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COMPUTING ECCENTRIC CONNECTIVITY INDEX OF A CLASS OF NANOSTAR DENDRIMERS

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ABSTRACT. Let G be a molecular graph. The eccentric connectivity index ξ(G) is defined as $\xi(G) = \sum_{u\in V(G)} \deg(u)\varepsilon(u)$, where deg(u) denotes the degree of vertex u and ε(u) is the largest distance between u and any other vertex v of G. In this paper, an exact formula for the eccentric connectivity index of a class of dendrimers is given. The correctness of this formula is investigated by computing the layer matrix of this class of dendrimers.

Keywords: Dendrimer, molecular graph, eccentric connectivity index.

INTRODUCTION

Dendrimers are highly branched macromolecules. They are being investigated for possible uses in nanotechnology, gene therapy, and other fields. Each dendrimer consists of a multifunctional core molecule with a dendritic wedge attached to each functional site. The core molecule without surrounding dendrons is usually referred to as zeros generation. Each successive repeat unit along all branches forms the next generation, 1st generation and 2nd generation and so on until the terminating generation. The topological study of these macromolecules is the aim of this article, see [1-4] for details.

We now describe some notations which will be kept throughout. The distance d(u,v) between two vertices u and v of a graph G is defined as the length of a shortest path connecting them. The summation of these numbers over all edges of G is called the Wiener index of G [5]. For a given vertex u of V(G) its eccentricity, ε(u), is the largest distance between u and any other vertex v of G. The maximum eccentricity over all vertices of G is called the diameter of G and denoted by D(G). The eccentric connectivity index ξ(G) is defined as $\xi(G) = \sum_{\mathbf{u}\in V(G)} \mathbf{deg(u)\varepsilon(u)}$, [6]. Some chemical application of this new proposed topological index are reported in [7−16] and its mathematical properties are studied in [17−21].

This paper addresses the problem of computing the eccentric connectivity index of nanostar dendrimers. Our notation is standard and taken mainly from [22] and the standard books of graph theory.

MAIN RESULT AND DISCUSSION

Let G be an n-vertex graph. Layer matrices have been proposed in connection to the sequences of walks: *DDS* (Distance Degree Sequence), *PDS* (Path Degree Sequence), and *WS* (Walk Sequence). They are built up on the layer partitions in G. A layer partition G(i) with respect to the vertex i, in G, is defined as

$$G(i) = \{G(v)j \mid j \in [0,\varepsilon(i)] \text{ and } v \in G(v)j \Leftrightarrow d(i,v) = j\}.$$

The entries in a layer matrix, LM, collect the property M_v (topological or chemical) for all vertices v belonging to the layer $G(v)_j$, $[LM]_{ij} = \sum_{v \in G(v)_j} M_v$. The matrix LM can be written as $LM(G) = \{ [LM]_{ij} \mid i \in V(G);\ j \in [0, D(G)]\}$. The dimensions of such a matrix are $n \times (D(G)+1)$, see [22] for details.

Suppose NS[n] denotes the molecular graph of a dendrimer with exactly n generations depicted in Fig. 1. The aim of this paper is to compute the eccentric connectivity index of this dendrimer.

