mathematics

Article

Some Reverse Degree-Based Topological Indices and Polynomials of Dendrimers

Wei Gao [1], Muhammad Younas [2], Adeel Farooq [2], Abaid ur Rehman Virk [3] and Waqas Nazeer [4,*]

1 School of Information Science and Technology, Yunnan Normal University, Kunming 650500, China; gaowei@ynnu.edu.cn
2 Department of Mathematics, COMSATS University Islamabad, Lahore Campus, Lahore 54000, Pakistan; muhammadyounas@cuilahore.edu.pk (M.Y.); adeelfarooq@cuilahore.edu.pk (A.F.)
3 Department of Mathematics, University of Management and Technology, Lahore 54770, Pakistan; abaid.math@gmail.com
4 Division of Science and Technology, University of Education, Lahore 54000, Pakistan
* Correspondence: nazeer.waqas@ue.edu.pk; Tel.: +92-321-470-7379

Received: 10 September 2018; Accepted: 18 October 2018; Published: 22 October 2018

Abstract: Topological indices collect information from the graph of molecule and help to predict properties of the underlying molecule. Zagreb indices are among the most studied topological indices due to their applications in chemistry. In this paper, we compute first and second reverse Zagreb indices, reverse hyper-Zagreb indices and their polynomials of Prophyrin, Propyl ether imine, Zinc Porphyrin and Poly (ethylene amido amine) dendrimers.

Keywords: reverse Zagreb index; reverse hyper-Zagreb index; reverse Zagreb polynomials; prophyrin; propyl ether imine; zinc porphyrin and poly (ethylene amido amine)

MSC: 26A51; 26A33; 33E12

1. Introduction

Dendrimers, from a Greek word that translates to "trees" [1,2], are repetitively branched molecules. Dendrimers are generally symmetrical about the core and generally adopt a spherical three-dimensional morphology. Word dendrites are also often encountered. Dendrites usually contain a single chemically addressable group called the focus or core. The first dendrimer was made by Fritz Vogtle [3] using different synthetic methods, such as by RG Denkewalter at Allied [4,5] and Donald Tomalia at Dow Chemical [6–8]. George R. Newkome, Craig Hawker and Jean Frechet in 1990 [9] introduced a fusion synthesis method. The popularity of dendrimers has greatly increased. By 2005, there were more than 5000 scientific papers and patents.

Uses of dendrimers include conjugating other chemical species to the dendrimer surface that can work as distinguishing operators, (for example, a dye molecule), targeting components, affinity ligands, imaging agents, radioligands or pharmaceutical compounds. Dendrimers have exceptionally solid potential for these applications as their structure can prompt multivalent systems. As such, one dendrimer particle has several conceivable sites to couple to an active species. Scientists expected to use the hydrophobic environments of the dendritic media to conduct photochemical reactions that create the items that are synthetically challenged. Carboxylic acid and phenol-terminated water–solvent dendrimers have been incorporated to set up their utility in tranquilizer conveyance, leading to compound responses in their insides. This may enable specialists to connect both focusing molecules and drug molecules to the same dendrimer, which could lessen negative symptoms of medications on healthy cells. Due to these applications, dendrimers are extensively studied [10–16].

Here, we study Prophyrin, Propyl ether imine, Zinc Porphyrin and Poly(ethylene amido amine) dendrimers (Figures 1–4).

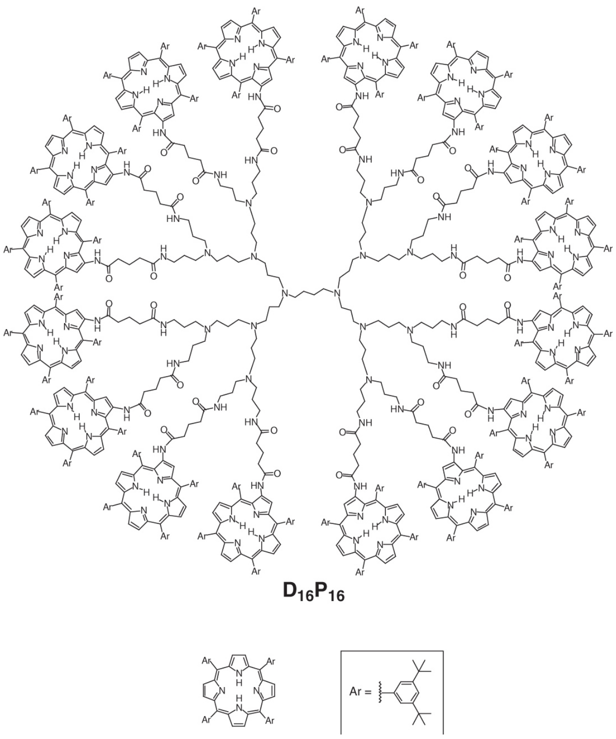

Figure 1. Prophyrin Dendrimer D_nP_n.

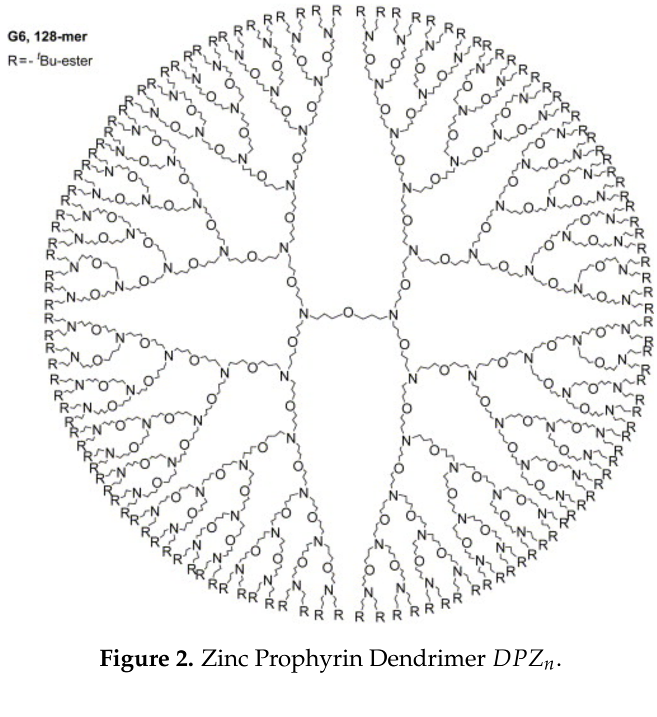

Figure 2. Zinc Prophyrin Dendrimer DPZ_n.

