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On Eccentricity-Based Topological Indices and Polynomials of Phosphorus-Containing Dendrimers

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Abstract: In the study of the quantitative structure–activity relationship and quantitative structure–property relationships, the eccentric-connectivity index has a very important place among the other topological descriptors due to its high degree of predictability for pharmaceutical properties. In this paper, we compute the exact formulas of the eccentric-connectivity index and its corresponding polynomial, the total eccentric-connectivity index and its corresponding polynomial, the first Zagreb eccentricity index, the augmented eccentric-connectivity index, and the modified eccentric-connectivity index and its corresponding polynomial for a class of phosphorus containing dendrimers.

Keywords: eccentric-connectivity index; augmented eccentric-connectivity index; molecular graph; phosphorus containing dendrimers

MSC: 05C90

1. Introduction

Dendrimers are synthetic polymers with highly branched structures, consisting of multiple branched monomers radiating from a central core. Layers of monomers are attached stepwise during synthesis, with the number of branch points defining the generation of a dendrimer [1]. Different kinds of experiments have proved that these polymers with well-defined dimensional structures and topological architectures have an array of applications in medicine [2]. Nowadays, dendrimers are currently attracting the interest of a great number of scientists because of their unusual physical and chemical properties and their wide range of potential applications in different fields, such as physics, biology, chemistry, engineering, and medicine [3]. 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 structures that correlate a chemical structure with various physical properties, biological activities or chemical reactivities. A topological index is an invariant of a graph, G_1; that is, if $Top(G_1)$ denotes a topological index of graph G_1, and if G_2 is another graph such that $G_1 \cong G_2$, then $Top(G_1) = Top(G_2)$. In chemistry, biochemistry and nanotechnology, distance-based topological indices of graphs are useful in isomer discrimination, structure–property relationships and structure–activity relationships.

2. Definitions and Notations

Let G be a connected and simple molecular graph with vertex set, $V(G)$, and edge set, $E(G)$. The vertices of G correspond to atoms, and an edge between two vertices corresponds to the chemical bond between these vertices. In graph G, two vertices, u and v, are adjacent, if and only if, they are the end vertices of an edge, $e \in E(G)$, and we write $e = uv$ or $e = vu$. For a vertex, u, the set of neighbor vertices is denoted by N_u and is defined as $N_u = \{v \in V(G) : uv \in E(G)\}$. The degree of vertex $u \in V(G)$ is denoted by d_u and is defined as $d_u = |N_u|$. Let S_u denote the sum of the degrees of all neighbors of vertex u, that is $S_u = \sum_{v \in N_u} d_v$. A (u_1, u_n)-path on n vertices is defined as a graph with vertex set, $\{u_i : 1 \leq i \leq n\}$, and edge set, $\{u_i u_{i+1} : 1 \leq i \leq n-1\}$. The distance, $d(u,v)$, between two vertices, $u, v \in V(G)$, is defined as the length of the shortest (u,v)-path in G. For a given vertex, $v \in V(G)$, the eccentricity, $\varepsilon(v)$, is defined as the largest distance between v and any other vertex, u in G. In 1947, Harold Wiener published a paper entitled "Structural Determination of Paraffin Boiling Points" [4]. In this work, the quantity, W_e, eventually named the Wiener index or Wiener number, was introduced for the first time, and he showed that there are excellent correlations between W_e and a variety of physico-chemical properties of organic compounds. Another distance-based topological index of the graph G is the eccentric-connectivity index, $\xi(G)$, which is defined as [5]

$$\xi(G) = \sum_{u \in V(G)} \varepsilon(u) d_u. \tag{1}$$

Different applications and mathematical properties of this index were discussed in [6–9]. For a graph, G, the eccentric-connectivity polynomial in variable y is defined as [10]

$$ECP(G,y) = \sum_{u \in V(G)} d_u y^{\varepsilon(u)}. \tag{2}$$

The total eccentricity index of a graph, G, is expressed as follows:

$$\varsigma(G) = \sum_{u \in V(G)} \varepsilon(u). \tag{3}$$

The total eccentric-connectivity polynomial in variable y of a graph, G, is defined as [10]

