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MULTIPLICATIVE ATOM-BOND CONNECTIVITY AND MULTIPLICATIVE GEOMETRIC-ARITHMETIC INDICES OF CHEMICAL STRUCTURES IN DRUGS

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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, biological characteristics and medical information of drugs. They are also used in the nanoscience engineering applications. In this paper, the first multiplicative atom bond connectivity and multiplicative geometric-arithmetic indices of some important nanostar dendrimers which appeared in nanoscience. These results have a wide application prospect in medical, nanoscience and pharmaceutical engineering.

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

Mathematics Subject Classification: *05C05, 05C12, 05C35.*

1. INTRODUCTION

In the field of nanoscience, many researchers found that there is a close relationship between the biological and chemical characteristics and the molecular graph structure of nanomaterial itself. Therefore it emerges as a new branch of Theoretical Chemistry and it depends on the calculation of topological index to compute the characteristics of nanomaterials. A molecular graph is a simple graph related to the structure of a nanomaterial. Each vertex of a molecular structure of drug can be expressed by a molecular graph represents an atom of the molecule and its edges to the bonds between atoms. Then chemical molecular structure of drug can be expressed by a molecular graph. Concerning the definition of the topological index on the molecular graph, and corresponding medical, chemical properties of drugs can be studied by the topological index calculation. To understand the nature of the drug, this procedure does not depend on the laboratory equipments and reagents, that it saves the cost.

In this paper, we consider only a finite, simple connected graph G with vertex set $V(G)$ and edge set $E(G)$. A single number that can be used to characterize some property of the molecular graph is called a topological index. Several degree based topological indices like Randić index, sum connectivity index, product connectivity Revan index, sum connectivity Revan index and so on. There are some contributions on degree based indices of certain molecular structures and they can be referred to Alikhani *et al.* [1], Ashrafi *et al.* [2], Das *et al.* [3], Estrada *et al.* [5], Gao *et al.* [6,7], Husin *et al*. [11], Kulli [17] and Zhao *et al.* [25].

In [12], Kulli introduced the first multiplicative atom bond connectivity index and multiplicative geometric- arithmetic index of a graph as follows:

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

$$ABC_1II(G)=\prod_{uv\in E(G)}\sqrt{\frac{d_G(u)+d_G(v)-2}{d_G(u)d_G(v)}}. \tag{1}$$

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

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

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Several papers contributed to different kinds of multiplicative connectivity indices of special molecular structures, and they can be referred to Gao *et al.* [8], Gao *et al.* [9], Gao *et al.* [10], Liu *et al.* [24], and Kulli [13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23].

In this paper, the first multiplicative atom bond connectivity and multiplicative geometric-arithmetic indices for certain infinite families of nanostar dendrimers are computed. For more information about nanostar dendrimers see [4].

2. RESULTS FOR $NS_1[n]$ DENDRIMER NANOSTARS

In this section, we focus on the first class of nanostar dendrimer, denoted by $NS_1[n]$, where n is the steps of growth in this type of dendrimer. The graph of $NS_1[n]$ nanostar dendrimer is presented in Figure 1.

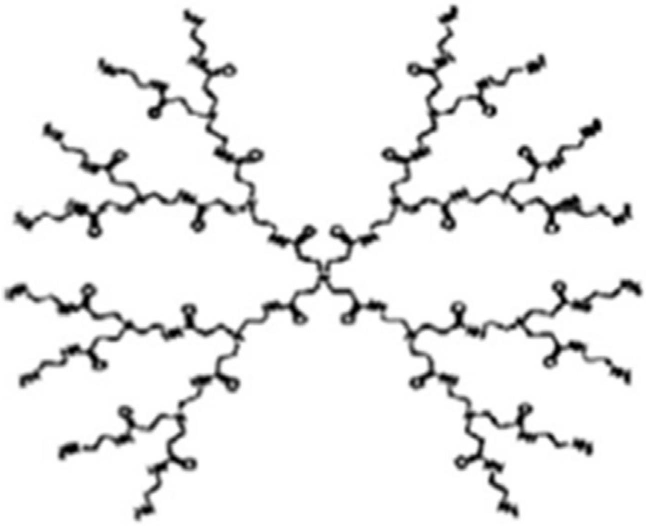

Figure-1: The molecular graph of $NS_1[n]$

Let G be the molecular graph of $NS_1[n]$ polypropylenimine octaamine dendrimer. By calculation, we obtain that G has $32 \times 2^n - 29$ edges. Also by calculation, we obtain that G has four types of edges based on the degree of end vertices of each edge as given in Table 1.

