Iranian Journal of Mathematical Chemistry, Vol. 3, Supplement 1, December 2012, pp. s7 – s18 **IJMC**

Eccentric Connectivity Index of Some Dendrimer Graphs

MODJTABA GHORBANI•, KHADIJEH MALEKJANI AND ALI KHAKI

Department of Mathematics, Faculty of Science, Shahid Rajaee Teacher Training University, Tehran, 16785 – 136, I. R. Iran;

(*Received March 6, 2011*)

ABSTRACT

The eccentricity connectivity index of a molecular graph G is defined as $\xi(G) = \Sigma_{a\in V(G)} \deg(a)\varepsilon(a)$, where $\varepsilon(a)$ is defined as the length of a maximal path connecting a to other vertices of G and $\deg(a)$ is degree of vertex a. Here, we compute this topological index for some infinite classes of dendrimer graphs.

Keywords: Eccentricity, topological index, dendrimer graphs.

1. INTRODUCTION

By a graph means a set of vertices and edges which denotes by $V(G)$ and $E(G)$, respectively. If e is an edge of G, connecting the vertices u and v, then we write $e = uv$ and say "u and v are adjacent". A connected graph is a graph such that there is a path between all pairs of vertices. Throughout this paper all graphs are simple and connected.

Molecular descriptors play a prominent map in chemistry, pharmacology, etc. Among them, topological indices are very important, [1]. Let $\sum$ be the class of finite graphs. A topological index is a function Top from $\sum$ into real numbers with this property that $Top(G) = Top(H)$, if G and H are isomorphic. Obviously, the number of vertices and the number of edges are topological index. If $x, y \in V(G)$ then the distance $d_G(x, y)$ between x and y is defined as the length of any shortest path in G connecting x and y. For a vertex u of $V(G)$, its eccentricity $\varepsilon(u)$ is the largest distance between u and any other vertex v of G,

•*Corresponding author*. (*E-mail: mghorbani@srttu.edu*)

$\varepsilon(u) = \max_{v\in V(G)} d_G(u,v)$. The maximum eccentricity over all vertices of G is called the diameter of G and denoted by $D(G)$. The eccentric connectivity index [2-6] $\xi^C(x)$ of a graph G is defined as $\xi^C(x) = \sum_{u\in V(G)} \deg(u)\varepsilon(u)$, where $\deg(u)$ denotes the degree of vertex u in G, *i. e.*, the number of its neighbors in G. The aim of this paper is to compute the eccentric of some infinite families of dendrimers. Then by using this value we can compute eccentric connectivity index and diameter of these dendrimer graphs. Throughout this paper our notations are standard and mainly taken from standard books of graph theory such as [7, 8]. The reader is encouraged to consult the Refs [9 – 16], for background materials as well as basic computational techniques.

2. RESULTS AND DISCUSSIONS

Before going to calculate this polynomial for an infinite class of fullerenes, we must compute $\xi^C(x)$, for some well-known class of graphs.

Lemma 1. The ξ - index for a k- regular graph is: $\xi^C(x) = k\sum_{a\in V(G)} \varepsilon(a)$.

Example 2. Suppose K_n denotes the complete graph on n vertices. Then for any vertex $v \in V(K_n)$, $\deg(v)= n-1$ and $\varepsilon(v)=1$. So, $\xi^C(x) = (n-1)\sum_{a\in V(G)} 1 = n(n-1)$.

An automorphism of the graph $G = (V, E)$ is a bijection σ on V which preserves the edge set E, *i. e*, if $e = uv$ is an edge, then $\sigma(e) = \sigma(u)\sigma(v)$ is an edge of E. Here the image of vertex u is denoted by $\sigma(u)$. The set of all automorphisms of G under the composition of mappings forms a group which is denoted by $Aut(G)$. $Aut(G)$ acts transitively on V if for any vertices u and v in V there is $\alpha \in Aut(G)$ such that $\alpha(u) = v$. Similarly $G = (V, E)$ is called edge-transitive graph if for any two edges $e_1 = uv$ and $e_2 = xy$ in E there is an element $\beta \in Aut(G)$ such that $\beta(e_1) = e_2$, where $\beta(e_1) = \beta(u)\beta(v)$. By means of group action the proof of the following Lemma is clear:

Lemma 3. If $Aut(G)$ on V has orbits V_i $(1 \le i \le s)$ and u_i be an arbitrary vertex of V_i, then:

$$\xi^C(G[1]) = \sum_{i=1}^{s}\sum_{u\in V_i} \deg(u_i)\varepsilon(u_i) = \sum_{i=1}^{s} |V_i| \deg(u_i)\varepsilon(u_i).$$

