Eccentricity based topological indices of a hetrofunctional dendrimer

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In a molecular graph G with vertex set V, the eccentricity $ec(u)$ of a vertex $u \in V$ is the maximum distance between u and any other vertex of G. The eccentric connectivity index $\xi(G)$ of G is defined by $\sum_{v \in V} d(v)ec(v)$, where $d(v)$ is a degree of vertex $v \in V$. In this paper, we consider a hetrofunctional dendrimer HFD(ei) and compute its eccentric connectivity index. Moreover, we compute some eccentricity based Zagreb indices of this dendrimer.

1. Introduction

Dendrimers are macromolecules which are highly branched and possess large number of functional group distributed over dendritic framework. Due to this feature, compared to linear polymer of same molecular weight, dendrimers exhibited an array of applications such as cancer therapy and biosensors for diagnostics. Hetrofunctional dendrimers have ability to include a large and exact number of different functional group within framework without compromising the structural features. Hetrofunctional dendrimers (HFD) are today considered to have large number of potential applications than traditional dendrimers [12]. A molecular graph represents the topology a molecule, where vertices represent the atoms and edges represent the covalent bonds. Through numerical graph-theoretic invariants, one can derive chemical information which are useful in chemical documentation, structural-property correlations and chemical structural-biological activity relationships [4]. For several years, many such graphs-theoretic invarients have been studied. These graph-theocratic invarients are called topological indicies which are molecular descriptors derived from information on connectivity and composition of molecules and are used for the mathematical characterization of molecules [9]. Recently, many researchers focussed to conjecture topological indices of nanostructures by using computational tools [2, 10, 11].

Let G be an n-vertex molecular graph with vertex set $V(G)$ and edge set $E(G)$. The order and size of G are $|V(G)|$ and $|E(G)|$, respectively. The distance $d(u,v)$ between two vertices $u, v \in V(G)$ is the length of a shortest path from u to v. The eccentricity $ec(u)$ of a vertex $u \in V(G)$ is defined as

$$ec(u) = \max\{d(u,v) \,|\, v \in V(G)\}. \qquad (1)$$

One of the oldest distance based topological index is the Wiener index [13] which is defined as half sum of the distances between all pairs of vertices in a graph. Another distance based topological index of the graph G is the eccentric-connectivity index $\xi(G)$ which is defined as:

$$\xi(G) = \sum_{v \in V(G)} ec(u)d(u),$$

where $d(u)$ is the degree of a vertex $u \in V(G)$. For further detail on these and some other topological indices, we refer [1, 7, 14]. Gutman and Trinajstic [8] introduced Zagreb indices which are defined as:

$$M_1(G) = \sum_{v \in V(G)} (d(v))^2, \qquad (2)$$

$$M_2(G) = \sum_{uv \in E(G)} d(u)d(v). \qquad (3)$$

Ghorbani and Hosseinzadeh [6] introduced some same new versions of Zagreb indices which are based on eccentricity and are defined as:

$$M_1^*(G) = \sum_{v \in V(G)} (ec(v))^2, \qquad (4)$$

$$M_2^*(G) = \sum_{uv \in E(G)} ec(u)ec(v). \qquad (5)$$

Farooq and Malik [5] computed the eccentric-connectivity index and eccentricity based Zagreb indices for some infinite families of nanostar dendrimers. Ashrafi and Saheli [3] also obtained the eccentric connectivity index of some families of nanostar

dendrimers. In this paper, we select the interior and exterior HFD(ei) possessed internal hydroxyl group and peripheral allyls group and compute its eccentric connectivity index ξ. Moreover, we also compute eccentricity based Zagreb indices M_1^* and M_2^* of this dendrimer.

2. HFD(ei) dendrimer

HFD are considered as state-of-art macromolecules having a large number of potential applications. With respect to positions of hetrofunctional group in HFD, there are following three possibilities: external (e); internal (i); or combination of external and internal (ei). In this paper, we select a HFD(ei)-G3-e(allyl)16-i-(hydroxyl)28 denoted by $D[n]$ and shown in Fig. 1, which is an HFD with internal hydroxyl and peripheral allyl group. The graphs corresponding to different growth stages are shown in Fig. $2-3$. It is evident that order and size of $D[n]$ are equal. The order and size of $D[n]$ is given below:

