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COMPUTING EDGE VERSION OF ECCENTRIC CONNECTIVITY INDEX OF NANOSTAR DENDRIMERS

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ABSTRACT. Let G be a molecular graph, the *edge version of eccentric connectivity index* of *G* are defined as $\xi_e^c(G)=\sum_{f\in E(G)}\deg(f)\cdot ecc(f)$, where $\deg(f)$ denotes the degree of an edge f and $ecc(f)$ is the largest distance between f and any other edge g of G, namely, eccentricity of f. In this paper exact formulas for the edge version of eccentric connectivity index of two classes of nanostar dendrimers were computed.

Keywords: edge eccentric connectivity index, nanostar dendrimers, topological index.

INTRODUCTION

Molecular descriptors are playing significant role in chemistry, pharmacology, etc. Among them, topological indices have a prominent place (TODESCHINI and CONSONNI, 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 the reader to consult papers (SHARMA *et al.*,1997; SARDANA and MADAN, 2001, 2002; LATHER and MADAN, 2005; DUREJA and MADAN, 2005, 2006, 2009; KUMAR and MADAN, 2007) for some applications and papers (MORGAN *et al.*, 2010; ZHOU, 2010; ASHRAFI *et al.*, 2011; ILIĆ and GUTMAN, 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 this article, see (ASHRAFI and MIRZARGAR, 2008; KHORAMDEL *et al.*, 2008; YOUSEFI-AZARI *et al.*, 2008; KARBASIOUN and ASHRAFI, 2009) 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 its eccentricity. Let $f=uv$ be an edge in $E(G)$. Then the degree of the edge f is defined to be $\deg(u)+\deg(v)-2$. For two edges $f_1=u_1v_1$, $f_1=u_2v_2$ in $E(G)$, the distance between $f_1$and f_2, denoted by $d(f_1,f_2)$, is defined to be
$d(f_1,f_2)=\min\{d(u_1,u_2),d(u_1,v_2),d(v_1,u_2),d(v_1,v_2)\}$. The *eccentricity* of an edge f, denoted by $ecc(f)$, is defined as

$$ecc(f)=\max\{d(f,e) \mid e\in E(G)\}$$

The *edge eccentric connectivity index* of G (XU and GUO, 2012), denoted by $\xi_e^{\,c}(G)$, is defined as

$$\xi_e^{\,c}(G)=\sum_{f\in E(G)}\deg(f)\cdot ecc(f)$$

The second and third author of this paper in some joint works computed the edge version of modified eccentric connectivity index of some molecular graphs (NEJATI and ALAEIYAN, 2014, 2015). In this paper exact formulas for the edge version of eccentric connectivity index of two classes nanostar dendrimers were computed.

MAIN RESULT AND DISCUSION

Suppose $NS(n)$ denotes the molecular graph of a dendrimer with exactly n generations depicted in Figure 1. The eccentric connectivity index of $NS(n)$ were obtained in (ASHRAFI and SAHELI, 2012). In the following theorem we calculate the edge eccentric connectivity index of $NS(n)$.

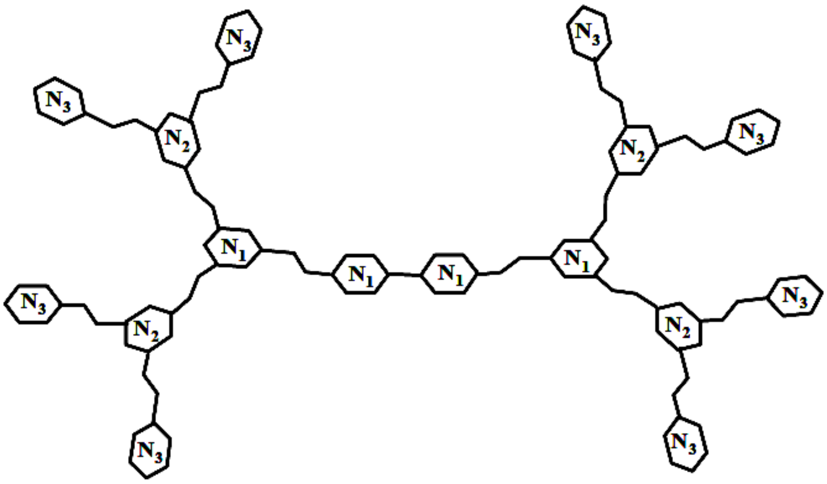

Figure 1. The molecular graph of $NS(3)$.

