



Article

On Eccentricity-Based Topological Indices Study of a Class of Porphyrin-Cored Dendrimers

Wei Gao ¹, Zahid Iqbal ² , Muhammad Ishaq ², Rabia Sarfraz ², Muhammad Aamir ^{3,4} 
and Adnan Aslam ^{5,*}

¹ School of Information Science and Technology, Yunnan Normal University, Kunming 650500, China; gaowei@ynnu.edu.cn

² School of Natural Sciences, National University of Sciences and Technology, Sector H-12, Islamabad 44000, Pakistan; 786zahidwarraich@gmail.com (Z.I.); ishaq_maths@yahoo.com (M.I.); sarfaraz_rabia@yahoo.com (R.S.)

³ Faculty of Physical and Numerical Sciences, Abdul Wali Khan University Mardan, Mardan, Pakistan; aamirkhan@awkum.edu.pk

⁴ Department of Mathematical Sciences, Faculty of Science, Universiti Teknologi Malaysia, Johor Bahru 81310, Malaysia

⁵ Department of Natural Sciences and Humanities, University of Engineering and Technology, Lahore 54000, Pakistan

* Correspondence: adnanaslam15@yahoo.com; Tel.: +92-332-544-2627

Received: 11 June 2018; Accepted: 1 August 2018; Published: 7 August 2018



Abstract: It is revealed from the previous studies that there is a strong relation between the chemical characteristic of a chemical compound and its molecular structure. Topological indices defined on the molecular structure of biomolecules can help to gain a better understanding of their physical features and biological activities. Eccentricity connectivity indices are distance-based molecular structure descriptors that have been used for the mathematical modeling of biological activities of diverse nature. As the porphyrin has photofunctional properties, such as a large absorption cross-section, fluorescence emission, and photosensitizing properties, due to these properties, porphyrin dendrimers can be used as photofunctional nanodevices. In this paper, we compute the exact formulae of different versions of eccentric connectivity index and their corresponding polynomials for a class of porphyrin-cored dendrimers. The results obtained can be used in computer-aided molecular design methods applied to pharmaceutical engineering.

Keywords: porphyrin-cored dendrimers; eccentric connectivity index; total eccentric connectivity index; augmented eccentric connectivity index

1. Introduction

In this era of rapid technological development, a large number of new nanomaterials, crystalline materials, and drugs emerge every year. To determine the chemical properties of such a large number of new compounds and new drugs requires a large amount of chemical experiments, thereby greatly increasing the workload of the chemical and pharmaceutical researchers. In this regard, computing different types of topological indices has provided the insights into medicinal behaviour of several compounds and drugs [1,2]. The computation method of topological indices has proven its worth by yielding medical information of drugs with less use of chemical-related equipment [3,4].

In chemical graph theory, various graphical invariants are used for establishing correlations of chemical structures with various physical properties, chemical reactivity, or biological activity [5,6]. These graphical invariants are called topological indices of molecular graphs in this field. There is a large family of distance-based topological indices of molecular graphs in chemical graph theory.

In chemistry, biochemistry and nanotechnology, distance-based topological indices of a graph are found to be useful in isomer discrimination, structure–property relationships and structure–activity relationships [7,8].

Dendrimers are synthetic polymers, of diverse initiator core, branches and the peripheral groups have been extensively synthesized in the last two decades [9]. Numerous kinds of experiments have proven that these polymers with well-defined structures and topological architectures exhibited an array of applications in medicine [10]. In these times, dendrimers are inviting the interest of a great number of researchers because of their remarkable physical and chemical properties and the wide range of promising applications in different fields [11–13]. Until now, the study of the eccentricity based topological indices for special chemical and nanostructures has been largely limited. Thus, we have been attracted to studying the mathematical properties of the eccentricity based topological indices and their polynomial versions of a class of dendrimers.

Now, we introduce some notations and definitions, which will be needed throughout this monograph. In a theoretical chemistry setting, chemical compounds are expressed as graphs. Let $G = (V(G), E(G))$ be a molecular graph, where $V(G)$, and $E(G)$ appear for the vertex and edge set, respectively. Vertices of G correlate with the atoms, and edges correspond to the chemical bonds between atoms. In a graph G , if two vertices s and t are end vertices of an edge $e \in E(G)$, then they are called adjacent, and we write this edge as $e = st$ or $e = ts$. For a vertex t , the set of neighbor vertices is denoted by N_t and is defined as $N_t = \{s \in V(G) : st \in E(G)\}$. The degree of a vertex $t \in V(G)$ is represented by d_t and is expressed as the number of edges connecting it. Let S_t denote the sum of the degrees of neighboring vertices of vertex t , which is $S_t = \sum_{s \in N_t} d_s$. A (t_1, t_n) -path on n vertices is defined as a graph with vertex set $\{t_1, \dots, t_n\}$ and edge set $\{t_i t_{i+1} : 1 \leq i \leq n - 1\}$. The distance between two vertices $s, t \in V(G)$ is represented by $d(s, t)$ and defined as the length of the shortest (s, t) -path in G . For a given vertex $t \in V(G)$, the eccentricity $\varepsilon(t)$ is defined as the maximum distance between t and any other vertex in G .