Example 4. Consider the dendrimer graph $G[1]$ depicted in Figure 1. It is easy to see that:

$$\xi^C(G) = 2\times2\times7 + 2\times2\times8 + 2\times3\times9 + 4\times2\times10 + 4\times2\times11 + 4\times2\times12 + 4\times1\times13 = 430$$

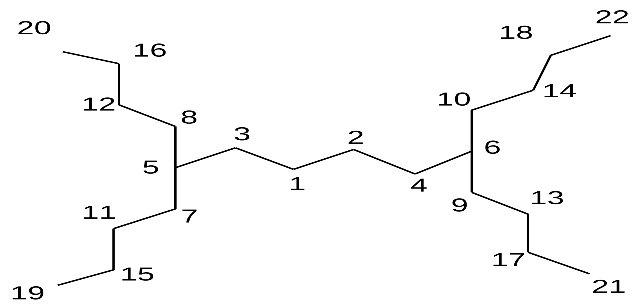

Figure 1. 2 – D Presentation of Dendrimer Graph *G*[1].

Example 5. Consider dendrimer graphs *G*[2] and *G*[3] depicted in Figures 2,3. By computing their eccentricity one can see that:

$$\xi^{C}(G[2]) = 2\times2\times11 + 2\times2\times12 + 2\times3\times13 + 4\times2\times15 + 4\times2\times16 + 4\times2\times12 + 4\times3\times17 + 8\times2\times18 + 8\times2\times19 + 8\times2\times20 + 8\times1\times21 = 1814,$$

and

$$\xi^{C}(G[3]) = 2\times2\times15 + 2\times2\times16 + 2\times3\times17 + 4\times2\times18 + 4\times2\times19 + 4\times2\times20 + 4\times3\times21 + 8\times2\times22 + 8\times2\times23 + 8\times2\times24 + 8\times3\times25 + 16\times2\times26 + 16\times2\times27 + 16\times2\times28 + 16\times1\times29 = 5694.$$

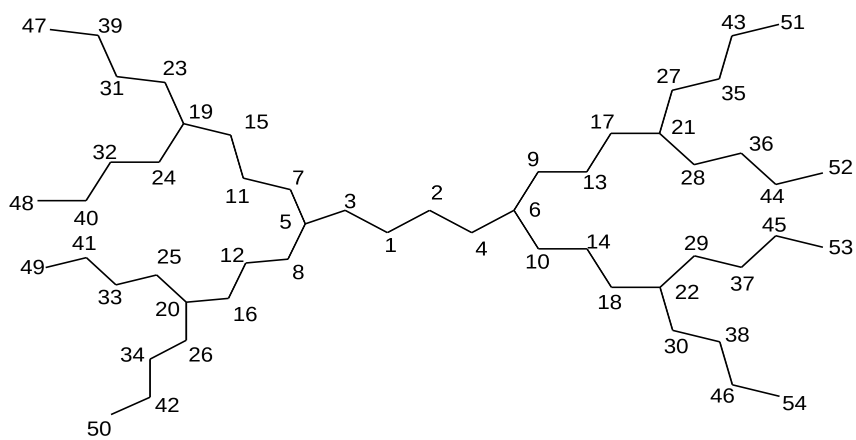

Figure 2. 2 – D Presentation of Dendrimer Graph *G*[2].

Theorem 6. Let *G*[*n*] be the dendrimer graph depicted in Figure 4, with exactly *n* levels. Then

$$\xi^{C}(G[n]) = 50\varepsilon + 184 + \sum_{i=2}^{n-1} 2^{i+1}[9\varepsilon + 36(i-1) + 42] + 2^{n+1}[7\varepsilon + 28(n-1) + 30],$$

where $\varepsilon = 4n+3$.

Proof. Using Figure 4 and Table 1 one can see there are n types of vertices in $V(G[n])$ and $\varepsilon = 4n+3$.