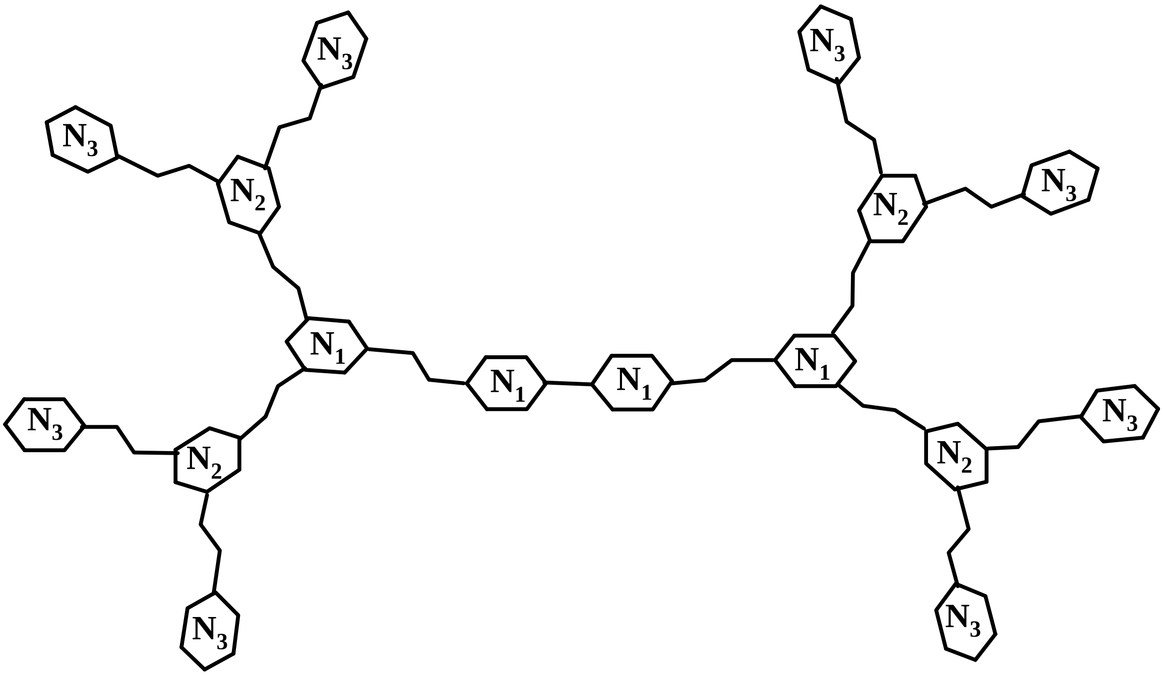

Fig. 1. – The Nanostar Dendrimer NS[2].

We first compute the eccentric connectivity index of NS[n] and then we check our calculations by computing the layer matrix of this dendrimer. Consider the core of NS[n] depicted in Fig. 2.

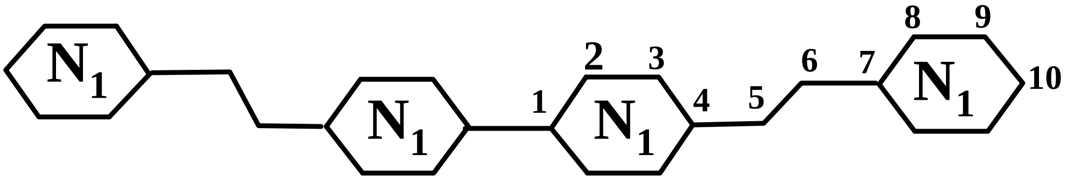

Fig. 2. – The Core of Dendrimer NS[2].

From the molecular graph of this dendrimer, one can see that some vertices of the graph have the same degree and the same eccentricity. So for computing the eccentric connectivity index of NS[n], it is enough to compute the eccentricity of a set of representatives. At first, one can see that NS[n] has exactly $2^{n+4} - 4$ vertices. By a simple calculation, we have:

$$\begin{aligned} \xi(NS[1]) &= (2\times3\times10) + (4\times2\times11) + (4\times2\times12) + (2\times3\times13) + (2\times2\times14) \\ &+ (2\times2\times15) + (2\times3\times16) + (4\times2\times17) + (4\times2\times18) + (2\times2\times19) \\ &= 890. \end{aligned}$$

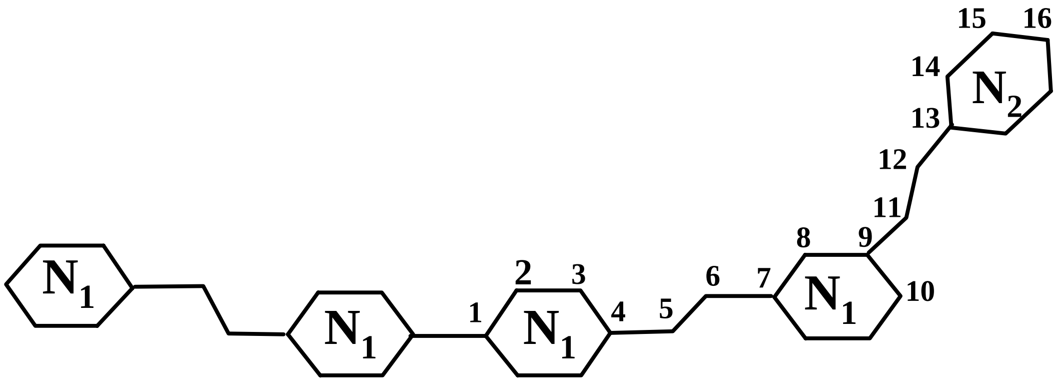

Fig. 3. – The Subgraph of NS[n] Constructed in the First Generation.

In the second step (when n = 2) we will find four new subgraphs containing a hexagon and a path of length 3 are added. We label the representative vertices of NS[2] by 11, 12, 13, 14, 15 and 16, Fig. 3. By a simple calculation, we can see that there are 2^{i+1} vertices of type 11 with eccentricity $1 + 5 \times (i - 1) + 17 + 5 \times (n - 1) + 1 = 5n + 5i + 9$. In Table 1, the degrees, frequencies and eccentricities of these vertices are computed.