$$TECP(G,y) = \sum_{u \in V(G)} y^{\varepsilon(u)}. \tag{4}$$

The first Zagreb index of a graph, G, in terms of eccentricity was given by Ghorbani and Hosseinzadeh [11], as follows:

$$M_1^{**}(G) = \sum_{u \in V(G)} (\varepsilon(u))^2. \tag{5}$$

Gupta and his co-authors [12] introduced the augmented eccentric-connectivity index of a graph, G, and it is defined as

$$^{A}\varepsilon(G) = \sum_{u \in V(G)} \frac{M(u)}{\varepsilon(u)}, \tag{6}$$

where $M(u)$ denotes the product of degrees of all neighbors of vertex u. Various properties of this index have been studied in [13,14]. For a graph, G, the modified versions of the eccentric-connectivity index and its polynomial are defined as follows

$$\Lambda(G) = \sum_{u \in V(G)} S_u \varepsilon(u), \tag{7}$$

$$MECP(G,y) = \sum_{u \in V(G)} S_u y^{\varepsilon(u)}. \tag{8}$$

Several mathematical and chemical properties of the modified eccentric-connectivity index and its polynomial were studied in [10,15]. 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 [16–18]. For a study of distance-based topological indices, see [19–21]. In this paper, we compute several distance-based indices, namely, the eccentric-connectivity index, the total eccentric-connectivity index, and the modified eccentric-connectivity index for the phosphorus-containing dendrimer Cyclotriphosphazene (N_3P_3) [22]. We also compute the corresponding polynomials of these indices for the same dendrimer. We also compute the first Zagreb eccentricity index and the augmented eccentric-connectivity index for the said dendrimer.

3. The Eccentricity-Based Indices and Polynomials for the Molecular Graph

Let the molecular graph of this dendrimer be $D(n)$, where the generation stage of $D(n)$ is represented by n. The first and second generations are shown in Figures 1 and 2 respectively.

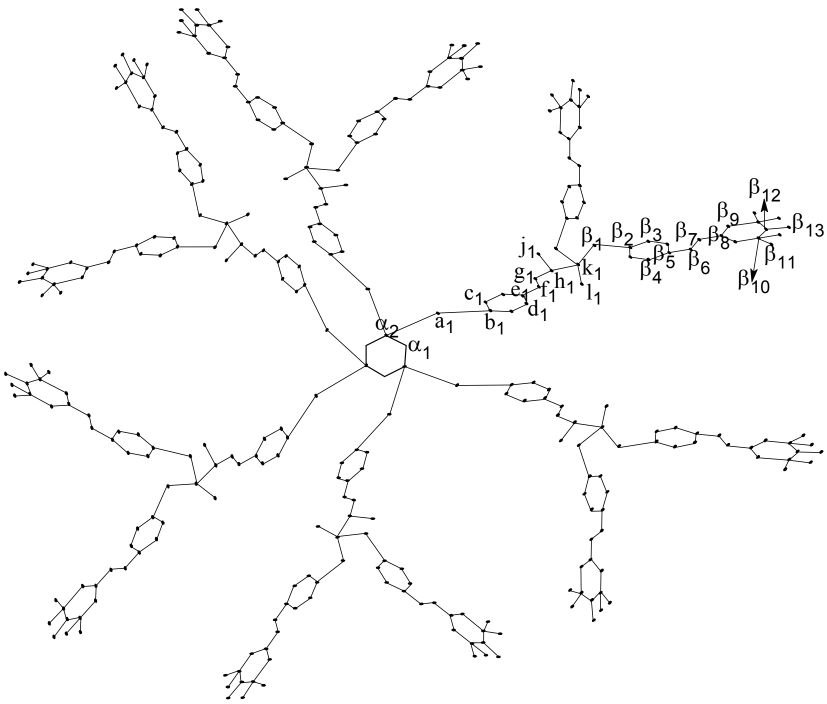

Figure 1. First generation.