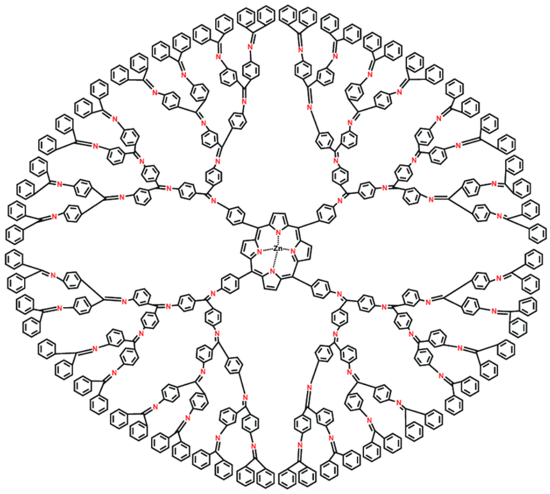

Figure 3. Propyl Ether Imine Dendrimer $(PETIM)$.

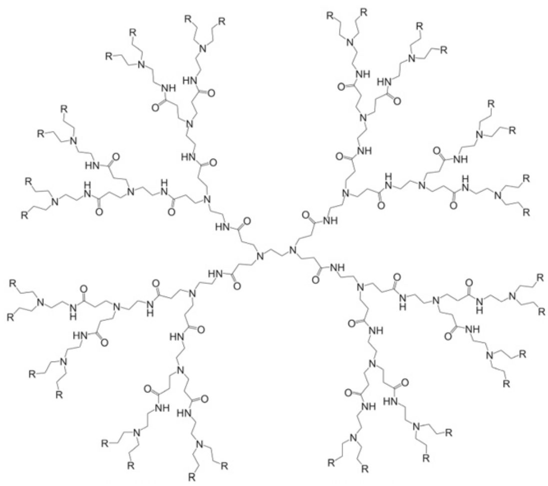

Figure 4. Poly(EThylene Amide Amine) Dendrimer $PETAA$.

Aslam et al. [16] studied three New/Old vertex-degree-based topological indices of these dendrimers. Gao et al., in 2018, ref. [17] computed eccentricity-based topological indices of Porphyrin-cored dendrimers. In the same year, Kang et al. [18] computed eccentricity-based topological indices of phosphorus-containing dendrimers. Some other degree-based topological indices of these dendrimers have been computed [19]. Figures 1–4 are taken from [17–19].

Topological indices correspond to certain physicochemical properties such as boiling point, stability, strain energy and so forth of a chemical compound. Currently, there are more than 148 topological indices and none of them completely describe all properties of the molecular compounds under study, so there is always room to define new topological indices. Our aim was to study Prophyrin, Propyl ether imine, Zinc Porphyrin and Poly(ethylene amido amine) dendrimers. We computed the first and second reverse Zagreb indices, reverse hyper-Zagreb indices and their polynomials of these dendrimers. Graphical comparison of our results is also presented.

2. Preliminaries

A graph having no loop or multiple edges is known as a simple graph. A molecular graph is a simple graph in which atoms and bonds are represented by vertices and edges, respectively. The degree of a vertex v is the number of edges attached with it and is denoted by d_v. The maximum degree of vertex among the vertices of a graph is denoted by $\Delta(G)$. Kulli [20] introduced the concept of reverse vertex degree c_v, as $c_v = \Delta(G) - d_v) + 1$. Throughout this paper, G denotes the simple graph, E denotes the edge set of G, V denotes the vertex set of G and $|X|$ denotes the cardinality of any set X.

In discrete mathematics, graph theory is not only the study of different properties of objects but also tells us about objects having same properties as investigating object [21]. In particular, graph polynomials related to graph are rich in information [22–27]. Mathematical tools such as polynomials and topological based numbers have significant importance to collect information about properties of chemical compounds [28–30]. We can find out hidden information about compounds through theses tools. Multifold graph polynomials are present in the literature. Actually, topological indices are numeric quantities that tell us about the whole structure of graph. There are many topological indices [31–34] that help us to study physical, chemical reactivities and biological properties. Wiener [35], in 1947, firstly introduced the concept of topological index while working on boiling point. Hosoya polynomial [22] plays an important role in the area of distance-based topological indices; we can find Wiener index, Hyper Wiener index and Tratch–Stankevich–Zefirove index from Hosoya polynomial. Randić index defined by Milan Randić [36] in 1975 is one of the oldest degree based topological indices and has been extensively studied by mathematician and chemists [37–41]. Later, Gutman et al. introduced the first and second Zagreb indices as

$$M_1(G) = \sum_{uv \epsilon E(G)} (d_u + d_v),$$

and

$$M_2(G) = \sum_{uv \epsilon E(G)} (d_u.d_v),$$

respectively.

Zagreb indices help us in finding Π electronic energy [42]. Many papers [43–48], surveys [42,49] and many modification of Zagreb indices are presented in the literature [20,50–54]. First and second Zagreb polynomials were defined in [26] as:

$$M_1(G,x) = \sum_{uv \epsilon E(G)} x^{(d_u + d_v)},$$

and

$$M_2(G,x) = \sum_{uv \epsilon E(G)} x^{(d_u.d_v)},$$

respectively.

Shirdel et al. [55] proposed the first and second hyper-Zagreb indices as:

$$H_1(G) = \sum_{uv \epsilon E(G)} (d_u + d_v)^2,$$

and

$$H_2(G) = \sum_{uv \epsilon E(G)} (d_u.d_v)^2.$$

Motivated by these indices, the first and second reverse Zagreb indices was defined in [20] as:

$$CM_1(G) = \sum_{uv \epsilon E(G)} (c_u + c_v),$$

and

$$CM_2(G) = \sum_{uv \epsilon E(G)} (c_u.c_v).$$

The first and second Reverse hyper-Zagreb indices was also defined in the same paper as:

$$HCM_1(G) = \sum_{uv \epsilon E(G)} (c_u + c_v)^2,$$

and

$$HCM_2(G) = \sum_{uv\epsilon E(G)} (c_u.c_v)^2.$$

With the help of reverse Zagreb and hyper-Zagreb indices, we are now able to define the reverse Zagreb and reverse hyper-Zagreb polynomials. For a simply connected graph G, the first and second reverse Zagreb polynomials are defined as:

$$CM_1(G,x) = \sum_{uv\epsilon E(G)} x^{(c_u+c_v)},$$

and

$$CM_2(G,x) = \sum_{uv\epsilon E(G)} x^{(c_u.c_v)}$$

and the first and second hyper-Zagreb polynomials are defined as:

$$HCM_1(G,x) = \sum_{uv\epsilon E(G)} x^{(c_u+c_v)^2},$$

and

$$HCM_2(G,x) = \sum_{uv\epsilon E(G)} x^{(c_u.c_v)^2}.$$

3. Main Results

In this section, we compute reverse Zagreb and reverse hyper-Zagreb indices of Prophyrin, Propyl ether imine, Zinc Porphyrin and Poly(ethylene amido amine) dendrimers.

