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Computing eccentric connectivity index of nanostar dendrimers

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Abstract: Let G be a molecular graph, the *eccentric connectivity index* of G is defined as $\xi^c(G) = \sum_{u \in V(G)} \deg(u) \cdot ecc(u)$, where $\deg(u)$ denotes the degree of vertex u and $ecc(u)$ is the largest distance between u and any other vertex v of G, namely, eccentricity of u. In this study, we present exact expressions for the eccentric connectivity index of two infinite classes of nanostar dendrimers.

Keywords: eccentric connectivity index, nanostar dendrimers, topological index, eccentricity

Introduction

Molecular descriptors are playing significant role in chemistry, pharmacology, etc. Among them, topological indices have a prominent place (Todeschini et al., 2000). There are numerous of topological descriptors that have found some applications in theoretical chemistry, especially in QSPR/QSAR research.

More recently, a new topological index, *eccentric connectivity index*, has been investigated. This topological model has been shown to give a high degree of predictability of pharmaceutical properties, and may provide leads for the development of safe and potent anti-HIV compounds. We encourage readers to consult papers (Dureja et al., 2005, 2006, 2009; Kumar et al., 2006, 2007; Lather et al., 2005; Sardana et al., 2001, 2002; Sharma et al., 1997) for some applications and papers (Morgan et al., 2010; Ilic et al., 2001; Xu X; Zhou et al., 2010; Ashrafi et al., 2011) for the mathematical properties of this topological index.

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 following articles, see (Khoramdel et al., 2008; Ashrafi et al., 2008; Karbasioun et al., 2009; Yousefi-Azari et al., 2008) for details.

Now, we introduce some notation and terminology. Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. Let $\deg(u)$ denote the degree of the vertex u in G. If $\deg(u) = 1$, then u is said to be a *pendent vertex*. An edge incident to a pendent vertex is said to be a *pendent edge*. For two vertices u and v in $V(G)$, we denote by $d(u, v)$ the distance between u and v, i.e., the length of the shortest path connecting u and v. The *eccentricity* of a vertex u in $V(G)$, denoted by $ecc(u)$, is defined to be

$ecc(u) = \max\{d(u, v) \mid v \in V(G)\}$

The *diameter* of a graph G is defined to be $\max\{ecc(u) \mid u \in V(G)\}$. The *eccentric connectivity index*, $\xi^c(G)$, of a graph G is defined as

$\xi^c(G) = \sum_{u \in V(G)} \deg(u) \cdot ecc(u)$

where $\deg(u)$ is the the degree of a vertex u and $ecc(u)$ is it's eccentricity.

The second author of this paper in some joint works computed some toplological indices of some molecular graphs related to eccentricity (Alaeiyan et al., 2013, 2015; Nejati et al., 2014, 2015). Yarahmadi investigated some topological indices of nanostar dendrimers in (Yarahmadi et al., 2010, 2011) and Ashrafi. A. R. in (Ashrafi et al., 2012) calculated eccentric connectivity index of a class of nanostar dendrimers. Also in (Nilanjan et al., 2016) Nilanjan presented exact expressions for the F-index and F-polynomial of six infinite classes of nanostar dendrimers. In this paper we computed the eccentric connectivity index of two infinite classes of nanostar dendrimers. Their structures are given in Figs. 1, 3.

Results

Suppose D_n denotes the molecular graph of a dendrimer with exactly generations depicted in Fig. 1 where $n \geq 1$. The total number of vertices and edges of D_n are calculated as $57 \times 2^{n-1} - 38$ and $33 \times 2^n - 45$ respectively. In the following theorem we calculate the eccentric connectivity index of D_n.

