



THE EDIZ ECCENTRIC CONNECTIVITY INDEX OF NANOSTAR DENDRIMER

$D_3[n]$

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ABSTRACT

A graph $G=(V,E)$ consists of a set of vertices $V(G)$ and a set of edges $E(G)$. In chemical graphs, the vertices and edges of the graph correspond to the atoms of the molecule and chemical bonds, respectively.

The *eccentric connectivity index* is equal to $\zeta(G)=\sum_{v \in V} d_v \times \varepsilon(v)$, where $\varepsilon(v)$ is the eccentricity of vertex v of G . In 2010, S. Ediz et al. defined *Ediz eccentric connectivity index* of G , ${}^E\zeta(G)$, is defined as $\sum_{v \in V(G)} \frac{S(v)}{\varepsilon(v)}$, where $S(v)$ is the sum of degrees of all vertices adjacent to vertex v . In

this paper, we compute the Ediz eccentric connectivity index of an infinite family of Nanostar Dendrimer $D_3[n]$ ($\forall n \geq 1$).

Keywords: Molecular graph, Eccentric connectivity index, Ediz eccentric connectivity index, Nanostar Dendrimer.

INTRODUCTION

Let $G=(V,E)$ be a graph, where $V(G)$ is a non-empty set of vertices and $E(G)$ is a set of edges. In chemical graphs, the vertices and edges of the graph correspond to the atoms of the molecule and chemical bonds, respectively. For $u \in V(G)$, defined d_u be degree of vertex u . If e is an edge of G , connecting the vertices u and v , then we write $e=uv \in E(G)$ and say u and v are adjacent and if there is a path between all pairs of vertices in G , then is a connected graph.

A molecular descriptors (or *Topological Index*) are a real number related to a molecular graph, which is a graph invariant. For two vertices $u, v \in V(G)$, the distance $d(u, v)$ is equal to the length of any shortest path in G connecting u and v . The *eccentric connectivity index* of the molecular graph G , $\xi(G)$, was proposed by *Sharma, Goswami and Madan* [1]. It is defined as

$$\xi(G) = \sum_{v \in V} d_v \times \varepsilon(v)$$

in which $\varepsilon(v)$ denoted the eccentricity of vertex v of G and eccentricity $\varepsilon(v)$ is the largest distance between v and any other vertex u of G or $\varepsilon(v) = \text{Max}\{d(v, u) | \forall v \in V(G)\}$. The radius $R(G)$ and diameter $D(G)$ are defined as the minimum and maximum eccentricity among vertices of G , respectively. In other works [1-17]:

$$D(G) = \text{Max}_{v \in V(G)} \{d(v, u) | \forall u \in V(G)\}.$$

$$R(G) = \text{Min}_{v \in V(G)} \{d(v, u) | \forall u \in V(G)\}.$$

Suppose $S(v)$ as the summation of degrees of all neighbors of vertex v in G . In other words, $S(u) = \sum_{v \in N_G(u)} d_v$ and $N_G(u) = \{v \in V(G) | uv \text{ in } E(G)\}$. In 2010, *S. Ediz* defined *Ediz eccentric connectivity index* of G is defined as

$$\xi^E(G) = \sum_{v \in V(G)} \frac{S(v)}{\varepsilon(v)}$$

where $S(v)$ is the sum of degrees of all vertices adjacent to vertex v and $\varepsilon(v)$ is the eccentricity of vertex v of G [18-20].

RESULTS AND DISCUSSION

In this section, we compute *Ediz eccentric connectivity index* for an infinite family of Nanostar Dendrimer $D_3[n]$.

Dendrimers are hyper-branched macromolecules, with a rigorously tailored architecture and are one of the main objects of Nano biotechnology. They can be synthesized, in a controlled manner, either by a divergent or a convergent procedure. Dendrimers have gained a wide range of applications in supra-molecular chemistry, particularly in host guest reactions and self-assembly processes. Their applications in chemistry, biology and nano-science are unlimited. Recently, the topological indices of some Dendrimer Nanostars have been investigated in [21-35]. See Figure 1, which show the kind of 3th growth of Dendrimer.

In this paper, we denote the n^{th} growth of Nanostar Dendrimer by $D_3[n] \forall n \in \mathbb{N}$.

From Figure 1 and [31-55], one can see that the Dendrimer Nanostars $D_3[n]$ has $|V(D_3[n])|=21(2^{n+1})-20$ vertices/atoms. Because in the structure of Dendrimer Nanostar $D_3[n]$ (Figure 1), there are $3(2^n)$ vertices/atoms with degree 1 (all Hydrogen atoms), $12(2^{n+1}-1)$ vertices of $D_3[n]$ with degree 2 and $15(2^n)-8$ vertices with degree

three. And also, there are $|E(D_3[n])|=1/2[1 \times 3(2^n) + 2 \times 12(2^{n+1}-1) + 3 \times 15(2^n)] = 24(2^{n+1}-1)$ edges/bonds in the Nanostar Dendrimer $D_3[n]$.