Theorem 1. The edge eccentric connectivity index of $NS(n)$ is computed as

$$\xi_e^c(NS(n)) = (480 \times 2^n - 80)n - 22 \times 2^n + 168 .$$

Proof. Considering Figure 2 and Table 1 we have $5n+5$ types of edges in $NS(n)$, based on their eccentricities. We have 2^{n+1} numbers of edges of type1 with maximum eccentricity equals to $10n+7$ (red edges). Also we have 2^{n+1} numbers of edges of types 2, 3 with eccentricity equals to $10n+6$ and $10n+5$ respectively. The number of edges of type 4 is 2^n and their eccentricity is $10n+4$ and so it continues until we have 4 edges of type $5n+4$ with eccentricity equals to $5n+4$ and finally there is one edge of type $5n+5$ with minimum edge eccentric connectivity equals to $5n+3$ (blue edge). Also it is clear that for any edge u in $NS(n)$, $\deg(u)=2$ or $\deg(u)=3$ except the last type of edges with minimum eccentricity such that it's degree is 4. (See Table 1).

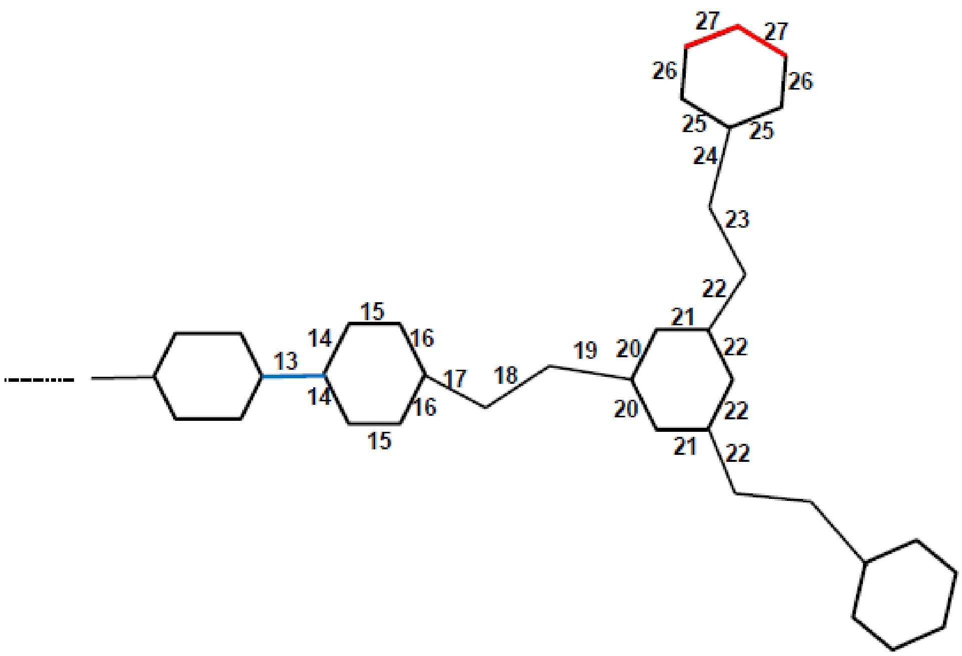

Figure 2. The eccentricity of edges in a half of $NS(2)$.