3.1. Prophyrin Dendrimer D_nP_n

Theorem 1. *Let D_nP_n be a prophyrin Dendrimer. Then, the first and second reverse Zagreb indices are*

1. $CM_1(D_nP_n) = 508n - 60.$
2. $CM_2(D_nP_n) = 558n - 81.$

Proof. In the Prophyrin dendrimer D_nP_n, there are $96n - 10$ vertices and $105n - 11$ edges. Based on the degree of end vertices, the edge set of D_nP_n can be divided into following sic classes

$$E_1(D_nP_n) = \{uv\epsilon E(D_nP_n); d_u = 1, d_v = 3\},$$

$$E_2(D_nP_n) = \{uv\epsilon E(D_nP_n); d_u = 1, d_v = 4\},$$

$$E_3(D_nP_n) = \{uv\epsilon E(D_nP_n); d_u = 2, d_v = 2\},$$

$$E_4(D_nP_n) = \{uv\epsilon E(D_nP_n); d_u = 2, d_v = 3\},$$

$$E_5(D_nP_n) = \{uv\epsilon E(D_nP_n); d_u = 3, d_v = 3\},$$

$$E_6(D_nP_n) = \{uv\epsilon E(D_nP_n); d_u = 3, d_v = 4\}.$$

In Figure 1, one can count easily that $|E_1(D_nP_n)| = 2n$, $|E_2(D_nP_n)| = 24n$, $|E_3(D_nP_n)| = 10n - 5$, $|E_4(D_nP_n)| = 48n - 6$, $|E_5(D_nP_n)| = 13n$ and $|E_6(D_nP_n)| = 8n$.

The maximum vertex degree $\Delta(G)$ in D_nP_n is 4, so we have following six types of reverse edges in D_nP_n.

$$CE_1(D_nP_n) = \{uv\epsilon E(D_nP_n); d_u = 4, d_v = 2\},$$

$$CE_2(D_nP_n) = \{uv\epsilon E(D_nP_n); d_u = 4, d_v = 1\},$$

$$CE_3(D_nP_n) = \{uv\epsilon E(D_nP_n); d_u = 3, d_v = 3\},$$
$$CE_4(D_nP_n) = \{uv\epsilon E(D_nP_n); d_u = 3, d_v = 2\},$$
$$CE_5(D_nP_n) = \{uv\epsilon E(D_nP_n); d_u = 2, d_v = 2\},$$
$$CE_6(D_nP_n) = \{uv\epsilon E(D_nP_n); d_u = 2, d_v = 1\}.$$

In addition, $|CE_1(D_nP_n)| = 2n$, $|CE_2(D_nP_n)| = 24n$, $|CE_3(D_nP_n)| = 10n - 5$, $|CE_4(D_nP_n)| = 48n - 6$, $|CE_5(D_nP_n)| = 13n$ and $|CE_6(D_nP_n)| = 8n$.

(i) Now, using the definition of reverse first Zagreb index, we have

$$\begin{aligned} CM_1(D_nP_n) &= \sum_{uv\epsilon E(G)} (c_u + c_v) \\ &= (4+2)(2n) + (4+1)(24n) + (3+3)(10n-5) \\ &\quad (3+2)(18n-6) + (2+2)(13n) + (2+1)(8n) \\ &= 508n - 60. \end{aligned}$$

(ii) Using the definition of reverse second Zagreb index, we have

$$\begin{aligned} CM_2(D_nP_n) &= \sum_{uv\epsilon E(G)} (c_u.c_v) \\ &= (4.2)(2n) + (4.1)(24n) + (3.3)(10n-5) \\ &\quad +(3.2)(18n-6) + (2.2)(13n) + (2.1)(8n) \\ &= 558n - 81. \end{aligned}$$

□

Theorem 2. *The first and second reverse Zagreb polynomials of D_nP_n are*

1. $CM_1(D_nP_n, x) = (12n-5)x^6 + (72n-6)x^5 + 13nx^4 + 8nx^3$.
2. $CM_2(D_nP_n, x) = (10n-5)x^9 + 2nx^8 + (48n-6)x^6 + 37nx^4 + 8nx^2$.

Proof.

(i) Using the information given in Theorem 1 and definition of reverse first Zagreb polynomial, we have

$$\begin{aligned} CM_1(D_nP_n, x) &= \sum_{uv\epsilon E(G)} x^{(c_u+c_v)} \\ &= (2n)x^{(4+2)} + (24n)x^{(4+1)} + (10n-5)x^{(3+3)} \\ &\quad +(18n-6)x^{(3+2)} + (13n)x^{(2+2)} + (8n)x^{(2+1)} \\ &= (12n-5)x^6 + (72n-6)x^5 + 13nx^4 + 8nx^3. \end{aligned}$$

(ii) Using the information given in Theorem 1 and definition of reverse second Zagreb polynomial, we have

$$\begin{aligned} CM_2(D_nP_n, x) &= \sum_{uv\epsilon E(G)} x^{(c_u.c_v)} \\ &= (2n)x^{(4.2)} + (24n)x^{(4.1)} + (10n-5)x^{(3.3)} \\ &\quad +(18n-6)x^{(3.2)} + (13n)x^{(2.2)} + (8n)x^{(2.1)} \\ &= (10n-5)x^9 + 2nx^8 + (48n-6)x^6 + 37nx^4 + 8nx^2. \end{aligned}$$

□

Theorem 3. *The first and second reverse hyper-Zagreb indices of prophyrin Dendrimer D_nP_n are*

1. $HCM_1(D_nP_n) = 2512n - 330.$
2. $HCM_2(D_nP_n) = 3290n - 621.$

Proof.

