

# SOME TOPOLOGICAL INDICES OF PHOSPHORUS CONTAINING DENDRIMERS

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**Abstract** Dendrimers are generally considered as a special class of polymers. It is globular in size, monodisperse, hyperbranched and have perfectly defined structures and synthesized step-by- step. The graph theory is used to establish correlations between chemical structures and various physical properties, chemical reactivity, or biological activity with the help of graphical invariants. The evaluation of the quantitative structure–activity and quantitative structure–property relationships, the eccentric-connectivity index has a very important place among the various topological descriptors due to its high degree of predictability for pharmaceutical properties. In this paper the first and second Zagreb indices, first and second Zagreb eccentricity indices, first and second Zagreb degree eccentricity indices, eccentric connectivity index and modified versions of eccentric-connectivity index of the molecular graph of phosphorus containing dendrimers are computed.

## 1 Introduction

Dendrimers are globular in size, macromolecules, hyperbranched and perfectly defined structures. In these all bonds emerge radially from a central focal point with a regular branching pattern and with repeat units that each contribute a branch point. The majority dendrimers are organic compounds, but dendrimers containing heteroatoms are very much attractive in present research due to its potential application in different fields such as Physics, Biology, Chemistry, Engineering, and Medicine. Among heteroatoms containing dendrimers, phosphorus derivatives have special attraction of a great number of scientists because of their unusual physical and chemical properties[8].

Phosphorus-containing dendrimers have already been used as reusable and efficient catalysts, for the elaboration of nanomaterials, as fluorescent agents for bio-imaging, and as drugs by themselves, to name as a few uses. All these properties pave the way for the search of other properties, which will surely benefit from the tools already elaborated for having two types of functional groups, in precise positions of dendritic structures[4].

A topological index sometimes known as a graph theoretic index, is a numerical invariant of a chemical graph. Topological indices are the mathematical measures associated with molecular graph structure that correlate the chemical structure with various physical properties, biological activity or chemical reactivity. In this paper we consider the following topological indices.

## 2 Definitions and Notations

All the graphs  $G = (V, E)$  considered in this paper are simple, undirected and connected graphs. For any vertices  $u, v \in V(G)$ , the distance  $d(u, v)$  is defined as the length of any shortest path connecting  $u$  and  $v$  in  $G$ . For any vertex  $u$  in  $G$ , the degree  $d(u)$  of  $u$  is the number of edges incident with  $u$  in  $G$  and the eccentricity  $e(u)$  of  $u$  is the largest distance between  $u$  and any other vertex of  $G$  [5].

In this paper we consider the following topological indices. Firstly the Zagreb indices were introduced by Gutman and Trinajstić in 1972 [7]. Recently, the Zagreb indices and their variants have been used to study molecular complexity, chirality, ZE-isomerism and heterosystems whilst the overall Zagreb indices exhibited a potential applicability for deriving multilinear regression models. Zagreb indices are also used by various researchers in their QSPR and QSAR studies. The main properties of  $M_1(G)$  and  $M_2(G)$  were summarized in [10].

The first Zagreb index  $M_1(G)$  is defined as

$$M_1(G) = \sum_{u \in V(G)} d(u)^2. \quad (2.1)$$

The second Zagreb index  $M_2(G)$  is defined as

$$M_2(G) = \sum_{uv \in E(G)} d(u)d(v). \quad (2.2)$$

The invariants based on vertex eccentricities attracted some attention in Chemistry. In an analogy with the first and the second Zagreb indices, M. Ghorbani et al. and D. Vukičević et al. introduced the first and second Zagreb eccentricity indices [6, 15]. The first Zagreb eccentricity ( $E_1$ ) and the second Zagreb eccentricity ( $E_2$ ) indices of a graph  $G$  are defined as

$$E_1(G) = \sum_{u \in V(G)} e(u)^2 \quad (2.3)$$

and

$$E_2(G) = \sum_{uv \in E(G)} e(u)e(v). \quad (2.4)$$

The eccentric connectivity index is a parameter recently introduced in [13]. The eccentric connectivity index of a connected graph  $G$  is defined as

$$\xi^c(G) = \sum_{u \in V(G)} d(u)e(u) \quad (2.5)$$

The modified versions of eccentric-connectivity index is introduced by A. R. Ashrafi and M. Ghorbani[2]. Distinct mathematical and chemical properties of the modified eccentric-connectivity index and its polynomial were studied in[1, 3]. The modified versions of eccentric-connectivity index is defined as

$$\Lambda(G) = \sum_{u \in V(G)} S_u e(u) \quad (2.6)$$

where,  $S_u$  is sum of the degrees of all neighbors of vertex  $u$  in  $G$ .