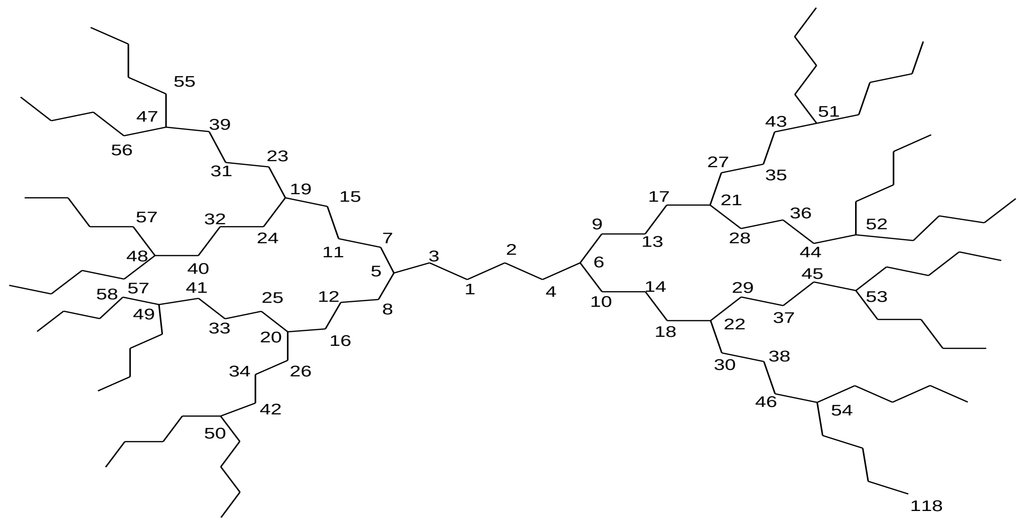

Figure 3. 2 – D Presentation of Dendrimer Graph $G[3]$.

By summation the values of eccentricity listed in Table 1 the proof is completed.

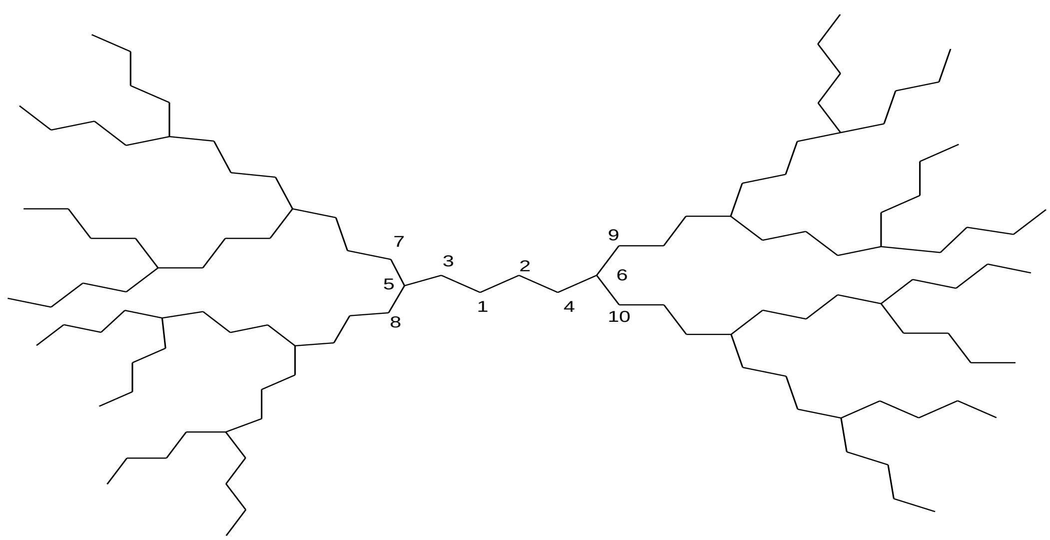

Figure 4. 2 – D Presentation of Dendrimer Graph $G[n]$.

Example 7. Consider the dendrimer graph $H[1]$, depicted in Figure 5. It is easy to see that

$$\xi^{C}(H[1]) = 2\times2\times9+2\times3\times10+4\times2\times11+4\times2\times12+4\times2\times13+4\times2\times14+4\times2\times15+ 8\times2\times16+4\times1\times17=812$$

Table 1. The Eccentricity of the Vertices of $G[n]$.