$d_G(u),\ d_G(v) \setminus uv \in E(G)$	(1, 2)	(1, 3)	(2,2)	(2,3)
Number of edges	2×2^n	$4 \times 2^n - 4$	$12 \times 2^n - 11$	$14 \times 2^n - 14$

Table-1: Edge partition of $NS_1[n]$

In the following theorems, we compute the first multiplicative *ABC* index and multiplicative *GA* index of $NS_1[n]$.

Theorem 1: The first multiplicative atom bond connectivity index of polypropylenimine octaamine dendrimer $NS_1[n]$ is

$$ABC_1II\left(NS_1[n]\right) = \left(\frac{1}{\sqrt{2}}\right)^{28\times 2^n - 25} \times \left(\frac{2}{3}\right)^{2\times 2^n - 2}.$$

Proof: From equation (1) and using Table 1, we deduce

$$ABC_1II\left(NS_1[n]\right) = \prod_{uv\in E(G)} \sqrt{\frac{d_G(u)+d_G(v)-2}{d_G(u)d_G(v)}}$$

$$= \left(\sqrt{\frac{1+2-2}{1\times 2}}\right)^{2\times 2^n} \times \left(\sqrt{\frac{1+3-2}{1\times 3}}\right)^{4\times 2^n - 4} \times \left(\sqrt{\frac{2+2-2}{2\times 2}}\right)^{12\times 2^n - 11} \times \left(\sqrt{\frac{2+3-2}{2\times 3}}\right)^{14\times 2^n - 14}$$

$$= \left(\frac{1}{\sqrt{2}}\right)^{28\times 2^n - 25} \times \left(\frac{2}{3}\right)^{2\times 2^n - 2}.$$

Theorem 2: The multiplicative geometric-arithmetic index of polypropylenimine octaamine $NS_1[n]$ dendrimer nanostar is

$$GAII\left(NS_1[n]\right) = \left(\frac{2\sqrt{2}}{3}\right)^{2\times 2^n} \times \left(\frac{\sqrt{3}}{2}\right)^{4\times 2^n - 4} \times \left(\frac{2\sqrt{6}}{5}\right)^{14\times 2^n - 14}.$$

Proof: From equation (2) and using Table (1), we deduce

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

$$= \left(\frac{2\sqrt{1\times 2}}{1+2}\right)^{2\times 2^n} \times \left(\frac{2\sqrt{1\times 3}}{1+3}\right)^{4\times 2^n-4} \times \left(\frac{2\sqrt{2\times 2}}{2+2}\right)^{12\times 2^n-11} \times \left(\frac{2\sqrt{2\times 3}}{2+3}\right)^{14\times 2^n-14}$$

$$= \left(\frac{2\sqrt{2}}{3}\right)^{2\times 2^n} \times \left(\frac{\sqrt{3}}{2}\right)^{4\times 2^n-4} \times \left(\frac{2\sqrt{6}}{5}\right)^{14\times 2^n-14}.$$

3. RESULTS FOR $NS_2[n]$ NANOSTAR DENDRIMERS

In this section, we focus on the second class of nanostar dendrimer, denoted by $NS_2[n]$, where n is the steps of growth in this type of dendrimer. The graph of $NS_2[n]$ nanostar dendrimer is shown in Figure 2.