$$|V(D[n])| = |E(D[n])| = \begin{cases} 16 \times 2^{t+1} + 8 \times 2^t - 38 & \text{if } n = 2t, t \geq 1 \\ 24 \times 2^{t+1} - 38 & \text{if } n = 2t+1, t \geq 0. \end{cases}$$
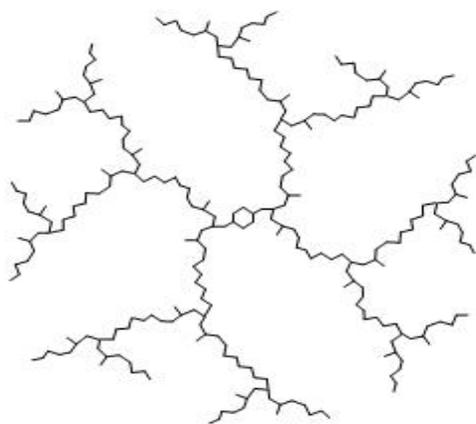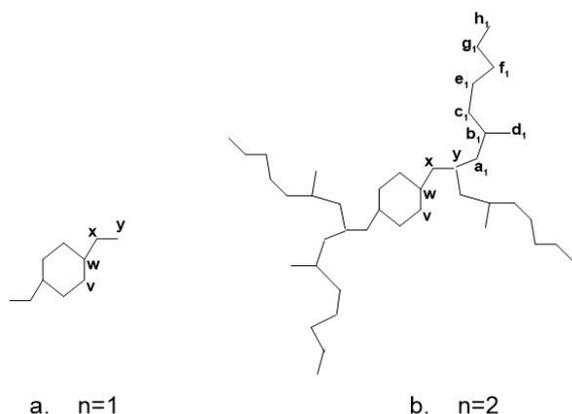

Fig. 1: $D[n]$ with $n = 6$.

a. n=1   b. n=2

Fig. 2: $D[n]$ with the $n = 1$ (the core) and $n = 2$.

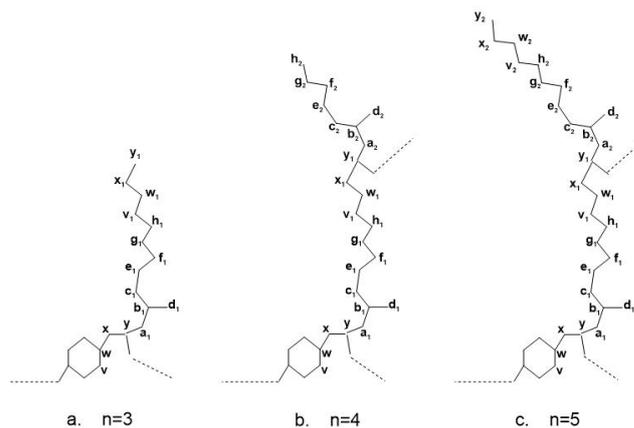a. n=3   b. n=4   c. n=5

Fig. 3: One branch of $D[n]$ with $n = 3, 4$ and 5.

3. The eccentric connectivity index

This section is devoted to the computation of the eccentric connectivity index of the dendrimer $D[n]$ shown in Fig. 1.

Theorem 3.1 The eccentric connectivity index of $D[n]$ for $n = 2t+1$ where $t \geq 0$ is given by

$$\xi(D[n]) = 2112t \times 2^t - 936 \times 2^t - 836t + 1036. \quad (6)$$

Proof. Using symmetry of the nanostar dendrimer $D[n]$, we use only one branch of $D[n]$ as labeled in Fig. $2-3$. We take one representative from a set of vertices which have same degree and eccentricity. These representatives are labeled by v, w, x, y, a_i, b_i, c_i, d_i, e_i, f_i, g_i, h_i, v_i, w_i, x_i, y_i. Here $1 \leq i \leq \dfrac{n-1}{2}$ when $n \geq 3$. The representatives of vertices of $D[n]$ with their degrees, eccentricities and frequencies of occurrence are given as follows.

Table 1: The vertices introduced for the core (first generation) with their degree, eccentricity and frequency for $n \geq 1$,

Representative	Degree	Eccentricity	Frequency
v	2	$11t+4$	4
w	3	$11t+5$	2
x	2	$11t+6$	2
y $(n=1)$	1	7	2
y $(n \neq 1)$	3	$11t+7$	2

where n is odd.