Step	***Vertex***	***Num***	***δ(u)***	***ε(u)***	$\sum \delta(u)\varepsilon(u)$
	v_1	2	2	ε	
	v_3	2	2	$\varepsilon + 1$	
	v_5	2	3	$\varepsilon + 2$	
1	v_7	4	2	$\varepsilon + 3$	$50\varepsilon + 184$
	v_{11}	4	2	$\varepsilon + 4$	
	v_{15}	4	2	$\varepsilon + 5$	
	v_{19}	4	3	$\varepsilon + 6$	
	v_1	8	2	$\varepsilon + 7$	
2	v_9	8	2	$\varepsilon + 8$	$72\varepsilon + 624$
	v_{17}	8	2	$\varepsilon + 9$	
	v_{25}	8	3	$\varepsilon + 10$	
⋮	v_1	2^{i+1}	2	$\varepsilon + 4(i-1) + 3$	
	$v_{2^{i+1}+1}$	2^{i+1}	2	$\varepsilon + 4(i-1) + 4$	
i	$v_{2^{i+2}+1}$	2^{i+1}	2	$\varepsilon + 4(i-1) + 5$	$2^{i+1}[9\varepsilon+36(i-1) + 42]$
⋮	$v_{3\times 2^{i+1}+1}$	2^{i+1}	3	$\varepsilon + 4(i-1) + 6$	
	v_1	2^{n+1}	2	$\varepsilon + 4(n-1) + 3$	
	$v_{2^{n+1}+1}$	2^{n+1}	2	$\varepsilon + 4(n-1) + 4$	
n	$v_{2^{n+2}+1}$	2^{n+1}	2	$\varepsilon + 4(n-1) + 5$	$2^{n+1}[7\varepsilon+28(n-1)+30]$
	$v_{3\times 2^{n+1}+1}$	2^{n+1}	1	$\varepsilon + 4(n-1) + 6$	

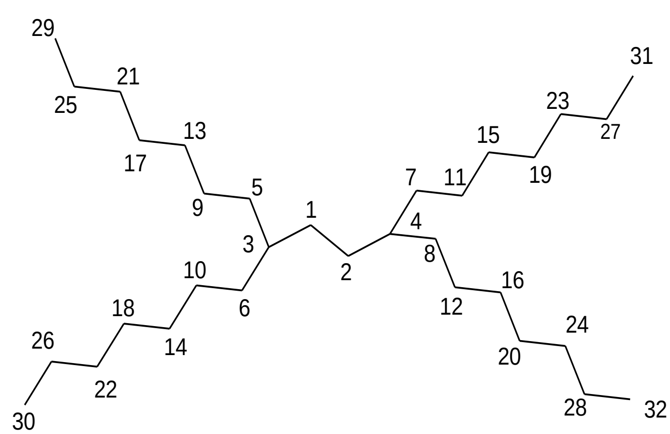

Figure 5. 2 – D Presentation of Dendrimer Graph $H[1]$.

Also, for n = 2, 3 $H[2]$ and $H[3]$ are depicted in Figures 6, 7 and we have:

$$\xi^C(H[2]) = 2\times2\times16 + 2\times3\times17 + 4\times3\times18 + 4\times2\times19 + 4\times2\times20 + 4\times2\times21 + 4\times2\times22 + 4\times2\times23 + 4\times3\times24 + 8\times2\times25 + 8\times2\times26 + 8\times2\times27 + 8\times2\times28 + 8\times2\times29 + 8\times2\times30 + 8\times1\times31 = 4326,$$

$$\xi^C(H[3]) = 2\times2\times23 + 2\times3\times24 + 4\times2\times25 + 4\times2\times26 + 4\times2\times27 + 4\times2\times28 + 4\times2\times29 + 4\times2\times30 + 4\times3\times31 + 8\times2\times32 + 8\times2\times33 + 8\times2\times34 + 8\times2\times35 + 8\times2\times36 + 8\times2\times37 + 8\times3\times38 + 16\times2\times39 + 16\times2\times40 + 16\times2\times41 + 16\times2\times42 + 16\times2\times43 + 16\times2\times44 + {}+16\times1\times45 = 14840.$$