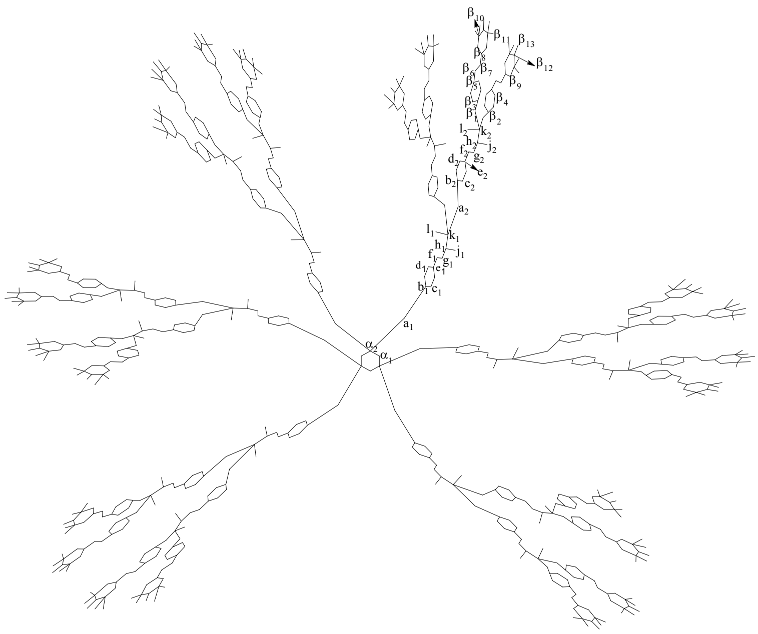

Figure 2. Second generation.

The size and order of graph $D(n)$ are $6(9 \times 2^{n+2} - 13)$ and $9(-8 + 11 \times 2^n)$, respectively. To compute the eccentricity-based indices and polynomials of $D(n)$, it is enough to compute the required information for a set of representatives of $V(D(n))$. We will compute the required information by using computational arguments. We make three sets of representatives of $V(D(n))$, say $A = \{\alpha_1, \alpha_2\}$, $B = \{\beta_1, \beta_2, \ldots, \beta_{13}\}$ and $C = \{a_i, b_i, c_i, d_i, e_i, f_i, g_i, h_i, j_i, k_i, l_i\}$ where $1 \leq i \leq n$, as shown in Figures 1 and 2. The degree, S_u, $M(u)$, and eccentricity for each u for the sets A, B, and C are shown in Tables 1 and 2. For simplicity, we assume $\gamma = 9n + 9i$ throughout the paper. By using Tables 1 and 2, we calculate the different eccentricity-based indices and their corresponding polynomials. In the following theorem, we determine the eccentric-connectivity index of $D(n)$.

Table 1. Sets A and B with their degrees, S_u, $M(u)$, eccentricities, and frequencies.

Representative	Degree	S_u	$M(u)$	Eccentricity	Frequency
α_1	2	8	16	$9n + 15$	3
α_2	4	8	16	$9n + 14$	3
β_1	2	7	12	$9n + 15$	$3 \times 2^{n+1}$
β_2	3	6	8	$9n + 16$	$3 \times 2^{n+1}$
β_3	2	5	6	$9n + 17$	$3 \times 2^{n+2}$
β_4	2	5	6	$9n + 18$	$3 \times 2^{n+2}$
β_5	3	6	8	$9n + 19$	$3 \times 2^{n+1}$
β_6	2	5	6	$9n + 20$	$3 \times 2^{n+1}$
β_7	2	5	6	$9n + 21$	$3 \times 2^{n+1}$
β_8	3	6	8	$9n + 22$	$3 \times 2^{n+1}$
β_9	2	7	12	$9n + 23$	$3 \times 2^{n+2}$
β_{10}	4	7	6	$9n + 24$	$3 \times 2^{n+2}$
β_{11}	1	4	4	$9n + 25$	$3 \times 2^{n+3}$
β_{12}	3	9	16	$9n + 25$	$3 \times 2^{n+1}$
β_{13}	1	3	3	$9n + 26$	$3 \times 2^{n+1}$

Table 2. Set C with degrees, S_u, $M(u)$, eccentricities, and frequencies.