Theorem 1. The eccentric connectivity index of D_n is computed as

$$\xi^c(D_n) = (1188 \times 2^n - 810)n - 1485 \times 2^n + 1665.$$

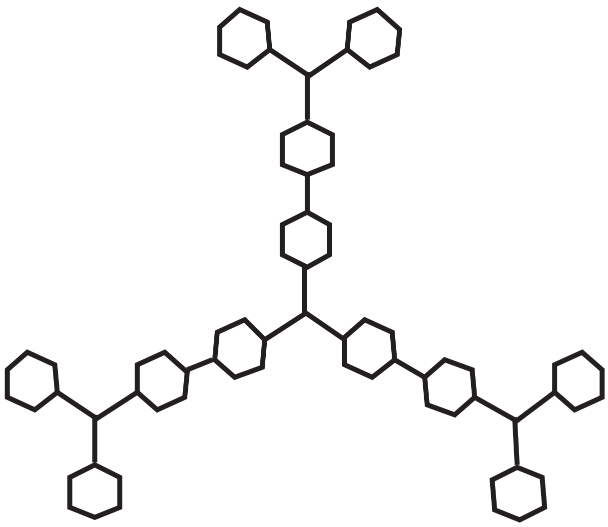

Fig. 1. The nanostar dendrimer $D_n(n = 2)$.

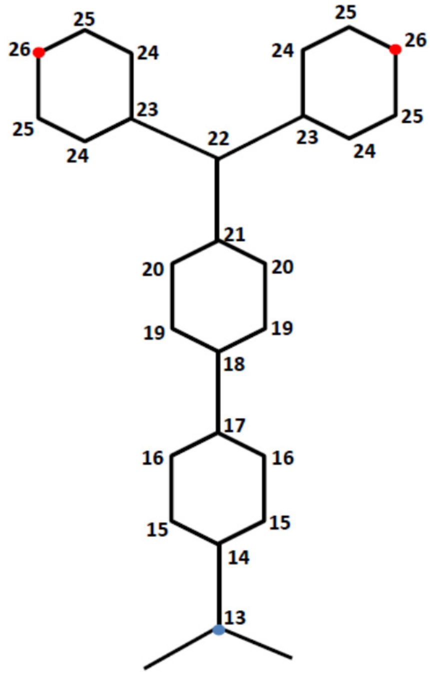

Fig. 2. The eccentricities in a third of D_2.

Proof . Considering Fig. 2 and Table. 1, it can be seen that, we have 9n-4 types of vertices in D_n, based on their eccentricities. We have $3 \times 2^{n-1}$ numbers of vertices of type1 with maximum eccentric connectivity equals to 18n-10 (red vertices). The number of vertices of type 2, 3 is 3×2^{n} and their eccentricities are 18n-11 and 18n-12 repectively. Also we have $3 \times 2^{n-1}$ numbers of vertices of type 4 with eccentric connectivity equals to 18n-13 and so it continues until we have three vertices of type 9n-5 with eccentric connectivity equals to 9n-4 and finally there is a vertex of type 9n-4 with minimum eccentric connectivity equals to 9n-5 (blue vertex). It is clear that for any vertex u in D_n, $\deg(u) = 2$ or $\deg(u) = 3$ (see Table. 1). Therefore we have

$$\xi^c(D_n) = \sum\nolimits_{u\in V(G)} \deg(u)\cdot ecc(u) =$$
$$= 2\times 3\times 2^{n-1}\times(18n-10)$$
$$+3\times 2^{n}\times 2\times(18n-11)+3\times 2^{n}\times 2\times(18n-12)$$
$$+3\times 2^{n-1}\times 3\times(18n-13)+3\times 1\times(9n-5)$$
$$+\sum_{k=0}^{n-2}\left(3\times 2^{n-2-k}\times 3\times(18n-14-9k)\right)$$
$$+\sum_{k=0}^{n-2}\left(3\times 2^{n-2-k}\times 3\times(18n-15-9k)\right)$$
$$+\sum_{k=0}^{n-2}\left(3\times 2^{n-1-k}\times 2\times(18n-16-9k)\right)$$
$$+\sum_{k=0}^{n-2}\left(3\times 2^{n-1-k}\times 2\times(18n-17-9k)\right)$$
$$+\sum_{k=0}^{n-2}\left(3\times 2^{n-2-k}\times 3\times(18n-18-9k)\right)$$
$$+\sum_{k=0}^{n-2}\left(3\times 2^{n-2-k}\times 3\times(18n-19-9k)\right)$$
$$+\sum_{k=0}^{n-2}\left(3\times 2^{n-1-k}\times 2\times(18n-20-9k)\right)$$
$$+\sum_{k=0}^{n-2}\left(3\times 2^{n-1-k}\times 2\times(18n-21-9k)\right)$$
$$+\sum_{k=0}^{n-2}\left(3\times 2^{n-2-k}\times 3\times(18n-22-9k)\right)$$
$$= 6\times 2^{n-1}\times(18n-10)+6\times 2^{n}\times(18n-11)$$
$$+6\times 2^{n}\times(18n-12)+9\times 2^{n-1}\times(18n-13)$$
$$+3\times(9n-5)+\sum_{k=0}^{n-2}\left[9\times 2^{n-2-k}\times(90n-45k-80)\right.$$
$$\left.+6\times 2^{n-1-k}\times(72n-36k-74)\right].$$