The history of topological indices goes back to 1947, when Harold Wiener put forward the study of first distance-based topological index, known as Wiener index [14]. Sharma, Goswami, and Madan [15] initiated the study of another distance-based topological index, termed as the eccentric connectivity index, of the graph G , described as

$$\zeta(G) = \sum_{u \in V(G)} \varepsilon(u) d_u, \quad (1)$$

which has been employed usefully for the buildup of various mathematical models for the prediction of biological activities of distinct nature. Some applications and mathematical properties of this index have been discussed by several authors [16–19]. For a graph G , Ashrafi and Jalali extended the study of the eccentric connectivity index by introducing the eccentric connectivity polynomial in [20]:

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

If we consider only the eccentricity of the vertices, then we obtain the total eccentricity index of the graph G , which is expressed as follows:

$$\zeta(G) = \sum_{t \in V(G)} \varepsilon(t). \quad (3)$$

For a graph G , the polynomial version of the total eccentricity index is described by Ashrafi et al. [20]:

$$TECP(G, x) = \sum_{t \in V(G)} x^{\varepsilon(t)}. \quad (4)$$

Ghorbani and Hosseinzadeh in [21] presented the first Zagreb index of a graph G in terms of eccentricity by replacing the vertex degrees with the vertex eccentricities in the following way:

$$M_1(G) = \sum_{t \in V(G)} (\varepsilon(t))^2. \quad (5)$$

Gupta, Singh and Madan [22] introduced the augmented eccentric connectivity index of a graph G , as a generalization of the eccentric connectivity index as follows:

$$A_\varepsilon(G) = \sum_{t \in V(G)} \frac{M(t)}{\varepsilon(t)}, \quad (6)$$

where $M(t)$ represents the product of degrees of all neighbors of vertex t . Various properties of this index have been examined in previous articles [23–25]. For a graph G , the modified versions of eccentric connectivity index and polynomial are defined as follows:

$$\Lambda(G) = \sum_{t \in V(G)} S_t \varepsilon(t), \quad (7)$$

$$MECP(G, x) = \sum_{t \in V(G)} S_t x^{\varepsilon(t)}. \quad (8)$$

Several mathematical and chemical properties of these modified versions have been studied [4,20]. For detailed results on the topological indices of graphs, the readers may refer to the previous reports [26–33]. As the porphyrin has unique photofunctional properties, such as a fluorescence emission, large absorption cross-section, and photosensitizing properties; so porphyrin dendrimers can be used as photofunctional nano-devices. The high solubility of porphyrin dendrimers permits their use in photodynamic therapy, a promising technology for fewer invasive cancer treatments [34]. In this paper, we will study the different topological indices and polynomials of the molecular graph of porphyrin-cored 2,2-bis (methylol) propionic acid dendrimers. Figure 1 depicts the molecular graph of the porphyrin-cored 2,2-bis (methylol) propionic acid dendrimer with the fourth growth stage. The synthesis and characterization of this dendrimer are described by Vestberg et al. (see [35]).

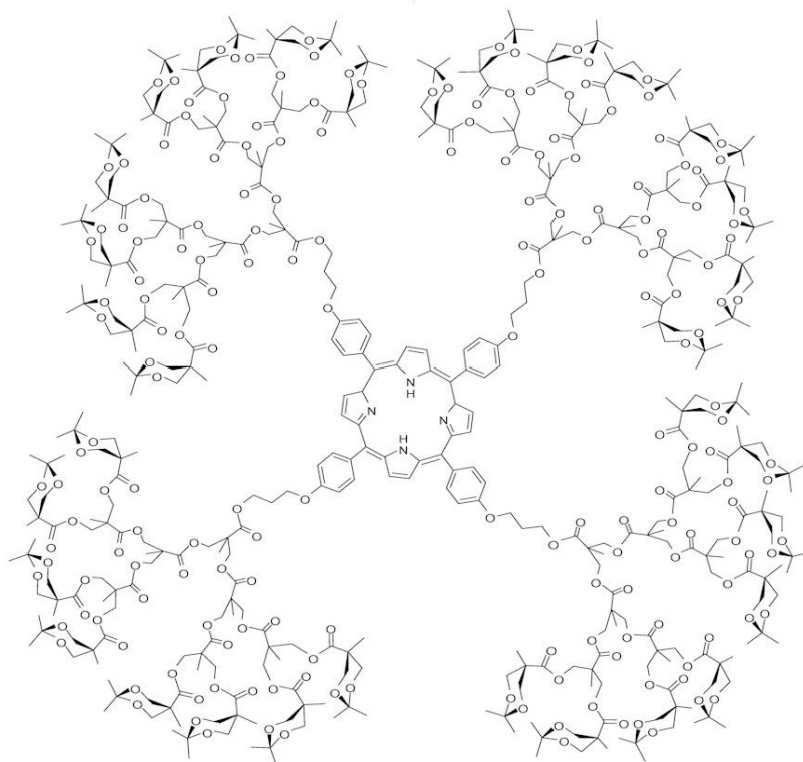


Figure 1. Porphyrin-cored 2,2-bis (methylol) propionic acid dendrimers for $n = 4$.