Representative	Degree	S_u	$M(u)$	Eccentricity	Frequency
a_i	2	7	12	$9n+9i+6=\gamma+6$	3×2^i
b_i	3	6	8	$\gamma+7$	3×2^i
c_i	2	5	6	$\gamma+8$	$3\times 2^{i+1}$
d_i	2	5	6	$\gamma+9$	$3\times 2^{i+1}$
e_i	3	6	8	$\gamma+10$	3×2^i
f_i	2	5	6	$\gamma+11$	3×2^i
g_i	2	5	6	$\gamma+12$	3×2^i
h_i	3	7	8	$\gamma+13$	3×2^i
j_i	1	3	3	$\gamma+14$	3×2^i
k_i	4	8	12	$\gamma+14$	3×2^i
l_i	1	4	4	$\gamma+15$	3×2^i

Theorem 1. *For graph $D(n)$, the eccentric-connectivity index is given by*

$$\xi(D(n)) = 18(2^{n+2}\times 79 - 78n + 2^n \times 303n + 1).$$

Proof. By putting the values of Tables 1 and 2 into Equation (1), the eccentric-connectivity index of $D(n)$ can be written as follows:

$$\begin{aligned}
\xi(D(n)) = \xi(A)+\xi(B)+\xi(C) &= \sum_{u\in A}\varepsilon(u)d_u + \sum_{u\in B}\varepsilon(u)d_u + \sum_{u\in C}\varepsilon(u)d_u \\
&= (2\times 3)(9n+15) + (3\times 4)(9n+14) + (3\times 2^{n+1}\times 2)(9n+15) \\
&+ (3\times 2^{n+1}\times 3)(9n+16) + (2\times 2^{n+2}\times 3)(9n+17) + (2\times 2^{n+2}\times 3)(9n+18) \\
&+ (3\times 2^{n+1}\times 3)(9n+19) + (2\times 2^{n+1}\times 3)(9n+20) + (2\times 2^{n+1}\times 3)(9n+21) \\
&+ (2\times 2^{n+2}\times 3)(9n+23) + (4\times 2^{n+2}\times 3)(9n+24) + (1\times 2^{n+3}\times 3)(9n+25) \\
&+ (3\times 2^{n+1}\times 3)(9n+22) + (3\times 2^{n+1}\times 3)(9n+25) + (1\times 2^{n+1}\times 3)(9n+26)
\end{aligned}$$

$$\begin{aligned}
&+ \sum_{i=1}^{n}\Big((2\times 2^i\times 3)(\gamma+6) + (3\times 2^i\times 3)(\gamma+7) + (2\times 2^{i+1}\times 3)(\gamma+8) \\
&+ (2^{i+2}\times 3)(\gamma+9) + (3\times 2^i\times 3)(\gamma+10) + (3\times 2^{i+1})(\gamma+11) + (2^{i+1}\times 3)(\gamma+12) \\
&+ (3\times 2^i\times 3)(\gamma+13) + (2^i\times 3)(\gamma+14) + (4\times 2^i\times 3)(\gamma+14) + (2^i\times 3)(\gamma+15)\Big).
\end{aligned}$$

After some calculations, we get

$$\xi(D(n)) = 18(2^{n+2}\times 79 - 78n + 2^n \times 303n + 1),$$

which completes the theorem. □

When the degrees of vertices are not taken into account, then by using the values of Tables 1 and 2 in (3), we have the following result.

Corollary 1. *For graph $D(n)$, the total eccentric-connectivity index is given by*

$$\varsigma(D(n)) = 9(2^{n+2}\times 69n + 2^{n+1}\times 149 - 72n - 3).$$

In the next theorem, the eccentric-connectivity polynomial for the molecular graph is derived.

Theorem 2. *For graph $D(n)$, the eccentric-connectivity polynomial is given by*

$$ECP(D(n),y) = 6y^{9n+14}(y+2) + 3\times 2^{n+1}y^{9n+15}(y^{11}+7y^{10}+8y^9+4y^8+3y^7+2y^6+2y^5 + 3y^4+4y^3+4y^2+3y+2) + \frac{6(y^3+5y^2+3y+2)\times y^{9n+21}(2^n y^{9n}-1)}{2y^9-1} + \frac{6(2y^5+3y^4+4y^3+4y^2+3y+2)\times y^{9n+15}(2^n y^{9n}-1)}{2y^9-1}.$$

