# *The First Geometric–Arithmetic Index of Some Nanostar Dendrimers*

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**ABSTRACT.** Dendrimers are highly branched organic macromolecules with successive layers or generations of branch units surrounding a central core [1, 4]. These are key molecules in nanotechnology and can be put to good use. In this article, we compute the first geometric-arithmetic index of two infinite classes of dendrimers.

**Keywords:** nanostar dendrimer, the first geometric-arithmetic index.



## 1. INTRODUCTION

Investigations of topological indices based on end–vertex degrees of edges have been conducted over 35 years. One of them is the first geometric–arithmetic index $(GA_1)$. The $(GA_1)$ index defined as:

$$GA_1(G) = \sum_{uv \in E(G)} \frac{\sqrt{d_u d_v}}{\frac{1}{2}(d_u + d_v)}$$

has been introduced less that a year ago [2, 3, 5]. Here $d_u$ denotes degree of vertex $u$ and so on.

Dendrimer is a synthetic 3-dimentional macromolecule that is prepared in a step-wise fashion from simple branched monomer units. The nanostar dendrimer is a part of a new group of macromolecules that appear to photon funnels just like artificial antennas. In this article many attempt have been made to compute the first geometric-arithmetic index for two types of nanostar dendrimers.

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*Received: March 25, 2013; Accepted: May 1, 2014.*

## 2. RESULTS AND DISCUSSION

**Lemma 1.** Consider the complete graph $K_n$ of order *n*. The first geometric-arithmetic index of this graph is computed as follow:

$$GA_1(K_n) = \frac{1}{2}n(n-1).$$

**Proof**. The degree of all the vertices of a complete graph of order *n* is *n-1* and the number of edges for $K_n$ is equal $\frac{1}{2}n(n-1)$, Thus

$$GA_1(K_n) = \sum_{uv\in E(K_n)} \frac{\sqrt{d_u d_v}}{\frac{1}{2}(d_u+d_v)} = \frac{1}{2}n(n-1)\frac{\sqrt{(n-1)^2}}{\frac{1}{2}2(n-1)} = \frac{1}{2}n(n-1).$$

**Lemma 2.** If *G* is a regular graph of degree *r>0,* then

$$GA_1(G) = \frac{nr}{2}.$$

**Proof**. A regular graph *G* on *n* vertices, having degree *r*, possesses $\frac{nr}{2}$ edges, thus

$$GA_1(G) = \sum_{uv\in E(G)} \frac{\sqrt{d_u d_v}}{\frac{1}{2}(d_u+d_v)} = \frac{nr}{2}\frac{\sqrt{r^2}}{\frac{1}{2}2(r+r)} = \frac{nr}{2}.$$

**Lemma 3.** Let $S_n$ be a star on *n+1* vertices (Figure 1), then

$$GA_1(S_n) = \frac{2n\sqrt{n}}{n+1}.$$

**Proof**. It is easily seen that there are *n* vertices of degree 1 and a vertex of degree *n*. Therefore,

$$GA_1(S_n) = \sum_{uv\in E(K_n)} \frac{\sqrt{d_u d_v}}{\frac{1}{2}(d_u+d_v)} = \frac{2n\sqrt{n}}{n+1}.$$

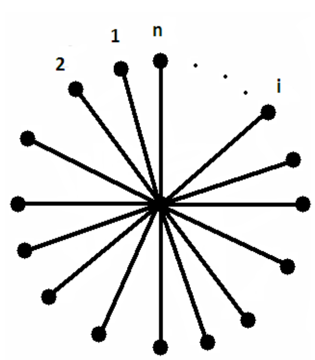


**Figure 1.** Star graph with *n*+1 vertices.

### *2.1 The First Geometric-arithmetic Index of the First Class of Nanostar Dendrimers*

Consider a graph G on n vertices, where $n \geq 2$. The maximum possible vertex degree in such a graph is *n–1*. Suppose $d_{ij}$ denote the number of edges of *G* connecting vertices of degrees *i* and *j*. Clearly, $d_{ij} = d_{ji}$. We now consider two infinite classes $NS_1[n]$ and $NS_2[n]$ of nanostar dendrimers, Figures 2 and 3. The aim is to compute the first geometric-arithmetic index for two of these nanostar dendrimers.

We consider the molecular graph of $K(n) = NS_1[n]$ with four similar branches and three extra edges, where *n* is steps of growth in this type of dendrimer nanostars (Figure 2). Define $d_{23}$ to be the number of edges connecting a vertex of degree *2* with a vertex of degree *3*, $d_{13}$ to be the number of edges connecting a vertex of degree *1* with a vertex of degree *3*, $d_{22}$ to be the number of edges connecting two vertices of degree *2* and $d_{12}$ to be the number of edges connecting a vertex of degree *1* with a vertex of degree *2*. Also $d_{ij}^{'}$ denote the number of edges connecting vertices of degrees i and j in each branch ($i, j \leq 4$). It is obvious that $d_{12} = 4d_{22}^{'} + 1$, $d_{22} = 4d_{22}^{'} + 1$, $d_{13} = 4$, $d_{13}^{'}$ and $d_{23} = 4d_{23}^{'} + 2$. On the other hand a simple calculation shows that $d_{12}^{'} = 2^{n-1}$. Therefore, $d_{12} = 4d_{12}^{'} = 2.2^n$. Using a similar argument, one can see that $d_{22}^{'} = 3(n-1)$ then $d_{22} = 12.2^n - 11$, $d_{13}^{'} = 2^n - 1$ then $d_{13} = 4, d_{13}^{'} = 4.2^n - 4$ and finally $d_{23}^{'} = 3(2^n - 1) + (2^{n-1} - 1)$ then $d_{23} = 4d_{23}^{'} + 2 = 14.2^n - 14$.

