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The Geometric-Arithmetic Index of an Infinite Class $NS_1[n]$of Dendrimer Nanostars

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ABSTRACT*:* A topological index of a graph G is a numeric quantity related to G which is describe molecular graph G. The nanostar dendrimer is an artificially manufactured or synthesized molecule built up from branched units called monomers [5]. In this paper the Geometric-arithmetic (GA) index of some graphs and an infinite class of nanostar dendrimers are computed.

KEYWORDS: Geometric-arithmetic index, Molecular Graph, *Dendrimer*, Nanostar

I. INTRODUCTION

Molecular descriptors have found a wide application in QSPR/QSAR studies [1]. Among them, topological indices have a prominent place. One of the best known and widely used is the connectivity index χ introduced in 1975 by Milan Randić [2, 3], who has shown this index to reflect molecular branching. To keep the spirit of the Randić index, and motivated by the definition of Randić connectivity index based on the end-vertex degrees of edges in a graph, Vukičevič and Furtula [4] proposed a topological index named the *geometric-arithmetic index GA*. The introduction of graph theoretic concepts in chemistry is well known and the reader is referred to the following references for definitions and notations [5, 6].

Let *G* be a connected graph with the vertex set $V(G)$ and edge-set $E(G)$, respectively.$|V(G)| = n$, $|E(G)| = m$ and n are the number of vertices and edges. The degree of a vertex $v \in V(G)$ is the number of vertices joining to v and denoted by deg(v)($or\ simply\ as\ d_v$). The *geometric-arithmetic index* of *G* is defined as

$$\mathrm{GA}(G) = \sum_{uv\in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v} \qquad \text{eq.(1)}$$

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II. RELATED WORK

For Physico-chemical properties such as entropy, enthalpy of vaporization, standard enthalpy of vaporization, enthalpy of formation, and acentric factor, it is noted in [7] that the predictive power of *GA* index is somewhat better than predictive power of the Randić connectivity index. In [8], Vukičevič and Furtula gave the lower and upper bounds for the *GA* index, determined the trees with the minimum, the second and the third minimum, as well as the second and the third maximum *GA* indices.

In this report, we investigate the Geometric-arithmetic (GA) index of some graphs and an infinite class of nanostar dendrimers

III. DENDRIMER NANOSTARS

Nano biotechnology is a rapidly advancing area of scientific and technological opportunity that applies the tools and processes of nanofabrication to build devices for studying biosystems. Dendrimers are one of the main objects of this new area of science. A dendrimer is an artificially manufactured or synthesized molecule built up from

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branched units called monomers using a nanoscale fabrication process. Dendrimers are highly ordered branched macromolecules which have attracted much theoretical and experimental attention. The topological study of these macromolecules is a new subject of research [12, 13] Dendrimers are recognized as one of the major commercially available nanoscale building blocks, large and complex molecules with very well defined chemical structure. From a polymer chemistry point of view, dendrimers are nearly perfect monodisperse macromolecules with a regular and highly branched three dimensional architecture. They consist of three major architectural components: core, branches and end groups. New branches emitting from a central core are added in steps until a tree-like structure is created. The nanostar dendrimer is a part of a new group of macroparticles that appear to be photon funnels just like artificial antennas. These macromolecules and more precisely those containing phosphorus are used in the formation of nanotubes, micro and macrocapsules, nanolatex, coloured glasses, chemical sensors, modified electrodes and so on [10, 11]

IV. MAIN RESULTS AND DISCUSSION

Lemma 1 : Consider the complete graph K_n of order n . The Geometric-arithmetic (GA) Index of this is computed as follows:

$$\mathrm{GA}(K_n) = \frac{n(n-1)}{2} \qquad \text{eq.(2)}$$

Proof. The degree of all the vertices of a complete graph K_n of order n is $n-1$ and the number of edges for K_n is equal to $\frac{1}{2}\, n(n-1)$ i,e., $|E(K_n)| = \frac{1}{2}\, n(n-1)$.