Therefore, we have

$$\xi_e^c(NS(n)) = \sum_{f\in E(G)} \deg(f)\cdot ecc(f) = 2^{n+1}\times 2\times(10n+7) + 2^{n+1}\times 2\times(10n+6)$$

$$2^{n+1}\times 3\times(10n+5) + \sum_{k=1}^{n-1}\left(\frac{2^n}{2^{k-1}}\times 3\times(10n-5k+9)\right)$$

$$+\sum_{k=1}^{n-1}\left(\frac{2^n}{2^{k-1}}\times 2\times(10n-5k+8)\right) + \sum_{k=1}^{n-1}\left(\frac{2^{n+1}}{2^{k-1}}\times 3\times(10n-5k+7)\right)$$

$$+\sum_{k=1}^{n-1}\left(\frac{2^n}{2^{k-1}}\times 3\times(10n-5k+6)\right) + \sum_{k=1}^{n-1}\left(\frac{2^n}{2^{k-1}}\times 3\times(10n-5k+5)\right)$$

$$+(2)(3)(5n+9)+(2)(2)(5n+8)+(2)(3)(5n+7)+(4)(3)(5n+6)+(4)(2)(5n+5)$$

$$+(4)(3)(5n+4)+(1)(4)(5n+3).$$

Thus, we have

$$\xi_e^c(NS(n)) = (480\times 2^n - 80)n - 22\times 2^n + 168.$$

Then this proof is completed.

Table 1. Types of edges in $NS(n)$.

Types of edges	**Num**	**ecc(f)**	**deg(f)**
1	2^{n+1}	$10n+7$	**2**
2	2^{n+1}	$10n+6$	**2**
3	2^{n+1}	$10n+5$	**3**
4	2^n	$10n+4$	**3**
5	2^n	$10n+3$	**2**
6	2^{n+1}	$10n+2$	**3**
...	**...**	**...**	**...**
5n - 2	**4**	$5n+10$	**3**
5n - 1	**2**	$5n+9$	**3**
5n	**2**	$5n+8$	**2**
5n + 1	**2**	$5n+7$	**3**
5n + 2	**4**	$5n+6$	**3**
5n + 3	**4**	$5n+5$	**2**
5n + 4	**4**	$5n+4$	**3**
5n + 5	**1**	$5n+3$	**4**

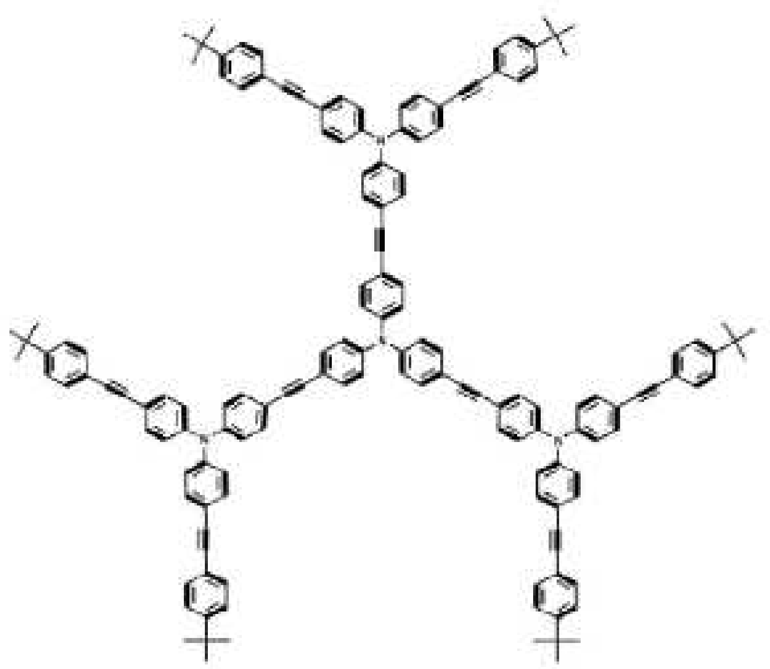

Figure 3. The molecular graph of $NSB(1)$.