Table 2: *The vertices introduced at second generation with their degree, eccentricity and frequency for* $n \geq 3$*, where* n *is odd.*

Representative	Degree	Eccentricity	Frequency
a_i	2	$11t + 11i - 3$	2^{i+1}
b_i	3	$11t + 11i - 2$	2^{i+1}
c_i	2	$11t + 11i - 1$	2^{i+1}
d_i	1	$11t + 11i - 1$	2^{i+1}
e_i	2	$11t + 11i$	2^{i+1}
f_i	2	$11t + 11i + 1$	2^{i+1}
g_i	2	$11t + 11i + 2$	2^{i+1}
h_i	2	$11t + 11i + 3$	2^{i+1}

Table 3: *The vertices introduced at third generation with their degree, eccentricity and frequency for* $n \geq 3$*, where* n *is odd.*

Representative	Degree	Eccentricity	Frequency
v_i	2	$11t + 11i + 4$	2^{i+1}
w_i	2	$11t + 11i + 5$	2^{i+1}
x_i	2	$11t + 11i + 6$	2^{i+1}
$y_i(i = t)$	1	$11t + 11i + 7$	2^{i+1}
$y_i(i \neq t)$	3	$11t + 11i + 7$	2^{i+1}

When $n = 1$ then $t = 0$. Using Table 1, the eccentric connectivity index of $D[1]$ can be written as follows:

$$\xi(D[1]) = \sum_{u \in D[n]} d(u)\varepsilon(u)$$
$$= (4 \times 2 \times 4) + (2 \times 3 \times 5) + (2 \times 2 \times 6) + (2 \times 1 \times 7)$$
$$= 100$$
$$= 2112(0) \times 2^0 - 936 \times 2^0 - 836(0) + 1036.$$

When $n = 3$ then $t = 1$. Using Tables 1 and 2, the eccentric connectivity index of $D[3]$ can be written as follows:

$$\xi(D[3]) = \sum_{u \in D[n]} d(u)\varepsilon(u)$$
$$= ((4 \times 2 \times 15) + (2 \times 3 \times 16) + (2 \times 2 \times 17) + (2 \times 3 \times 18)) + ((4 \times 2 \times 19) + (4 \times 3 \times 20)$$
$$+ (4 \times 2 \times 21) + (4 \times 1 \times 21) + (4 \times 2 \times 22) + (4 \times 2 \times 23) + (4 \times 2 \times 24) + (4 \times 2 \times 25))$$
$$+ ((4 \times 2 \times 26) + (4 \times 2 \times 27) + (4 \times 2 \times 28) + (4 \times 1 \times 29))$$
$$= 2552$$
$$= 2112(1) \times 2^1 - 936 \times 2^1 - 836(1) + 1036.$$

When $n \geq 5$, then using Tables $1 - 3$, the eccentric connectivity index is obtained as follows:

$$\xi(D[n]) = \sum_{u \in D[n]} d(u)ec(u)$$

$$= ((2 \times 4) \times (11t + 4) + (3 \times 2) \times (11t + 5) + (2 \times 2) \times (11t + 6)$$
$$+ (3 \times 2) \times (11t + 7)) + \sum_{i=1}^{t} (2 \times 2^{i+1} \times (11t + 11i - 3)$$
$$+ 3 \times 2^{i+1} \times (11t + 11i - 2) + 2 \times 2^{i+1} \times (11t + 11i - 1)$$
$$+ 2^{i+1} \times (11t + 11i - 1) + 2 \times 2^{i+1} \times (11t + 11i)$$
$$+ 2 \times 2^{i+1} \times (11t + 11i + 1) + 2 \times 2^{i+1} \times (11t + 11i + 2)$$
$$+ 2 \times 2^{i+1} \times (11t + 11i + 3)) + \sum_{i=1}^{t} (2 \times 2^{i+1} \times (11t + 11i + 4)$$

$$+ 2 \times 2^{i+1} \times (11t + 11i + 5) + 2 \times 2^{i+1} \times (11t + 11i + 6))$$
$$+ \sum_{i=1}^{t-1} (3 \times 2^{i+1} \times (11t + 11i + 7) + 1 \times 2^{t+1} \times (22t + 7))$$
$$= 2112t \times 2^t - 936 \times 2^t - 836t + 1036.$$

The proof is complete.

Theorem 3.2 *The eccentric connectivity index of* $D[n]$, *for* $n = 2t$*, where* $t \geq 1$ *is given by*

$$\xi(D[n]) = 1760t \times 2^t - 1336 \times 2^t - 836 \times t + 1340. \ (7)$$

Proof. Using symmetry of the nanostar dendrimer $D[n]$, we use only one branch of $D[n]$ as labeled in Fig. $2 - 3$. We take one representative from a set of vertices which have same degree and eccentricity. These representatives

are labeled by v, w, x, y, a_i, b_i, c_i, d_i, e_i, f_i, g_i, h_i. Here $1 \le i \le \dfrac{n}{2}$.