The Zagreb degree eccentricity indices are introduced in[12]. Further studies on Zagreb degree eccentricity index can be found in[11, 14]. First Zagreb degree eccentricity ( $DE_1$ ) and second zagreb degree eccentricity ( $DE_2$ ) indices of a graph  $G$  are defined as

$$DE_1 = \sum_{u \in V(G)} (e(u) + d(u))^2 \quad (2.7)$$

and

$$DE_2(G) = \sum_{uv \in E(G)} (e(u) + d(u))(e(v) + d(v)) \quad (2.8)$$

Some major types of topological indices of graphs are degree-based, distance-based, and counting-related. Some degree-based topological indices have been computed for some classes of dendrimers, see for instance[9]. In this paper, we compute several distance and eccentricity based topological indices, namely, the first and second Zagreb indices, first and second Zagreb eccentricity indices, first and second Zagreb degree eccentricity indices, eccentric connectivity index and modified versions of eccentric-connectivity index of Phosphorus containing dendrimers.

### 3 Main Results

The molecular structure of Phosphorus containing dendrimer of first generation is shown in the Figure 1. Let the molecular graph of this dendrimer be denoted by  $D(n)$ , where the generation stage of  $D(n)$  is represented by  $n$ .

The first and second generation of  $D(n)$  are shown in Figure 2 and Figure 3. The size and order of the graph  $D(n)$  are  $6[33 \times 2^n - 12]$  and  $6[35 \times 2^n - 13]$ , respectively. We make three sets of representatives of  $V(D(n))$ , say  $A = \{u_1, u_2\}$   $B = \{v_1, v_2, v_3, \dots, v_{11}\}$  and  $C = \{a_i, b_i, c_i, d_i, e_i, f_i, g_i, h_i, j_i, k_i\}$  where  $1 \leq i \leq n$ , as shown in Figures 2 and 3. The degree,  $S_u$  and eccentricity for each  $u$  for the sets  $A, B$  and  $C$  are shown in Tables 1 and 2. For simplicity, we assume  $\alpha = 9n + 9i + 4$  throughout the paper.