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

A hydrogen-depleted molecular graph is the molecular graph with hydrogen vertices deleted. The characterization of a molecule by an associated graph leads to a large number of powerful and useful discriminators called topological indices. In chemical graph theory, usually a topological index is a numerical parameter mathematically derived from the hydrogen-suppressed molecular graph [36–38]. Although it is customary to use hydrogen-suppressed molecular graphs, there exist graph descriptors and topological indices that are computed from the whole, hydrogen-containing molecular graph [39]. We denote the hydrogen-suppressed molecular graph of this dendrimer with $D(n)$, where the generation stage of $D(n)$ is represented by n (see Figure 1). The graph of the dendrimer $D(n)$ consists of a central core with 68 vertices and four branches with each branch having $2^3(1 + 2 + 2^2 + \dots + 2^{n-1}) = 2^{n+3} - 8$ vertices. Hence, a simple calculation shows that the order of $D(n)$ is $4(9 + 2^{n+3})$. In addition, each branch consist of $2^{n+3} - 8$ edges. This gives the total number of edges in $D(n)$ are $4(11 + 2^{n+3})$. To work out the eccentricity-based indices and polynomials of $D(n)$, it is sufficient to determine the desired data for the sets of representatives. We partition the molecular graph $D(n)$ into two parts, one of them is core C and other is subgraph $Z(n)$ of $D(n)$ having four similar branches with vertex set $V(D(n)) - V(C)$. The molecular graphs of cores and the first generation of dendrimers are shown in Figure 2. The sets of representatives from a set of vertices of the core and subgraph of $D(n)$, with their degrees, S_t , $M(t)$ and eccentricity for each t are given in Tables 1 and 2, respectively. For the core, these representatives are labelled by α_l , where $1 \leq l \leq 12$ as shown in Figure 2. For $Z(n)$, where $n \geq 1$, these representatives are labelled by $a_i, b_i, c_i, d_i, e_i, f_i, a_{n+1}$, where $1 \leq i \leq n$ as shown in Figure 2. For our convenience, throughout this paper, we use $\gamma = 4n + 4i$.

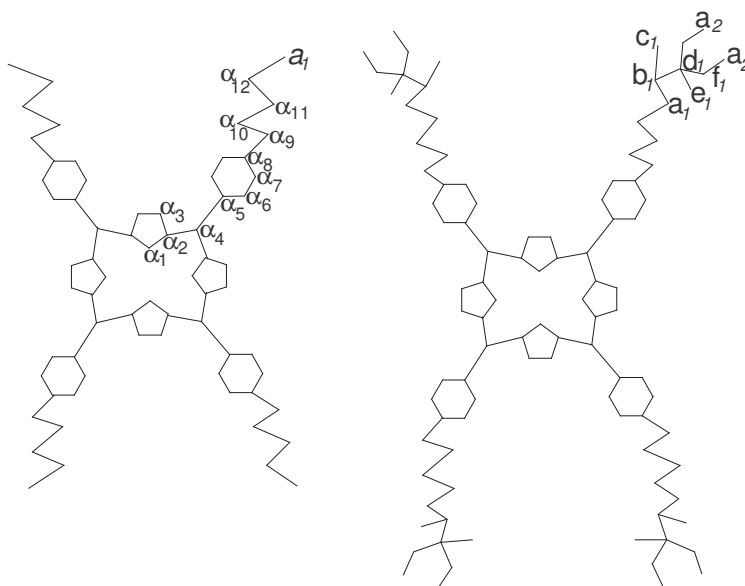


Figure 2. Core of the dendrimer $D(n)$; first generation of the dendrimer $D(n)$.

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. The set of representatives of the core with their degrees, S_t , $M(t)$, eccentricities and frequencies.

| Representative | Degree | S_t | $M(t)$ | Eccentricity | Frequency |
|----------------|--------|-------|--------|--------------|-----------|
| α_1 | 2 | 6 | 9 | $4n + 15$ | 4 |
| α_2 | 3 | 7 | 12 | $4n + 16$ | 8 |
| α_3 | 2 | 5 | 6 | $4n + 16$ | 8 |
| α_4 | 3 | 9 | 27 | $4n + 17$ | 4 |
| α_5 | 3 | 7 | 12 | $4n + 18$ | 4 |
| α_6 | 2 | 5 | 6 | $4n + 19$ | 8 |
| α_7 | 2 | 5 | 6 | $4n + 20$ | 8 |
| α_8 | 3 | 6 | 8 | $4n + 21$ | 4 |
| α_9 | 2 | 5 | 6 | $4n + 22$ | 4 |
| α_{10} | 2 | 4 | 4 | $4n + 23$ | 4 |
| α_{11} | 2 | 4 | 4 | $4n + 24$ | 4 |
| α_{12} | 2 | 3 | 2 | $4n + 25$ | 4 |