Table 4: The vertices introduced for the core (first generation)
with their degree, eccentricity and frequency
for $n \ge 2$, where n is even

Representative	Degree	Eccentricity	Frequency
v	2	$11t$	4
w	3	$11t+1$	2
x	2	$11t+2$	2
y	3	$11t+3$	2

Table 5: The vertices introduced at second generation with their
degree, eccentricity and frequency for $n \ge 2$, where n is even

Representative	Degree	Eccentricity	Frequency
a_i	2	$11t+11i-7$	2^{i+1}
b_i	3	$11t+11i-6$	2^{i+1}
c_i	2	$11t+11i-5$	2^{i+1}
d_i	1	$11t+11i-5$	2^{i+1}
e_i	2	$11t+11i-4$	2^{i+1}

Representative	Degree	Eccentricity	Frequency
f_i	2	$11t+11i-3$	2^{i+1}
g_i	2	$11t+11i-2$	2^{i+1}
$h_i\,(i=t)$	1	$11t+11i-1$	2^{i+1}
$h_i\,(i \ne t)$	2	$11t+11i-1$	2^{i+1}

Now we take representative from a set of vertices which are introduce at $n = 3$ and have same degree and eccentricity also. These representatives are labeled v_i, w_i, x_i, y_i. Here $1 \le i \le t-1$ and $t = n/2$.

Table 6: The vertices introduced at third generation with their
degree, eccentricity and frequency for $n \ge 4$, where n is even

Representative	Degree	Eccentricity	Frequency
v_i	2	$11t+11i$	2^{i+1}
w_i	2	$11t+11i+1$	2^{i+1}
x_i	2	$11t+11i+2$	2^{i+1}
y_i	3	$11t+11i+3$	2^{i+1}

When $n = 2$ then $t = 1$. Using Table 4, we get

$$
\begin{aligned}
\xi(D[2]) &= \sum_{u \in V(D[n])} d(u)ec(u) \\
&= ((4\times 2\times 11)+(2\times 3\times 12)+(2\times 2\times 13)+(2\times 3\times 14))+((4\times 2\times 15)+(4\times 3\times 16) \\
&\quad +(4\times 2\times 17)+(4\times 1\times 17)+(4\times 2\times 18)+(4\times 2\times 19)+(4\times 2\times 20)+(4\times 1\times 21)) \\
&= 1352 \\
&= 1760(1)\times 2^1 - 1336\times 2^1 - 836\times 1 + 1340.
\end{aligned}
$$

When $n \ge 4$, then using Tables $4-6$, the eccentric connectivity index of $D[n]$ can be written as follows.

$$
\begin{aligned}
\xi(D[n]) &= \sum_{u \in D[n]} d(u)ec(u) \\
&= (2\times 4\times 11t+(3\times 2)\times(11t+1)+(2\times 2)\times(11t+2)+(3\times 2)\times(11t+3)) \\
&\quad +(\sum_{i=1}^{t}(2\times 2^{i+1}\times(11t+11i-7)+3\times 2^{i+1}\times(11t+11i-6) \\
&\quad +2\times 2^{i+1}\times(11t+11i-5)+1\times 2^{i+1}\times(11t+11i-5)+2\times 2^{i+1}\times(11t+11i-4) \\
&\quad +2\times 2^{i+1}\times(11t+11i-3)+2\times 2^{i+1}\times(11t+11i-2)) \\
&\quad +\sum_{t=1}^{t-1}(2\times 2^{i+1}\times(11t+11i-1))+(1\times 2^{t+1}\times(22t-1))) \\
&\quad +(\sum_{i=1}^{t-1}(2\times 2^{i+1}\times(11t+11i)+2\times 2^{i+1}\times(11t+11i+1) \\
&\quad +2\times 2^{i+1}\times(11t+11i+2)+3\times 2^{i+1}\times(11t+11i+3))), \\
&= 1760t\times 2^t - 1336\times 2^t - 836\times t + 1340.
\end{aligned}
$$

The proof is complete.

4. Eccentricity based Zagreb indices

This section deals with some eccentricity based Zagreb indices defined by Equations (4) and (5).