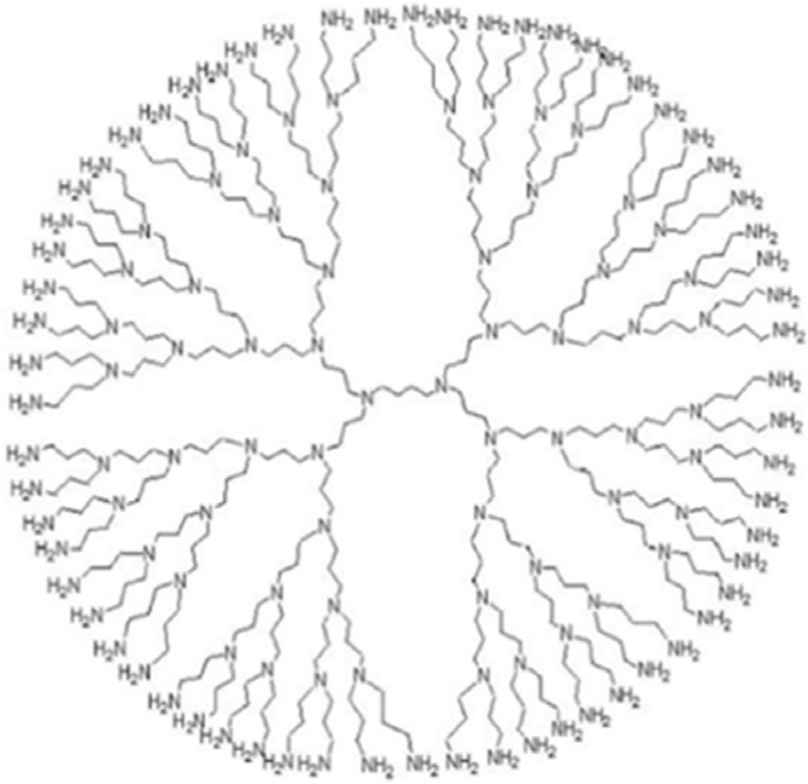

Figure-2: The structure of $NS_2[n]$

Let G be the molecular graph of $NS_2[n]$ polypropylenimine octaamine dendrimer. By calculation, we obtain that G has $16 \times 2^n - 11$ edges. Also by calculation, we obtain that G has three types of edges based on the degree of end vertices of each edge as given Table 2.

$d_G(u),\ d_G(v) \setminus uv \in E(G)$	(1, 2)	(2,2)	(2,3)
Number of edges	2×2^n	$8 \times 2^n - 5$	$6 \times 2^n - 6$

Table-2: Edge partition of $NS_2[n]$

In the following theorems, we derive the first multiplicative ABC index and multiplicative GA index of $NS_2[n]$.

Theorem 3: The first multiplicative atom bond connectivity index of polypropyleninine octaamine dendrimer $NS_2[n]$ is

$$ABC_1II\left(NS_2[n]\right) = \left(\sqrt{\frac{1}{2}}\right)^{16\times 2^n-11}.$$

Proof: Using equation (1) and Table 2, we derive

$$ABC_1II\left(NS_2[n]\right)=\prod_{uv\in E(G)}\sqrt{\frac{d_G(u)+d_G(v)-2}{d_G(u)d_G(v)}}$$

$$=\left(\sqrt{\frac{1+2-2}{1\times 2}}\right)^{2\times 2^n}\times\left(\sqrt{\frac{2+2-2}{2\times 2}}\right)^{8\times 2^n-5}\left(\sqrt{\frac{2+3-2}{2\times 3}}\right)^{6\times 2^n-6}=\left(\sqrt{\frac{1}{2}}\right)^{16\times 2^n-11}.$$

Theorem 4: The multiplicative geometric-arithmetic index of polypropyleninine octaamine dendrimer $NS_2[n]$ is

$$GAII\left(NS_2[n]\right)=\left(\frac{2\sqrt{2}}{3}\right)^{2\times 2^n}\times\left(\frac{2\sqrt{6}}{5}\right)^{6\times 2^n-6}.$$