(i) Using the information given in Theorem 1 and definition of reverse first hyper-Zagreb index, we have

$$\begin{aligned} HCM_1(D_nP_n) &= \sum_{uv\epsilon E(G)} (c_u + c_v)^2 \\ &= (4+2)^2(2n) + (4+1)^2(24n) + (3+3)^2(10n-5) \\ &\quad +(3+2)^2(18n-6) + (2+2)^2(13n) + (2+1)^2(8n) \\ &= 2512n - 330. \end{aligned}$$

(ii) Using the information given in Theorem 1 and definition of reverse second hyper-Zagreb index, we have

$$\begin{aligned} HCM_2(D_nP_n) &= \sum_{uv\epsilon E(G)} (c_u.c_v)^2 \\ &= (4.2)^2(2n) + (4.1)^2(24n) + (3.3)^2(10n-5) \\ &\quad +(3.2)^2(18n-6) + (2.2)^2(13n) + (2.1)^2(8n) \\ &= 3290n - 621 \end{aligned}$$

□

Theorem 4. *The first and second reverse hyper-Zagreb polynomials of D_nP_n are*

1. $HCM_1(D_nP_n, x) = (12n-5)x^{36} + (72n-6)x^{25} + 13nx^{16} + 8nx^9.$
2. $HCM_1(D_nP_n, x) = (10n-5)x^{81} + 2nx^{64} + (48n-6)x^{36} + 37nx^{16} + 8nx^4.$

Proof.

(i) Using the information given in Theorem 1 and definition of reverse first hyper-Zagreb polynomial, we have

$$\begin{aligned} CM_1(D_nP_n, x) &= \sum_{uv\epsilon E(G)} x^{(c_u+c_v)^2} \\ &= (2n)x^{(4+2)^2} + (24n)x^{(4+1)^2} + (10n-5)x^{(3+3)^2} \\ &\quad +(18n-6)x^{(3+2)^2} + (13n)x^{(2+2)^2} + (8n)x^{(2+1)^2} \\ &= (12n-5)x^{36} + (72n-6)x^{25} + 13nx^{16} + 8nx^9. \end{aligned}$$

(ii) Using the information given in Theorem 1 and definition of reverse second hyper-Zagreb polynomial, we have

$$\begin{aligned} CM_2(D_nP_n, x) &= \sum_{uv\epsilon E(G)} x^{(c_u.c_v)^2} \\ &= (2n)x^{(4.2)^2} + (24n)x^{(4.1)^2} + (10n-5)x^{(3.3)^2} \\ &\quad +(18n-6)x^{(3.2)^2} + (13n)x^{(2.2)^2} + (8n)x^{(2.1)^2} \\ &= (10n-5)x^{81} + 2nx^{64} + (48n-6)x^{36} + 37nx^4 + 8nx^4. \end{aligned}$$

□

The values of first and second reverse Zagreb indices and first and second reverse hyper-Zagreb indices of D_nP_n for specific values of n are given in Table 1.

Table 1. Topological indices of D_nP_n.

	n = 1	n = 2	n = 3	n = 4	n = 5	n = 6	n = 7	n = 8	n = 9
First Reverse Zagreb Index	448	956	1464	1972	2480	2988	3496	4004	4512
Second Reverse Zagreb Index	497	1055	1613	2171	2729	3287	3845	4403	4961
First Reverse Hyper-Zagreb Index	2182	4694	7206	9718	12,230	14,742	17,254	19,766	22,278
Second Reverse Hyper-Zagreb Index	2669	5959	9249	12,539	15,829	19,119	22,409	25,699	28,989

3.2. Propyl Ether Imine Dendrimer ($PETIM$)

In this section, we compute reverse Zagreb indices, reverse Zagreb polynomials, reverse hyper-Zagreb indices and reverse hyper-Zagreb polynomials of Propyl Ether Imine dendrimer $PETIM$.

Theorem 5. *The first and second reverse Zagreb indices of $PETIM$ are*

1. $CM_1(PETIM) = 4.2^{n+4} + 3.2^{n+1} + 3.2^n - 102.$
2. $CM_2(PETIM) = 4.2^{n+4} + 2.2^{n+1} + 36.2^n - 108.$

Proof. In Propyl Ether Imine dendrimer $PETIM$, there are $24.2^n - 23$ vertices and $24.2^n - 24$ edges. Based on the degree of end vertices, the edge set of $PETIM$ can be divided into following three classes.

$$E_1(PETIM) = \{uv \epsilon E(PETIM); d_u = 1, d_v = 2\},$$

$$E_2(PETIM) = \{uv \epsilon E(PETIM); d_u = 2, d_v = 2\},$$

$$E_3(PETIM) = \{uv \epsilon E(PETIM); d_u = 2, d_v = 3\}.$$

In Figure 2, one can count easily that $|E_1(PETIM)| = 2^{n+1}$, $|E_1(PETIM)| = 2^{n+4} - 18$ and $|E_1(PETIM)| = 6.2^n - 6$.

The maximum vertex degree $\Delta(G)$ of $PETIM$ is 3, so we have following types of reverse edges.

$$CE_1(PETIM) = \{uv \epsilon CE(PETIM); c_u = 3, c_v = 2\}.$$

$$CE_2(PETIM) = \{uv \epsilon CE(PETIM); c_u = 2, c_v = 2\}.$$

$$CE_3(PETIM) = \{uv \epsilon CE(PETIM); c_u = 2, c_v = 1\}.$$

Obviously, we have $|CE_1(PETIM)| = 2^{n+1}$, $|CE_1(PETIM)| = 2^{n+4} - 18$ and $|CE_1(PETIM)| = 6.2^n - 6$.

(i) Now, from the definition of reverse first Zagreb index, we have

$$\begin{aligned} CM_1(PETIM) &= \sum_{uv \epsilon E(G)} (c_u + c_v) \\ &= (1+2)(2^{n+1}) + (2+2)(2^{n+4} - 18) + (2+3)(6.2^n - 6) \\ &= 4.2^{n+4} + 3.2^{n+1} + 3.2^n - 102. \end{aligned}$$

(ii) From the definition of reverse second Zagreb index, we have

$$\begin{aligned} CM_2(PETIM) &= \sum_{uv\epsilon E(G)} (c_u.c_v) \\ &= (1.2)(2^{n+1}) + (2.2)(2^{n+4} - 18) + (2.3)(6.2^n - 6) \\ &= 4.2^{n+4} + 2.2^{n+1} + 36.2^n - 108. \end{aligned}$$

□

Theorem 6. *The first and second reverse Zagreb polynomials of* $(PETIM)$ *are,*

1. $CM_1(PETIM, x) = (6.2^n - 6)x^5 + (2^{(n+4)} - 18)x^4 + (2^{n+1})x^3.$
2. $CM_2(PETIM, x) = (6.2^n - 6)x^6 + (2^{(n+4)} - 18)x^4 + (2^{n+1})x^2.$

Proof.