Now with simplification in MATLAB software (Matlab et al., 2012) we have

$$\xi^c(D_n) = \left(1188\times 2^{n}-810\right)n-1485\times 2^{n}+1665.$$

Then this proof is completed.

Now we consider another class of dendrimer, denoted as $NS_5(n)$ denotes the molecular graph of a dendrimer with exactly n generations depicted in Fig. 3 where $n \geq 1$.

In the following theorem we calculate the eccentric connectivity index of $NS_5(n)$.

Theorem 2. The eccentric connectivity index of $NS_5(n)$ is computed as

$$\xi^c\left(NS_5(n)\right) = \left(1200\times 2^{n}+270\right)n+2544\times 2^{n}+1275.$$

Proof . Considering Fig. 4 and Table. 2, it can be seen that, we have 5n+14 types of vertices in

Table 1. Types of vertices in D_n.

Types of Vertices	Num	*ecc*(*u*)	deg(*u*)
1	$2^{n-1} \times 3$	$18n - 10$	2
2	$2^{n} \times 3$	$18n - 11$	2
3	$2^{n} \times 3$	$18n - 12$	2
4	$2^{n-1} \times 3$	$18n - 13$	3
5	$2^{n-2} \times 3$	$18n - 14$	3
6	$2^{n-2} \times 3$	$18n - 15$	3
...	...	...	...
$9n - 6$	6	$9n - 3$	2
$9n - 5$	3	$9n - 4$	3
$9n - 4$	1	$9n - 5$	3

$NS_5(n)$, based on their eccentricities. We have 9×2^n numbers of vertices of type1 with maximum eccentric connectivity equals to 10n+28 (red vertices). Also we have 3×2^n numbers of vertices of types 2, 3 with eccentric connectivity equals to 10n+27 and 10n+26 respectively. The number of vertices of type 4 is 3×2^n and their eccentricity is 10n+25 and so it continues until we have six vertices of type 5n+13 with eccentric connectivity equals to 5n+16 and finally there are three vertices of type 5n+14 with minimum eccentric connectivity equals to 5n+15 (blue vertices). It is clear that for any vertex u in $NS_5(n)$, deg(u) = 1 or deg(u) = 2 or deg(u) = 3. (See Table. 2). Therefore we have