Proof. By using Tables 1 and 2 in (2), we have

$$\begin{aligned}
ECP(D(n),y) &= ECP(A,y) + ECP(B,y) + ECP(C,y) \\
&= \sum_{u\in A} d_u y^{\varepsilon(u)} + \sum_{u\in B} d_u y^{\varepsilon(u)} + \sum_{u\in C} d_u y^{\varepsilon(u)} \\
&= (2\times 3)y^{9n+15} + (4\times 3)y^{9n+14} + (3\times 2^{n+2})y^{9n+15} + (3\times 3\times 2^{n+1})y^{9n+16} \\
&+ (2\times 3\times 2^{n+2})y^{9n+17} + (2\times 3\times 2^{n+2})y^{9n+18} + (3\times 3\times 2^{n+1})y^{9n+19} \\
&+ (2\times 3\times 2^{n+1})y^{9n+20} + (2\times 3\times 2^{n+1})y^{9n+21} + (3\times 3\times 2^{n+1})y^{9n+22} \\
&+ (2\times 3\times 2^{n+2})y^{9n+23} + (4\times 3\times 2^{n+2})y^{9n+24} + (1\times 3\times 2^{n+3})y^{9n+25} \\
&+ (3\times 3\times 2^{n+1})y^{9n+25} + (1\times 3\times 2^{n+1})y^{9n+26} + \sum_{i=1}^{n}\Big((2\times 3\times 2^i)y^{\gamma+6} \\
&+ (2\times 3\times 2^{i+1})y^{\gamma+8} + (2\times 3\times 2^{i+1})y^{\gamma+9} + (3\times 3\times 2^i)y^{\gamma+10} \\
&+ (2\times 3\times 2^i)y^{\gamma+11} + (3\times 3\times 2^i)y^{\gamma+7} + (2\times 3\times 2^i)y^{\gamma+12} \\
&+ (3\times 3\times 2^i)y^{\gamma+13} + (3\times 2^i)y^{\gamma+14} + (4\times 3\times 2^i)y^{\gamma+14} + (3\times 2^i)y^{\gamma+15}\Big).
\end{aligned}$$

After some calculations, we get the required result. □

By putting the values of Tables 1 and 2 into (4), we get the following result.

Corollary 2. *For graph $D(n)$, the total eccentric-connectivity polynomial is given by*

$$TECP(D(n),y) = 3y^{9n+14}(y+1) + 3\times 2^{n+1}y^{9n+15}(y^{11}+5y^{10}+2y^9+2y^8+y^7+y^6+y^5 + y^4+2y^3+2y^2+y+1) + \frac{6(y^3+2y^2+y+1)\times y^{9n+21}(2^n y^{9n}-1)}{2y^9-1} + \frac{6(y+1)(y^2+1)^2\times y^{9n+15}(2^n y^{9n}-1)}{2y^9-1}.$$

In the next theorem, we compute the closed formula for the first Zagreb eccentricity index.

Theorem 3. *For graph $D(n)$, the first Zagreb eccentricity index is given by*

$$M_1^{**}(D(n)) = 3(2^{n+4}\times 7295n^2 + 2^{n+3}\times 2097n - 1944n^2 - 162n + 2^{n+1}\times 11641 - 4053).$$

Proof. By using the values of Tables 1 and 2 in (5), we compute the first Zagreb eccentricity index of $D(n)$ as follows:

$$\begin{aligned} M_1^{**}(D(n)) &= M_1^{**}(A) + M_1^{**}(B) + M_1^{**}(C) = \sum_{v\in A}[\varepsilon(v)]^2 + \sum_{v\in B}[\varepsilon(v)]^2 + \sum_{v\in C}[\varepsilon(v)]^2 \\ &= 3(9n+15)^2 + 3(9n+14)^2 + (3\times 2^{n+1})(9n+15)^2 + (3\times 2^{n+1})(9n+16)^2 \\ &+ (3\times 2^{n+2})(9n+17)^2 + (3\times 2^{n+2})(9n+18)^2 + (3\times 2^{n+1})(9n+19)^2 \\ &+ (3\times 2^{n+1})(9n+20)^2 + (3\times 2^{n+1})(9n+21)^2 + (3\times 2^{n+1})(9n+22)^2 \\ &+ (3\times 2^{n+2})(9n+23)^2 + (3\times 2^{n+2})(9n+24)^2 + (3\times 2^{n+3})(9n+25)^2 \\ &+ (3\times 2^{n+1})(9n+25)^2 + (3\times 2^{n+1})(9n+26)^2 + \sum_{i=1}^{n}\Big((3\times 2^i)(\gamma+6)^2 \\ &+ (3\times 2^i)(\gamma+7)^2 + (3\times 2^{i+1})(\gamma+8)^2 + (3\times 2^{i+1})(\gamma+9)^2 + (3\times 2^i)(\gamma+10)^2 \\ &+ (3\times 2^i)(\gamma+11)^2 + (3\times 2^i)(\gamma+12)^2 + (3\times 2^i)(\gamma+13)^2 + (3\times 2^i)(\gamma+14)^2 \\ &+ (3\times 2^i)(\gamma+14)^2 + (3\times 2^i)(\gamma+15)^2\Big). \end{aligned}$$

After some calculations, we obtain

$$M_1^{**}(D(n)) = 3(2^{n+4}\times 7295n^2 + 2^{n+3}\times 2097n - 1944n^2 - 162n + 2^{n+1}\times 11,641 - 4053),$$

which finishes the theorem. □

We determine the augmented eccentric-connectivity index in the next theorem.

Theorem 4. *For graph $D(n)$, the augmented eccentric-connectivity index is given by*

$$\begin{aligned} {}^{A}\varepsilon(D(n)) &= \frac{48}{9n+15} + \frac{48}{9n+14} + \frac{36\times 2^{n+1}}{9n+15} + \frac{24\times 2^{n+1}}{9n+16} + \frac{18\times 2^{n+2}}{9n+17} + \frac{18\times 2^{n+2}}{9n+18} \\ &+ \frac{24\times 2^{n+1}}{9n+19} + \frac{18\times 2^{n+1}}{9n+20} + \frac{18\times 2^{n+1}}{9n+21} + \frac{24\times 2^{n+1}}{9n+22} + \frac{36\times 2^{n+2}}{9n+23} + \frac{18\times 2^{n+2}}{9n+24} \\ &+ \frac{12\times 2^{n+3}}{9n+25} + \frac{48\times 2^{n+1}}{9n+25} + \frac{9\times 2^{n+1}}{9n+26} + \left(\frac{72}{9n+15} + \cdots + \frac{36\times 2^{n}}{18n+6}\right) \\ &+ \left(\frac{48}{9n+16} + \cdots + \frac{24\times 2^{n}}{18n+7}\right) + \left(\frac{72}{9n+17} + \cdots + \frac{18\times 2^{n+1}}{18n+8}\right) \\ &+ \left(\frac{72}{9n+18} + \cdots + \frac{18\times 2^{n+1}}{18n+9}\right) + \left(\frac{48}{9n+19} + \cdots + \frac{24\times 2^{n}}{18n+10}\right) \\ &+ \left(\frac{36}{9n+20} + \cdots + \frac{18\times 2^{n}}{18n+11}\right) + \left(\frac{36}{9n+21} + \cdots + \frac{18\times 2^{n}}{18n+12}\right) \\ &+ \left(\frac{48}{9n+22} + \cdots + \frac{24\times 2^{n}}{18n+13}\right) + \left(\frac{18}{9n+23} + \cdots + \frac{9\times 2^{n}}{18n+14}\right) \\ &+ \left(\frac{72}{9n+23} + \cdots + \frac{36\times 2^{n}}{18n+14}\right) + \left(\frac{24}{9n+24} + \cdots + \frac{12\times 2^{n}}{18n+15}\right). \end{aligned}$$

