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SOME TOPOLOGICAL INDICES FOR THEORETICAL STUDY OF TWO TYPES OF NANOSTAR DENDERIMERS

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In this paper we compute three indices (first geometric-arithmetic index (GA_1), Randic index $R(G)$ and sum-connectivity index $\chi(G)$) for two types of Nanostar Denderimers. Geometric-arithmetic, Randic and sum-connectivity are some of the topological indices that they are numerical values associated with chemical constitution purporting for correlation of chemical structure with various physical properties, chemical reactivity or biological activity. The Nanostar Dendrimers is part of a new group of macromolecules that appear to be photon funnels just like artificial antennas.

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1. Introduction

Let G be a simple graph, the vertex and edge sets of which are represented by $V(G)$ and $E(G)$, respectively. Denote by du the degree of the vertex u of graph G.

Nanostar Dendrimers are one of the main objects of nanobiotechnology. They possess a well defined molecular topology. Their step-wise growth follows a mathematical progression. In an exact phrase, Nanostar Dendrimers are hyperbranched macromolecules, showing a rigorous, aesthetically appealing architecture. The Nanostar Dendrimer is part of a new group of macromolecules having great applications but the structure must be understood [1].

A topological index is a real number related to a molecular graph. There are several topological indices already defined. The Geometric-arithmetic index is a topological index. A class of geometric-arithmetic topological indices may be defined as [2],

$$GA_{general}(G) = \sum_{uv\in E} \frac{2\sqrt{Q_u Q_v}}{Q_u + Q_v},$$

where Q_u is some quantity that in a unique manner can be associated with the vertex u of the graph G. The name geometric-arithmetic comes from of the fact that $\sqrt{Q_u Q_v}$ and $\frac{(Q_u + Q_v)}{2}$ are the geometric and arithmetic means respectively, of the numbers Q_u and Q_v.

In the general case, $\sqrt{Q_u Q_v} \le \frac{(Q_u + Q_v)}{2}$ with equality if and only if $Q_u = Q_v$. The first member of this class was considered by Vukicevic and Furtula [3] by setting Q_u to be the degree d_u of the vertex u of the graph G and we called first geometric-arithmetic index:

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

The lower and upper bounds for the GA_1 index of any graphs, tree and molecular tree have given [3, 4].

The product-connectivity index, also called Randic index $R(G)$ of a graph G is defined as follows:

$$R(G)=\sum_{uv\in E}\frac{1}{\sqrt{d_u d_v}},$$

where d_u denotes the degree of a vertex u and the summation runs over all edges uv of G. This topological index was first proposed by Randic [5] in 1975.
The sum-connectivity index was recently proposed [6]. The sum-connectivity index of the graph G is defined as

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

where d_u denotes the degree of a vertex u and the summation runs over all edges uv of G.
Ashrafi and co-author have computed the product-connectivity index for three types of the Nanostar Dendrimer [7].

The Szeged and PI indices are some of important indices that computed for some classes of Nanostar Dendrimer by Ashrafi with co-authors [8-14] and Iranmanesh with co-authers [15, 16].

In this paper, we calculate $(GA_1), R(G)$ and $\chi(G)$ for two types of the Nanostar Dendrimer.

Main results

Let G be a simple graph without directed and multiple edges and without loops, on n vertices and $n\geq 2$. The maximum possible vertex degree in such a graph G is $n-1$. Suppose $x_{i,j}$ denote the number of edges of graph G connecting vertices of degrees i and j. Clearly, $x_{i,j}=x_{j,i}$ and $x_{i,j}\geq 0$. Denote by n_i the number of vertices of degree i in graph G. Clearly, $n_0=0$ and $n_1+n_2+\cdots+n_{n-1}=n$. Now, the first geometric-arithmetic index, Randic index and sum-connectivity index can be written as

$$GA_1(G)=\sum_{1\leq i\leq j\leq n-1}\frac{2\sqrt{ij}}{i+j}x_{i,j}, \qquad (1)$$

$$R(G)=\sum_{1\leq i\leq j\leq n-1}\frac{1}{\sqrt{ij}}x_{i,j}, \qquad (2)$$

$$\chi(G)=\sum_{1\leq i\leq j\leq n-1}\frac{1}{\sqrt{i+j}}x_{i,j}. \qquad (3)$$

Counting the edges incident to vertices of degree i we arrive at the identity

$$x_{1,i}+x_{2,i}+\ldots+x_{i-1,i}+2x_{i,i}+x_{i,i+1}+\ldots+x_{n-1}=in_i,$$

which holds for $i = 1, 2, \ldots, n-1$.

Two infinite classes $NSC_5C_6[n]$ and $NSD[n]$ of Nanostar Dendrimers were considered (Figures 1 and 2). In this section the first geometric-arithmetic index, Randic index and sum-connectivity index were computed for these Nanostar Dendrimers.