Proof: Using equation (2) and Table 2, we have

$$GII(NS_2[n])=\prod_{uv\in E(G)}\frac{2\sqrt{d_G(u)d_G(v)}}{d_G(u)+d_G(v)}$$

$$=\left(\frac{2\sqrt{1\times 2}}{1+2}\right)^{2\times 2^n}\times\left(\frac{2\sqrt{2\times 2}}{2+2}\right)^{8\times 2^n-5}\times\left(\frac{2\sqrt{2\times 3}}{2+3}\right)^{6\times 2^n-6}$$

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

4. RESULTS FOR $NS_3[n]$ POLYMER DENDRIMERS

In this section, we focus on the class of nanostar dendrimer, denoted by $NS_3[n]$, where n is the steps of growth in this type of dendrimer. The graph of $NS_3[n]$ polymer dendrimer is presented in Figure 3.

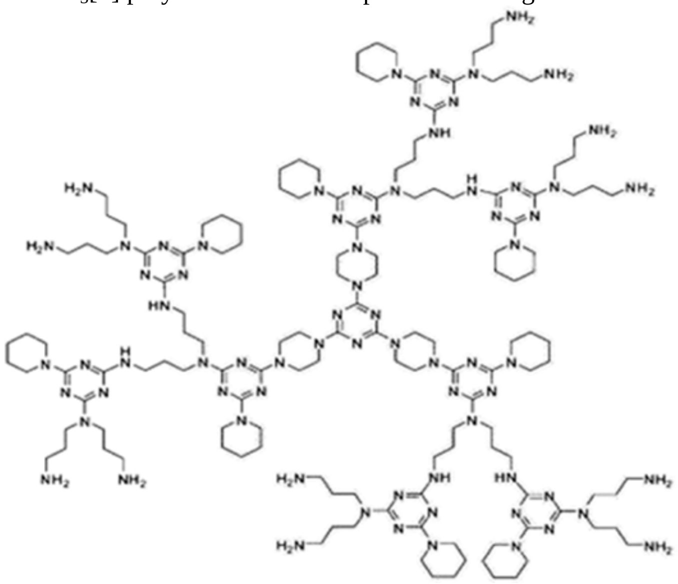

Figure-3: The structure of polymer dendrimer $NS_3[n]$

Let G be the molecular graph of $NS_3[n]$ polymer dendrimer. By calculation, we obtain that $|E(NS_3[n])| = 69\times 2^n + 90$. Also by calculation, we obtain that G has four types of edges based on the degree of the end vertices of each edge as given in Table 3.

$d_G(u),\ d_G(v)\setminus uv\in E(G)$	(1, 2)	(2, 2)	(2,3)	(3,3)
Number of edges	3×2^n	$27\times 2^n-24$	$33\times 2^n+114$	6×2^n

Table-3: Edge partition of $NS_3[n]$

We now compute the first multiplicative *ABC* index and multiplicative *GA* index of $NS_3[n]$.

Theorem 5: The first multiplicative atom bond connectivity index of polymer dendrimer $NS_3[n]$ is

$$ABCII\left(NS_3[n]\right)=\left(\frac{1}{\sqrt{2}}\right)^{63\times 2^n+90}\times\left(\frac{2}{3}\right)^{6\times 2^n}.$$

Proof: From equation (1) and using Table 3, we obtain

$$ABC_1II\left(NS_3[n]\right)=\prod_{uv\in E(G)}\sqrt{\frac{d_G(u)+d_G(v)-2}{d_G(u)d_G(v)}}$$

$$=\left(\sqrt{\frac{1+2-2}{1\times 2}}\right)^{3\times 2^n}\times\left(\sqrt{\frac{2+2-2}{2\times 2}}\right)^{27\times 2^n-24}\times\left(\sqrt{\frac{2+3-2}{2\times 3}}\right)^{33\times 2^n+114}\times\left(\sqrt{\frac{3+3-2}{3\times 3}}\right)^{6\times 2^n}$$

$$=\left(\frac{1}{\sqrt{2}}\right)^{63\times 2^n+90}\times\left(\frac{2}{3}\right)^{6\times 2^n}.$$