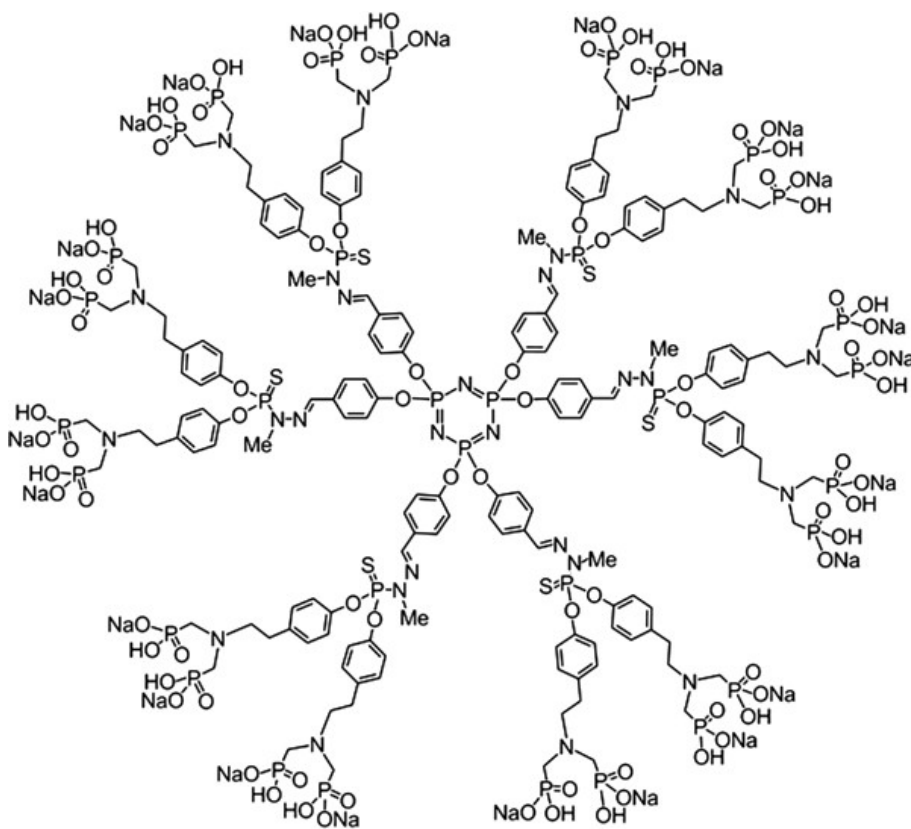


Figure 1: Molecular structure of  $D(n)$

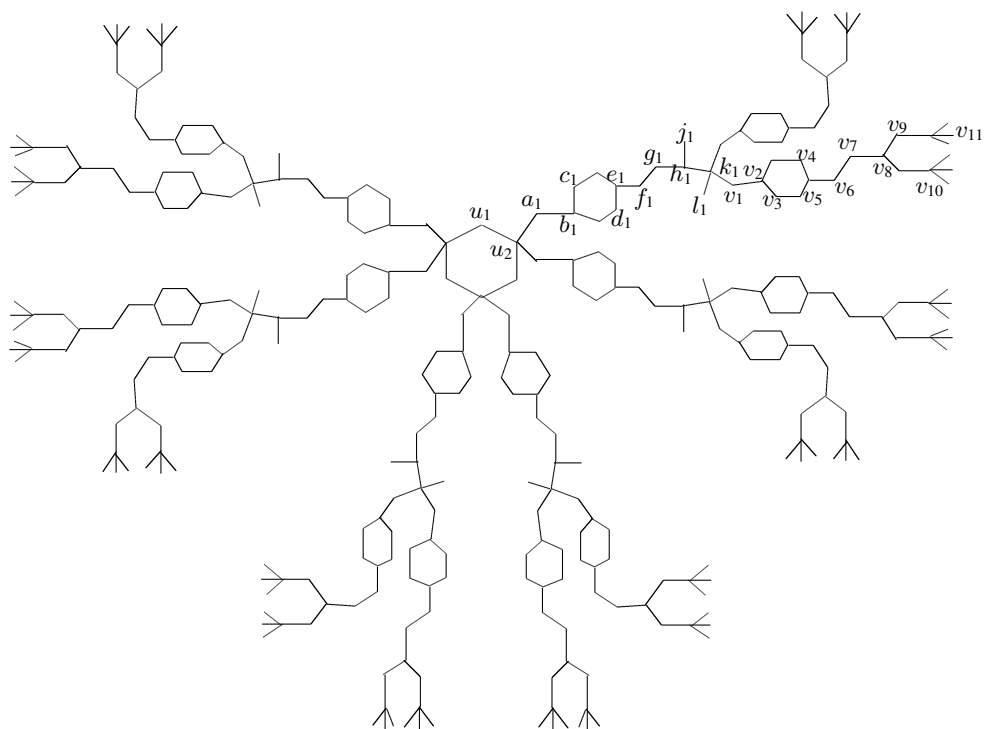


Figure 2: First generation

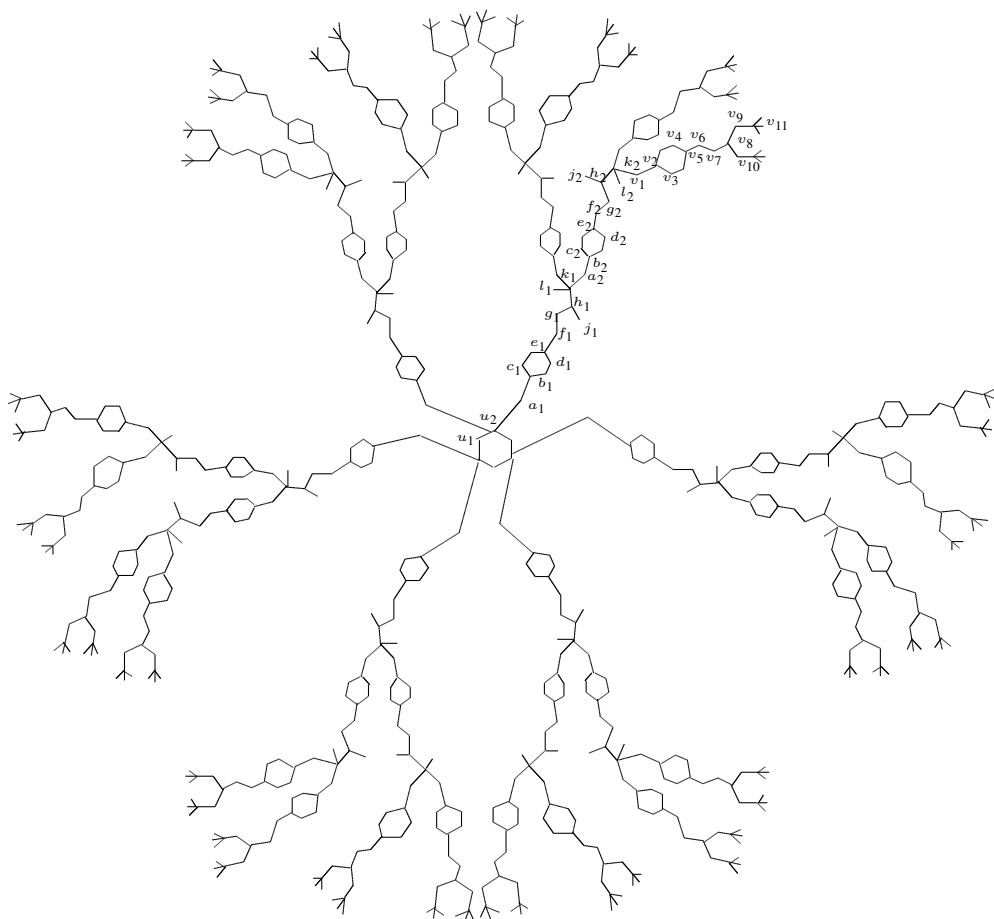


Figure 3: Second generation

Vertex representative	Degree	$S_u$	Eccentricity	Frequency
$u_1$	2	8	$9n+14$	3
$u_2$	4	8	$9n+13$	3
$v_1$	2	7	$18n+14$	$3 \times 2^{n+1}$
$v_2$	3	6	$18n+15$	$3 \times 2^{n+1}$
$v_3$	2	5	$18n+16$	$3 \times 2^{n+2}$
$v_4$	2	5	$18n+17$	$3 \times 2^{n+2}$
$v_5$	3	6	$18n+18$	$3 \times 2^{n+1}$
$v_6$	2	5	$18n+19$	$3 \times 2^{n+1}$
$v_7$	2	5	$18n+20$	$3 \times 2^{n+1}$
$v_8$	3	6	$18n+21$	$3 \times 2^{n+1}$
$v_9$	2	7	$18n+22$	$3 \times 2^{n+2}$
$v_{10}$	4	5	$18n+23$	$3 \times 2^{n+2}$
$v_{11}$	1	4	$18n+24$	$3 \times 3 \times 2^{n+2}$

Table 1: Sets  $A$  and  $B$  with their degrees,  $S_u$ , eccentricity and frequencies.

vertex representative	Degree	$S_u$	Eccentricity	Frequency
$a_i$	2	7	$\alpha + 1$	$3 \times 2^i$
$b_i$	3	6	$\alpha + 2$	$3 \times 2^i$
$c_i$	2	5	$\alpha + 3$	$3 \times 2^{i+1}$
$d_i$	2	5	$\alpha + 4$	$3 \times 2^{i+1}$
$e_i$	3	6	$\alpha + 5$	$3 \times 2^i$
$f_i$	2	5	$\alpha + 6$	$3 \times 2^i$
$g_i$	2	5	$\alpha + 7$	$3 \times 2^i$
$h_i$	3	7	$\alpha + 8$	$3 \times 2^i$
$j_i$	1	3	$\alpha + 9$	$3 \times 2^i$
$k_i$	4	8	$\alpha + 9$	$3 \times 2^i$
$l_i$	1	4	$\alpha + 10$	$3 \times 2^i$