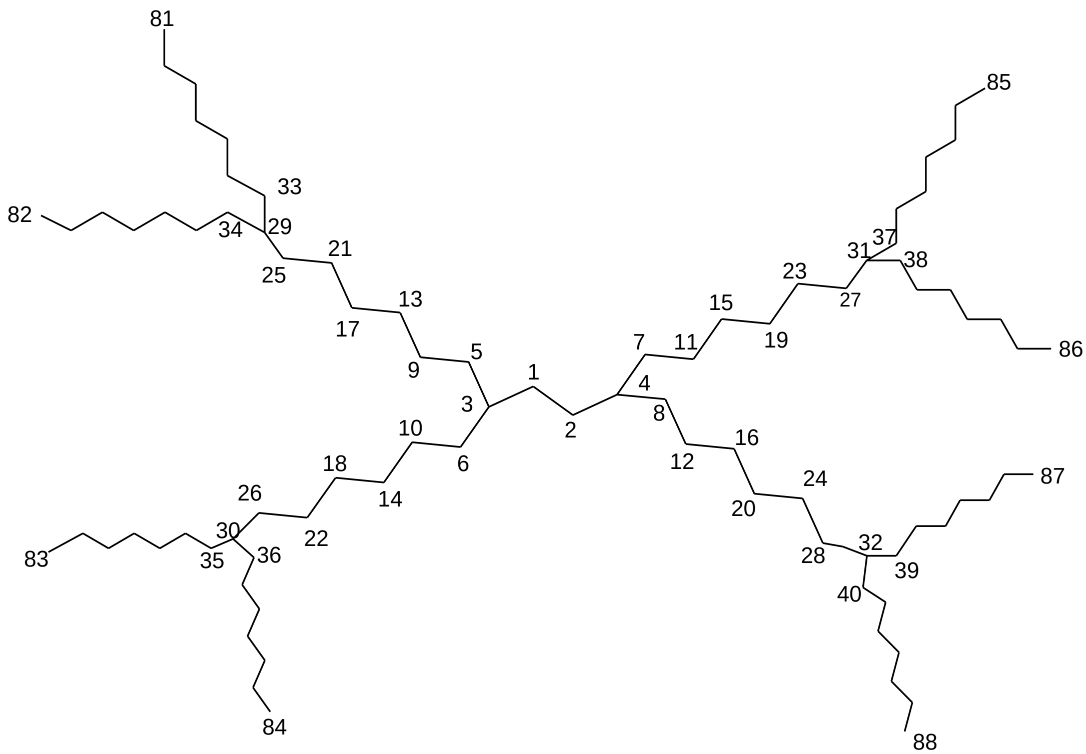

Figure 6. 2 – D Presentation of Dendrimer Graph *H*[2].

In generally we have the following Theorem:

Theorem 8. Let *H*[*n*] be a dendrimer graph on *n* levels, see Figure 8. Then

$$\xi^C(H[n]) = 70\varepsilon + 286 + \sum_{i=2}^{n-1} 2^{i+1}[15\varepsilon + 105(i-1) + 78] + 2^{n+1}[13\varepsilon + 91(n-1) + 62],$$

where $\varepsilon = 7n+2$.

Proof. Similar to proof of Theorem 6, one can see that we can divide the vertices of graph *H*[*n*] to *n* types, see Table 2:

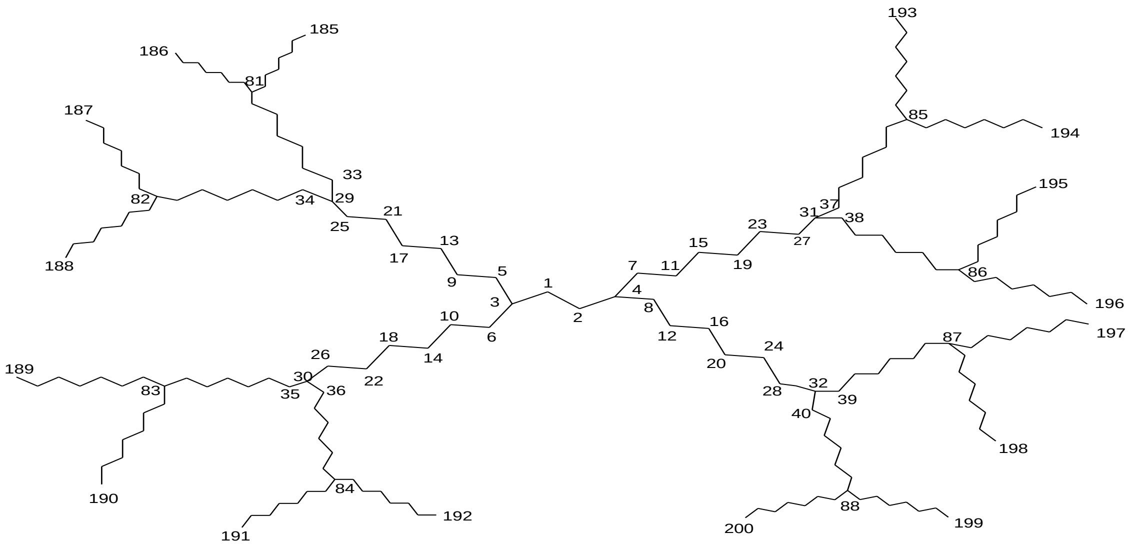

Figure 7. 2 – D Presentation of Dendrimer Graph $H[3]$.

Table 2. The Eccentricity of the Vertices of $H[n]$.