Theorem 4.1 *The second Zagreb eccentricity index* M_1^* *of* $D[n]$, *for* $n = 2t+1$, *where* $t \geq 0$ *is given by*

$$M_1^*(D[n]) = 23232t^2 \times 2^t - 19536t \times 2^t - 4598t^2 + 16196 \times 2^t + 10912t - 15912. \qquad (8)$$

Proof. When $n = 1$ then $t = 0$. We use Table 1 to get

$$M_1^*(D[1]) = \sum_{v \in V(D[1])} (ec(v))^2$$
$$= 4 \times (4)^2 + 2 \times (5)^2 + 2 \times (6)^2 + 2 \times (7)^2$$
$$= 284$$
$$= 23232(0^2) \times 2^0 - 19536(0) \times 2^0 - 4598(0^2) + 16196 \times 2^0 + 10912(0) - 15912.$$

When $n = 3$ then $t = 1$. We use Tables 1-2 to get

$$M_1^*(D[3]) = \sum_{v \in V(D[3])} (ec(v))^2$$
$$= (4 \times (15)^2 + 2 \times (16)^2 + 2 \times (17)^2 + 2 \times (18)^2) + (4 \times (19)^2 + 4 \times (20)^2 +$$
$$4 \times (21)^2 + 4 \times (21)^2 + 4 \times (22)^2 + 4 \times (23)^2 + 4 \times (24)^2 + 4 \times (25)^2) +$$
$$(4 \times (26)^2 + 4 \times (27)^2 + 4 \times (28)^2 + 4 \times (29)^2)$$
$$= 30186$$
$$= 23232(1^2) \times 2^1 - 19536(1) \times 2^1 - 4598(1^2) + 16196 \times 2^1 + 10912(1) - 15912.$$

When $n \geq 5$, then we use Tables $1-3$ to get

$$M_1^*(D[n]) = \sum_{v \in V(D[n])} (ec(v))^2$$
$$= (4 \times (11t+4)^2 + 2 \times (11t+5)^2 + 2 \times (11t+6)^2 + 2 \times (11t+7)^2)$$
$$+ (\sum_{i=1}^{t} (2^{i+1} \times (11t+11i-3)^2 + 2^{i+1} \times (11t+11i-2)^2 +$$
$$2^{i+1} \times (11t+11i-1)^2 + 2^{i+1} \times (11t+11i-1)^2 + 2^{i+1} \times (11t+11i)^2 +$$
$$2^{i+1} \times (11t+11i+1)^2 + 2^{i+1} \times (11t+11i+2)^2 + 2^{i+1} \times (11t+11i+3)^2))$$
$$+ (\sum_{i=1}^{t} (2^{i+1} \times (11t+11i+4)^2 + 2^{i+1} \times (11t+11i+5)^2 + 2^{i+1} \times (11t+11i+6)^2) +$$
$$\sum_{i=1}^{t-1} (2^{i+1} \times (11t+11i+7)^2) + (2^{t+1} \times (22t+7)^2))$$
$$= 23232t^2 \times 2^t - 19536t \times 2^t - 4598t^2 + 16196 \times 2^t + 10912t - 15912.$$

The proof is complete.

Theorem 4.2 *The second Zagreb-eccentricity index* M_1^* *of* $D[n]$, *for* $n = 2t$, *where* $t \geq 1$ *is given by*

$$M_1^*(D[n]) = 19360t^2 \times 2^t - 28512t \times 2^t - 4598t^2 + 20488 \times 2^t + 14256t - 20488. \qquad (9)$$

Proof. When $n = 2$ then $t = 1$. Using Table 4, we get

$$M_1^*(D[2]) = \sum_{v \in V} [ec(v)]^2$$

$$= (4 \times (11)^2 + 2 \times (12)^2 + 2 \times (13)^2 + 2 \times (14)^2) + (4 \times (15)^2 + 4 \times (16)^2 +$$
$$4 \times (17)^2 + 4 \times (17)^2 + 4 \times (18)^2 + 4 \times (19)^2 + 4 \times (20)^2 + 4 \times (21)^2) +$$
$$= 11824$$
$$= 19360(1^2) \times 2^1 - 28512(1) \times 2^1 - 4598(1^2) + 20488 \times 2^1 + 14256(1) - 20488.$$

When $n \geq 4$, the using Tables $4-6$, we get

$$M_1^*(D[n]) = \sum_{v \in V(D[n])} (ec(v))^2$$

$$= (4 \times (11t)^2 + 2 \times (11t+1)^2 + 2 \times (11t+2)^2 + 2 \times (11t+3)^2) +$$

$$(\sum_{i=1}^{t} (2^{i+1} \times (11t+11i-7)^2 + 2^{i+1} \times (11t+11i-6)^2 +$$

$$2^{i+1} \times (11t+11i-5)^2 + 2^{i+1} \times (11t+11i-5)^2 +$$

$$2^{i+1} \times (11t+11i-4)^2 + 2^{i+1} \times (11t+11i-3)^2 +$$

$$2^{i+1} \times (11t+11i-2)^2) + \sum_{i=1}^{t-1} (2^{i+1} \times (11t+11i-1)^2)$$

$$+ (1 \times 2^{t+1} \times (22t-1)^2)) + (\sum_{i=1}^{t-1} (2^{i+1} \times (11t+11i)^2 +$$

$$2^{i+1} \times (11t+11i+1)^2 + 2^{i+1} \times (11t+11i+2)^2 +$$

$$+ 2^{i+1} \times (11t+11i+3)^2))$$
$$= 19360t^2 \times 2^t - 28512t \times 2^t - 4598t^2 + 20488 \times 2^t + 14256t - 20488.$$

The proof is complete.

