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Computing GA_4 index of an infinite class of nanostar dendrimers

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Let G be a connected graph, the GA index (Geometric-Arithmetic index) is a topological index was defined as $GA(G)=\sum_{uv\in E(G)}\frac{\sqrt{d_u d_v}}{\frac{1}{2}(d_u+d_v)}$ where d_u denotes degree of u. Now we define a new version of GA index as $GA_4(G)=\sum_{uv\in E(G)}\frac{\sqrt{\varepsilon(u)\varepsilon(v)}}{\frac{1}{2}(\varepsilon(u)+\varepsilon(v))}$ where $\varepsilon(v)$ is the largest distance between v and any other vertex u of G or the eccentricity of v. In this paper an exact formula for the GA_4 index of an infinite class of nanostar dendrimers is given.

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1. Introduction

Nanobiotechnology 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. Here a dendrimer is a synthetic 3-dimensional macromolecule that is prepared in a step-wise fashion from simple branched monomer units, the nature and functionality of which can be easily controlled and varied. The nanostar dendrimer is part of a new group of macromolecules that the structure and the energy transfer mechanism must be understood.

A map taking graphs as arguments is called a graph invariant or topological index if it assigns equal values to isomorphic graphs. There are several topological indices have been defined and many of them have found applications as means to model chemical, pharmaceutical and other properties of molecules.

The GA index is a topological index introduced by Vukicevic and Furtula [1]. And the GA_2 and the GA_3 indices was introduced by Zhou et al [2]. The aim of this paper is to present a new GA_4 index and computing this topological index for an infinite class nanostar dendrimers.

2. Definitions

Some algebraic definitions used for the study are given. Let G be a graph with vertex and edge sets *V(G)* and *E(G)*, respectively. As usual, the distance between the vertices u and v of G is denoted by *d(u,v)* and it is defined as the number of edges in a minimal path connecting the vertices u and v.

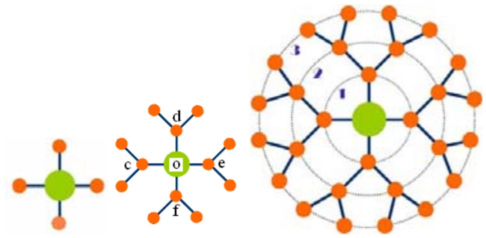
A molecular graph is a graph such that vertices represent atoms and edges represent bonds. These graphs have been used for affinity diagrams showing a relationship between chemical substances. Obviously, the degree of each atom in a molecular graph is at most four.

The Wiener index is the first distance based topological index was introduced in 1947 by chemist Harold Wiener 3] as the half-sum of all topological distances in the hydrogen-depleted graph representing the skeleton of the molecule. The GA index is another topological index introduced by Vukicevic and Furtula [1] . The GA_2 and the GA_3 indices was introduced by Zhou et al [2]. To define a new the GA_4 index of a graph G, we assume that $\varepsilon(v)$ is the largest distance between v and any other vertex u of G or the eccentricity of v. Now we define a new version of GA index as

$$GA_4(G)=\sum_{uv\in E(G)}\frac{\sqrt{\varepsilon(u)\varepsilon(v)}}{\frac{1}{2}(\varepsilon(u)+\varepsilon(v))}.$$

Our notation are standard and taken mainly from the standard book of graph theory.

In this paper we investigate the GA_4 index for an infinite family of dendrimers which are used Ahmadi and Seif [4]. Structure of dendrimers, which are used in this study is as depicted in Fig. 1. Here n is the step of growth in the type of dendrimer.



D[1] D[2] D[3]

Fig. 1. Structures of the dendrimers used in this study.

3. Theorem and proof

In recent research in mathematical chemistry, particular attention is paid to distance-based graph invariants. Throughout this section D[n] denotes the molecular graph of a nanostar dendrimer with exactly *n* generation. Notice that Fig. 1, we can list the eccentricities of the vertices D[1], D[2], D[3] and D[n] in Table 1.

Table 1. Dendrimers and its eccentricities.

Dendrimers	Eccentricities
D[1]	1,2
D[2]	2,3,4
D[3]	3,4,5,6
D[4]	4,5,6,7,8
…	…
D[n]	n,n+1,…,2n

Also in Fig. 1, we can easily see that the number of neighbouring vertices and its eccentricities. And we list them in Table 2.

Table 2. Dendrimers with the number of neighbouring eccentric vertices.

Dendrimers	The number of neighbouring eccentric vertices
D[1]	$(1,2)\rightarrow 2^2$
D[2]	$(2,3)\rightarrow 2^2$, $(3,4)\rightarrow 2^3$
D[3]	$(3,4)\rightarrow 2^2$, $(4,5)\rightarrow 2^3$, $(5,6)\rightarrow 2^4$
D[4]	$(4,5)\rightarrow 2^2$, $(5,6)\rightarrow 2^3$, $(6,7)\rightarrow 2^4$, $(7,8)\rightarrow 2^5$
…	…
D[n]	$(n,n+1)\rightarrow 2^2$, $(n+1,n+2)\rightarrow 2^3$, …., $(2n-1,2n)\rightarrow 2^{n+1}$.

In the light of these observations we can state our our main result.

Theorem. The GA_4 index of the nanostar dendrimer D[n] is computed as;

$$GA_4(D[n]) = 2^3\frac{\sqrt{n(n+1)}}{2n+1} + 2^4\frac{\sqrt{(n+1)(n+2)}}{2n+3} + \ldots + 2^{n+2}\frac{\sqrt{(2n-1)2n}}{4n-1}.$$

Proof. We can write directly from definition;

$$GA_4(D[n]) = \sum_{uv\in E(D[n])}\frac{\sqrt{\varepsilon_u\varepsilon_v}}{\frac{1}{2}(\varepsilon_u+\varepsilon_v)}$$

$$= 2^2\frac{\sqrt{n(n+1)}}{\frac{1}{2}(n+(n+1))} + 2^3\frac{\sqrt{(n+1)(n+2)}}{\frac{1}{2}((n+1)+(n+2))} + \ldots + 2^{n+1}\frac{\sqrt{(2n-1)2n}}{\frac{1}{2}((2n-1)+2n)}$$

$$= 2^3\frac{\sqrt{n(n+1)}}{2n+1} + 2^4\frac{\sqrt{(n+1)(n+2)}}{2n+3} + \ldots + 2^{n+2}\frac{\sqrt{(2n-1)2n}}{4n-1}.$$

And this completes the proof.

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