(i) From the information given in Theorem 5 and by the definition of reverse first Zagreb polynomial, we have

$$\begin{aligned} CM_1(PETIM, x) &= \sum_{uv\epsilon E(G)} x^{(c_u+c_v)} \\ &= (2^{n+1})x^{(1+2)} + (2^{(n+4)} - 18)x^{(2+2)} + (6.2^n - 6)x^{(2+3)} \\ &= (6.2^n - 6)x^5 + (2^{(n+4)} - 18)x^4 + (2^{n+1})x^3. \end{aligned}$$

(ii) From the information given in Theorem 5 and by the definition of reverse second Zagreb polynomial, we have

$$\begin{aligned} CM_2(PETIM, x) &= \sum_{uv\epsilon E(G)} x^{(c_u.c_v)} \\ &= (2^{n+1})x^{(1.2)} + (2^{(n+4)} - 18)x^{(2.2)} + (6.2^n - 6)x^{(2.3)} \\ &= (6.2^n - 6)x^6 + (2^{(n+4)} - 18)x^4 + (2^{n+1})x^2. \end{aligned}$$

□

Theorem 7. *The first and second reverse hyper-Zagreb indices of prophyrin Dendrimer* $PETIM$ *are*

1. $HCM_1(PETIM) = 16.2^{n+4} + 9.2^{n+1} + 150.2^n - 438,$
2. $HCM_2(PETIM) = 16.2^{n+4} + 4.2^{n+1} + 216.2^n - 504.$

Proof.

(i) From the information given in Theorem 5 and by the definition of reverse first hyper-Zagreb index, we have

$$\begin{aligned} HCM_1(PETIM) &= \sum_{uv\epsilon E(G)} (c_u + c_v)^2 \\ &= (1+2)^2(2^{n+1}) + (2+2)^2(2^{n+4} - 18) + (2+3)^2(6.2^n - 6) \\ &= 16.2^{n+4} + 9.2^{n+1} + 150.2^n - 438. \end{aligned}$$

(ii) From the information given in Theorem 5 and by the definition of reverse second hyper-Zagreb index, we have

$$\begin{aligned} HCM_2(PETIM) &= \sum_{uv\epsilon E(G)} (c_u.c_v)^2 \\ &= (1.2)^2(2^{n+1}) + (2.2)^2(2^{n+4} - 18) + (2.3)^2(6.2^n - 6) \\ &= 16.2^{n+4} + 4.2^{n+1} + 216.2^n - 504. \end{aligned}$$

□

Theorem 8. *The first and second reverse hyper-Zagreb polynomials of $PETIM$ are*

1. $HCM_1(PETIM, x) = (6.2^n - 6)x^{25} + (2^{(n+4)} - 18)x^{16} + (2^{n+1})x^9.$
2. $HCM_2(PETIM, x) = (6.2^n - 6)x^{36} + (2^{(n+4)} - 18)x^{16} + (2^{n+1})x^4.$

Proof.

(i) From the information given in Theorem 5 and by the definition of reverse first hyper-Zagreb polynomial, we have

$$\begin{aligned} HCM_1(PETIM, x) &= \sum_{uv\epsilon E(G)} x^{(c_u+c_v)^2} \\ &= (2^{n+1})x^{(1+2)^2} + (2^{n+4} - 18)x^{(2+2)^2} + (6.2^n - 6)x^{(2+3)^2} \\ &= (6.2^n - 6)x^{25} + (2^{(n+4)} - 18)x^{16} + (2^{n+1})x^9. \end{aligned}$$

(ii) From the information given in Theorem 5 and by the definition of reverse second hyper-Zagreb polynomial, we have

$$\begin{aligned} HCM_2(PETIM, x) &= \sum_{uv\epsilon E(G)} x^{(c_u.c_v)^2} \\ &= (2^{n+1})x^{(1.2)^2} + (2^{n+4} - 18)x^{(2.2)^2} + (6.2^n - 6)x^{(2.3)^2} \\ &= (6.2^n - 6)x^{36} + (2^{(n+4)} - 18)x^{16} + (2^{n+1})x^4. \end{aligned}$$

□

The values of first and second reverse Zagreb indices and first and second reverse hyper-Zagreb indices of $PETIM$ for specific values of n are given in Table 2.

Table 2. Topological indices of $PETIM$.

	$n = 1$	$n = 2$	$n = 3$	$n = 4$	$n = 5$	$n = 6$	$n = 7$	$n = 8$	$n = 9$
First Reverse Zagreb Index	44	190	482	1066	2234	4570	9242	18,586	37,274
Second Reverse Zagreb Index	100	308	724	1556	3220	6548	13,204	26,516	53,140
First Reverse Hyper-Zagreb Index	410	1258	2954	6346	13,130	26,698	53,834	108,106	216,650
Second Reverse Hyper-Zagreb Index	456	1416	3336	7176	14,856	30,216	60,936	122,376	245,256

3.3. *Zinc Prophyrin Dendrimer DPZ_n*

In this section, we compute reverse Zagreb indices, reverse Zagreb polynomials, reverse hyper-Zagreb indices and reverse hyper-Zagreb polynomials of Zinc Prophyrin Dendrimer DPZ_n.

Theorem 9. *Let DPZ_n be a Zinc Prophyrin Dendrimer. Then, the first and second reverse Zagreb indices are*

1. $CM_1(DPZ_n) = 328.2^n - 156$,
2. $CM_2(DPZ_n) = 416.2^n - 188$.

Proof. In Zinc Prophyrin dendrimer DPZ_n, there are $96n - 10$ vertices and $105n - 11$ edges. The edge set of DPZ_n can be divided into following four classes by mean of the degree of end vertices.

$$E_1(DPZ_n) = \{uv\epsilon E(DPZ_n); d_u = 2, d_v = 2\},$$

$$E_2(DPZ_n) = \{uv\epsilon E(DPZ_n); d_u = 2, d_v = 3\},$$
$$E_3(DPZ_n) = \{uv\epsilon E(DPZ_n); d_u = 3, d_v = 3\},$$
$$E_4(DPZ_n) = \{uv\epsilon E(DPZ_n); d_u = 3, d_v = 4\}.$$

In Figure 3, one can count easily that $|E_1(DPZ_n)| = 16.2^n - 4$, $|E_2(DPZ_n)| = 40.2^n - 16$, $|E_3(DPZ_n)| = 8.2^n - 16$ and $|E_4(DPZ_n)| = 4$.

The maximum vertex degree $\Delta(G)$ of DPZ_n is 4, so

$$CE_1(DPZ_n) = \{uv\epsilon E(DPZ_n); d_u = 3, d_v = 3\},$$
$$CE_2(DPZ_n) = \{uv\epsilon E(DPZ_n); d_u = 3, d_v = 2\},$$
$$CE_3(DPZ_n) = \{uv\epsilon E(DPZ_n); d_u = 2, d_v = 2\},$$
$$CE_4(DPZ_n) = \{uv\epsilon E(DPZ_n); d_u = 2, d_v = 1\}.$$

In addition, $|E_1(DPZ_n)| = 16.2^n - 4$, $|E_2(DPZ_n)| = 40.2^n - 16$, $|E_3(DPZ_n)| = 8.2^n - 16$ and $|E_4(DPZ_n)| = 4$.