Three topological index of the Nanostar Dendrimer $NSC_5C_6[n]$

Consider the molecular graph of $G[n] = NSC_5C_6[n]$, where n are steps of growth in this type of Nanostar Dendrimer, see Figure 1. The number of vertices and edges for Nanostar Dendrimer $NSC_5C_6[n]$ were calculated by using a simple method ($|V(NSC_5C_6[n])| = 9\times 2^{n+2} - 44$ and $|E(NSC_5C_6[n])| = 10\times 2^{n+2} - 50$). We begin by computing values of n_1, n_2, n_3 and n_4 for the Nanostar Dendrimer $NSC_5C_6[n]$.

$n_1 = 2\times 2^{n+2} - 6,$ $\quad n_2 = 7\times 2^{n+1} - 20,$

$n_3 = 6\times 2^{n+1} - 18,$ $\quad n_4 = 2^{n+1}.$

Now we compute $x_{i,j}$ for $1 \le i \le j \le 4$,

$x_{1,3} = 2^{n+2} - 6,$ $\quad x_{1,4} = 2^{n+2},$

$x_{2,2} = 2^{n+2} - 6,$ $\quad x_{2,3} = 9\times 2^{n+1} - 28,$

$x_{2,4} = 2^{n+1},$ $\quad x_{3,3} = 4\times 2^{n+1} - 2^n - 10,$

$x_{4,4} = 2^n.$

Theorem 1: The first geometric-arithmetic index, Randic index and sum-connectivity index of the Nanostar Dendrimer $G[n] = NSC_5C_6[n]$ are computed as follows:

$$GA_1(G[n]) = 38.1860\times 2^n - 48.6304,$$
$$R(G[n]) = 16.9483\times 2^n - 21.2284,$$
$$\chi(G[n]) = 17.8665\times 2^n - 22.6045.$$

Proof:

Put $a_{i,j} = \frac{2\sqrt{ij}}{i+j}$, $b_{i,j} = \frac{1}{\sqrt{ij}}$ and $c_{i,j} = \frac{1}{\sqrt{i+j}}$. Now, by our calculations given in last paragraph and Eq. (1), (2) and (3) we have:

$$GA_1(G[n]) = \sum_{1\le i\le j\le 4} a_{i,j}x_{i,j} = a_{1,3}x_{1,3} + a_{1,4}x_{1,4} + a_{2,2}x_{2,2} + a_{2,3}x_{2,3} + a_{2,4}x_{2,4} + a_{3,3}x_{3,3} + a_{4,4}x_{4,4}.$$

After substitution $x_{i,j}$ for $1 \le i \le j \le 4$, and computed $a_{i,j}$ for $1 \le i \le j \le 4$ we obtain:

$GA_1(G[n]) = 38.1860\times 2^n - 48.6304.$

And,

$$R(G[n]) = \sum_{1\le i\le j\le 4} b_{i,j}x_{i,j} = b_{1,3}x_{1,3} + b_{1,4}x_{1,4} + b_{2,2}x_{2,2} + b_{2,3}x_{2,3} + b_{2,4}x_{2,4} + b_{3,3}x_{3,3} + b_{4,4}x_{4,4}.$$

After substitution $x_{i,j}$ for $1 \le i \le j \le 4$, and computed $b_{i,j}$ for $1 \le i \le j \le 4$ we obtain:

$R(G[n]) = 16.9483\times 2^n - 21.2284.$

And,

$$\chi(G[n]) = \sum_{1\le i\le j\le 4} c_{i,j}x_{i,j} = c_{1,3}x_{1,3} + c_{1,4}x_{1,4} + c_{2,2}x_{2,2} + c_{2,3}x_{2,3} + c_{2,4}x_{2,4} + c_{3,3}x_{3,3} + c_{4,4}x_{4,4}.$$

After substitution $x_{i,j}$ for $1 \le i \le j \le 4$, and computed $c_{i,j}$ for $1 \le i \le j \le 4$ we obtain:

$\chi(G[n]) = 17.8665\times 2^n - 22.6045.$

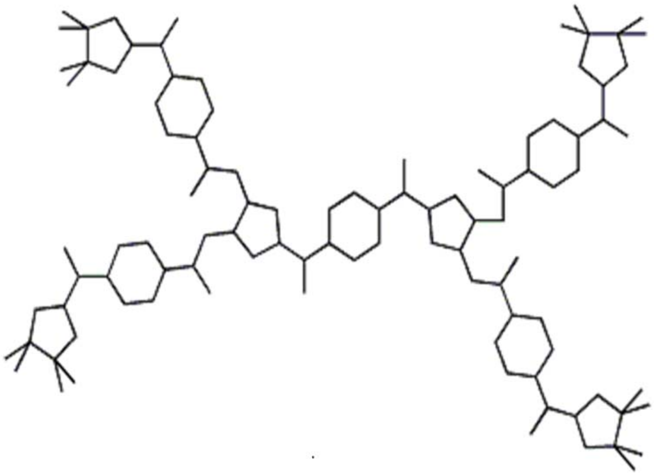

Fig. 1. The Nanostar Dendrimer $NSC_5C_6[2]$

Three topological index of the Nanostar Dendrimer $NSD[n]$

Consider the molecular graph of $H[n] = NSD[n]$, where n are steps of growth in this type of Nanostar Dendrimer, see Figure 2. The number of vertices and edges for Nanostar Dendrimer $NSD[n]$ were calculated by using a simple method ($|V(NSC_5C_6[n])| = 120\times 2^n - 108$ and $|E(NSC_5C_6[n])| = 140\times 2^n - 127$). We begin by computing values of n_2 and n_3 for the Nanostar Dendrimer $NSD[n]$.