Table 2: Set  $C$  with degrees,  $S_u$ , eccentricity and frequencies.

**Theorem 3.1.** First Zagreb index of graph  $D(n)$  is  $M_1(D(n)) = 261 \times 2^{n+2} - 378$

**Proof.** By using values of Tables 1 and 2 in equation 2.1, we compute the First Zagreb index of graph  $D(n)$  in the following way

$$\begin{aligned}
 M_1(D(n)) &= \sum_{u \in V(D(n))} d(u)^2 \\
 &= \sum_{u \in A} d(u)^2 + \sum_{u \in B} d(u)^2 + \sum_{u \in C} d(u)^2 \\
 &= 3(2^2) + 3(4^2) + 3 \times 2^{n+1}(2^2) + 3 \times 2^{n+1}(3^2) + 3 \times 2^{n+2}(2^2) + 3 \times 2^{n+2}(2^2) \\
 &\quad + 3 \times 2^{n+1}(3^2) + 3 \times 2^{n+1}(2^2) + 3 \times 2^{n+1}(2^2) + 3 \times 2^{n+1}(3^2) + 3 \times 2^{n+2}(2^2) \\
 &\quad + 3 \times 2^{n+2}(4^2) + 3 \times 3 \times 2^{n+2}(1^2) \\
 &\quad + \sum_{i=1}^n [3 \times 2^i(2^2) + 3 \times 2^i(3^2) + 3 \times 2^{i+1}(2^2) + 3 \times 2^{i+1}(2^2) + 3 \times 2^i(3^2) \\
 &\quad + 3 \times 2^i(2^2) + 3 \times 2^i(2^2) + 3 \times 2^i(3^2) + 3 \times 2^i(1^2) + 3 \times 2^i(4^2) + 3 \times 2^i(1^2)] \\
 &= 261 \times 2^{n+2} - 378. \quad \square
 \end{aligned}$$

**Theorem 3.2.** First Zagreb eccentricity index of graph  $D(n)$  is  $E_1(D(n)) = 2^{n+1}[32076n^2 + 44604n + 32193] - 5832n^2 + 810n - 12177$

**Proof.** Substituting the values of Tables 1 and 2 in equation 2.3, we compute the First Zagreb eccentricity index of  $D(n)$  as follows.