Thus

$$\mathrm{GA}(K_n) = \frac{n(n-1)}{2} \; \frac{2\sqrt{(n-1)^2}}{2(n-1)} = \frac{n(n-1)}{2} \qquad \text{eq.(3)}$$

Lemma 2:

Suppose C_n is a cycle of length n labeled by $1,2,\ldots,n$. Then the Geometric-arithmetic (GA) Index of this cycle is

$$\mathrm{GA(C_n)} = \mathrm{n} \qquad \text{eq.(4)}$$

Proof. The degree of all the vertices of C_n is two, so we can write

$$\mathrm{GA(C_n)} = \mathrm{n}\left(\frac{2\sqrt{2.2}}{2+2}\right) = n \qquad \text{eq. (5)}$$

Lemma 3: Suppose S_n is the star on n vertices, then the Geometric-arithmetic (GA) Index of this is computed as follows:

$$\mathrm{GA(S_n)} = \frac{2(\mathrm{n}-1)^{\frac{3}{2}}}{n} \qquad \text{eq.(6)}$$

Proof :

In a star S_n all the leaves are of degree 1 and the degree of internal node is $n-1$.Also the number of edges for S_n is $n-1$ i,e., $|E(S_n)| = (n-1)$. Hence the Geometric-arithmetic (GA) Index is computed as:

$$GA(S_n) = n-1\left(\frac{2\sqrt{1.(n-1)}}{1+(n-1)}\right) = \frac{2(\mathrm{n}-1)^{\frac{3}{2}}}{n}$$

Lemma 4: If G is a regular graph of degree $r > 0$, then

$$\mathrm{GA(G)} = \frac{\mathrm{nr}}{2} \qquad \text{eq.(7)}$$

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

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$$GA(G) = \frac{\mathrm{nr}}{2}\left(\frac{2\sqrt{\mathrm{r.r}}}{\mathrm{r+r}}\right) = \frac{\mathrm{nr}}{2}.$$

V. GA INDEX FOR INFINITE CLASS $NS_1[n]$ OF DENDRIMER NANOSTARS

Consider the molecular graph $G(n) = NS_1[n]$, where n is steps of growth in this type of dendrimer nanostars, see Fig. 1. $NS_1[n]$ can be divided to three parts in each step. Define d_{ij} to be the number of edges connecting a vertex of degree *i* with a vertex of degree *j*. Also $d_{ij}^{(n)}$ means the value of d_{ij} in the n^{th} step.

Using a simple calculation, we can show that $|V(NS_1[n])| = 24 \times 2^n - 4$ and

$|E(NS_1[n])| = 27 \times 2^n - 5$.

Theorem 4: The Geometric-arithmetic (GA) Index of $G(n) = NS_1[n]$ is computed as follows

$$GA(NS_1[n]) = \frac{4}{5} + \frac{12\sqrt{3}}{7} + \frac{[6+9\sum_{i=1}^{n} 2^i]2\sqrt{6}}{5} + [6 + 3(2^{n+1} + \sum_{i=1}^{n} 2^{i-1})] \qquad \text{eq.(8)}$$

Proof: There is only one vertex of degree 1, and the number of vertices of degree 4 is also 1. Since there is an edge between the vertices of degree one and four, we have $d_{14}^{(n)} = 1$ (for all n)
and it is easy to see that $d_{34} = 3$ for all the steps of growth. On the other hand the number of the new branches in n^{th} step is equal to $3 \times 2^{n-1}$ (the number of new branches in each step organize a geometric progression).
We can show that $d_{22}^{(n)} = 6 + 3(2^{n+1} + \sum_{i=1}^{n} 2^{i-1})$, because $NS_1[n]$ can be divided to exactly three parts in each step and the number of edges connecting two vertices of degree 2 (except the edges of the hexagon) in each part is 3, on the other hand the number of the new hexagon in each step is $3 \times 2^{n-1}$ and each of them has 4 edges that connecting two vertices of degree 2, also there are three hexagons in all of the steps and each of them have 2 edges that connecting two vertices of degree 2. So we have

$$d_{22}^{(n)} = 3 \times 2 + 3 \times 4 \times 2^{n-1} + 3\sum_{i=1}^{n} 2^{i-1} = 6 + 3\left(2^{n+1} + \sum_{i=1}^{n} 2^{i-1}\right).$$