**Theorem 4**. The first geometric-arithmetic index of $K(n) = NS_1[n]$ is

$$GA_1(K(n)) = (\frac{4\sqrt{2}}{3} + 12 + 2\sqrt{3} + \frac{28\sqrt{6}}{5})2^n - (11 + 2\sqrt{3} + \frac{28\sqrt{6}}{5}).$$

**Proof.** We have $GA_1(K(n)) = \sum_{uv \in E(K(n))} \frac{\sqrt{d_u d_v}}{\frac{1}{2}(d_u + d_v)}$. Then

$$GA_1(K(n)) = (2.2^n)\frac{2\sqrt{2}}{3} + (12.2^n - 11) + (4.2^n - 4)\frac{\sqrt{3}}{2} + (14.2^n - 4)\frac{2\sqrt{6}}{5}$$
$$= GA_1(K(n)) = (\frac{4\sqrt{2}}{3} + 12 + 2\sqrt{3} + \frac{28\sqrt{6}}{5})2^n - (11 + 2\sqrt{3} + \frac{28\sqrt{6}}{5}).$$

### *2.2 The First Geometric-arithmetic Index of the Second Class of Nanostar Dendrimers*

We consider the second class $H(n) = NS_2[n]$, where *n* is steps of growth. Since the molecular graph of *H* has four similar branches and five extra edges **(**Figure 3), $d_{12} = 4d_{12}^{'}$,

$d_{22} = 4d'_{22} + 3$ and $d_{23} = 4d'_{23} + 2$. By a routine calculation we have $d'_{12} = 2^{n-1}$, $d'_{22} = 2(2^n - 1)$ and $d'_{23} = 3.2^{n-1} - 2$. One can prove that $d_{12} = 2^{n+1}$, $d_{22} + 8.2^n - 5$ and $d_{23} = 6.2^n - 6$.

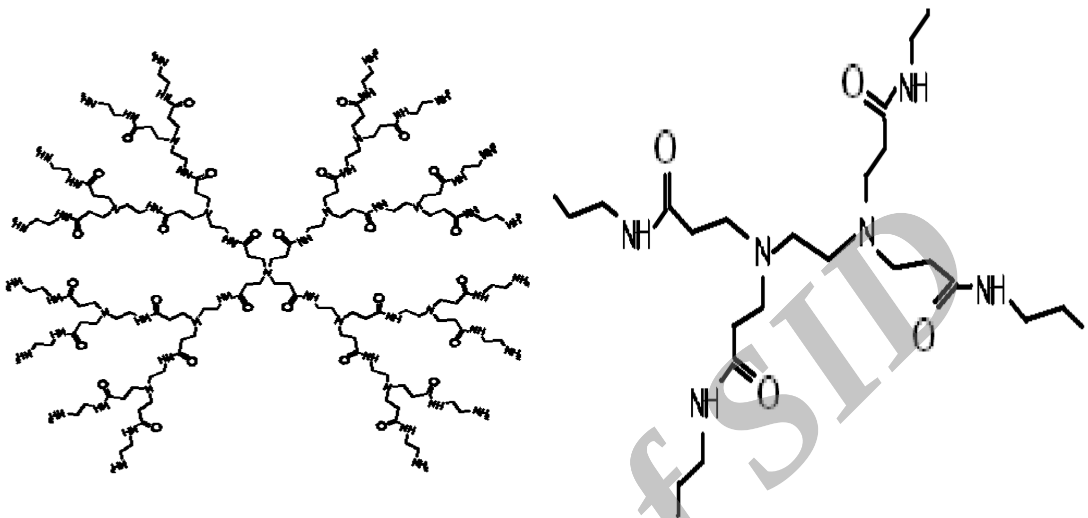

**Figure 2**. $NS_1[1]$ and $NS_1[n]$ PAMAM Dendrimer.

**Theorem 5.** The first geometric-arithmetic index of $H(n) = NS_2[n]$ is computed as follows:

$$GA_1(H(n)) = (\frac{4\sqrt{2}}{3} + 8 + \frac{12\sqrt{6}}{5})2^n - (5 + \frac{12\sqrt{6}}{5})$$

**Proof.** By definition, we have:

$$\begin{aligned} GA_1(H(n)) &= \sum_{uv\in E(H(n))} \frac{\sqrt{d_u d_v}}{\frac{1}{2}(d_u + d_v)} \\ &= 2^{n+1}\frac{2\sqrt{2}}{3} + (8.2^n - 5) + (6.2^n - 6)\frac{2\sqrt{6}}{5} \\ &= (\frac{4\sqrt{2}}{3} + 8 + \frac{12\sqrt{6}}{5})2^n - (5 + \frac{12\sqrt{6}}{5}). \end{aligned}$$

