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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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,

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

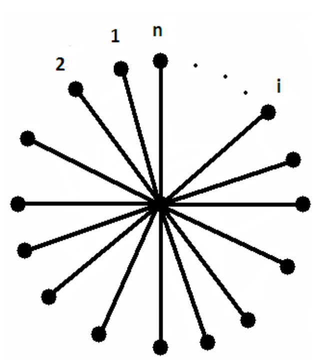

Figure 1. Star graph with *n*+1 vertices.

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 $d_{23}=6.2^n-6$.

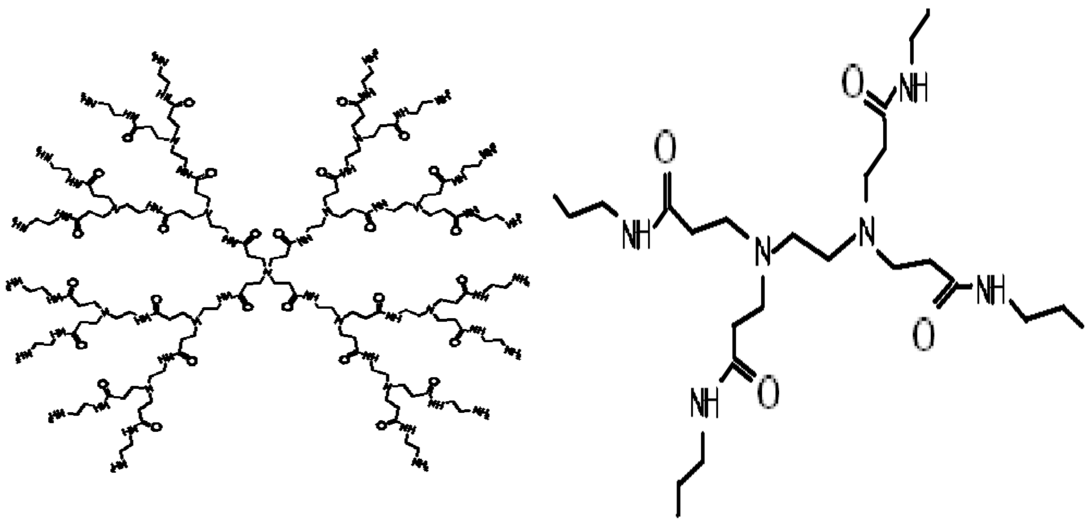

Figure 2. $NS_1[1]$ and $NS_1[n]$ PAMAM Dendrimer.

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:

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

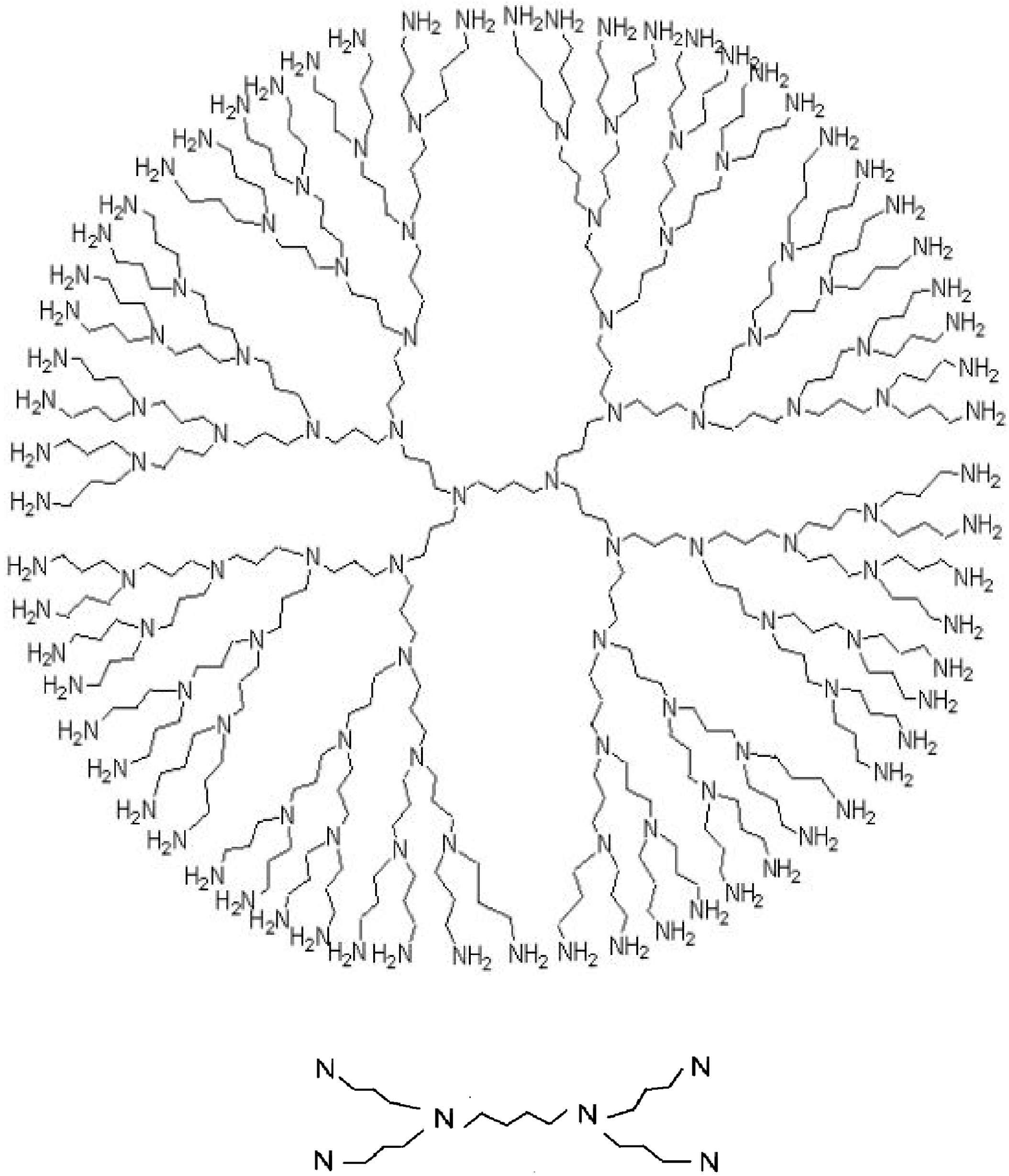

Figure 3. $NS_2[1]$ and $NS_2[n]$ Polypropylenimin octaamin Dendrimer.

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

REFERENCES

1. A. R. Ashrafi and P. Nikzad, Connectivity index of the family of dendrimer nanostar, *Digest Journal of Nanomaterials and Biostructures* **4** (2009) 269–273.
2. G. Fath–Tabar, B. Furtula and I. Gutman, A new geometric–arithmetic index, *J. Math. Chem.* **47** (2010) 477–486.
3. D. Vukičević and B. Furtula, Topological index based on the ratios of geometrical and arithmetical means of end–vertex degree of edges, *J. Math. Chem.* **46** (2009) 1368–1376.
4. K. Yamamoto, M. Higuchi, S. Shiki, M. Tsuruta and H. Chiba, Stepwise radial complexation of imine groups in phenylazomethine dendrimers, *Nature* **415** (2002) 509-511.
5. M. Ghorbani and M. Jalali, Computing a new topological index of nano structures, *Digest Journal of Nanomaterials and Biostructures* **4** (2009) 681–685.