Table 2. The set of representatives of the subgraph $Z(n)$ of $D(n)$ with degrees, S_t , $M(t)$, eccentricities and frequencies.

| Representative | Degree | S_t | $M(t)$ | Eccentricity | Frequency |
|----------------|--------|-------|--------|---------------|-----------|
| a_{n+1} | 1 | 2 | 2 | $8n + 26$ | 2^{n+2} |
| a_i | 2 | 5 | 6 | $\gamma + 22$ | 2^{i+1} |
| b_i | 3 | 7 | 8 | $\gamma + 23$ | 2^{i+1} |
| c_i | 1 | 3 | 3 | $\gamma + 24$ | 2^{i+1} |
| d_i | 4 | 8 | 12 | $\gamma + 24$ | 2^{i+1} |
| e_i | 1 | 4 | 4 | $\gamma + 25$ | 2^{i+1} |
| f_i | 2 | 5 | 4 | $\gamma + 25$ | 2^{i+2} |

Theorem 1. The eccentric connectivity index for the molecular graph $D(n)$ is given by

$$\zeta(D(n)) = 16(2^{n+5} \times n + 22n + 2^n \times 81 + 101).$$

Proof. By using the values of Tables 1 and 2 in the definition of eccentricity connectivity index given by Equation (1), the eccentric connectivity index of $D(n)$ can be computed as follows:

$$\begin{aligned} \zeta(D(n)) &= \zeta(C) + \zeta(Z(n)) = \sum_{t \in V(C)} \varepsilon(t)d_t + \sum_{t \in V(Z(n))} \varepsilon(t)d_t \\ &= (2 \times 4)(4n + 15) + (3 \times 8)(4n + 16) + (2 \times 8)(4n + 16) + (3 \times 4)(4n + 17) \\ &\quad + (3 \times 4)(4n + 18) + (2 \times 8)(4n + 19) + (2 \times 8)(4n + 20) + (3 \times 4)(4n + 21) \\ &\quad + (2 \times 4)(4n + 22) + (2 \times 4)(4n + 23) + (2 \times 4)(4n + 24) + (2 \times 4)(4n + 25) \\ &\quad + (1 \times 2^{n+2})(8n + 26) + \sum_{i=1}^n \left((2 \times 2^{i+1})(\gamma + 22) + (3 \times 2^{i+1})(\gamma + 23) \right. \\ &\quad \left. + (1 \times 2^{i+1})(\gamma + 24) + (4 \times 2^{i+1})(\gamma + 24) + (1 \times 2^{i+1})(\gamma + 25) + (2 \times 2^{i+2})(\gamma + 25) \right). \end{aligned}$$

After some calculations, we get

$$\zeta(D(n)) = 16(2^{n+5} \times n + 22n + 2^n \times 81 + 101),$$

which proves the theorem. \square

In the similar way, by putting the values of Tables 1 and 2 in Equation (3), we have the following result.

Corollary 1. The total eccentric connectivity index of $D(n)$ is given by

$$\zeta(D(n)) = 4(2^{n+6} \times n + 2^{n+1} \times 83 + 36n + 167).$$

In the upcoming theorem, the absolute formula for the eccentric connectivity polynomial for $D(n)$ has been obtained.

Theorem 2. The eccentric connectivity polynomial for $D(n)$ is given by

$$\begin{aligned} ECP(D(n), x) &= 4x^{4n+15}(2x^{10} + 2x^9 + 2x^8 + 2x^7 + 3x^6 + 4x^5 + 4x^4 + 3x^3 + 3x^2 \\ &\quad + 10x + 2) + 2^{n+2}x^{2(4n+13)} + \frac{4(5x^3 + 5x^2 + 3x + 2) \times x^{4n+26}(2^n x^{4n} - 1)}{2x^4 - 1}. \end{aligned}$$

Proof. By using the values of Tables 1 and 2 in Equation (2), we have

$$\begin{aligned} ECP(D(n), x) &= ECP(C, x) + ECP(Z(n), x) = \sum_{t \in V(C)} d_t x^{\varepsilon(t)} + \sum_{t \in V(Z(n))} d_t x^{\varepsilon(t)} \\ &= (2 \times 4)x^{4n+15} + (8 \times 3)x^{4n+16} + (8 \times 2)x^{4n+16} + (4 \times 3)x^{4n+17} \\ &\quad + (4 \times 3)x^{4n+18} + (8 \times 2)x^{4n+19} + (8 \times 2)x^{4n+20} + (4 \times 3)x^{4n+21} \\ &\quad + (4 \times 2)x^{4n+22} + (4 \times 2)x^{4n+23} + (4 \times 2)x^{4n+24} + (4 \times 2)x^{4n+25} \\ &\quad + (1 \times 2^{n+2})x^{8n+26} + \sum_{i=1}^n \left((2 \times 2^{i+1})x^{\gamma+22} + (3 \times 2^{i+1})x^{\gamma+23} \right. \\ &\quad \left. + (1 \times 2^{i+1})x^{\gamma+24} + (4 \times 2^{i+1})x^{\gamma+24} + (1 \times 2^{i+1})x^{\gamma+25} + (2 \times 2^{i+2})x^{\gamma+25} \right). \end{aligned}$$

After several calculation steps, we obtain the desired result. \square

The total eccentric connectivity polynomial of $D(n)$ can be calculated by using the values of Tables 1 and 2 in Equation (4). We have the following result.