Step	*Vertex*	*Num*	*δ(u)*	*ε(u)*	$\sum \delta(u)\varepsilon(u)$
	v_1	2	2	ε	
	v_3	2	3	$\varepsilon+1$	
	v_5	4	2	$\varepsilon+2$	
1	v_9	4	2	$\varepsilon+3$	$70\varepsilon+256$
	⋮	⋮	⋮	⋮	
	v_{25}	4	2	$\varepsilon+7$	
	v_{29}	4	3	$\varepsilon+8$	
	v_1	8	2	$\varepsilon+9$	
	v_9	8	2	$\varepsilon+10$	
2	⋮	⋮	⋮	⋮	$120\varepsilon+1464$
	v_{41}	8	2	$\varepsilon+14$	
	v_{49}	8	3	$\varepsilon+15$	
⋮	v_1	2^{i+1}	2	$\varepsilon+7(i-1)+2$	
	$v_{2^{i+1}+1}$	2^{i+1}	2	$\varepsilon+7(i-1)+3$	
i	$v_{2^{i+2}+1}$	2^{i+1}	2	$\varepsilon+7(i-1)+4$	$2^{i+1}[15\varepsilon+105(i-1)+78]$
	⋮	⋮	⋮	⋮	
⋮	$v_{6\times2^{i+1}+1}$	2^{i+1}	3	$\varepsilon+7(i-1)+8$	
	v_1	2^{n+1}	2	$\varepsilon+7(n-1)+2$	
	$v_{2^{n+1}+1}$	2^{n+1}	2	$\varepsilon+7(n-1)+3$	
n	$v_{2^{n+2}+1}$	2^{n+1}	2	$\varepsilon+7(n-1)+4$	$2^{n+1}[13\varepsilon+91(n-1)+62]$
	⋮	⋮	⋮	⋮	
	$v_{6\times2^{n+1}+1}$	2^{n+1}	1	$\varepsilon+7(n-1)+8$	

where ε = 7n+2. By summation the eccentricities of vertices in Table 2 the proof is completed.

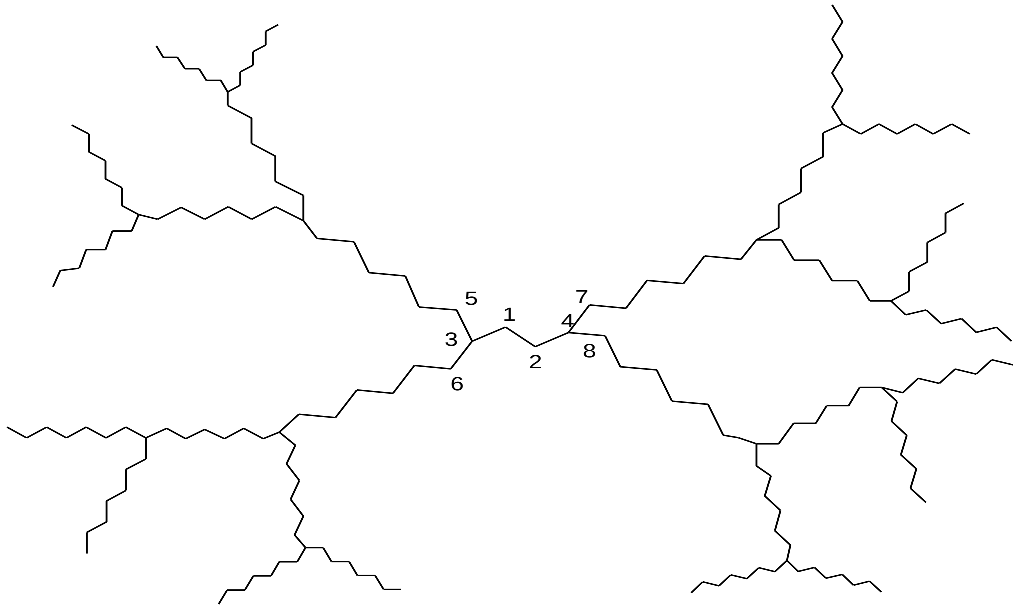

Figure 8. 2 – D Presentation of Dendrimer Graph *H*[n].

Finally, we are ready to compute the eccentric connectivity index of dendrimer graph *K*[*n*] depicted in Figure 11. To do this at the first step, we assume *n* = 1, see Figure 9 and we have:

$$\xi^C(G) = 2\times2\times14 + 2\times3\times13 + 4\times2\times12 + 4\times3\times11 + 2\times3\times10 + 2\times3\times10 + 2\times3\times11 + 2\times3\times10 + 2\times2\times12 + 2\times2\times11 + 2\times2\times13 + 2\times2\times12 + 2\times2\times15 + 2\times3\times16 + 4\times2\times17 + 4\times3\times18 + 2\times2\times19 + 4\times1\times19 = 1460.$$