Proof. By using the values of Tables 1 and 2 in (6), we compute the augumented eccentric-connectivity index of $D(n)$ in the following way:

$$\begin{aligned}
{}^{A}\varepsilon(D(n)) &= {}^{A}\varepsilon(A) + {}^{A}\varepsilon(B) + {}^{A}\varepsilon(C) = \sum_{u\in A}\frac{M(u)}{\varepsilon(u)} + \sum_{u\in B}\frac{M(u)}{\varepsilon(u)} + \sum_{u\in C}\frac{M(u)}{\varepsilon(u)} \\
&= \frac{3\times 16}{9n+15} + \frac{3\times 16}{9n+14} + \frac{3\times 2^{n+1}\times 12}{9n+15} + \frac{3\times 2^{n+1}\times 8}{9n+16} + \frac{3\times 2^{n+2}\times 6}{9n+17} \\
&+ \frac{3\times 2^{n+2}\times 6}{9n+18} + \frac{3\times 2^{n+1}\times 8}{9n+19} + \frac{3\times 2^{n+1}\times 6}{9n+20} + \frac{3\times 2^{n+1}\times 6}{9n+21} \\
&+ \frac{3\times 2^{n+1}\times 8}{9n+22} + \frac{3\times 2^{n+2}\times 12}{9n+23} + \frac{3\times 2^{n+2}\times 6}{9n+24} + \frac{3\times 2^{n+3}\times 4}{9n+25} \\
&+ \frac{3\times 2^{n+1}\times 16}{9n+25} + \frac{3\times 2^{n+1}\times 3}{9n+26} + \sum_{i=1}^{n}\Big(\frac{3\times 2^{i}\times 12}{\gamma+6} + \frac{3\times 2^{i}\times 8}{\gamma+7} \\
&+ \frac{3\times 2^{i+1}\times 6}{\gamma+8} + \frac{3\times 2^{i+1}\times 6}{\gamma+9} + \frac{3\times 2^{i}\times 8}{\gamma+10} + \frac{3\times 2^{i}\times 6}{\gamma+11} + \frac{3\times 2^{i}\times 6}{\gamma+12} \\
&+ \frac{3\times 2^{i}\times 8}{\gamma+13} + \frac{3\times 2^{i}\times 3}{\gamma+14} + \frac{3\times 2^{i}\times 12}{\gamma+14} + \frac{3\times 2^{i}\times 4}{\gamma+15}\Big).
\end{aligned}$$

After some calculations, we obtain the required result. □

Now, we compute the closed formula for the modified eccentric-connectivity index.

Theorem 5. *For graph $D(n)$, the modified eccentric-connectivity index is given by*

$$\Lambda(D(n)) = 6(2^{n}\times 2277n - 567n + 2^{n+1}\times 1229 + 21).$$

Proof. By using the values of Tables 1 and 2 in (7), we compute the modified eccentric-connectivity index of $D(n)$ in the following way:

$$\begin{aligned}
\Lambda(D(n)) &= \Lambda(A) + \Lambda(B) + \Lambda(C) = \sum_{u\in A} S_u\varepsilon(u) + \sum_{u\in B} S_u\varepsilon(u) + \sum_{u\in C} S_u\varepsilon(u) \\
&= (8\times 3)(9n+15) + (8\times 3)(9n+14) + (7\times 3\times 2^{n+1})(9n+15) \\
&+ (5\times 3\times 2^{n+2})(9n+17) + (5\times 3\times 2^{n+2})(9n+18) + (6\times 3\times 2^{n+1})(9n+19) \\
&+ (5\times 3\times 2^{n+1})(9n+20) + (5\times 3\times 2^{n+1})(9n+21) + (6\times 3\times 2^{n+1})(9n+22) \\
&+ (7\times 3\times 2^{n+2})(9n+23) + (7\times 3\times 2^{n+2})(9n+24) + (4\times 3\times 2^{n+3})(9n+25) \\
&+ (9\times 3\times 2^{n+1})(9n+25) + (3\times 3\times 2^{n+1})(9n+26) + (6\times 3\times 2^{n+1})(9n+16) \\
&+ \sum_{i=1}^{n}\Big((7\times 3\times 2^{i})(\gamma+6) + (6\times 3\times 2^{i})(\gamma+7) + (5\times 3\times 2^{i+1})(\gamma+8) \\
&+ (5\times 3\times 2^{i+1})(\gamma+9) + (6\times 3\times 2^{i})(\gamma+10) + (5\times 3\times 2^{i})(\gamma+11) \\
&+ (5\times 3\times 2^{i})(\gamma+12) + (7\times 3\times 2^{i})(\gamma+13) + (3\times 3\times 2^{i})(\gamma+14) \\
&+ (8\times 3\times 2^{i})(\gamma+14) + (4\times 3\times 2^{i})(\gamma+15)\Big).
\end{aligned}$$

After some calculations, we obtain

$$\Lambda(D(n)) = 6(2^{n}\times 2277n - 567n + 2^{n+1}\times 1229 + 21),$$

which completes the proof. □

Finally, we compute the closed formula for the modified eccentric-connectivity polynomial.