Corollary 2. *The total eccentric connectivity polynomial of $D(n)$ is given by*

$$TECP(D(n), x) = 4x^{4n+15}(x^{10} + x^9 + x^8 + x^7 + x^6 + 2x^5 + 2x^4 + x^3 + x^2 + 4x + 1) + 2^{n+2}x^{2(4n+13)} + \frac{4(3x^3 + 2x^2 + x + 1)x^{4n+26}(2^n x^{4n} - 1)}{2x^4 - 1}.$$

Now, we compute the precise value of first Zagreb eccentricity index.

Theorem 3. *The first Zagreb eccentricity index for the molecular graph $D(n)$ is given by*

$$M_1(D(n)) = 4(2^{n+9} \times n^2 + 2^{n+5} \times 83n + 2^{n+2} \times 927 + 144n^2 + 1336n + 3007).$$

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

$$\begin{aligned} M_1(D(n)) &= M_1(C) + M_1(Z(n)) = \sum_{v \in V(C)} [\varepsilon(v)]^2 + \sum_{v \in V(Z(n))} [\varepsilon(v)]^2 \\ &= 4(4n + 15)^2 + 8(4n + 16)^2 + 8(4n + 16)^2 + 4(4n + 17)^2 + 4(4n + 18)^2 \\ &\quad + 8(4n + 19)^2 + 8(4n + 20)^2 + 4(4n + 21)^2 + 4(4n + 22)^2 + 4(4n + 23)^2 \\ &\quad + 4(4n + 24)^2 + 4(4n + 25)^2 + 2^{n+2}(8n + 26)^2 + \sum_{i=1}^n \left(2^{i+1}(\gamma + 22)^2 \right. \\ &\quad \left. + 2^{i+1}(\gamma + 23)^2 + 2^{i+1}(\gamma + 24)^2 + 2^{i+1}(\gamma + 24)^2 + 2^{i+1}(\gamma + 25)^2 + 2^{i+2}(\gamma + 25)^2 \right). \end{aligned}$$

After some calculations, we have

$$M_1(D(n)) = 4(2^{n+9} \times n^2 + 2^{n+5} \times 83n + 2^{n+2} \times 927 + 144n^2 + 1336n + 3007),$$

which proves our theorem. \square

Theorem 4. *The augmented eccentric connectivity index for the molecular graph $D(n)$ is given by*

$$\begin{aligned} {}^A\varepsilon(D(n)) &= \frac{36}{4n + 15} + \frac{144}{4n + 16} + \frac{108}{4n + 17} + \frac{48}{4n + 18} + \frac{48}{4n + 19} + \frac{48}{4n + 20} \\ &\quad + \frac{32}{4n + 21} + \frac{24}{4n + 22} + \frac{16}{4n + 23} + \frac{16}{4n + 24} + \frac{8}{4n + 25} + \frac{2^{n+3}}{8n + 26} \\ &\quad + \left(\frac{24}{4n + 26} + \dots + \frac{3 \times 2^{n+2}}{8n + 22} \right) + \left(\frac{32}{4n + 27} + \dots + \frac{2^{n+4}}{8n + 23} \right) \\ &\quad + \left(\frac{12}{4n + 28} + \dots + \frac{3 \times 2^{n+1}}{8n + 24} \right) + \left(\frac{48}{4n + 28} + \dots + \frac{3 \times 2^{n+3}}{8n + 24} \right) \\ &\quad + \left(\frac{16}{4n + 29} + \dots + \frac{2^{n+3}}{8n + 25} \right) + \left(\frac{32}{4n + 29} + \dots + \frac{2^{n+4}}{8n + 25} \right). \end{aligned}$$

Proof. According to the values given in Tables 1 and 2 and Equation (6), we work out the augmented eccentric connectivity index of $D(n)$ in the following way:

$$\begin{aligned} {}^A\varepsilon(D(n)) &= {}^A\varepsilon(C) + {}^A\varepsilon(Z(n)) = \sum_{t \in V(C)} \frac{M(t)}{\varepsilon(t)} + \sum_{t \in V(Z(n))} \frac{M(t)}{\varepsilon(t)} \\ &= \frac{9 \times 4}{4n + 15} + \frac{12 \times 8}{4n + 16} + \frac{6 \times 8}{4n + 16} + \frac{27 \times 4}{4n + 17} + \frac{12 \times 4}{4n + 18} + \frac{6 \times 8}{4n + 19} \\ &\quad + \frac{6 \times 8}{4n + 20} + \frac{4 \times 8}{4n + 21} + \frac{6 \times 4}{4n + 22} + \frac{4 \times 4}{4n + 23} + \frac{4 \times 4}{4n + 24} + \frac{2 \times 4}{4n + 25} + \frac{2 \times 2^{n+2}}{8n + 26} \\ &\quad + \sum_{i=1}^n \left(\frac{6 \times 2^{i+1}}{\gamma + 22} + \frac{8 \times 2^{i+1}}{\gamma + 23} + \frac{3 \times 2^{i+1}}{\gamma + 24} + \frac{12 \times 2^{i+1}}{\gamma + 24} + \frac{4 \times 2^{i+1}}{\gamma + 25} + \frac{4 \times 2^{i+2}}{\gamma + 25} \right). \end{aligned}$$