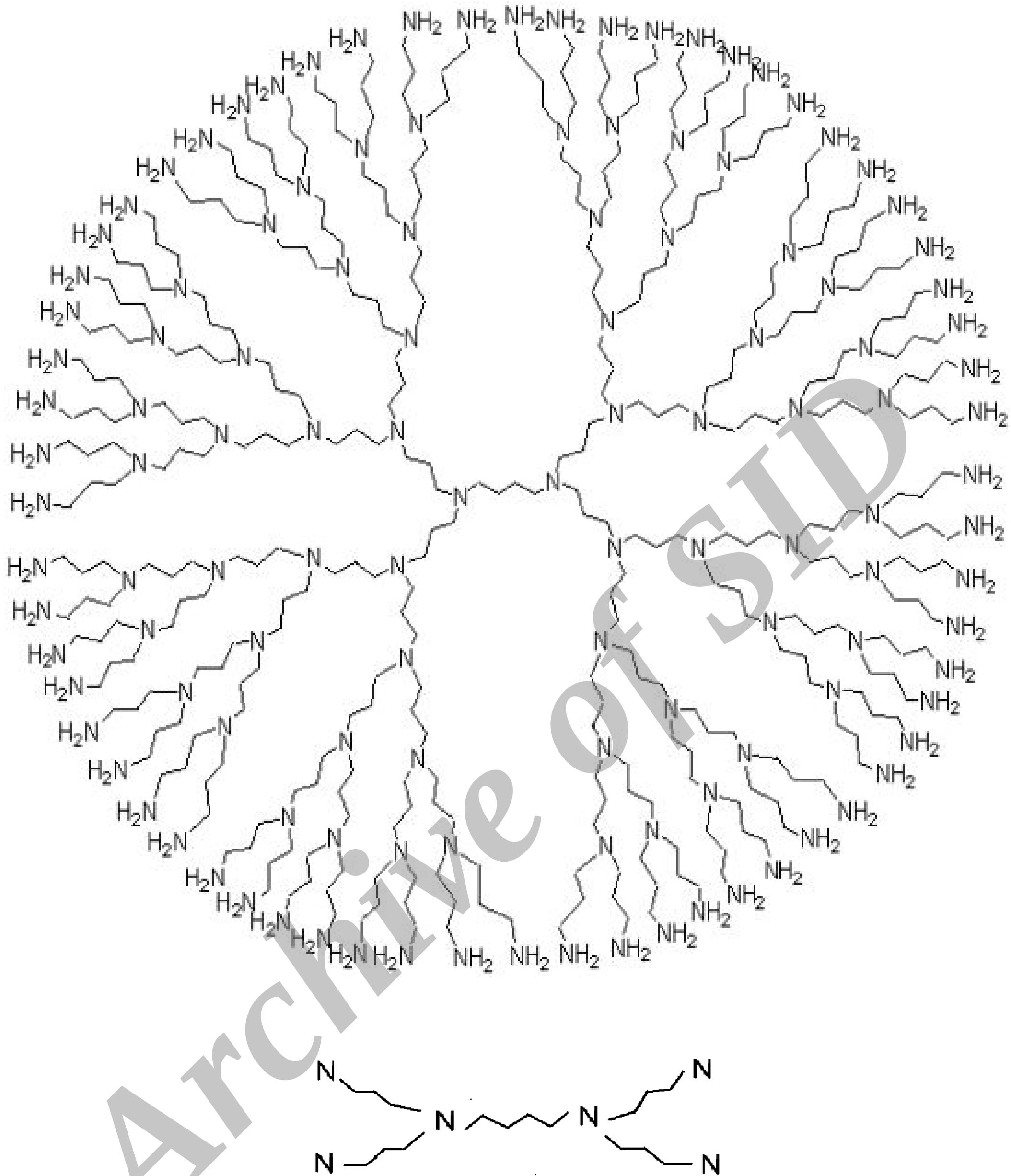



**Figure 3.** $NS_2[1]$ and $NS_2[n]$ Polypropylenimin octaamin Dendrimer.

In Table 1, this topological index are calculated for two classes of dendrimers.

**Table 1.** $GA_1$ Index for some Dendrimer Graphs.

| *n* | $GA_1$ **Index of** $NS_1[n]$ | $GA_1$ **Index of** $NS_2[n]$ |
|---|---|---|
| **1** | 33.9525 | 20.6500 |
| **2** | 96.0862 | 52.1788 |
| **3** | 220.3537 | 115.2364 |
| **4** | 468.8886 | 241.3515 |
| **5** | 965.9583 | 493.5818 |
| **6** | 1960.1000 | 998.0424 |
| **7** | 3948.4000 | 2007.0000 |
| **8** | 7924.9000 | 4024.8000 |
| **9** | 15878.0000 | 8060.5000 |
| **10** | 31784.0000 | 16132.0000 |



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