(i) Now, from the definition of reverse first Zagreb index, we have

$$\begin{aligned} CM_1(DPZ_n) &= \sum_{uv\epsilon E(G)} (c_u + c_v) \\ &= (3+3)(16.2^n - 4) + (3+2)(40.2^n - 16) \\ &\quad +(2+2)(8.2^n - 16) + (2+1)(4) \\ &= 328.2^n - 156. \end{aligned}$$

(ii) From the definition of reverse second Zagreb index, we have

$$\begin{aligned} CM_2(DPZ_n) &= \sum_{uv\epsilon E(G)} (c_u . c_v) \\ &= (3.3)(16.2^n - 4) + (3.2)(40.2^n - 16) \\ &\quad +(2.2)(8.2^n - 16) + (2.1)(4) \\ &= 416.2^n - 188. \end{aligned}$$

□

Theorem 10. *The first and second reverse Zagreb polynomials of* (DPZ_n) *are*

1. $CM_1(DPZ_n, x) = (16.2^n - 4)x^6 + (40.2^n - 16)x^5 + (8.2^n - 16)x^4 + (4)x^3$,
2. $CM_2(DPZ_n, x) = (16.2^n - 4)x^9 + (40.2^n - 16)x^6 + (8.2^n - 16)x^4 + (4)x^2$.

Proof.

(i) From the information given in Theorem 9 and by the definition of reverse first Zagreb polynomial, we have

$$\begin{aligned} CM_1(DPZ_n, x) &= \sum_{uv\epsilon E(G)} x^{(c_u+c_v)} \\ &= (16.2^n-4)x^{(3+3)} + (40.2^n-16)x^{(3+2)} \\ &\quad +(8.2^n-16)x^{(2+2)} + (4)x^{(2+1)} \\ &= (16.2^n-4)x^6 + (40.2^n-16)x^5 + (8.2^n-16)x^4 + (4)x^3. \end{aligned}$$

(ii) From the information given in Theorem 9 and by the definition of reverse second Zagreb polynomial, we have

$$\begin{aligned} CM_2(DPZ_n, x) &= \sum_{uv\epsilon E(G)} x^{(c_u.c_v)} \\ &= (16.2^n-4)x^{(3.3)} + (40.2^n-16)x^{(3.2)} \\ &\quad +(8.2^n-16)x^{(2.2)} + (4)x^{(2.1)} \\ &= (16.2^n-4)x^9 + (40.2^n-16)x^6 + (8.2^n-16)x^4 + (4)x^2. \end{aligned}$$

□

Theorem 11. *Let DPZ_n be a Zinc Prophyrin Dendrimer, the first and second reverse hyper-Zagreb indices are*

1. $HCM_1(DPZ_n) = 1704.2^n - 764$,
2. $HCM_2(DPZ_n) = 2964.2^n - 1140$.

Proof.

(i) From the information given in Theorem 9 and by the definition of reverse first hyper-Zagreb index, we have

$$\begin{aligned} HCM_1(DPZ_n) &= \sum_{uv\epsilon E(G)} (c_u+c_v)^2 \\ &= (3+3)^2(16.2^n-4) + (3+2)^2(40.2^n-16) \\ &\quad +(2+2)^2(8.2^n-16) + (2+1)^2(4) \\ &= 1704.2^n - 764. \end{aligned}$$

(ii) From the information given in Theorem 9 and by the definition of reverse first hyper-Zagreb index, we have

$$\begin{aligned} HCM_2(DPZ_n) &= \sum_{uv\epsilon E(G)} (c_u.c_v)^2 \\ &= (3.3)^2(16.2^n-4) + (3.2)^2(40.2^n-16) \\ &\quad +(2.2)^2(8.2^n-16) + (2.1)^2(4) \\ &= 2964.2^n - 1140. \end{aligned}$$

□

Theorem 12. *The first and second reverse hyper-Zagreb polynomials of (DPZ_n) are*

1. $HCM_1(DPZ_n, x) = (16.2^n-4)x^{36} + (40.2^n-16)x^{25} + (8.2^n-16)x^{16} + (4)x^9$,
2. $HCM_2(DPZ_n, x) = (16.2^n-4)x^{81} + (40.2^n-16)x^{36} + (8.2^n-16)x^{16} + (4)x^4$.

Proof.

(i) From the information given in Theorem 9 and by the definition of reverse first hyper-Zagreb polynomial, we have

$$\begin{aligned} HCM_1(DPZ_n, x) &= \sum_{uv\epsilon E(G)} x^{(c_u+c_v)^2} \\ &= (16.2^n-4)x^{(3+3)^2} + (40.2^n-16)x^{(3+2)^2} \\ &\quad +(8.2^n-16)x^{(2+2)^2} + (4)x^{(2+1)^2} \\ &= (16.2^n-4)x^{36} + (40.2^n-16)x^{25} + (8.2^n-16)x^{16} + (4)x^{9}. \end{aligned}$$

(ii) From the information given in Theorem 9 and by the definition of reverse second hyper-Zagreb polynomial, we have

$$\begin{aligned} HCM_2(DPZ_n, x) &= \sum_{uv\epsilon E(G)} x^{(c_u.c_v)^2} \\ &= (16.2^n-4)x^{(3.3)^2} + (40.2^n-16)x^{(3.2)^2} \\ &\quad +(8.2^n-16)x^{(2.2)^2} + (4)x^{(2.1)^2} \\ &= (16.2^n-4)x^{81} + (40.2^n-16)x^{36} + (8.2^n-16)x^{16} + (4)x^{4}. \end{aligned}$$

□

The values of first and second reverse Zagreb indices and first and second reverse hyper-Zagreb indices of (DPZ_n) for specific values of n are given in Table 3.

Table 3. Topological indices of (DPZ_n).