$$\begin{aligned} E_1(D(n)) &= \sum_{u \in V(D(n))} e(u)^2 \\ &= 3(9n + 14)^2 + 3(9n + 13)^2 + 3 \times 2^{n+1}(18n + 14)^2 + 3 \times 2^{n+1}(18n + 15)^2 \\ &\quad + 3 \times 2^{n+2}(18n + 16)^2 + 3 \times 2^{n+2}(18n + 17)^2 + 3 \times 2^{n+1}(18n + 18)^2 \\ &\quad + 3 \times 2^{n+1}(18n + 19)^2 + 3 \times 2^{n+1}(18n + 20)^2 + 3 \times 2^{n+1}(18n + 21)^2 \\ &\quad + 3 \times 2^{n+2}(18n + 22)^2 + 3 \times 2^{n+2}(18n + 23)^2 + 3 \times 3 \times 2^{n+2}(18n + 24)^2 \\ &\quad + \sum_{i=1}^n [3 \times 2^i(\alpha + 1)^2 + 3 \times 2^i(\alpha + 2)^2 + 3 \times 2^{i+1}(\alpha + 3)^2 + 3 \times 2^{i+1}(\alpha + 4)^2 \\ &\quad + 3 \times 2^i(\alpha + 5)^2 + 3 \times 2^i(\alpha + 6)^2 + 3 \times 2^i(\alpha + 7)^2 + 3 \times 2^i(\alpha + 8)^2 \\ &\quad + 3 \times 2^i(\alpha + 9)^2 + 3 \times 2^i(\alpha + 9)^2 + 3 \times 2^i(\alpha + 10)^2] \\ &= 2^{n+1}[32076n^2 + 44604n + 32193] - 5832n^2 + 810n - 12177. \quad \square \end{aligned}$$

**Theorem 3.3.** The eccentric connectivity index of  $D(n)$  is  $\xi^c(D(n)) = 2^{n+1}[3780n + 2481] - 1404n + 174$ .

**Proof.** The eccentric connectivity index of  $D(n)$  is given by  $\xi^c(D(n)) = \sum_{u \in V(D(n))} e(u)d(u)$ . By Tables 1 and 2, we get

$$\begin{aligned} \xi^c(D(n)) &= 3(9n + 14)2 + 3(9n + 13)4 + 3 \times 2^{n+1}(18n + 14)2 + 3 \times 2^{n+1}(18n + 15)3 \\ &\quad + 3 \times 2^{n+2}(18n + 16)2 + 3 \times 2^{n+2}(18n + 17)2 + 3 \times 2^{n+1}(18n + 18)3 \\ &\quad + 3 \times 2^{n+1}(18n + 19)2 + 3 \times 2^{n+1}(18n + 20)2 + 3 \times 2^{n+1}(18n + 21)3 \\ &\quad + 3 \times 2^{n+2}(18n + 22)2 + 3 \times 2^{n+2}(18n + 23)4 + 3 \times 3 \times 2^{n+2}(18n + 24)1 \\ &\quad + \sum_{i=1}^n [3 \times 2^i(\alpha + 1)2 + 3 \times 2^i(\alpha + 2)3 + 3 \times 2^{i+1}(\alpha + 3)2 + 3 \times 2^{i+1}(\alpha + 4)2 \\ &\quad + 3 \times 2^i(\alpha + 5)3 + 3 \times 2^i(\alpha + 6)2 + 3 \times 2^i(\alpha + 7)2 + 3 \times 2^i(\alpha + 8)3 \\ &\quad + 3 \times 2^i(\alpha + 9)1 + 3 \times 2^i(\alpha + 9)4 + 3 \times 2^i(\alpha + 10)1] \\ &= 2^{n+1}[3780n + 2481] - 1404n + 174. \quad \square \end{aligned}$$

**Theorem 3.4.** The modified versions of eccentric-connectivity index of  $D(n)$  is  $\Lambda(D(n)) = 2^{n+1}[9396n + 6255] - 3402n + 504$ .

**Proof.** Formula for the modified versions of eccentric-connectivity index of  $D(n)$  is given by  $\Lambda(D(n)) = \sum_{u \in V(D(n))} S_u e_u$ . Using the values of Tables 1 and 2 we have,

$$\begin{aligned} \Lambda(D(n)) &= 3 \times 8(9n + 14) + 3 \times 8(9n + 13) + 3 \times 2^{n+1} \times 7(18n + 14) + 3 \times 2^{n+1} \times 6(18n + 15) \\ &\quad + 3 \times 2^{n+2} \times 5(18n + 16) + 3 \times 2^{n+2} \times 5(18n + 17) + 3 \times 2^{n+1} \times 6(18n + 18) \\ &\quad + 3 \times 2^{n+1} \times 5(18n + 19) + 3 \times 2^{n+1} \times 5(18n + 20) + 3 \times 2^{n+1} \times 6(18n + 21) \\ &\quad + 3 \times 2^{n+2} \times 7(18n + 22) + 3 \times 2^{n+2} \times 5(18n + 23) + 3 \times 3 \times 2^{n+2} \times 4(18n + 24) \end{aligned}$$

$$\begin{aligned}
 &+ \sum_{i=1}^n [3 \times 2^i \times 7(\alpha + 1) + 3 \times 2^i \times 6(\alpha + 2) + 3 \times 2^{i+1} \times 5(\alpha + 3) + 3 \times 2^{i+1} \times 5(\alpha + 4) \\
 &+ 3 \times 2^i \times 6(\alpha + 5) + 3 \times 2^i \times 5(\alpha + 6) + 3 \times 2^i \times 5(\alpha + 7) + 3 \times 2^i \times 7(\alpha + 8) \\
 &+ 3 \times 2^i \times 3(\alpha + 9) + 3 \times 2^i \times 8(\alpha + 9) + 3 \times 2^i \times 4(\alpha + 10)] \\
 &= 2^{n+1}[9396n + 6255] - 3402n + 504. \quad \square
 \end{aligned}$$