From the structure of Dendrimer Nanostar $D_3[n]$ in Figure 1, we see that an element as Figure 2 (we called "Leaf") is added to $D_3[n-1]$ in the n^{th} growth of Nanostar Dendrimer.

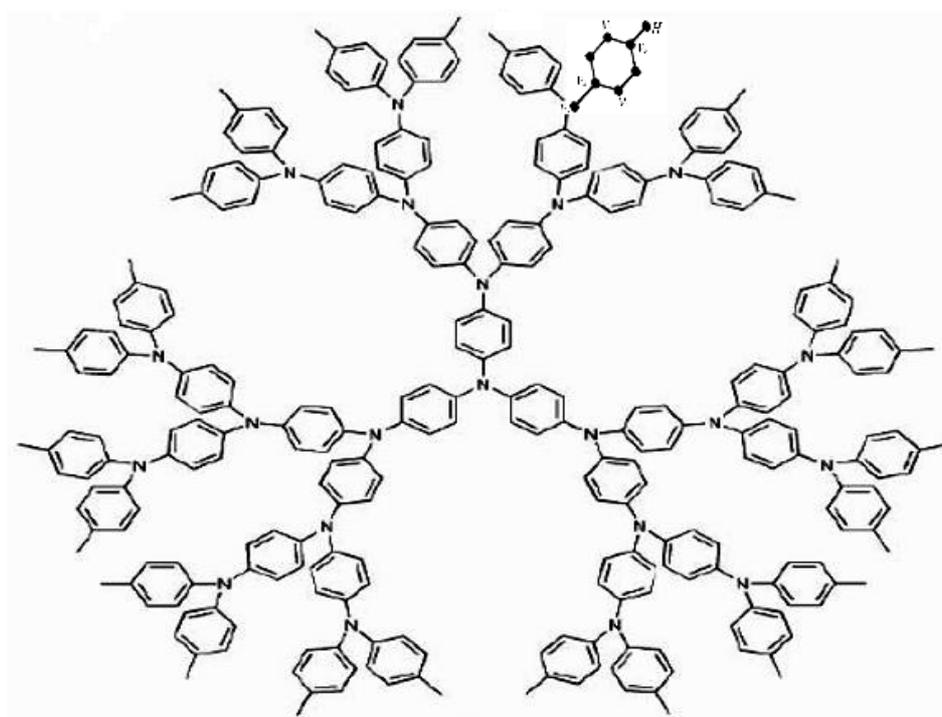


Figure 1: [31-35] An example of the Nanostar Dendrimer $D_3[n], \forall n \in \mathbb{N}$.

In Figure 2, we labeled vertices of an arbitrary added leaf in the n^{th} growth of Nanostar Dendrimer $D_3[n]$. Since the maximum eccentricity of this added leaf is 5, therefore the eccentricity of previous vertices increase 10. Thus, we can compute the eccentricity of all vertices v_1, v_2, \dots, v_5 (see Table 1).

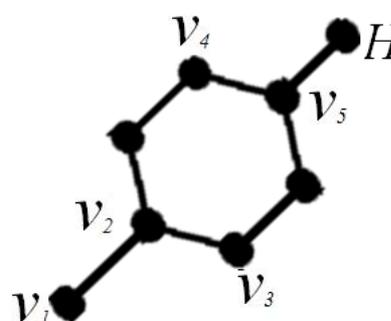


Figure 2: An added leaf in the n^{th} growth of Nanostar Dendrimer $D_3[n]$.

Now, on based the structure of Dendrimer Nanostar $D_3[n]$, one can see that the vertices v_1 (all Nitrogen atoms N), v_2 and v_5 have degree 3 and the vertices v_3 and v_4 have degree 2. Obviously all

Hydrogen atoms H have degree 1. The summation of degree $S(v)$ for all vertices of Dendrimer Nanostar $D_3[n]$ (see Figure 3 and Table 1).