Theorem 4.3 *The third Zagreb eccentricity index*
$M_2^*(D[n])$ *of* $D[n]$ *for* $n = 2t+1$, *is given by*

$$M_2^*(D[n]) = \begin{cases} 256 & \text{if } t = 0, \\ 23232t^2 \times 2^t - 20592t \times 2^t - 4598t^2 & \\ + 16640 \times 2^t + 11396t - 16384. & \text{if } t \geq 1. \end{cases}$$

Proof. Using symmetry of the nanostar dendrimer $D[n]$, we use only one branch of $D[n]$ as labeled in Fig. 2-3. We take one representative from a set of vertices which have same degree and eccentricity. These representatives are labeled by u, v, w, x, y, a_i, b_i, c_i, d_i, e_i, f_i, g_i, h_i.

Table 7: The edge partition of $D[n]$, with respect to the representatives of pair of end-vertices and their frequency of occurrence. The eccentricities are taken from Table 1, Table 2 and Table 3, Here n is odd, $t = \dfrac{n-1}{2}$, $1 \leq i \leq t-1$.

Representative	Eccentricity	Frequency
$[u,v]$	$[11t+4, 11t+4]$	2
$[v,w]$	$[11t+4, 11t+5]$	2^2
$[w,x]$	$[11t+5, 11t+6]$	2
$[x,y]$	$[11t+6, 11t+7]$	2
$[y,a_1]$	$[11t+7, 11t+8]$	2^2
$[a_1,b_1]$	$[11t+8, 11t+9]$	2^2
$[b_1,c_1]$	$[11t+9, 11t+10]$	2^3
$[c_1,e_1]$	$[11t+10, 11t+11]$	2^2
$[e_1,f_1]$	$[11t+11, 11t+12]$	2^2
$[f_1,g_1]$	$[11t+12, 11t+13]$	2^2
$[g_1,h_1]$	$[11t+13, 11t+14]$	2^2
$[h_1,v_1]$	$[11t+14, 11t+15]$	2^2
$[v_1,w_1]$	$[11t+15, 11t+16]$	2^2
$[w_1,x_1]$	$[11t+16, 11t+17]$	2^2
$[x_1,y_1]$	$[11t+17, 11t+18]$	2^2

Representative	Eccentricity	Frequency
$[y_i, a_{i+1}]$	$[11t+11i+7, 11t+11(i+1)-3]$	2^{i+2}
$[a_{i+1}, b_{i+1}]$	$[11t+11(i+1)-3, 11t+11(i+1)-2]$	2^{i+2}
$[b_{i+1}, c_{i+1}]$	$[11t+11(i+1)-2, 11t+11(i+1)-1]$	2^{i+3}
$[c_{i+1}, e_{i+1}]$	$[11t+11(i+1)-1, 11t+11(i+1)]$	2^{i+2}
$[e_{i+1}, f_{i+1}]$	$[11t+11(i+1), 11t+11(i+1)+1]$	2^{i+2}
$[f_{i+1}, g_{i+1}]$	$[11t+11(i+1)+1, 11t+11(i+1)+2]$	2^{i+2}
$[g_{i+1}, h_{i+1}]$	$[11t+11(i+1)+2, 11t+11(i+1)+3]$	2^{i+2}
$[h_{i+1}, v_{i+1}]$	$[11t+11(i+1)+3, 11t+11(i+1)+4]$	2^{i+2}
$[v_{i+1}, w_{i+1}]$	$[11t+11(i+1)+4, 11t+11(i+1)+5]$	2^{i+2}
$[w_{i+1}, x_{i+1}]$	$[11t+11(i+1)+5, 11t+11(i+1)+6]$	2^{i+2}
$[x_{i+1}, y_{i+1}]$	$[11t+11(i+1)+6, 11t+11(i+1)+7]$	2^{i+2}