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

$$GAII\left(NS_3[n]\right)=\left(\frac{2\sqrt{2}}{3}\right)^{3\times 2^n}\times\left(\frac{2\sqrt{6}}{5}\right)^{33\times 2^n+114}.$$

Proof: From equation (2) and using Table 3, we have

$$GII(NS_3[n])=\prod_{uv\in E(G)}\frac{2\sqrt{d_G(u)d_G(v)}}{d_G(u)+d_G(v)}$$

$$=\left(\frac{2\sqrt{1\times 2}}{1+2}\right)^{3\times 2^n}\times\left(\frac{2\sqrt{2\times 2}}{2+2}\right)^{27\times 2^n-24}\times\left(\frac{2\sqrt{2\times 3}}{2+3}\right)^{33\times 2^n+114}\times\left(\frac{2\sqrt{3\times 3}}{3+3}\right)^{6\times 2^n}$$

$$=\left(\frac{2\sqrt{2}}{3}\right)^{3\times 2^n}\times\left(\frac{2\sqrt{6}}{5}\right)^{33\times 2^n+114}.$$

5. RESULTS FOR $NS_4[n]$ FULLERENE DENDRIMERS

In this section, we consider the class of fullerene dendrimer, denoted by $NS_4[n]$, where n is the steps of growth in this type of dendrimer. The molecular graph of $NS_4[n]$ fullerene dendrimer is presented in Figure 4.

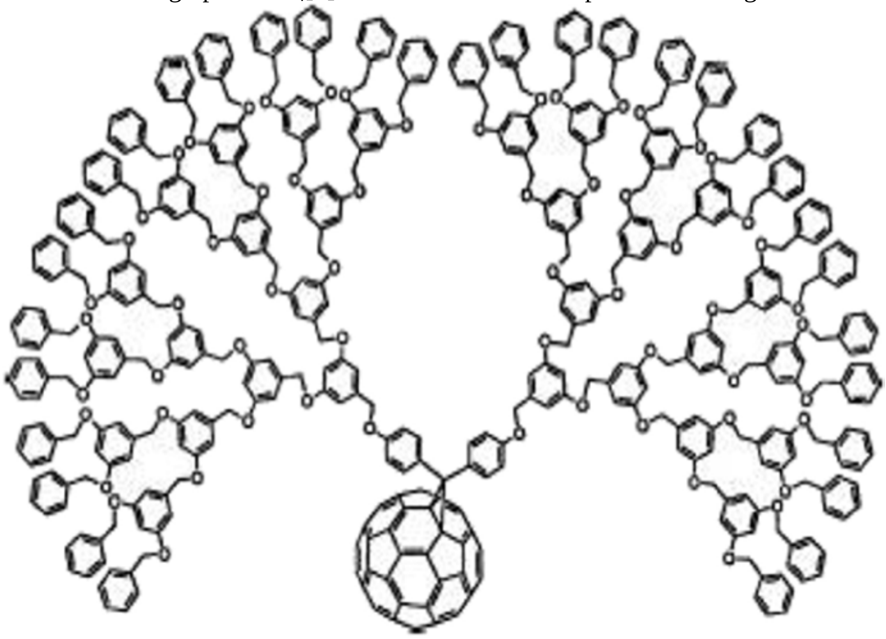

Figure-4: The structure of fullerene dendrimer $NS_4[n]$

Let G be the graph of $NS_4[n]$ fullerene dendrimer. By calculation, we obtain that G has $20 \times 2^n + 89$ edges. Also by calculation, we obtain that G has six types of edges based on the degree of the end vertices of each edge as given in Table 4.

$d_G(u),\ d_G(v) \setminus uv \in E(G)$	(1, 2)	(2, 2)	(2,3)	(3,3)	(3,4)	(4,4)
Number of edges	2×2^n	$2 \times 2^n + 2$	$16 \times 2^n - 8$	86	6	3

Table-4: Edge partition of $NS_4[n]$

We now compute the first multiplicative *ABC* index and multiplicative *GA* index of $NS_4[n]$.