After merging up the similar items in the above equation, we obtain the required result. \square

Now, we determine the accurate value of the modified eccentric connectivity index.

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

$$\Lambda(D(n)) = 4(2^{n+3} \times 39n + 204n + 2^n \times 789 + 905).$$

Proof. By inserting the values of Tables 1 and 2 in Equation (7), we determine the modified eccentric connectivity index of $D(n)$ as follows:

$$\begin{aligned} \Lambda(D(n)) &= \Lambda(C) + \Lambda(Z(n)) = \sum_{t \in V(C)} S_t \varepsilon(t) + \sum_{t \in V(Z(n))} S_t \varepsilon(t) \\ &= (6 \times 4)(4n + 15) + (7 \times 8)(4n + 16) + (5 \times 8)(4n + 16) \\ &\quad + (9 \times 4)(4n + 17) + (7 \times 4)(4n + 18) + (5 \times 8)(4n + 19) + (5 \times 8)(4n + 20) \\ &\quad + (6 \times 4)(4n + 21) + (5 \times 4)(4n + 22) + (4 \times 4)(4n + 23) + (4 \times 4)(4n + 24) \\ &\quad + (3 \times 4)(4n + 25) + (2 \times 2^{n+2})(8n + 26) + \sum_{i=1}^n \left((5 \times 2^{i+1})(\gamma + 22) + (7 \times 2^{i+1})(\gamma + 23) \right. \\ &\quad \left. + (3 \times 2^{i+1})(\gamma + 24) + (8 \times 2^{i+1})(\gamma + 24) + (4 \times 2^{i+1})(\gamma + 25) + (5 \times 2^{i+2})(\gamma + 25) \right). \end{aligned}$$

Clearly, the above equation is equal to

$$\Lambda(D(n)) = 4(2^{n+3} \times 39n + 204n + 2^n \times 789 + 905),$$

which implies the desired result. \square

In the following theorem, we compute the closed formula for the modified eccentric connectivity polynomial.

Theorem 6. The modified eccentric connectivity polynomial of $D(n)$ is given by

$$\begin{aligned} \Lambda(D(n)) &= 4x^{4n+15}(3x^{10} + 4x^9 + 4x^8 + 5x^7 + 6x^6 + 10x^5 + 10x^4 + 7x^3 \\ &\quad + 9x^2 + 24x + 6) + 2^{n+3}x^{2(4n+13)} + \frac{4(14x^3 + 11x^2 + 7x + 5)x^{4n+26}(2^n x^{4n} - 1)}{2x^4 - 1}. \end{aligned}$$

Proof. Followed by the values depicted in Tables 1 and 2, and the expression of the modified eccentric connectivity polynomial in Equation (8), the value of modified eccentric connectivity polynomial of $D(n)$ can be written as follows:

$$\begin{aligned} MECP(D(n), x) &= MECP(C, x) + MECP(Z(n), x) = \sum_{t \in V(C)} S_t x^{\epsilon(t)} + \sum_{t \in V(Z(n))} S_t x^{\epsilon(t)} \\ &= (6 \times 4)x^{4n+15} + (8 \times 7)x^{4n+16} + (8 \times 5)x^{4n+16} + (4 \times 9)x^{4n+17} \\ &\quad + (4 \times 7)x^{4n+18} + (8 \times 5)x^{4n+19} + (8 \times 5)x^{4n+20} + (4 \times 6)x^{4n+21} \\ &\quad + (4 \times 5)x^{4n+22} + (4 \times 4)x^{4n+23} + (4 \times 4)x^{4n+24} + (4 \times 3)x^{4n+25} \\ &\quad + (2 \times 2^{n+2})x^{8n+26} + \sum_{i=1}^n \left((5 \times 2^{i+1})x^{\gamma+22} + (7 \times 2^{i+1})x^{\gamma+23} \right. \\ &\quad \left. + (3 \times 2^{i+1})x^{\gamma+24} + (8 \times 2^{i+1})x^{\gamma+24} + (4 \times 2^{i+1})x^{\gamma+25} + (5 \times 2^{i+2})x^{\gamma+25} \right). \end{aligned}$$

By means of simple calculations, we obtain the required result. \square

3. Conclusions

With the remarkable growth in the field of computer technology and accompanied by the introduction of the utilization of it in pharmacology, chemistry, and biology, a set of methodologies like quantitative structure–activity relationship and quantitative structure–property relationships have been developed. These methodologies have been widely applied in medicinal chemistry for the interpretation of many chemical and biological processes. In this paper, by molecular structure analysis, eccentricity calculating and mathematical derivation, we have computed the precise values of different versions of eccentric connectivity indices and their corresponding polynomials for a class of porphyrin-cored dendrimers. The theoretical formulations obtained in our work illustrate the promising prospects of their application for the pharmacy and chemical engineering.