When $n=1$ then $t=0$. We use Table 1 to compute M_2^* as follows:

$$M_2^*(D[1]) = \sum_{uv \in E} ec(u)ec(v)$$

$$= 2 \times (4 \times 4) + 4 \times (4 \times 5) + 2 \times (5 \times 6) + 2 \times (6 \times 7)$$

$$= 256.$$

When $n=3$, we have $t=1$, Using Table 1 and Table 2, we compute M_2^* as follows:

$$M_2^*(D[3]) = \sum_{uv \in E} ec(u)ec(v)$$

$$= (2 \times (15 \times 15) + 4 \times (15 \times 16) + 2 \times (16 \times 17) + 2 \times (7 \times 18)) + (4 \times (18 \times 19) +$$
$$4 \times (19 \times 20) + 4 \times (20 \times 21) + 4 \times (20 \times 21) + 4 \times (21 \times 22) + 4 \times (22 \times 23) +$$
$$4 \times (23 \times 24) + 4 \times (24 \times 25)) + (4 \times (25 \times 26) + 4 \times (26 \times 27) + 4 \times (28 \times 29))$$

$$= 28974.$$

When $n \geq 5$, we use Tables $1-3$ to compute M_2^* as follows:

$$M_2^*(D[n]) = \sum_{uv \in E} ec(u)ec(v) = 2 \times (11t+4) \times (11t+4) + 4 \times (11t+4) \times (11t+5) +$$

$$2 \times (11t+5) \times (11t+6) + 2 \times (11t+6) \times (11t+7) + 4 \times (11t+7) \times (11t+8) + 2^2 \times (11t+8) \times (11t+9) +$$

$$2^3 \times (11t+9) \times (11t+10) + 2^2 \times (11t+10) \times (11t+11) + 2^2 \times (11t+11) \times (11t+12) + 2^2 \times (11t+12) \times (11t+13)$$

$$+ 2^2 \times (11t+13) \times (11t+14) + 2^2 \times (11t+14) \times (11t+15) + 2^2 \times (11t+15) \times (11t+16) + 2^2 \times (11t+16) \times (11t+17) +$$

$$2^2 \times (11t+17) \times (11t+18) + \sum_{i=1}^{t-1} (2^{i+2} \times (11t+11i+7) \times (11t+11(i+1)-3) +$$

$$2^{i+2} \times (11t+11(i+1)-3) \times (11t+11(i+1)-2) + 2^{i+3} \times (11t+11(i+1)-2) \times (11t+11 \times (i+1)-1) +$$

$$2^{i+2} \times (11t+11(i+1)-1) \times (11t+11(i+1)) + 2^{i+2} \times (11t+11(i+1)) \times (11t+11(i+1)+1) +$$

$$2^{i+2} \times (11t+11(i+1)+1) \times (11t+11(i+1)+2) + 2^{i+2} \times (11t+11(i+1)+2)(11t+11(i+1)+3) +$$

$$2^{i+2} \times (11t+11(i+1)+3) \times (11t+11(i+1)+4) + 2^{i+2} \times (11t+11(i+1)+4) \times (11t+11(i+1)+5) +$$

$$2^{i+2} \times (11t+11(i+1)+5) \times (11t+11(i+1)+6) + 2^{i+2} \times (11t+11(i+1)+6) \times (11t+11(i+1)+7))$$

$$= 23232t^2 \times 2^t - 20592t \times 2^t - 4598t^2 + 16640 \times 2^t + 11396t - 16384.$$

This completes the proof.

Theorem 4.4 *The third Zagreb eccentricity index of* $D[n]$

for $n = 2t$ *where* $t \geq 1$ *is given by*

$$M_2^*(D[n]) = \begin{cases} 11214 & \text{if } n = 2, \\ 19360t^2 \times 2^t - 29392t \times 2^t - 4598t^2 + 21136 \times 2^t + 14740t - 21136. & \text{if } n > 2. \end{cases}$$

Proof.

Table 8: The edge partition of $D[n]$ with respect to the representatives of pair of end-vertices and their frequency of occurrence.

The eccentricities are taken from Table 4, Table 5 and Table 6. Here n is even, $t = \dfrac{n}{2}$, $1 \leq i \leq t-1$.