**Theorem 3.5.** First Zagreb degree eccentricity index of  $D(n)$  is  $DE_1(D(n)) = 2^{n+1}(32076n^2 + 52164n + 37677) - 5832n^2 - 1998n - 12207$

**Proof.** The Tables 1 and 2 give the value of the First Zagreb degree eccentricity index of  $D(n)$  as below.

$$\begin{aligned}
 DE_1(D(n)) &= \sum_{u \in V(D(n))} (e(u) + d(u))^2 \\
 &= 3(9n + 14 + 2)^2 + 3(9n + 13 + 4)^2 + 3 \times 2^{n+1}(18n + 14 + 2)^2 \\
 &\quad + 3 \times 2^{n+1}(18n + 15 + 3)^2 + 3 \times 2^{n+2}(18n + 16 + 2)^2 + 3 \times 2^{n+2}(18n + 17 + 2)^2 \\
 &\quad + 3 \times 2^{n+1}(18n + 18 + 3)^2 + 3 \times 2^{n+1}(18n + 19 + 2)^2 + 3 \times 2^{n+1}(18n + 20 + 2)^2 \\
 &\quad + 3 \times 2^{n+1}(18n + 21 + 3)^2 + 3 \times 2^{n+2}(18n + 22 + 2)^2 + 3 \times 2^{n+2}(18n + 23 + 4)^2 \\
 &\quad + 3 \times 3 \times 2^{n+2}(18n + 24 + 1)^2 + \sum_{i=1}^n [3 \times 2^i(\alpha + 1 + 2)^2 + 3 \times 2^i(\alpha + 2 + 3)^2 \\
 &\quad + 3 \times 2^{i+1}(\alpha + 3 + 2)^2 + 3 \times 2^{i+1}(\alpha + 4 + 2)^2 + 3 \times 2^i(\alpha + 5 + 3)^2 \\
 &\quad + 3 \times 2^i(\alpha + 6 + 2)^2 + 3 \times 2^i(\alpha + 7 + 2)^2 + 3 \times 2^i(\alpha + 8 + 3)^2 \\
 &\quad + 3 \times 2^i(\alpha + 9 + 1)^2 + 3 \times 2^i(\alpha + 9 + 4)^2 + 3 \times 2^i(\alpha + 10 + 1)^2] \\
 &= 2^{n+1}(32076n^2 + 52164n + 37677) - 5832n^2 - 1998n - 12207. \quad \square
 \end{aligned}$$

**Theorem 3.6.** Second Zagreb eccentricity index of graph  $D(n)$  is  $E_2(D(n)) = 2^n(67068n^2 + 89316n + 64305) - 5832n^2 - 2538n - 11808$

**Proof.** The Second Zagreb eccentricity index of  $D(n)$  is calculated by substituting the values of Table 3 in 2.4 as below.

$$\begin{aligned}
 E_2(D(n)) &= \sum_{uv \in E(D(n))} e(u)e(v) \\
 &= 6(9n + 14)(9n + 13) + 6(9n + 13)(9n + 14) + (3 \times 2^{n+1})(18n + 13)(18n + 14) \\
 &\quad + (3 \times 2^{n+1})(18n + 14)(18n + 15) + (3 \times 2^{n+2})(18n + 15)(18n + 16) \\
 &\quad + (3 \times 2^{n+2})(18n + 16)(18n + 17) + (3 \times 2^{n+2})(18n + 17)(18n + 18) \\
 &\quad + (3 \times 2^{n+1})(18n + 18)(18n + 19) + (3 \times 2^{n+1})(18n + 19)(18n + 20) \\
 &\quad + (3 \times 2^{n+1})(18n + 20)(18n + 21) + (3 \times 2^{n+2})(18n + 21)(18n + 22) \\
 &\quad + (3 \times 2^{n+2})(18n + 22)(18n + 23) + (3 \times 3 \times 2^{n+2})(18n + 23)(18n + 24) \\
 &\quad + \sum_{i=1}^{n-1} 3 \times 2^i(\alpha + 9)(\alpha + 1) + \sum_{i=1}^n [3 \times 2^i(\alpha + 1)(\alpha + 2) + 3 \times 2^{i+1}(\alpha + 2)(\alpha + 3) \\
 &\quad + 3 \times 2^{i+1}(\alpha + 3)(\alpha + 4) + 3 \times 2^{i+1}(\alpha + 4)(\alpha + 5) + 3 \times 2^i(\alpha + 5)(\alpha + 6) \\
 &\quad + 3 \times 2^i(\alpha + 6)(\alpha + 7) + 3 \times 2^i(\alpha + 7)(\alpha + 8) + 3 \times 2^i(\alpha + 8)(\alpha + 9) \\
 &\quad + 3 \times 2^i(\alpha + 8)(\alpha + 9) + 3 \times 2^i(\alpha + 9)(\alpha + 10)] \\
 &= 2^n(67068n^2 + 89316n + 64305) - 5832n^2 - 2538n - 11808. \quad \square
 \end{aligned}$$

The degrees, eccentricity and frequencies of edges of  $D(n)$  are shown in Table 3.