Theorem 7: The first multiplicative atom bond connectivity index of fullerene dendrimer $NS_4[n]$ is

$$ABC_1II\left(NS_4[n]\right)=\left(\frac{1}{2}\right)^{10\times 2^n-3}\times\left(\frac{2}{3}\right)^{86}\times\left(\frac{5}{12}\right)^{3}\times\left(\frac{\sqrt{6}}{4}\right)^{3}.$$

Proof: From equation (1) and using Table 4, we derive

$$ABC_1II\left(NS_4[n]\right)=\prod_{uv\in E(G)}\sqrt{\frac{d_G(u)+d_G(v)-2}{d_G(u)d_G(v)}}$$

$$=\left(\sqrt{\frac{1+2-2}{1\times 2}}\right)^{2\times 2^n}\times\left(\sqrt{\frac{2+2-2}{2\times 2}}\right)^{2\times 2^n+2}\times\left(\sqrt{\frac{2+3-2}{2\times 3}}\right)^{16\times 2^n-8}\times\left(\sqrt{\frac{3+3-2}{3\times 3}}\right)^{86}\times\left(\sqrt{\frac{3+4-2}{3\times 4}}\right)^{6}\times\left(\sqrt{\frac{4+4-2}{4\times 4}}\right)^{3}$$

$$=\left(\frac{1}{2}\right)^{10\times 2^n-3}\times\left(\frac{2}{3}\right)^{6\times 2^n}\times\left(\frac{5}{12}\right)^{3}\times\left(\frac{\sqrt{6}}{4}\right)^{3}.$$

Theorem 8: The multiplicative geometric-arithmetic index of fullerene dendrimer $NS_4[n]$ is

$$GAII\left(NS_4[n]\right)=\left(\frac{2\sqrt{2}}{3}\right)^{2\times 2^n}\times\left(\frac{2\sqrt{6}}{5}\right)^{16\times 2^n-8}\times\left(\frac{4\sqrt{3}}{7}\right)^{6}.$$

Proof: From equation (2) and using Table 4, we derive

$$GAII\left(NS_4[n]\right)=\prod_{uv\in E(G)}\frac{2\sqrt{d_G(u)d_G(v)}}{d_G(u)+d_G(v)}$$

$$=\left(\frac{2\sqrt{1\times 2}}{1+2}\right)^{2\times 2^n}\times\left(\frac{2\sqrt{2\times 2}}{2+2}\right)^{2\times 2^n+2}\times\left(\frac{2\sqrt{2\times 3}}{2+3}\right)^{16\times 2^n-8}\times\left(\frac{2\sqrt{3\times 3}}{3+3}\right)^{86}\times\left(\frac{2\sqrt{3\times 4}}{3+4}\right)^{6}\times\left(\frac{2\sqrt{4\times 4}}{4+4}\right)^{3}$$

$$=\left(\frac{2\sqrt{2}}{3}\right)^{3\times 2^n}\times\left(\frac{2\sqrt{6}}{5}\right)^{16\times 2^n-8}\times\left(\frac{4\sqrt{3}}{7}\right)^{6}.$$

6. RESULTS FOR POLYMER DENDRIMERS $NS_5[n]$

In this section, we consider the class of polymer dendrimer $NS_5[n]$, where n is the steps of growth. The molecular graph of $NS_5[n]$ polymer dendrimer is shown in Figure 5.

