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Computing Ediz eccentric connectivity index of an infinite class of nanostar dendrimers

S. EDİZ
Department of Mathematics, Yüzüncü Yıl University, Van, Turkey

Let *G* be a molecular graph, we firstly define Ediz eccentric connectivity index as ${}^{E}\xi^{c}(G)=\sum_{i=1}^{n}\left(\frac{S_i}{E_i}\right)$ where S_i is the sum of degrees of all vertices v_j, adjacent to vertex v_i, E_i is the largest distance between v_i and any other vertex v_k of *G* or the eccentricity of v_i and *n* is the number of vertices in graph *G.* In this paper an exact formula for the Ediz eccentric connectivity 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 augmented eccentric connectivity index is a topological index introduced by Bajaj et al [1]. In this paper we firstly defined Ediz connectivity 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 [2] as the half-sum of all topological distances in the hydrogen-depleted graph representing the skeleton of the molecule. The augmented eccentric connectivity index is another topological index introduced by Bajaj et al [1] and defined as ${}^{A}\xi^{c}(G)=\sum_{i=1}^{n}\left(\frac{M_i}{E_i}\right)$ where M_i is the product of degrees of all vertices v_j, adjacent to vertex v_i, E_i is the largest distance between v_i and any other vertex v_k of *G* or the eccentricity of v_i and *n* is the number of vertices in graph *G*. In this paper we firstly define Ediz eccentric connectivity index as ${}^{E}\xi^{c}(G)=\sum_{i=1}^{n}\left(\frac{S_i}{E_i}\right)$ where S_i is the sum of degrees of all vertices v_j, adjacent to vertex v_i, E_i is the largest distance between v_i and any other vertex v_k of *G* or the eccentricity of v_i and *n* is the number of vertices in graph *G*. In this paper an exact formula for the Ediz eccentric connectivity index of an infinite class of nanostar dendrimers is given.

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

In this paper we investigate the augmented eccentric connectivity index for an infinite family of dendrimers which are used Ahmadi and Seif [3]. 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.

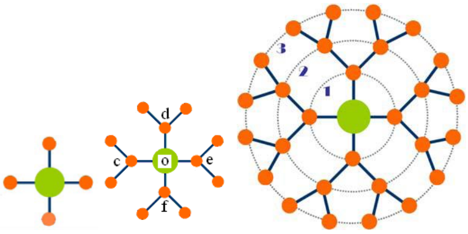

Fig. 1. Structures of the dendrimers used in this study

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

Theorem. Ediz eccentric connectivity index of the nanostar dendrimer D[n] $(n \geq 3)$ is computed as;

$$^{E}\xi^{c}(D[n]) = 2^{n+1}\frac{3}{2n} + 2^{n}\frac{5}{2n-1} + 2^{n-1}\frac{9}{2n-2} + 2^{n-2}\frac{9}{2n-1} + \ldots + 2^{4}\frac{9}{n+3} + 2^{3}\frac{9}{n+2} + 4\frac{10}{n+1} + \frac{12}{n}$$

Proof.

Note that Fig. 1, we can see each dendrimer except from D[1] consists of three degree conditions: 1, 3 and 4. And note that Fig. 1, the *n. level* vertices' degree are 1 and each of them has only one neighbour with degree 3. The number of *n.level* vertices are 2^{n+1}. And the *n-1. level* vertices' degree are 3 and each of of them has exactly two neighbours with degree 1 and one neighbour with degree 3. The number of *n-1* level vertices are 2^{n}. And the *n-2. level* vertices' degree are 3 and each of them has exactly three neighbours with degree 3. The number of *n-2* level vertices are 2^{n-1}. Proceeding in this manner, the *2.level* vertices' degree are 3 and each of them has excatly three neighbours with degree 3. And the *1.level* vertices' degree are 3 and each of them has two neighbours with degree 3 and one neighbour with degree 4. The number of *1.level* vertices are 4. And the *0.level* vertex degree is 4. And it has four neighbours with degree 3. In the light of these observations we can write directly from the definition of Ediz eccentric connectivity index:

$$^{E}\xi^{c}(D[n]) = \sum_{i=1}^{n}\left(\frac{S_i}{E_i}\right)$$

$$^{E}\xi^{c}(D[n]) = 2^{n+1}\frac{3}{2n} + 2^{n}\frac{5}{2n-1} + 2^{n-1}\frac{9}{2n-2} + 2^{n-2}\frac{9}{2n-1} + \ldots + 2^{4}\frac{9}{n+3} + 2^{3}\frac{9}{n+2} + 4\frac{10}{n+1} + \frac{12}{n}$$

And this completes the proof.

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*Corresponding author: ediz571@gmail.com