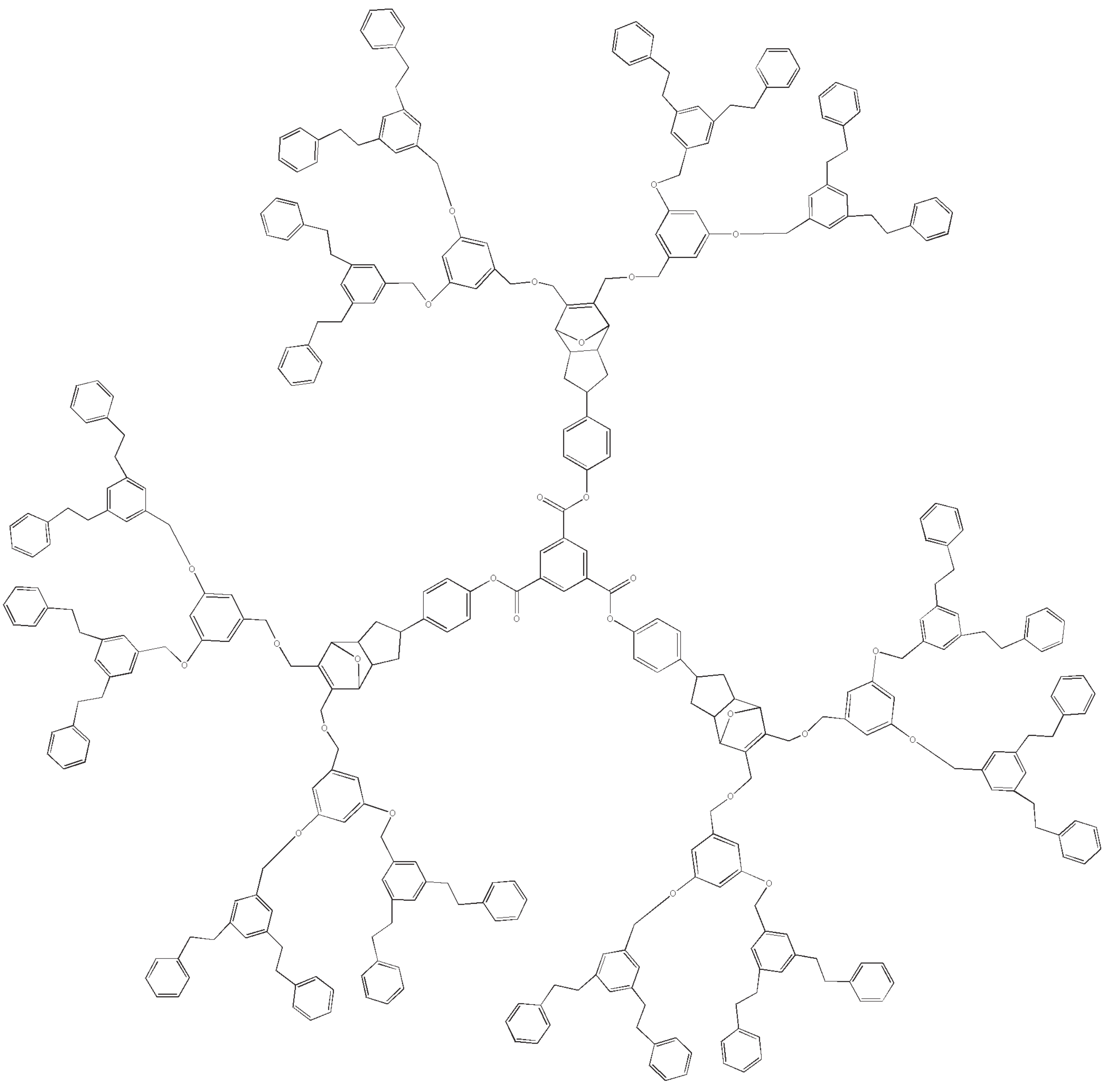

Fig. 3 Polymer dendrimer $NS_5(n)(n = 2)$.

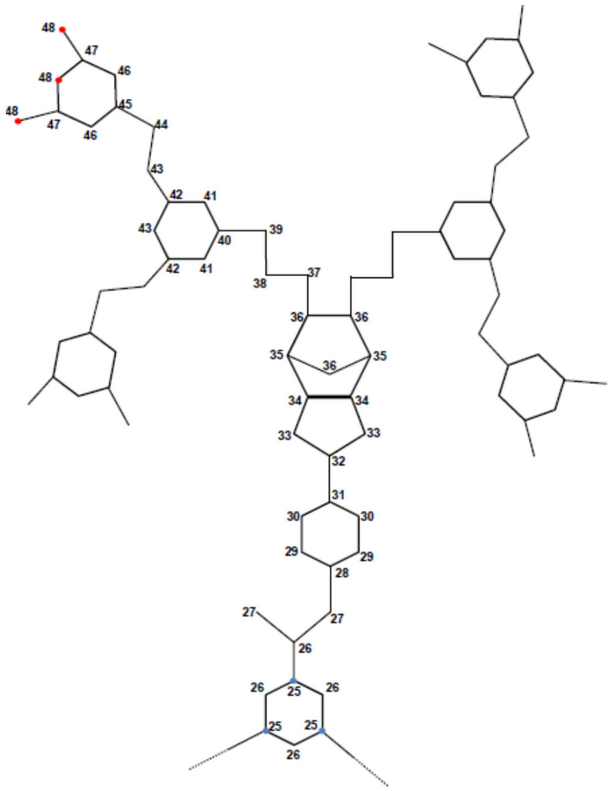

Fig. 4 The eccentricities in a third of $NS_5(2)$.