	$n = 1$	$n = 2$	$n = 3$	$n = 4$	$n = 5$	$n = 6$	$n = 7$	$n = 8$	$n = 9$
First Reverse Zagreb Index	500	1156	2468	5092	10,340	20,836	41,828	83,812	167,780
Second Reverse Zagreb Index	644	1476	3140	6468	13,124	26,436	53,060	106,308	212,804
First Reverse Hyper-Zagreb Index	2644	6052	12,868	26,500	53,764	108,292	217,348	435,460	871,684
Second Reverse Hyper-Zagreb Index	4788	10,716	22,572	46,284	93,708	188,556	378,252	757,644	1,516,428

3.4. Poly(EThylene Amide Amine) Dendrimer $PETAA$

In this section, we compute reverse Zagreb indices, reverse Zagreb polynomials, reverse hyper-Zagreb indices and reverse hyper-Zagreb polynomials of Poly(EThylene Amide Amine) Dendrimer $PETAA$.

Theorem 13. *Let $PETAA$ be a Poly(EThylene Amide Amine) Dendrimer, then the first and second reverse Zagreb indices are*

1. $CM_1(PETAA) = 100.2^n - 67.$
2. $CM_2(PETAA) = 100.2^n - 56.$

Proof. In Poly(EThylene Amide Amine) dendrimer $PETAA$, there are $44.2^n - 18$ vertices and $44.2^n - 19$ edges. Based on the degree of end vertices, the edge set of $PETAA$ can be divided into following four classes.

$$E_1(PETAA) = \{uv\epsilon E(PETAA); d_u = 1, d_v = 2\},$$

$$E_2(PETAA) = \{uv\epsilon E(PETAA); d_u = 1, d_v = 3\},$$

$$E_3(PETAA) = \{uv\epsilon E(PETAA); d_u = 2, d_v = 2\},$$
$$E_4(PETAA) = \{uv\epsilon E(PETAA); d_u = 2, d_v = 3\}.$$

In Figure 4, one can count easily that $|E_1(PETAA)| = 4.2^n$, $|E_2(PETAA)| = 4.2^n - 2$, $|E_3(PETAA)| = 16.2^n - 8$ and $|E_4(PETAA)| = 20.2^n - 9$.

The maximum vertex degree $\Delta(G)$ of $PETAA$ is 3. Thus,

$$CE_1(PETAA) = \{uv\epsilon E(PETAA); d_u = 3, d_v = 2\},$$
$$CE_2(PETAA) = \{uv\epsilon E(PETAA); d_u = 3, d_v = 1\},$$
$$CE_3(PETAA) = \{uv\epsilon E(PETAA); d_u = 2, d_v = 2\},$$
$$CE_4(PETAA) = \{uv\epsilon E(PETAA); d_u = 2, d_v = 1\}.$$

In addition, $|CE_1(PETAA)| = 4.2^n$, $|CE_2(PETAA)| = 4.2^n - 2$, $|CE_3(PETAA)| = 16.2^n - 8$ and $|CE_4(PETAA)| = 20.2^n - 9$.

(i) Now, from the definition of reverse first Zagreb index, we have
$$\begin{aligned} CM_1(PETAA) &= \sum_{uv\epsilon E(G)} (c_u + c_v) \\ &= (3+2)(4.2^n) + (3+1)(4.2^n - 2) + \\ &\quad (2+2)(16.2^n - 8) + (2+1)(20.2^n - 9) \\ &= 100.2^n - 67. \end{aligned}$$

(ii) From the definition of reverse Zagreb index, we have

$$\begin{aligned} CM_2(PETAA) &= \sum_{uv\epsilon E(G)} (c_u . c_v) \\ &= (3.2)(4.2^n) + (3.1)(4.2^n - 2) + \\ &\quad (2.2)(16.2^n - 8) + (2.1)(20.2^n - 9) \\ &= 100.2^n - 56. \end{aligned}$$

□

Theorem 14. *The first and second reverse Zagreb polynomal of Poly(EThylene Amide Amine) dendrimer $PETAAA$ are*

1. $CM_1(PETAA, x) = (4.2^n)x^5 + (20.2^n - 10)x^4 + (20.2^n - 9)x^3$,
2. $CM_2(PETAA, x) = (4.2^n)x^6 + (16.2^n - 8)x^4 + (24.2^n - 11)x^3$.

Proof.

(i) From the information given in Theorem 13 and by the definition of reverse first Zagreb polynomial, we have

$$\begin{aligned} CM_1(PETAA, x) &= \sum_{uv\epsilon E(G)} x^{(c_u + c_v)} \\ &= (4.2^n)x^{(3+2)} + (4.2^n - 2)x^{(3+1)} + \\ &\quad (16.2^n - 8)x^{(2+2)} + (20.2^n - 9)x^{(2+1)} \\ &= (4.2^n)x^5 + (20.2^n - 10)x^4 + (20.2^n - 9)x^3. \end{aligned}$$

(ii) From the information given in Theorem 13 and by the definition of reverse second Zagreb polynomial, we have

$$\begin{aligned} CM_2(PETAA,x) &= \sum_{uv\epsilon E(G)} x^{(c_u.c_v)} \\ &= (4.2^n)x^{(3.2)} + (4.2^n-2)x^{(3.1)} + \\ &\quad (16.2^n-8)x^{(2.2)} + (20.2^n-9)x^{(2.1)} \\ &= (4.2^n)x^6 + (16.2^n-8)x^4 + (24.2^n-11)x^3. \end{aligned}$$

□

Theorem 15. *Let PETAA be a Poly (EThylene Amide Amine) Dendrimer. Then, the first and second reverse hyper-Zagreb indices are*

1. $HCM_1(PETAA) = 420.2^n - 241$,
2. $HCM_2(PETAA) = 436.2^n - 182$.

Proof.

(i) From the information given in Theorem 13 and by the definition of reverse first hyper-Zagreb index, we have

$$\begin{aligned} HCM_1(PETAA) &= \sum_{uv\epsilon E(G)} (c_u+c_v)^2 \\ &= (3+2)^2(4.2^n) + (3+1)^2(4.2^n-2) + \\ &\quad (2+2)^2(16.2^n-8) + (2+1)^2(20.2^n-9) \\ &= 420.2^n - 241. \end{aligned}$$

(ii) From the information given in Theorem 13 and by the definition of reverse second hyper-Zagreb index, we have

$$\begin{aligned} HCM_2(PETAA) &= \sum_{uv\epsilon E(G)} (c_u.c_v)^2 \\ &= (3.2)^2(4.2^n) + (3.1)^2(4.2^n-2) + \\ &\quad (2.2)^2(16.2^n-8) + (2.1)^2(20.2^n-9) \\ &= 436.2^n - 182. \end{aligned}$$

□

Theorem 16. *The first and second reverse hyper-Zagreb polynomal of Poly(EThylene Amide Amine) dendrimer PETAAA are*

1. $HCM_1(PETAA,x) = (4.2^n)x^{25} + (20.2^n-10)x^{16} + (20.2^n-9)x^9$,
2. $HCM_2(PETAA,x) = (4.2^n)x^{36} + (16.2^n-8)x^{16} + (24.2^n-11)x^9$.