We now partition the molecular graph of NS[n] into two parts, one of them is the core C and other is the maximal subgraph T of NS[n] with vertex set V(NS[n]) – V(C). Then we have:

$$\xi(T) = 2\sum_{i=1}^{n-1} 2^{i+1}(5n + 5i + 9) + 2\sum_{i=1}^{n-1} 2^{i+1}(5n + 5i + 10) + 3\sum_{i=1}^{n-1} 2^{i+2}(5n + 5i + 11) + 2\times\sum_{i=1}^{n-1} 2^{i+2}(5n + 5i + 12) + 3\times\sum_{i=1}^{n-2} 2^{i+2}(5n + 5i + 13) + 2\times\sum_{i=1}^{n-1} 2^{i+1}(5n + 5i + 14) + 2\times 2^{n+1}(10n + 8) = 420n\times 2^n + 60\times 2^n - 440n - 592.$$

$$\xi(C) = 6\times(5n + 5) + 8\times(5n + 6) + 8\times(5n + 7) + 6\times(5n + 8) + 4\times(5n + 9) + 4\times(5n + 10) + 6\times(5n + 11) + 8\times(5n + 12) + 12\times(5n + 13) + 4\times(5n + 14) = 330n + 632.$$

Table 1. - The Frequencies and Eccentricities of Vertices 13, 14, 15, 16, 17 and 18.

No.	Degree	Frequency	Eccentricity
11	2	2^{i+1}	1+5(i–1) +17+5(n–1)+1
12	2	2^{i+1}	2+5(i–1)+17+5(n–1)+1
13	3	2^{i+1}	3+5(i–1)+17+5(n–1)+1
14	2	$2\times2^{i+1}$	4+5(i–1)+17+5(n–1)+1
15	3 or 2	$2\times2^{i+1}$ or 2×2^{n}	5+5(i-1)+17 +5(n-1)+1 or 5+5(n-2)+17+5(n–1)+1
16	2	2^{i+1}	6+5(i–1)+17+5(n–1)+1

Then $\xi(NS[n]) = 420n \times 2^n + 60 \times 2^n - 110n + 40$. In Table 2, the eccentric connectivity index of NS[n], $n \leq 12$, are computed.

Table 2. - The Eccentric Connectivity Index (ECI) of NS[n], $n \leq 12$.

No	1	2	3	4	5	6
ECI	890	3420	10270	27440	68610	164500
No	7	8	9	10	11	12
ECI	383270	874680	1965130	4361180	9583470	20888320

In what follows, the layer matrix of NS[n] is also computed. In this matrix the first column from left, denotes the frequencies of each representative, the first column from right is the number of non-zero entries in each row minus 1 and the second column is trivially the degree sequence of NS[n]. If we use this matrix to compute the eccentric connectivity index of NS[n], we will obtain the same equation for computing eccentric connectivity index of NS[n]. This shows that our calculations are correct.

$$
LM = \begin{array}{c}
2\\ 4\\ 4\\ 2\\ 2\\ 2\\ 2\\ 4\\ 4\\ 2\\ 2^{i+1}\\ 2^{i+1}\\ 2^{i+1}\\ 2^{i+2}\\ \begin{cases}2^{i+2}\\ 2^{n+1}\end{cases}\\ 2^{i+1}
\end{array}
\left[\begin{array}{cccccccccccccccccccc}
1 & 3 & \cdots & k & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
1 & 2 & & \cdots & k & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
1 & 2 & & \cdots & & k & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
1 & 3 & & & \cdots & & k & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
1 & 2 & & & \cdots & & & k & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
1 & 2 & & & & \cdots & & & k & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
1 & 3 & & & & \cdots & & & & k & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
1 & 2 & & & & & \cdots & & & & k & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
1 & 3 & & & & & \cdots & & & & & k & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
1 & 2 & & & & & & \cdots & & & & & k & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
1 & 2 & & & & & & \cdots & & & & & & \cdots & k & 0 & 0 & 0 & 0 & 0\\
1 & 2 & & & & & & & \cdots & & & & & & & k & 0 & 0 & 0 & 0\\
1 & 3 & & & & & & & \cdots & & & & & & & & k & 0 & 0 & 0\\
1 & 2 & & & & & & & & \cdots & & & & & & & & k & 0 & 0\\
1 & \begin{cases}3\\ 2\end{cases} & & & & & & & & \cdots & & & & & & & & & k & 0\\
1 & 2 & & & & & & & & & \cdots & & & & & & & & & k
\end{array}\right]
\begin{array}{c}
5n+5\\ 5n+6\\ 5n+7\\ 5n+8\\ 5n+9\\ 5n+10\\ 5n+11\\ 5n+12\\ 5n+13\\ 5n+14\\ 5n+5i+9\\ 5n+5i+10\\ 5n+5i+11\\ 5n+5i+12\\ \begin{cases}5n+5i+13\\ 10n+8\end{cases}\\ 5n+5i+14
\end{array}
$$

CONCLUSIONS

In this paper a method for computing layer matrix of a dendrimer is presented which is useful for computing eccentric connectivity index of dendrimers. This method is efficient for dendrimers. We applied our method on an infinite class of dendrimers.

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