By a similar way we can compute the eccentricity of vertices of *K*[*n*] depicted in Figure 9. A direct computation shows this topological index is as follows:

$$\xi^C(G) = 2\times2\times19 + 2\times3\times18 + 4\times2\times17 + 4\times3\times16 + 2\times3\times15 + 2\times3\times15 + 2\times3\times16 + 2\times3\times15 + 2\times2\times17 + 2\times2\times16 + 2\times2\times18 + 2\times2\times17 + 2\times2\times20 + 2\times3\times21 + 4\times2\times22 + 4\times3\times23 + 2\times2\times24 + 4\times2\times24 + 4\times2\times25 + 4\times3\times26 + 8\times2\times27 + 8\times3\times28 + 4\times2\times29 + 8\times1\times29 = 1460.$$

By using the Table 3 and Figure 11, similar to the last Theorems one can see there are *n* types of vertices in graph *K*[*n*], see Table 3. So, by summation of these values we can prove the following Theorem:

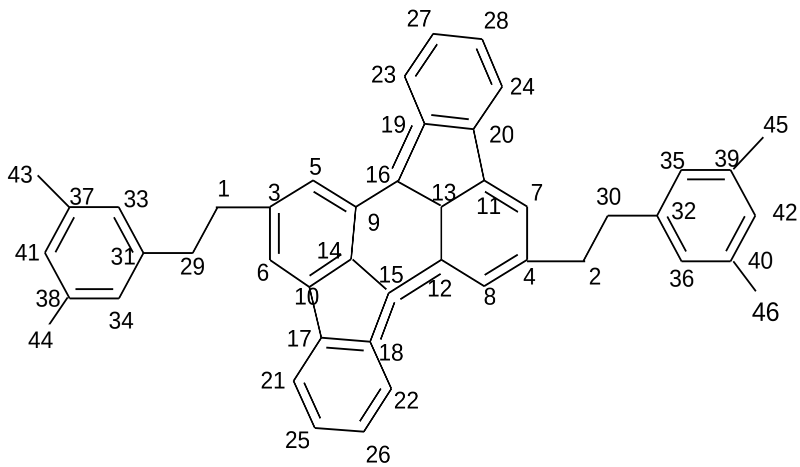

Figure 9. 2 – D Presentation of Dendrimer Graph *K*[1].

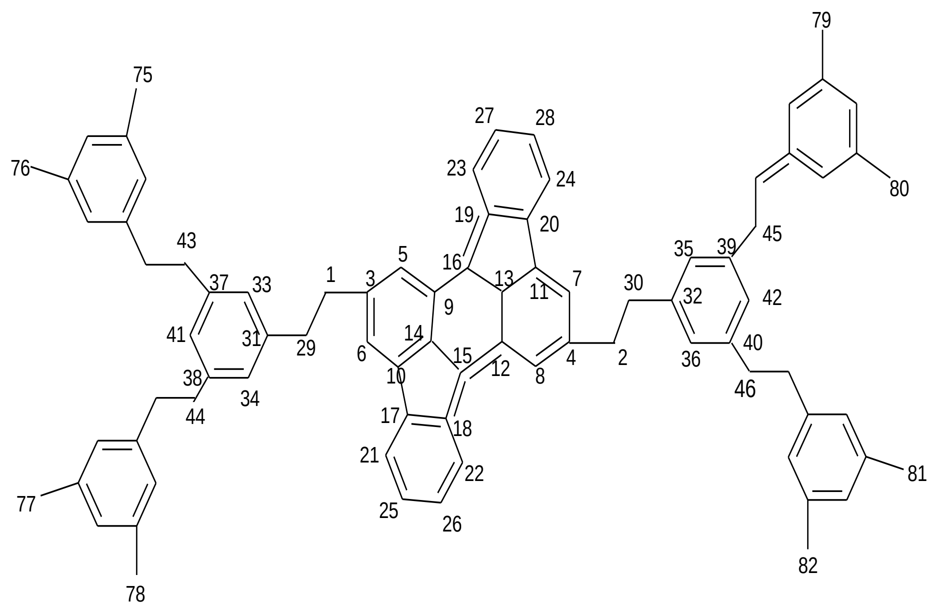

Figure 10. Dendrimer Graph *K*[2].

Theorem 9.

$$\xi^{C}(G) = 112\varepsilon - 32 + \sum_{i=2}^{n-1} 2^{i+1}[21\varepsilon + 105(i-1) + 74] + 2^{n+1}[19\varepsilon + 95(n-1) + 64],$$

where $\varepsilon = 5n+9$.