Author Contributions: Conceptualization, W.G.; Investigation, Z.I. and M.I.; Methodology, Z.I., M.I. and A.A.; Software, R.S.; Validation, R.S.; Writing–original draft, M.A.; Writing–review & editing, A.A.

Funding: This work was supported in part by the National Natural Science Foundation of China (no. 11761083).

Conflicts of Interest: The authors declare no conflict of interest.

References

- González-Díaz, H.; Vilar, S.; Santana, L.; Uriarte, E. Medicinal chemistry and bioinformatics-current trends in drugs discovery with networks topological indices. *Curr. Top. Med. Chem.* **2007**, *7*, 1025–1039. [[CrossRef](#)]
- Gozalbes, R.; Doucet, J.P.; Derouin, F. Application of topological descriptors in QSAR and drug design: History and new trends. *Curr. Drug Targets* **2002**, *2*, 93–102.
- Kier, L.B.; Hall, L.H. *Molecular Connectivity in Structure-Activity Analysis*; Jhon Wiley and Sons: New York, NY, USA, 1986.
- Alaeiyan, M.; Asadpour, J.; Mojarad, R. A numerical method for MEC polynomial and MEC index of one-pentagonal carbon nanocones. *Fuller. Nanotub. Carbon Nanostruct.* **2013**, *21*, 825–835. [[CrossRef](#)]
- Gutman, I.; Trinajstić, N. Graph theory and molecular orbitals Total φ -electron energy of alternant hydrocarbons. *Chem. Phys. Lett.* **1972**, *17*, 535–538. [[CrossRef](#)]
- Rücker, G.; Rücker, C. On topological indices, boiling points, and cycloalkanes. *J. Chem. Inf. Comput. Sci.* **1999**, *39*, 788–802. [[CrossRef](#)]
- Basak, S.C.; Magnuson, V.R.; Niemi, G.J.; Regal, R.R.; Veith, G.D. Topological indices: Their nature, mutual relatedness, and applications. *Math. Model.* **1987**, *8*, 300–305. [[CrossRef](#)]
- Duardo-Sanchez, A.; Patlewicz, G.; González-Díaz, H. A review of network topological indices from chem-bioinformatics to legal sciences and back. *Curr. Bioinform.* **2011**, *6*, 53–70. [[CrossRef](#)]
- Adronov, A.; Frechet, J.M.J. Light-harvesting dendrimers. *Chem. Commun.* **2000**, *33*, 1701–1710. [[CrossRef](#)]