Representative	Eccentricity	Frequency
$[u, v]$	$[11t, 11t]$	2
$[v, w]$	$[11t, 11t + 1]$	2^2
$[w, x]$	$[11t + 1, 11t + 2]$	2
$[x, y]$	$[11t + 2, 11t + 3]$	2
$[y, a_1]$	$[11t + 3, 11t + 4]$	2^2
$[a_i, b_i]$	$[11t + 11i - 7, 11t + 11i - 6]$	2^{i+1}
$[b_i, c_i]$	$[11t + 11i - 6, 11t + 11i - 5]$	2^{i+2}
$[c_i, e_i]$	$[11t + 11i - 5, 11t + 11i - 4]$	2^{i+1}
$[e_i, f_i]$	$[11t + 11i - 4, 11t + 11i - 3]$	2^{i+1}
$[f_i, g_i]$	$[11t + 11i - 3, 11t + 11i - 2]$	2^{i+1}
$[g_i, h_i]$	$[11t + 11i - 2, 11t + 11i - 1]$	2^{i+1}
$[h_i, v_i]$	$[11t + 11i - 1, 11t + 11i]$	2^{i+1}
$[v_i, w_i]$	$[11t + 11i, 11t + 11i + 1]$	2^{i+1}
$[w_i, x_i]$	$[11t + 11i + 1, 11t + 11i + 2]$	2^{i+1}
$[x_i, y_i]$	$[11t + 11i + 2, 11t + 11i + 3]$	2^{i+1}
$[y_i, a_{i+1}]$	$[11t + 11i + 3, 11t + 11(i+1) - 7]$	2^{i+2}
$[a_t, b_t]$	$[22t - 7, 22t - 6]$	2^{t+1}
$[b_t, c_t]$	$[22t - 6, 22t - 5]$	2^{t+2}
$[c_t, e_t]$	$[22t - 5, 22t - 4]$	2^{t+1}
$[e_t, f_t]$	$[22t - 4, 22t - 3]$	2^{t+1}
$[f_t, g_t]$	$[22t - 3, 22t - 2]$	2^{t+1}
$[g_t, h_t]$	$[22t - 2, 22t - 1]$	2^{t+1}

When $n = 2$ then $t = 1$. We have

$$M_2^*(D[2]) = \sum_{uv \in E(D[2])} ec(u)ec(v)$$

$= 2 \times (11 \times 11) + 4 \times (11 \times 12) + 2 \times (12 \times 13) + 2 \times (13 \times 14)$

$+ 4 \times (14 \times 15) + 4 \times (15 \times 16) + 8 \times (17 \times 18) + 4 \times (17 \times 18)$

$+ 4 \times (18 \times 19) + 4 \times (19 \times 20) + 4 \times (20 \times 21)$

$= 11214.$

When $n \geq 4$ then using Tables $4 - 6$, we have

$$M_2^*(D[n]) = \sum_{uv \in E(D[n])} ec(u)ec(v)$$

$$= 2 \times (11t) \times (11t) + 4 \times (11t) \times (11t+1) + 2 \times (11t+1) \times (11t+2)$$
$$+ 2 \times (11t+2) \times (11t+3) + 4 \times (11t+3) \times (11t+4)$$
$$+ \sum_{i=1}^{t-1} (2^{i+1} \times (11t+11i-7) \times (11t+11i-6)$$
$$+ 2^{i+2} \times (11t+11i-6) \times (11t+11i-5) + 2^{i+1} \times (11t+11i-5)$$
$$\times (11t+11i-4) + 2^{i+1} \times (11t+11i-4) \times (11t+11i-3)$$
$$+ 2^{i+1} \times (11t+11i-3) \times (11t+11i-2)$$
$$+ 2^{i+1} \times (11t+11i-2) \times (11t+11i-1) + 2^{i+1} \times (11t+11i-1)$$
$$\times (11t+11i) + 2^{i+1} \times (11t+11i) \times (11t+11i+1)$$
$$+ 2^{i+1} \times (11t+11i+1) \times (11t+11i+2) + 2^{i+1} \times (11t+11i+2)$$
$$\times (11t+11i+3) + 2^{i+2} \times (11t+11i+3) \times (11t+11(i+1)-7))$$
$$+ 2^{t+1} \times (11t+11t-7) \times (11t+11t-6) + 2^{t+2} \times (11t+11t-6)$$
$$\times (11t+11t-5) + 2^{t+1} \times (11t+11t-5) \times (11t+11t-4)$$
$$+ 2^{t+1} \times (11t+11t-4) \times (11t+11t-3) + 2^{t+1} \times (11t+11t-3)$$
$$\times (11t+11t-2) + 2^{t+1} \times (11t+11t-2) \times (11t+11t-1)$$
$$= 19360t^2 \times 2^t - 29392t \times 2^t - 4598t^2 + 21136 \times 2^t + 14740t - 21136.$$

This completes the proof.

5. Conclusion

In this paper, we consider a family of hetrofunctional dendrimer HFD(ei) and compute their eccentric connectivity indices. We also compute some eccentricity based Zagreb indices for this famly of nanosar dendrimer.

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