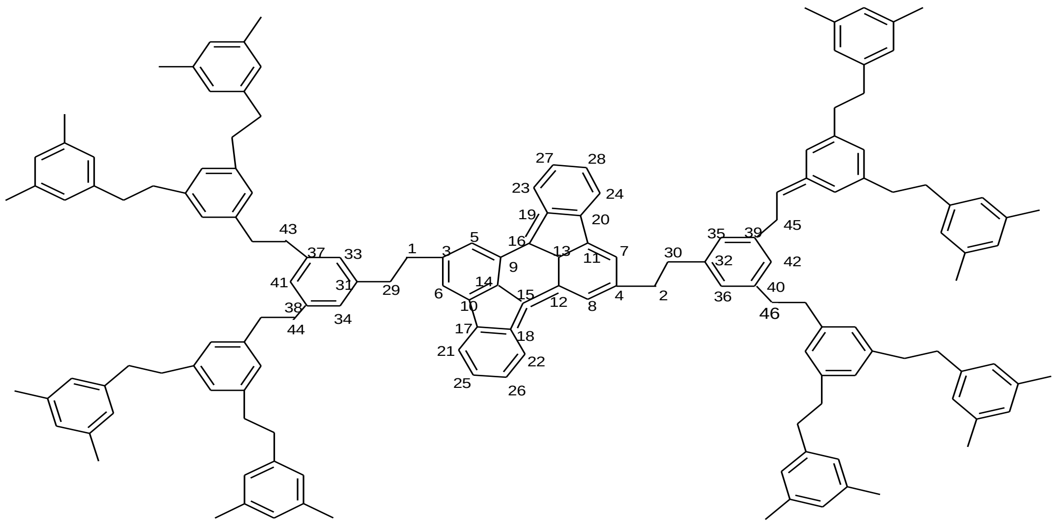

Figure 11. 2 – D Presentation of Dendrimer Graph $K[n]$.

Table 3. The Eccentricity of the Vertices of $K[n]$.

Step	*Vertex*	*Num*	$\delta(u)$	$\varepsilon(u)$	$\sum\delta(u)\varepsilon(u)$
1	v_1	2	2	ε	$112\varepsilon - 32$
	v_3	2	3	$\varepsilon - 1$	
	v_5	4	2	$\varepsilon - 2$	
	v_9	4	3	$\varepsilon - 3$	
	$\vdots$	$\vdots$	$\vdots$	$\vdots$	
	v_{41}	2	2	$\varepsilon + 5$	
	v_{43}	4	2	$\varepsilon + 5$	
2	v_1	4	2	$\varepsilon + 6$	$84\varepsilon + 716$
	v_5	4	3	$\varepsilon + 7$	
	v_9	8	2	$\varepsilon + 8$	
	v_{17}	8	3	$\varepsilon + 9$	
	v_{25}	4	2	$\varepsilon + 10$	
	v_{29}	8	3	$\varepsilon + 10$	
$\vdots$	v_1	2^i	2	$\varepsilon + 5(i - 1) + 1$	
	v_{2^i+1}	2^i	3	$\varepsilon + 5(i - 1) + 2$	
i	$v_{2^{i+2}+1}$	2^{i+1}	2	$\varepsilon + 5(i - 1) + 3$	$2^i[21\varepsilon+105(i - 1) + 74]$
	$v_{2^{i+2}+1}$	2^{i+1}	3	$\varepsilon + 5(i - 1) + 4$	
$\vdots$	$v_{3\times2^{i+2}+1}$	2^i	2	$\varepsilon + 5(i - 1) + 5$	
	$v_{3\times2^{i+2}+1}$	2^{i+1}	2	$\varepsilon + 5(i - 1) + 5$	
n	v_1	2^n	2	$\varepsilon + 5(n - 1) + 1$	$2^n\,[19\varepsilon+95(n - 1) + 64]$
	v_{2^n+1}	2^n	3	$\varepsilon + 5(n - 1) + 2$	
	$v_{2^{n+2}+1}$	2^{n+1}	2	$\varepsilon + 5(n - 1) + 3$	
	$v_{2^{n+2}+1}$	2^{n+1}	3	$\varepsilon + 5(n - 1) + 4$	
	$v_{3\times2^{n+2}+1}$	2^n	2	$\varepsilon + 5(n - 1) + 5$	
	$v_{3\times2^{n+2}+1}$	2^{n+1}	1	$\varepsilon + 5(n - 1) + 5$	

3. CONCLUSIONS

By using the definition of the eccentric connectivity index, we computed this new topological index for some classes of dendrimer graphs.

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