$n_2 = 80\times 2^n - 70,$ $\qquad$ $n_3 = 40\times 2^n - 38$.

Now we compute $x_{2,2}$, $x_{2,3}$ and $x_{3,3}$,

$x_{2,2} = 56\times 2^n - 48,$ $\qquad$ $x_{2,3} = 48\times 2^n - 44,$

$x_{3,3} = 36\times 2^n - 35$.

Theorem 2: The first geometric-arithmetic index, Randic index and sum-connectivity index of the Nanostar Dendrimer $H[n] = NSD[n]$ are computed as follows:

$$GA_1(H[n]) = 139.0302\times 2^n - 126.1110\ ,$$
$$R(H[n]) = 59.5959\times 2^n - 53.6296\ ,$$
$$\chi(H[n]) = 64.1632\times 2^n - 57.9661\ .$$

Proof:

Put $a_{i,j} = \frac{2\sqrt{ij}}{i+j}$, $b_{i,j} = \frac{1}{\sqrt{ij}}$ and $c_{i,j} = \frac{1}{\sqrt{i+j}}$. Now, by our calculations given in last paragraph and Eq. (1), (2) and (3) we have:

$$GA_1(H[n]) = \sum_{1\le i\le j\le 3} a_{i,j}.x_{i,j} = a_{2,2}x_{2,2} + a_{2,3}x_{2,3} + a_{3,3}x_{3,3}.$$

After substitution $x_{i,j}$ for $1\le i\le j\le 3$, and computed $a_{i,j}$ for $1\le i\le j\le 3$ we obtain:

$$GA_1(H[n]) = 139.03\times 2^n - 126.11.$$

And,

$$R(H[n]) = \sum_{1\le i\le j\le 3} b_{i,j}.x_{i,j} = b_{2,2}x_{2,2} + b_{2,3}x_{2,3} + b_{3,3}x_{3,3}.$$

After substitution $x_{i,j}$ for $1 \le i \le j \le 3$, and computed $b_{i,j}$ for $1 \le i \le j \le 3$ we obtain:

$R(H[n]) = 59.5959 \times 2^n - 53.6296$.

And,

$$\chi(H[n]) = \sum_{1 \le i \le j \le 3} c_{i,j} x_{i,j} = c_{2,2}x_{2,2} + c_{2,3}x_{2,3} + c_{3,3}x_{3,3}.$$

After substitution $x_{i,j}$ for $1 \le i \le j \le 3$, and computed $c_{i,j}$ for $1 \le i \le j \le 3$ we obtain:

$\chi(H[n]) = 64.1632 \times 2^n - 57.9661$.

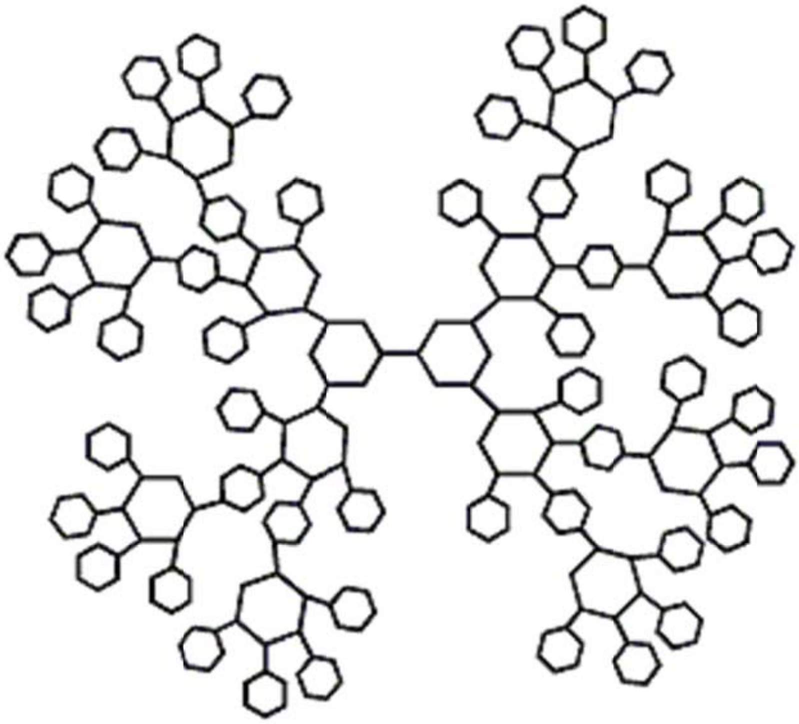

Fig. 2. The Nanostar Dendrimer $NSD[2]$

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