One type of nanostar dendrimers is N-branched phenylacetylenes and it is shown by $NSB(n)$, some topological indices were obtained in (YARAHMADI and FATH-TABAR, 2011; YARAHMADI, 2010). In Figure 3, the molecular graph of $NSB(n)$ are shown. In Theorem 2 we obtain the edge eccentric connectivity index of $NSB(n)$.

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

$$\xi_e^c(NSB(n)) = (5292\times 2^n - 1188)n + 1593\times 2^n + 660 .$$

Proof. Considering Figure 4 and Table 2, it can be seen that, we have $9n+10$ types of edges in $NSB(n)$, based on their eccentricities. We have 9×2^n numbers of edges of type1 with maximum eccentricity equals to $18n+18$ (red edges). Also we have 3×2^n numbers of edges of types 2 with eccentricity equals to $18n+17$ and $3\times 2^{n+1}$ numbers of edges are of type 3 and the eccentricity of them equals to $18n+16$. The number of edges of type 4 is $3\times 2^{n+1}$ and their eccentricity is $18n+15$ and so it continues until we have 6 edges of type $9n+9$ with eccentricity equals to $9n+10$ and finally there are three edges of type $9n+10$ with minimum edge eccentric connectivity equals to $9n+9$ (blue edges). Also it is clear that for any edge u in $NSB(n)$, $\deg(u)=2$ or $\deg(u)=3$ or $\deg(u)=4$ except the edges of type two such that the degree of each of them is 5. (See Table 2). Therefore, we have

$$\xi_e^c(NSB(n)) = \sum\nolimits_{f\in E(G)} \deg(f)\cdot ecc(f) = 9\times 2^n \times 3\times(18n+18) + 3\times 2^n \times 5\times(18n+17)$$
$$+\sum_{k=1}^{n}\left(\frac{3\times 2^{n-1}}{2^{k-1}}\times 4\times(18n-9k+17)\right)+\sum_{k=1}^{n+1}\left(\frac{3\times 2^{n+1}}{2^{k-1}}\times 3\times(18n-9k+25)\right)$$
$$+\sum_{k=1}^{n+1}\left(\frac{3\times 2^{n+1}}{2^{k-1}}\times 2\times(18n-9k+24)\right)+\sum_{k=1}^{n+1}\left(\frac{3\times 2^{n+1}}{2^{k-1}}\times 3\times(18n-9k+23)\right)$$
$$+\sum_{k=1}^{n+1}\left(\frac{3\times 2^{n}}{2^{k-1}}\times 4\times(18n-9k+22)\right)+\sum_{k=1}^{n+1}\left(\frac{3\times 2^{n+1}}{2^{k-1}}\times 3\times(18n-9k+21)\right)$$

$$+\sum_{k=1}^{n+1}\left(\frac{3\times 2^{n+1}}{2^{k-1}}\times 2\times(18n-9k+20)\right)+\sum_{k=1}^{n+1}\left(\frac{3\times 2^{n+1}}{2^{k-1}}\times 3\times(18n-9k+19)\right)$$
$$+\sum_{k=1}^{n+1}\left(\frac{3\times 2^{n}}{2^{k-1}}\times 4\times(18n-9k+18)\right).$$