10. Naka, K.; Tanaka, Y.; Chujo, Y. Effect of anionic starburst dendrimers on the crystallization of CaCO₃ in aqueous solution, Size control of spherical vaterite particles. *Langmuir* **2002**, *18*, 3655–3658. [[CrossRef](#)]
11. Suresh, R.; Singh, C.; Rewar, P. Dendrimers as carriers and its application in therapy. *Int. J. Anal. Pharm. Biomed. Sci.* **2015**, *4*, 15–23.
12. Zhao, Z.; Lou, S.; Hu, Y.; Zhu, J.; Zhang, C. A Nano-in-Nano Polymer-Dendrimer Nanoparticle-Based Nanosystem for Controlled Multidrug Delivery. *Mol. Pharm.* **2017**, *14*, 2697–2710. [[CrossRef](#)] [[PubMed](#)]
13. Abbasi, E.; Aval, S.F.; Akbarzadeh, A.; Milani, M.; Nasrabadi, H.T.; Joo, S.W.; Hanifehpour, Y.; Nejati-Koshki, K.; Pashaei-Asl, R. Dendrimers: Synthesis, applications and properties. *Nanoscale Res Lett.* **2014**, *9*, 247–256. [[CrossRef](#)] [[PubMed](#)]
14. Wiener, H. Structural determination of paraffin boiling points. *J. Am. Chem. Soc.* **1947**, *69*, 17–20. [[CrossRef](#)] [[PubMed](#)]
15. Sharma, V.; Goswami, R.; Madan, A.K. Eccentric connectivity index: A novel highly discriminating topological descriptor for structure property and structure activity studies. *J. Chem. Inf. Comput. Sci.* **1997**, *37*, 273–282. [[CrossRef](#)]
16. Dureja, H.; Madan, A.K. Topochemical models for prediction of cyclin-dependent kinase 2 inhibitory activity of indole-2-ones. *J. Mol. Model.* **2005**, *11*, 525–531. [[CrossRef](#)] [[PubMed](#)]
17. Ilic, A.; Gutman, I. Eccentric connectivity index of chemical trees. *MATCH Commun. Math. Comput. Chem.* **2011**, *65*, 731–744.
18. Kumar, V.; Madan, A.K. Application of graph theory: Prediction of cytosolic phospholipase A₂ inhibitory activity of propan-2-ones. *J. Math. Chem.* **2006**, *39*, 511–521. [[CrossRef](#)]
19. Zhou, B. On eccentric connectivity index. *MATCH Commun. Math. Comput. Chem.* **2010**, *63*, 181–198.
20. Ashrafi, A.R.; Ghorbani, M.; Hossein-Zadeh, M.A. The eccentric connectivity polynomial of some graph operations. *Serdica J. Comput.* **2011**, *5*, 101–116.
21. Ghorbani, M.; Hosseinzadeh, M.A. A new version of Zagreb indices. *Filomat* **2012**, *26*, 93–100. [[CrossRef](#)]
22. Gupta, S.; Singh, M.; Madan, A.K. Connective eccentricity index: A novel topological descriptor for predicting biological activity. *J. Mol. Graph. Model.* **2000**, *18*, 18–25. [[CrossRef](#)]
23. De, N. Relationship between augmented eccentric connectivity index and some other graph invariants. *Int. J. Adv. Math. Sci.* **2013**, *1*, 26–32. [[CrossRef](#)]
24. Došlić, T.; Saheli, M. Augmented eccentric connectivity index. *Miskolc Math. Notes.* **2011**, *12*, 149–157.
25. Sedlar, J. On augmented eccentric connectivity index of graphs and trees. *MATCH Commun. Math. Comput. Chem.* **2012**, *68*, 325–342.
26. Aslam, A.; Ahmed, S.; Gao, W. On topological indices of boron triangular nanotubes. *Z. Naturforsch.* **2017**, *72*, 711–716. [[CrossRef](#)]
27. Aslam, A.; Bashir, Y.; Ahmed, S.; Gao, W. On topological indices of certain dendrimer structures. *Z. Naturforsch.* **2017**, *72*, 559–566. [[CrossRef](#)]
28. Aslam, A.; Jamil, M.K.; Gao, W.; Nazeer, W. On topological aspects of some dendrimer structures. *Nanotechnol. Rev.* **2018**, *7*, 123–129. [[CrossRef](#)]
29. Aslam, A.; Guirao, J.L.; Ahmad, S.; Gao, W. Topological Indices of the Line Graph of Subdivision Graph of Complete Bipartite Graphs. *Appl. Math. Inf. Sci.* **2017**, *11*, 1631–1636. [[CrossRef](#)]
30. Farooq, R.; Malik, M.A. On some eccentricity based topological indices of nanostar dendrimers. *Optoelectron. Adv. Mater. Rapid Commun.* **2015**, *9*, 842–849.
31. Xu, K.; Li, X. Comparison between two eccentricity-based topological indices of graphs. *Croat. Chem. Acta* **2016**, *89*, 499–504. [[CrossRef](#)]
32. Bashir, Y.; Aslam, A.; Kamran, M.; Qureshi, I.; Jahangir, A.; Rafiq, M.; Bibi, N.; Muhammad, N. On forgotten topological indices of some dendrimers structure. *Molecules* **2017**, *22*, 867. [[CrossRef](#)] [[PubMed](#)]
33. Kang, S.M.; Iqbal, Z.; Ishaq, M.; Sarfraz, R.; Aslam, A.; Nazeer, W. On Eccentricity-Based Topological Indices and Polynomials of Phosphorus-Containing Dendrimers. *Symmetry* **2018**, *10*, 237–246. [[CrossRef](#)]
34. Jeong, Y.H.; Yoon, H.J.; Jang, W.D. Dendrimer porphyrin-based self-assembled nano-devices for biomedical applications. *Polym. J.* **2012**, *44*, 512–521. [[CrossRef](#)]
35. Vestberg, R.; Nyström, A.; Lindgren, M.; Malmström, E.; Hult, A. Porphyrin-cored 2,2-bis (methylol) propionic acid dendrimers. *Chem. Mater.* **2004**, *16*, 2794–2804. [[CrossRef](#)]
36. Nayak, A.; Stojmenovic, I. *Hand Book of Applied Algorithms: Solving Scientific, Engineering, and Practical Problems*; John Wiley and Sons: Hoboken, NJ, USA, 2007; 560p.

37. Sloot, P.; Bubak, M.; Sunderam, V.S.; Alexandrov, V.N.; Albada, G.D.; Dongarra, J.J. Part 3, Lecture notes in computer science. In *Computational Science-ICCS*; Springer: Krakow, Poland, 2004.
38. Trinajstić, N. *Computational Chemical Graph Theory: Characterization, Enumeration and Generation of Chemical Structures by Computer Methods*; Ellis Horwood Ltd.: New York, NY, USA, 1991.
39. Devillers, J.; Balaban, A.T. *Topological Indices and Related Descriptors in QSAR and QSPR*; CRC Press: Boca Raton, FL, USA, 2000; 811p.



© 2018 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (<http://creativecommons.org/licenses/by/4.0/>).