

The eccentric connectivity index of a new class of nanostar dendrimers

A. R. ASHRAFI*, M. SAHELI

Institute of Nanoscience and Nanotechnology, University of Kashan, Kashan 87317-51167, I.R. Iran

Let G be a molecular graph. The eccentric connectivity index $\xi(G)$ is defined as $\xi(G) = \sum_{u \in V(G)} \deg(u)\varepsilon(u)$, where $\deg(u)$ denotes the degree of vertex u and $\varepsilon(u)$ 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 new class of nanostar dendrimers is given.

(Received March 31, 2010; accepted June 16, 2010)

Keywords: Nanostar dendrimer, Molecular graph, Eccentric connectivity index

1. 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 zero 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, $\varepsilon(u)$, 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 $\xi(G)$ of is defined as $\xi(G) = \sum_{u \in V(G)} \deg(u)\varepsilon(u)$, [6–11]. The mathematical properties of this new topological index are studied in some recent papers [12–16].

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

2. Main results and discussion

Suppose $NS[n]$ denotes the molecular graph of a nanostar dendrimer with exactly n generations depicted in Fig. 1. Obviously, $|V(NS[n])| = 24 + \sum_{i=1}^{n-1} 18 \times 2^i = 18 \times$

$2^n - 12$ and $|EV(NS[n])| = 27 + \sum_{i=1}^{n-1} 21 \times 2^i = 21 \times 2^n - 15$. The aim of this section is to compute the eccentric connectivity index of this nanostar dendrimer.

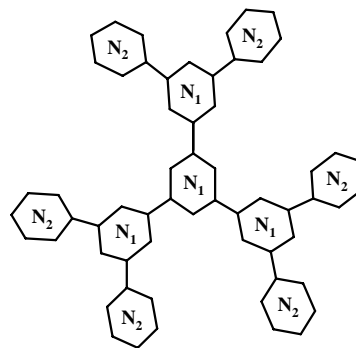


Fig. 1. The nanostar dendrimer $NS[2]$.

Consider the core of $NS[n]$ depicted in Fig. 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.

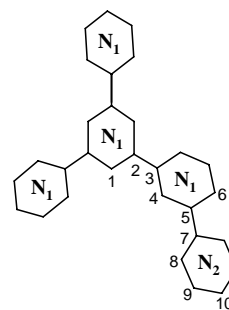


Fig. 2. The Core of dendrimer $NS[2]$.

We choose representatives from vertices of the same degree and eccentricity. In the core of NS[n], the representatives are labeled by 1, 2, 3, 4, 5 and 6, Fig. 2. By a simple calculation, we have:

$$\xi(\text{NS}[1]) = (3 \times 2 \times 7) + (3 \times 3 \times 6) + (3 \times 3 \times 7) + (6 \times 2 \times 8) + (6 \times 3 \times 9) + (3 \times 2 \times 10) = 406.$$

In the second step (when $n = 2$) we will find six new subgraphs containing a hexagon and an edge are added. We label the representative vertices of NS[2] by 7, 8, 9 and 10. In Table 1, the degrees, frequencies and eccentricities of these vertices are computed.

Table 1. The frequencies and eccentricities of vertices 7, 8, 9 and 10.

No.	Degree	Frequency	Eccentricity
7	2	3×2^i	$1+3(i-1)+3+2+3+3(n-1)+1$
8	2	$3 \times 2^{i+1}$	$2+5(i-1)+3+2+3+5(n-1)+1$
9	3 or 2	$3 \times 2^{i+1}$ or 3×2^n	$5+5(i-1)+3+2+3+5(n-1)+1$ or $5+5(n-2)+3+2+3+5(n-1)+1$
10	2	3×2^i	$6+5(i-1)+3+2+3+5(n-1)+1$

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 $V(\text{NS}[n]) - V(C)$. Then we have:

$$\begin{aligned} \xi(T) &= 9 \times \sum_{i=1}^{n-1} 2^{i+1} \times (3n + 3i + 10) + 6 \\ &\sum_{i=1}^{n-1} 2^{i+2} \times (3n + 3i + 11) + 6 \times 2^{n+1}(6n + 9) \\ &+ 9 \times \sum_{i=1}^{n-2} 2^{i+2} \times (3n + 3i + 12) + 6 \\ &\sum_{i=1}^{n-1} 2^{i+1} \times (3n + 3i + 13) \\ &= 504n \times 2^n + 438 \times 2^n - 540n - 1524. \end{aligned}$$

and,

$$\begin{aligned} \xi(C) &= 6 \times (3n + 7) + 9 \times (3n + 6) + 9 \times (3n + 7) + 12 \times \\ &(3n + 8) + 18 \times (3n + 9) \\ &+ 6 \times (3n + 10) = 180n + 477 \end{aligned}$$

From these calculations, we have $\xi(\text{NS}[n]) = 504n \times 2^n + 504 \times 2^n - 360n + 1047$.

3. Conclusions

In this paper a method for computing eccentric connectivity index of a new class of nanostar dendrimer is presented. This method is useful for working by all dendrimers. We applied our method on an infinite class of dendrimers.

References

- [1] M. H. Khalifeh, H. Yousefi-Azari, A. R. Ashrafi, Indian J. Chem. **47A**, 1503 (2008).
- [2] A. R. Ashrafi, M. Mirzargar, Indian J. Chem. **47A**, 538 (2008).
- [3] A. Karbasioun, A. R. Ashrafi, Macedonian J. Chem. Chem. Eng. **28**, 49 (2009).
- [4] H. Yousefi-Azari, A. R. Ashrafi, A. Bahrami, J. Yazdani, Asian J. Chem. **20**, 15 (2008).
- [5] H. Wiener, J. Am. Chem. Soc. **69**, 17 (1947).
- [6] V. Sharma, R. Goswami, A. K. Madan, J. Chem. Inf. Comput. Sci. **37**, 273 (1997).
- [7] S. Sardana, A. K. Madan, MATCH Commun. Math. Comput. Chem. **43**, 85 (2001).
- [8] S. Gupta, M. Singh, A. K. Madan, J. Math. Anal. Appl. **266**, 259 (2002).
- [9] M. Fischermann, A. Homann, D. Rautenbach, L. A. Szekely, L. Volkmann, Discrete Appl. Math. **122**, 127 (2002).
- [10] V. Kumar, S. Sardana, A. K. Madan, J. Mol. Model. **10**, 399 (2004).
- [11] H. Dureja, A. K. Madan, Med. Chem. Res. **16**, 331 (2007).
- [12] A. Ilic, I. Gutman, MATCH Commun. Math. Comput. Chem. (in press).
- [13] B. Zhou, Z. Du, MATCH Commun. Math. Comput. Chem. **63**, 181 (2010).
- [14] A. R. Ashrafi, T. Doslic, M. Saheli, MATCH Commun. Math. Comput. Chem. **65**, (2011), in press.
- [15] M. Ghorbani, A. R. Ashrafi, M. Hemmasi, Optoelectron. Adv. Mater.-Rapid Comm. **3**(12), 1306 (2009).
- [16] A. R. Ashrafi, M. Ghorbani, M. Jalali, Optoelectron. Adv. Mater.-Rapid Comm. **3**(8), 823 (2009).

*Corresponding author: ashrafi@kashanu.ac.ir