Thus, we have

$$\xi_e^c(NSB(n))=(5292\times 2^n-1188)n+1593\times 2^n+660.$$

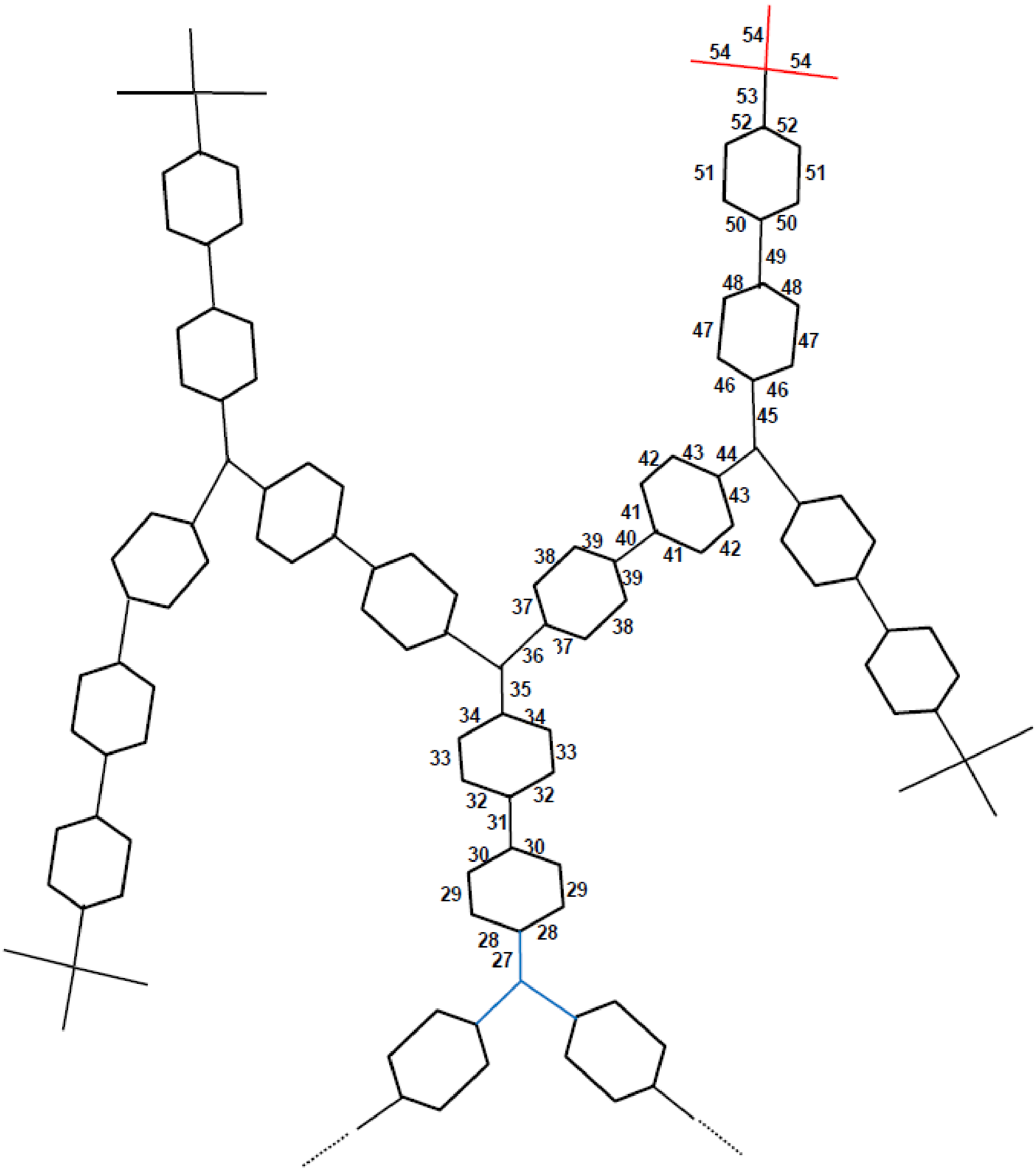

Figure 4. The eccentricity of edges in a third of $NSB(2)$.

Then this proof is completed.

Table 2. Types of edges in $NSB(n)$.

Types of edges	**Num**	$\mathbf{ecc(f)}$	$\mathbf{deg(f)}$
1	$2^n \times 9$	$18n+18$	**3**
2	$2^n \times 3$	$18n+17$	**5**
3	$2^{n+1} \times 3$	$18n+16$	**3**
4	$2^{n+1} \times 3$	$18n+15$	**2**
5	$2^{n+1} \times 3$	$18n+14$	**3**
6	$2^n \times 3$	$18n+13$	**4**
...	**...**	**...**	**...**
9n + 7	**6**	$9n+12$	**3**
9n + 8	**6**	$9n+11$	**2**
9n + 9	**6**	$9n+10$	**3**
9n + 10	**3**	$9n+9$	**4**

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