Also the number of edges connecting a vertex of degree 2 with a vertex of degree 3 in each branch of each step is 6 (see Fig. 1), and there are 6 joint edges that connect a vertex of degree 2 with a vertex of degree 3, so we have

$$d_{23}^{(n)} = 6 + 6\sum_{i=1}^{n} 3 \times 2^{i-1} = 6 + 9\sum_{i=1}^{n} 2^i.$$

Thus we have

$$GA(NS_1[n]) = \frac{4}{5} + \frac{12\sqrt{3}}{7} + \frac{[6 + 9\sum_{i=1}^{n} 2^i]2\sqrt{6}}{5} + \left[6 + 3\left(2^{n+1} + \sum_{i=1}^{n} 2^{i-1}\right)\right]$$

The following table gives the values of GA index of Nanostar Dendrimer $NS_1[i], i = 1\ to\ 5$ from which we can observe n values as in eq.(8) .

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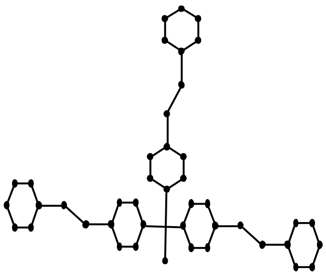
	d_{14}	d_{34}	d_{22}	d_{23}	$GA(NS_1[n])$
$NS_1[1]$	1	3	21	24	48.339
$NS_1[2]$	1	3	39	60	101.56
$NS_1[3]$	1	3	75	132	208.10
$NS_1[4]$	1	3	147	276	421.19
$NS_1[5]$	1	3	291	564	847.37

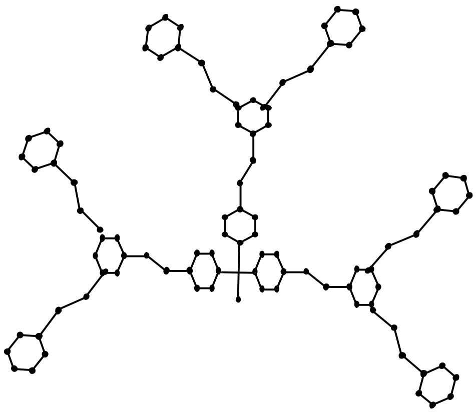
Table 1. Computing GA index for $NS_1[i]$ i≤ 5

The following is the pictorial representation of Nanostar Dendrimer $NS_1[i], i = 1 \, to \, 3$, from which the corresponding values of GA can be computed as in the above table 1.

Fig.1.The molecular graph of $NS_1[n]$



a. $NS_1[1]$



b. $NS_1[2]$

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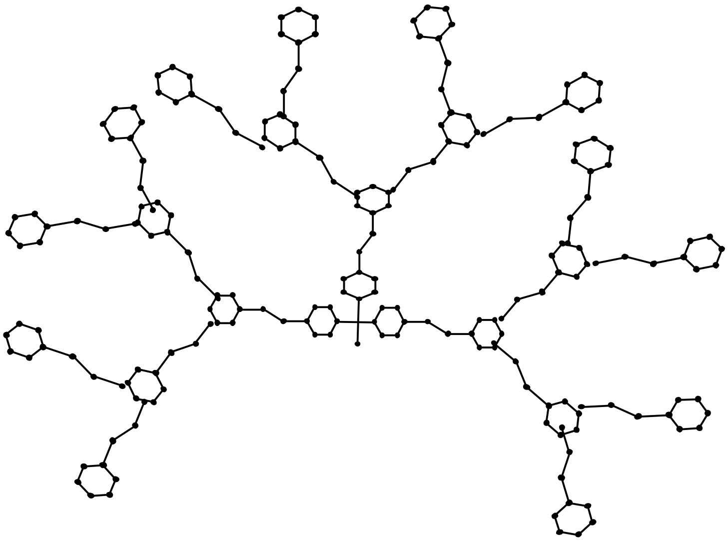

c. $NS_1[3]$

VI. Conclusion and Future Work

The future study can be made by comparing the topological indices on Dendrimer Nanostars. Also higher orders may be calculated.

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