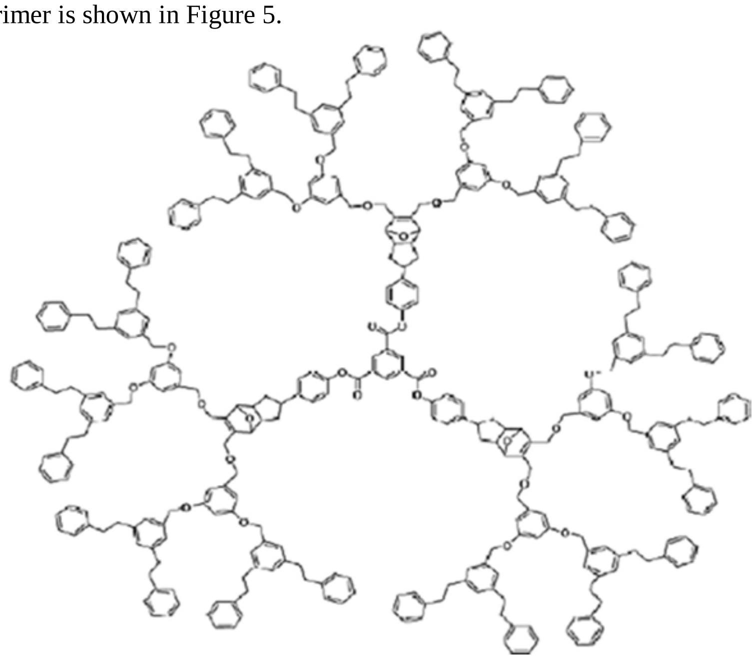

Figure-5: The structure of polymer dendrimer $NS_5[n]$

Let G be the graph of $NS_5[n]$ polymer dendrimer. By calculation, we obtain that $NS_5[n]$ has $60 \times 2^n + 27$ edges. Also by calculation, we obtain that $E(NS_5[n])$ can be divided into four partitions as given in Table 5.

$d_G(u),\ d_G(v) \setminus uv \in E(G)$	(1, 3)	(2, 2)	(2,3)	(3,3)
Number of edges	$6 \times 2^n + 3$	$6 \times 2^n + 6$	$48 \times 2^n - 6$	24

Table-5: Edge partition of $NS_5[n]$

We now compute the first multiplicative *ABC* index and multiplicative *GA* index of $NS_5[n]$.

Theorem 9: The first multiplicative atom bond connectivity index of polymer dendrimer $NS_5[n]$ is

$$ABC_1II(NS_5[n]) = \left(\sqrt{\frac{2}{3}}\right)^{6\times 2^n+51} \times \left(\frac{1}{2}\right)^{27\times 2^n}.$$

Proof: From equation (1) and using Table 5, we deduce

$$ABC_1II(NS_5[n]) = \prod_{uv\in E(G)} \sqrt{\frac{d_G(u)+d_G(v)-2}{d_G(u)d_G(v)}}$$

$$= \left(\sqrt{\frac{1+3-2}{1\times 3}}\right)^{6\times 2^n+3} \times \left(\sqrt{\frac{2+2-2}{2\times 2}}\right)^{6\times 2^n+6} \times \left(\sqrt{\frac{2+3-2}{2\times 3}}\right)^{48\times 2^n-6} \times \left(\sqrt{\frac{3+3-2}{3\times 3}}\right)^{24}$$

$$= \left(\sqrt{\frac{2}{3}}\right)^{6\times 2^n+51} \times \left(\frac{1}{2}\right)^{27\times 2^n}.$$

Theorem 10: The multiplicative geometric-arithmetic index of polymer dendrimer $NS_5[n]$ is

$$GAII(NS_5[n]) = \left(\frac{\sqrt{3}}{2}\right)^{6\times 2^n+3} \times \left(\frac{2\sqrt{6}}{5}\right)^{48\times 2^n-6}.$$

Proof: Using equation (2) and using Table 5, we deduce

$$GAII(NS_5[n]) = \prod_{uv\in E(G)} \frac{2\sqrt{d_G(u)d_G(v)}}{d_G(u)+d_G(v)}$$

$$= \left(\frac{2\sqrt{1\times 3}}{1+3}\right)^{6\times 2^n+3} \times \left(\frac{2\sqrt{2\times 2}}{2+2}\right)^{6\times 2^n+6} \times \left(\frac{2\sqrt{2\times 3}}{2+3}\right)^{48\times 2^n-6} \times \left(\frac{2\sqrt{3\times 3}}{3+3}\right)^{24}$$

$$= \left(\frac{\sqrt{3}}{2}\right)^{6\times 2^n+3} \times \left(\frac{2\sqrt{6}}{5}\right)^{48\times 2^n-6}.$$

7. RESULTS FOR NANOSTAR DENDRIMERS D_n

We now focus on the class of nanostar dendrimer, denoted by D_n, where n is the steps of growth. The graph of D_n nanostar dendrimer is depicted in Figure 6.