$$\xi^c\left(NS_5(n)\right)=$$

$$=\sum\nolimits_{u\in V(G)}\deg(u).ecc(u)=3\times 2^{n+1}\times(10n+28)$$

$$+3\times 2^n\times(2)\times(10n+28)+\sum_{k=1}^{n-1}\frac{3\times 2^{n+1}}{2^{k-1}}(3)(10n-5k+32)$$

$$+\sum_{k=1}^{n-1}\frac{3\times 2^{n+1}}{2^{k-1}}(2)(10n-5k+31)+$$

$$+\sum_{k=1}^{n-1}\frac{3\times 2^{n}}{2^{k-1}}(3)(10n-5k+30)$$

$$+\sum_{k=1}^{n-1}\frac{3\times 2^{n}}{2^{k-1}}(2)(10n-5k+29)+$$

$$+\sum_{k=1}^{n-1}\frac{9\times 2^{n-1}}{2^{k-1}}(2)(10n-5k+28)$$

$$+\sum_{k=1}^{2}(4-k)(12)(5n-k+33)+\sum_{k=1}^{3}(6)(2)(5n-k+30)$$

$$+\sum_{k=1}^{2}(6)(3)(5n-4k+34)+\sum_{k=1}^{2}(2)(3k)(5n-3k+29)$$

$$+\sum_{k=1}^{2}(6)(3)(5n-k+26)+\sum_{k=1}^{2}(3)(3)(5n-k+23)$$

$$+\sum_{k=1}^{2}(2)(6)(5n-k+21)+\sum_{k=1}^{2}(3)(3)(5n-2k+20)$$

$$+\sum_{k=1}^{2}(2)(3)(5n-k+18)+$$

$$+(3)(1)(5n+17)+(3)(3)(5n+15)$$

$$=12\times 2^n\times(10n+28)$$

$$+\sum_{k=1}^{n-1}\left[\frac{2^{n+1}}{2^{k-1}}(150n-75k+476)+\right.$$

$$+\frac{2^n}{2^{k-1}}(150n-75k+444)$$

$$\left.+\frac{2^{n-1}}{2^{k-1}}(180n-90k+504)\right]+\sum_{k=1}^{3}12(5n-k+30)$$

$$+\sum_{k=1}^{2}\left(600n-405k-30kn-6k^2+3411\right)+3\times(5n+17)$$

$$+9\times(5n+15).$$

Now with simplification in MATLAB software (Matlab et al,. 2012) we have

$$\xi^c\left(NS_5(n)\right)=\left(1200\times 2^n+270\right)n+2544\times 2^n+1275.$$

Then this proof is completed.

Table 2. Types of vertices in $NS_5(n)$.

Types of Vertices	Num	*ecc*(*u*)	deg(*u*)
1	$3\times 2^{n+1}$	$10n+28$	1
1	3×2^{n}	$10n+28$	2
2	$3\times 2^{n+1}$	$10n+27$	3
3	$3\times 2^{n+1}$	$10n+26$	2
4	3×2^{n}	$10n+25$	3
5	3×2^{n}	$10n+24$	2
...	...	...	...
$5n+11$	3	$5n+18$	3
$5n+12$	3	$5n+17$	2
$5n+12$	3	$5n+17$	1
$5n+13$	3	$5n+16$	3
$5n+13$	3	$5n+16$	2
$5n+14$	3	$5n+15$	3

Conclusions

The eccentric connectivity index has been employed successfully for the development of numerous mathematical models for the prediction of biological activities of diverse nature. Dendrimers are large and complex molecules with well tailored chemical structures. In this paper, exact formulas for the eccentric connectivity index of two infinite classes of nanostar dendrimers are given. It would be interesting for future study to investigate other topological indices such as edge version of eccentric connectivity index of these nanostar dendrimers.

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