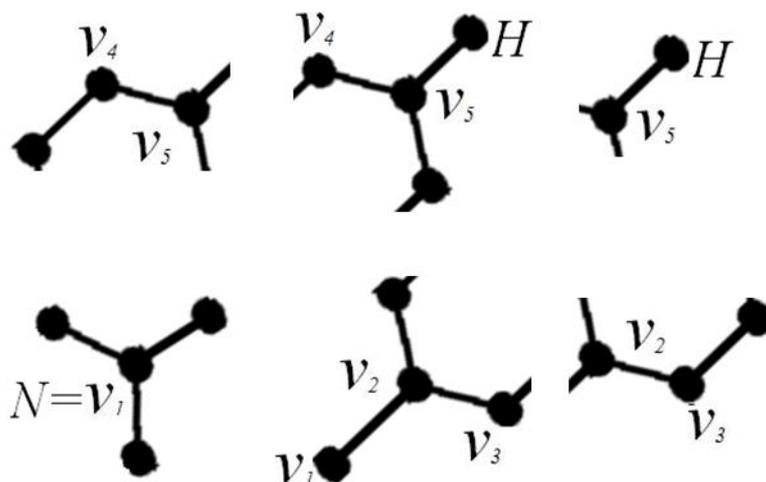


Figure 3: Vertices in an added leaf of $D_3[n]$ with all their adjacent.

Table 1: The number, eccentricity $\epsilon(v)$ and summation of degree $S(v)$ for vertices of an leaf in Nanostar Dendrimer $D_3[n]$.

Vertices in an added leaf in $D_3[n]$	The eccentricity of v in the i^{th} growth of $D_3[n]$	The summation of degree $S(v)$	The number of these vertices
v_1 (Nitrogen atoms N)	$5i+5n+5$	9	$3(2^{n-1})$
v_2	$5i+5n+6$	7	$3(2^n)$
v_3	$5i+5n+7$	5	$3(2^{n+1})$
v_4	$5i+5n+8$	5	$3(2^{n+1})$
v_5	$5i+5n+9$	5	$3(2^n)$
Hydrogen atoms H	$10n+10$	3	$3(2^n)$

Now, we can compute the Ediz eccentric connectivity index of an infinite family of Nanostar Dendrimer $D_3[n]$ ($\forall n \geq 1$) as:

$$\begin{aligned}
 E_{\zeta}^{\infty}(D_3[n]) &= \sum_{v \in (D_3[n])} \frac{S(v)}{\epsilon(v)} \\
 &= \sum_{\substack{v_1 \in D_3[i] \\ i=1, \dots, n}} \frac{S(v_1)}{\epsilon(v_1)} + \sum_{\substack{v_2 \in D_3[i] \\ i=1, \dots, n}} \frac{S(v_2)}{\epsilon(v_2)} + \sum_{\substack{v_3 \in D_3[i] \\ i=1, \dots, n}} \frac{S(v_3)}{\epsilon(v_3)} + \sum_{\substack{v_4 \in D_3[i] \\ i=1, \dots, n}} \frac{S(v_4)}{\epsilon(v_4)} + \sum_{\substack{v_5 \in D_3[i] \\ i=1, \dots, n}} \frac{S(v_5)}{\epsilon(v_5)} \\
 &+ \sum_{\substack{\text{Hydrogen atoms} \\ \text{of } D_3[n]}} \frac{S(H)}{\epsilon(H)}
 \end{aligned}$$

$$\begin{aligned}
 &= \frac{9}{5n+5} + \sum_{\substack{v_1 \text{ in } D_3[i] \\ i=2, \dots, n}} \frac{9}{5i+5n+5} + \sum_{\substack{v_2 \text{ in } D_3[i] \\ i=1, \dots, n}} \frac{7}{5i+5n+6} + \sum_{\substack{v_3 \text{ in } D_3[i] \\ i=1, \dots, n}} \frac{5}{5i+5n+7} \\
 &+ \sum_{\substack{v_4 \text{ in } D_3[i] \\ i=1, \dots, n}} \frac{5}{5i+5n+8} + \sum_{\substack{v_4 \text{ in } D_3[i] \\ i=1, \dots, n}} \frac{5}{5i+5n+9} + \sum_{\substack{\text{Hydrogen atoms} \\ \text{of } D_3[n]}} \frac{3}{10(n+1)} \\
 &= \frac{-9}{5(n+2)} + \sum_{i=1}^n \frac{27(2^{i-1})}{5i+5n+5} + \sum_{i=1}^n \frac{21(2^i)}{5i+5n+6} + \sum_{i=1}^n \frac{15(2^{i+1})}{5i+5n+7} + \sum_{i=1}^n \frac{15(2^{i+1})}{5i+5n+8} \\
 &+ \sum_{i=1}^n \frac{15(2^i)}{5i+5n+9} + \frac{3(2^n)}{10(n+1)} \\
 &= \sum_{i=1}^n \left(\frac{27(2^{i-1})}{5i+5(n+1)} + \frac{21(2^i)}{5i+1+5(n+1)} + \frac{15(2^{i+1})}{5i+2+5(n+1)} + \frac{15(2^{i+1})}{5i+3+5(n+1)} + \frac{15(2^i)}{5i+4+5(n+1)} \right) \\
 &+ \frac{3}{5} \left(\frac{2^{n-1}}{n+1} - \frac{3}{n+2} \right)
 \end{aligned}$$

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