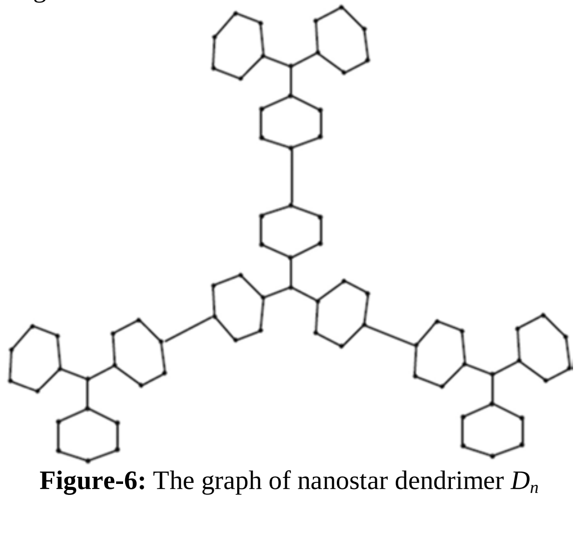

Figure-6: The graph of nanostar dendrimer D_n

Let G be the graph of D_n nanostar dendrimer. The graph G has $33 \times 2^n - 45$ edges. By calculation, we obtain that the edge set $E(D_n)$ can be divided into three partitions as given Table 6.

$d_G(u),\ d_G(v) \setminus uv \in E(G)$	(2, 2)	(2,3)	(3,3)
Number of edges	$12\times2^n - 12$	$15 \times 2^n - 24$	$6 \times 2^n - 9$

Table-6: Edge partition of D_n

In the following theorems, we determine the first multiplicative *ABC* index and multiplicative *GA* index of D_n.

Theorem 11: The first multiplicative atom bond connectivity index of nanostar dendrimer D_n is

$$ABC_1II(D_n) = \left(\sqrt{\frac{1}{2}}\right)^{27\times2^n-36} \times \left(\frac{2}{3}\right)^{6\times2^n-9}.$$

Proof: Using equation (1) and using Table 6, we obtain

$$ABC_1II(D_n) = \prod_{uv\in E(G)} \sqrt{\frac{d_G(u)+d_G(v)-2}{d_G(u)d_G(v)}}$$

$$= \left(\sqrt{\frac{2+2-2}{2\times2}}\right)^{12\times2^n-12} \times \left(\sqrt{\frac{2+3-2}{2\times3}}\right)^{15\times2^n-24} \left(\sqrt{\frac{3+3-2}{3\times3}}\right)^{6\times2^n-9}$$

$$= \left(\sqrt{\frac{1}{2}}\right)^{27\times2^n-36} \times \left(\frac{2}{3}\right)^{6\times2^n-9}.$$

Theorem 12: The multiplicative geometric-arithmetic index of nanostar dendrimer D_n is

$$GAII(D_n) = \left(\frac{2\sqrt{6}}{5}\right)^{15\times2^n-24}.$$

Proof: Using equation (2) and Table 6, we obtain

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

$$= \left(\frac{2\sqrt{2\times2}}{2+2}\right)^{12\times2^n-12} \times \left(\frac{2\sqrt{2\times3}}{2+3}\right)^{15\times2^n-24} \times \left(\frac{2\sqrt{3\times3}}{3+3}\right)^{6\times2^n-9}$$

$$= \left(\frac{2\sqrt{6}}{5}\right)^{15\times2^n-24}.$$

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