Edge representative	Degree	Eccentricity	Frequency
$(u_1, u_2)$	(2,4)	$(9n+14, 9n+13)$	6
$(u_2, a_1)$	(4,2)	$(9n+13, 9n+14)$	6
$(k_n, v_1)$	(4,2)	$(18n+13, 18n+14)$	$3 \times 2^{n+1}$
$(v_1, v_2)$	(2,3)	$(18n+14, 18n+15)$	$3 \times 2^{n+1}$
$(v_2, v_3)$	(3,2)	$(18n+15, 18n+16)$	$3 \times 2^{n+2}$
$(v_3, v_4)$	(2,2)	$(18n+16, 18n+17)$	$3 \times 2^{n+2}$
$(v_4, v_5)$	(2,3)	$(18n+17, 18n+18)$	$3 \times 2^{n+2}$
$(v_5, v_6)$	(3,2)	$(18n+18, 18n+19)$	$3 \times 2^{n+1}$
$(v_6, v_7)$	(2,2)	$(18n+19, 18n+20)$	$3 \times 2^{n+1}$
$(v_7, v_8)$	(2,3)	$(18n+20, 18n+21)$	$3 \times 2^{n+1}$
$(v_8, v_9)$	(3,2)	$(18n+21, 18n+22)$	$3 \times 2^{n+2}$
$(v_9, v_{10})$	(2,4)	$(18n+22, 18n+23)$	$3 \times 2^{n+2}$
$(v_{10}, v_{11})$	(4,1)	$(18n+23, 18n+24)$	$3 \times 3 \times 2^{n+2}$
$(k_i, a_{i+1}), i > n$	(4,2)	$(\alpha + 9, \alpha + 1)$	$3 \times 2^i$
$(a_i, b_i)$	(2,3)	$(\alpha + 1, \alpha + 2)$	$3 \times 2^i$
$(b_i, c_i)$	(3,2)	$(\alpha + 2, \alpha + 3)$	$3 \times 2^{i+1}$
$(c_i, d_i)$	(2,2)	$(\alpha + 3, \alpha + 4)$	$3 \times 2^{i+1}$
$(d_i, e_i)$	(2,3)	$(\alpha + 4, \alpha + 5)$	$3 \times 2^{i+1}$
$(e_i, f_i)$	(3,2)	$(\alpha + 5, \alpha + 6)$	$3 \times 2^i$
$(f_i, g_i)$	(2,2)	$(\alpha + 6, \alpha + 7)$	$3 \times 2^i$
$(g_i, h_i)$	(2,3)	$(\alpha + 7, \alpha + 8)$	$3 \times 2^i$
$(h_i, j_i)$	(3,1)	$(\alpha + 8, \alpha + 9)$	$3 \times 2^i$
$(h_i, k_i)$	(3,4)	$(\alpha + 8, \alpha + 9)$	$3 \times 2^i$
$(k_i, l_i)$	(4,1)	$(\alpha + 9, \alpha + 10)$	$3 \times 2^i$

Table 3: Degrees, eccentricity and frequencies of edges of  $D(n)$ .

**Theorem 3.7.** *Second Zagreb degree eccentricity index of graph  $D(n)$  is  $DE_2(D(n)) = 2^n(26244n^2 + 6912n + 14217) - 6804n^2 - 4104n - 14574$*

**Proof.** By equation 2.8, the Second Zagreb degree eccentricity index of  $D(n)$  is given by  $DE_2(D(n)) = \sum_{uv \in E(D(n))} (e(u) + d(u))(e(v) + d(v))$ . Using Table 3 we have,

$$\begin{aligned}
 DE_2(D(n)) = & 6(9n + 14 + 2)(9n + 13 + 4) + 6(9n + 13 + 4)(9n + 14 + 2) \\
 & + (3 \times 2^{n+1})(18n + 13 + 4)(18n + 14 + 2) + (3 \times 2^{n+1})(18n + 14 + 2)(18n + 15 + 3) \\
 & + (3 \times 2^{n+2})(18n + 15 + 3)(18n + 16 + 2) + (3 \times 2^{n+2})(18n + 16 + 2)(18n + 17 + 2) \\
 & + (3 \times 2^{n+2})(18n + 17 + 2)(18n + 18 + 3) + (3 \times 2^{n+1})(18n + 18 + 3)(18n + 19 + 2) \\
 & + (3 \times 2^{n+1})(18n + 19 + 2)(18n + 20 + 2) + (3 \times 2^{n+1})(18n + 20 + 2)(18n + 21 + 3) \\
 & + (3 \times 2^{n+2})(18n + 21 + 3)(18n + 22 + 2) + (3 \times 2^{n+2})(18n + 22 + 2)(18n + 23 + 4) \\
 & + (3 \times 3 \times 2^{n+2})(18n + 23 + 4)(18n + 24 + 1) + \sum_{i=1}^{n-1} 3 \times 2^i (\alpha + 9 + 4)(\alpha + 1 + 2)
 \end{aligned}$$