Theorem 6. *For graph $D(n)$, the modified eccentric-connectivity polynomial is given by*

$$\begin{aligned} MECP(D(n),y) &= 24y^{9n+14}(y+1) + 2^{n+1} \times y^{9n+15}(9y^{11} + 75y^{10} + 42y^9 + 42y^8 \\ &+ 18y^7 + 15y^6 + 15y^5 + 18y^4 + 30y^3 + 30y^2 + 18y + 21) \\ &+ \frac{6(5y^5 + 6y^4 + 10y^3 + 10y^2 + 6y + 7)y^{9n+15}(2^n y^{9n} - 1)}{2y^9 - 1} \\ &+ \frac{6(4y^3 + 11y^2 + 7y + 5)y^{9n+21}(2^n y^{9n} - 1)}{2y^9 - 1}. \end{aligned}$$

Proof. By using the values of Tables 1 and 2 in (8), we compute the modified eccentric-connectivity polynomial of $D(n)$ in the following way:

$$\begin{aligned} MECP(D(n),y) &= MECP(A,y) + MECP(B,y) + MECP(C,y) \\ &= \sum_{u \in A} S_u y^{\varepsilon(u)} + \sum_{u \in B} S_u y^{\varepsilon(u)} + \sum_{u \in C} S_u y^{\varepsilon(u)} \\ &= (8 \times 3)y^{9n+15} + (8 \times 3)y^{9n+14} + (7 \times 3 \times 2^{n+1})y^{9n+15} \\ &+ (6 \times 3 \times 2^{n+1})y^{9n+16} + (5 \times 3 \times 2^{n+2})y^{9n+17} + (5 \times 3 \times 2^{n+2})y^{9n+18} \\ &+ (6 \times 3 \times 2^{n+1})y^{9n+19} + (5 \times 3 \times 2^{n+1})y^{9n+20} + (5 \times 3 \times 2^{n+1})y^{9n+21} \\ &+ (6 \times 3 \times 2^{n+1})y^{9n+22} + (7 \times 3 \times 2^{n+2})y^{9n+23} + (7 \times 3 \times 2^{n+2})y^{9n+24} \\ &+ (4 \times 3 \times 2^{n+3})y^{9n+25} + (9 \times 3 \times 2^{n+1})y^{9n+25} + (3 \times 3 \times 2^{n+1})y^{9n+26} \\ &+ \sum_{i=1}^{n} \Big((7 \times 3 \times 2^i)(y^{\gamma+6}) + (6 \times 3 \times 2^i)(y^{\gamma+7}) + (5 \times 3 \times 2^{i+1})(y^{\gamma+8}) \\ &+ (5 \times 3 \times 2^{i+1})(y^{\gamma+9}) + (6 \times 3 \times 2^i)(y^{\gamma+10}) + (5 \times 3 \times 2^i)(y^{\gamma+11}) \\ &+ (5 \times 3 \times 2^i)(y^{\gamma+12}) + (7 \times 3 \times 2^i)(y^{\gamma+13}) + (3 \times 3 \times 2^i)(y^{\gamma+14}) \\ &+ (8 \times 3 \times 2^i)(y^{\gamma+14}) + (4 \times 3 \times 2^i)(y^{\gamma+15}) \Big). \end{aligned}$$

After some calculations, we obtain the required result. □

4. Conclusions

In this paper we discussed the theoretical topics in molecular science and computed the eccentric topological indices for a class of phosphorus-containing dendrimers in regard to their molecular structure analysis, distance computing and mathematical derivation. Phosphorus-containing dendrimers have various applications in nanomedicine and materials science; therefore, these theoretical results could have applications in medical science.

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