=\left(\sqrt{\frac{1+3-2}{1\times 3}}\right)^{2^{n+1}}\times\left(\sqrt{\frac{2+2-2}{2\times 2}}\right)^{22\times 2^n-7}\times\left(\sqrt{\frac{2+3-2}{2\times 3}}\right)^{28\times 2^n-6}\times\left(\sqrt{\frac{3+3-2}{3\times 3}}\right)^{6\times 2^n}$$

$$=\left(\frac{2}{3}\right)^{7\times 2^n}\times\left(\frac{1}{\sqrt{2}}\right)^{50\times 2^n-13}.$$

In the following theorem, we compute the multiplicative geometric-arithmetic index of $NS_3[n]$ dendrimer nanostars.

Theorem 6. The multiplicative geometric-arithmetic index of $NS_3[n]$ dendrimer nanostar is

$$GAII\left(NS_3[n]\right)=\left(\frac{\sqrt{3}}{2}\right)^{2^{n+1}}\times\left(\frac{2\sqrt{6}}{5}\right)^{28\times 2^n-6}.$$

Proof: By definition, we have $GAII(G)=\prod_{uv\in E(G)}\frac{2\sqrt{d_G(u)d_G(v)}}{d_G(u)+d_G(v)}$

Thus

$$GAII\left(NS_3[n]\right)=\left(\frac{2\sqrt{1\times 3}}{1+3}\right)^{2^{n+1}}\times\left(\frac{2\sqrt{2\times 2}}{2+2}\right)^{22\times 2^n-7}\times\left(\frac{2\sqrt{2\times 3}}{2+3}\right)^{28\times 2^n-6}\times\left(\frac{2\sqrt{3\times 3}}{3+3}\right)^{6\times 2^n}$$

$$=\left(\frac{\sqrt{3}}{2}\right)^{2^{n+1}}\times\left(\frac{2\sqrt{6}}{5}\right)^{28\times 2^n-6}.$$

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