$$\begin{aligned}
 &+ \sum_{i=1}^n [3 \times 2^i(\alpha + 1 + 2)(\alpha + 2 + 3) + 3 \times 2^{i+1}(\alpha + 2 + 3)(\alpha + 3 + 2) \\
 &+ 3 \times 2^{i+1}(\alpha + 3 + 2)(\alpha + 4 + 2) + 3 \times 2^{i+1}(\alpha + 4 + 2)(\alpha + 5 + 3) \\
 &+ 3 \times 2^i(\alpha + 5 + 3)(\alpha + 6 + 2) + 3 \times 2^i(\alpha + 6 + 2)(\alpha + 7 + 2) \\
 &+ 3 \times 2^i(\alpha + 7 + 2)(\alpha + 8 + 3) + 3 \times 2^i(\alpha + 8 + 3)(\alpha + 9 + 1) \\
 &+ 3 \times 2^i(\alpha + 8 + 3)(\alpha + 9 + 4) + 3 \times 2^i(\alpha + 9 + 4)(\alpha + 10 + 1)] \\
 &= 2^n(26244n^2 + 6912n + 14217) - 6804n^2 - 4104n - 14574. \quad \square
 \end{aligned}$$

### Graphical comparison

Graph theory as a tool has been extensively used to molecular topology theory of chemical computation. The findings are helps significantly in the engineering application. In this paper, several important chemical structures are examined, and by means of first and second Zagreb indices, first and second Zagreb degree eccentricity indices, eccentric connectivity index and modified versions of eccentric-connectivity index for a class of Phosphorus containing dendrimers are calculated. Our calculated results, for example the eccentric-connectivity index is currently being used for the modeling of biological activities of a chemical compound and it is useful for determining reflect molecular branching. However, many physico-chemical properties are dependent on factors rather different than branching.

The pictorial representation of the comparison of the first and second Zagreb indices, first and second Zagreb eccentricity indices, first and second Zagreb degree eccentricity indices, eccentric connectivity index and modified versions of eccentric-connectivity index for  $D(n)$ . is shown in Figure 4. Now we give geometric comparison of the result. Figure 4 illustrate that class of Phosphorus containing dendrimers has greatest value of first and second Zagreb eccentricity indices and second Zagreb degree eccentricity index and have the least value of first Zagreb index, eccentric connectivity index and modified versions of eccentric-connectivity index.

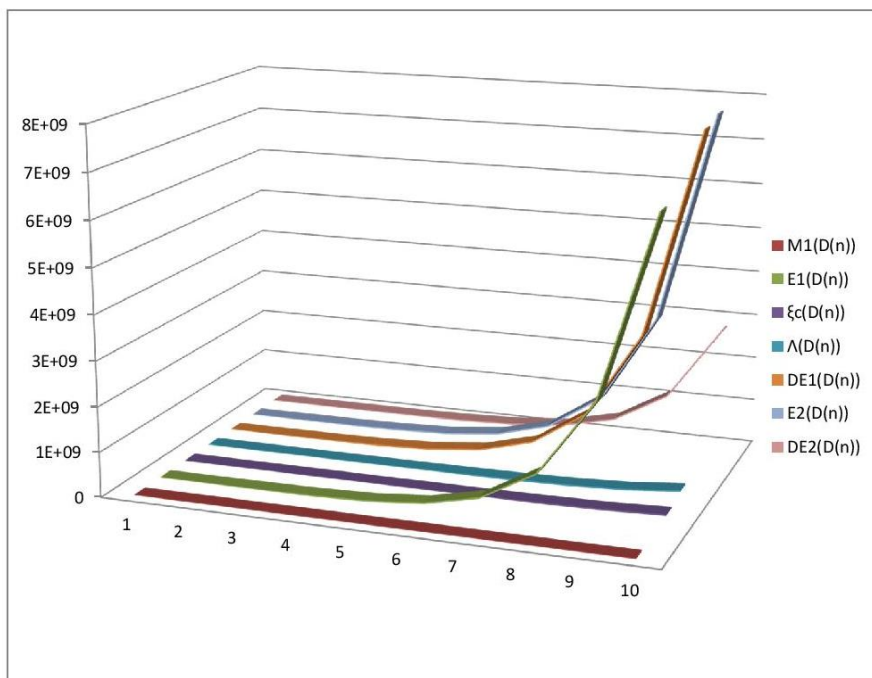


Figure 4

## Conclusion

In this paper, we compute the precise values of first and second Zagreb indices, first and second Zagreb eccentricity indices, first and second Zagreb degree eccentricity indices, eccentric connectivity index and modified versions of eccentric-connectivity index for a class of Phosphorus containing dendrimers.

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