Proof.

(i) From the information given in Theorem 13 and by the definition of reverse first hyper-Zagreb polynomial, we have

$$\begin{aligned} HCM_1(PETAA,x) &= \sum_{uv\epsilon E(G)} x^{(c_u+c_v)^2} \\ &= (4.2^n)x^{(3+2)^2} + (4.2^n-2)x^{(3+1)^2} + \\ &\quad (16.2^n-8)x^{(2+2)^2} + (20.2^n-9)x^{(2+1)^2} \\ &= (4.2^n)x^{25} + (20.2^n-10)x^{16} + (20.2^n-9)x^9. \end{aligned}$$

(ii) From the information given in Theorem 13 and by the definition of reverse second hyper-Zagreb polynomial, we have

$$
\begin{aligned}
HCM_2(PETAA, x) &= \sum_{uv \epsilon E(G)} x^{(c_u . c_v)^2} \\
&= (4.2^n) x^{(3.2)^2} + (4.2^n - 2) x^{(3.1)^2} + \\
&\quad (16.2^n - 8) x^{(2.2)^2} + (20.2^n - 9) x^{(2.1)^2} \\
&= (4.2^n) x^{36} + (16.2^n - 8) x^{16} + (24.2^n - 11) x^9 .
\end{aligned}
$$

□

The values of first and second reverse Zagreb indices and first and second reverse hyper-Zagreb indices of Poly(EThylene Amide Amine) dendrimer for specific values of n are given in Table 4.

Table 4. Topological indices of Poly (EThylene Amide Amine) dendrimer.

	n = 1	**n = 2**	**n = 3**	**n = 4**	**n = 5**	**n = 6**	**n = 7**	**n = 8**	**n = 9**
First Reverse Zagreb Index	133	333	733	1533	3133	6333	12,733	25,533	51,133
Second Reverse Zagreb Index	144	344	744	1544	3144	6344	12,744	25,544	51,144
First Reverse Hyper-Zagreb Index	599	1439	3119	6479	13,199	26,639	53,519	107,279	214,799
Second Reverse Hyper-Zagreb Index	690	1562	3306	6794	13,770	27,722	55,626	111,434	223,050

4. Graphical Comparison and Concluding Remarks

There are many application of dendrimers, typically involve conjugating other chemical species to the dendrimer surface that can function as detecting agents (such as a dye molecule), affinity ligands, targeting components, radioligands, imaging agents, or pharmaceutically active compounds. Topological indices of dendrimers are useful in theoretical chemistry, pharmacology, toxicology, and environmental chemistry [56,57]. In this paper, we compute reverse first Zagreb index, reverse second Zagreb index, reverse first hyper-Zagreb index, reverse second hyper-Zagreb index, reverse first Zagreb polynomial, reverse second Zargeb polynomial, reverse first hyper-Zagreb polynomial and reverse second hyper-Zagreb polynomial of Prophyrin, Propyl ether imine, Zinc Porphyrin and Poly(ethylene amido amine) dendrimers. Figure 5 shows that Zinc Porphyrin dendrimers get highest value of first reverse Zagreb index and Prophyrin get least value of first reverse Zagreb index. In Figures 6–8, we can choose the dendrimers having largest and least values of second reverse Zagreb, first reverse hyper-Zagreb and second reverse hyper-Zagreb index, respectively.

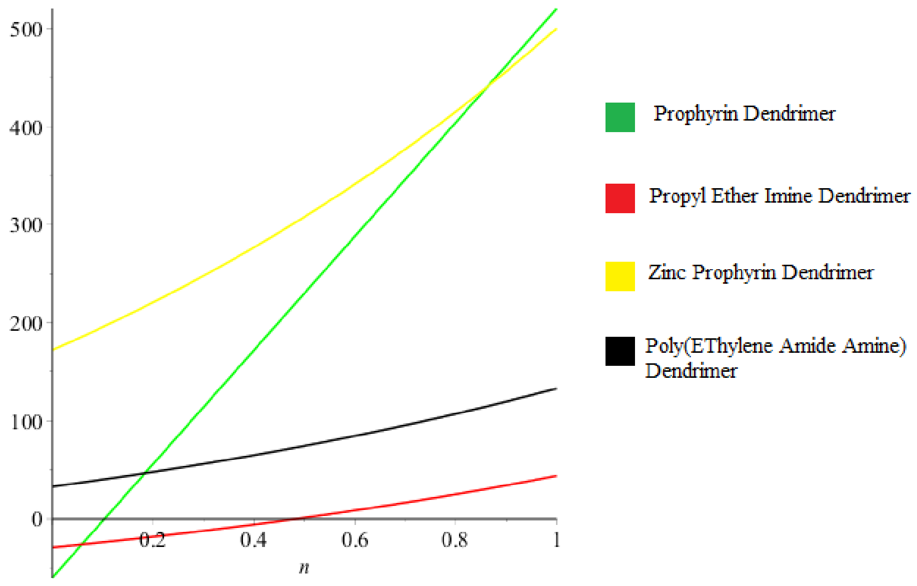

Figure 5. First reverse Zagreb indices.

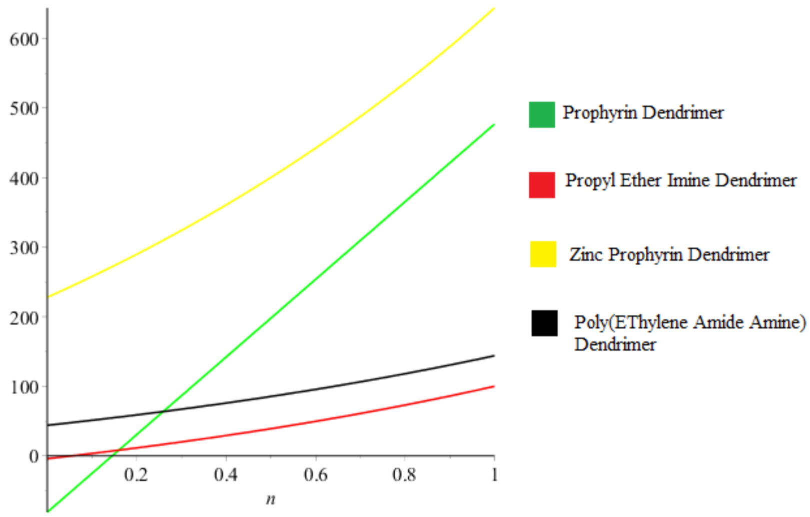

Figure 6. Second reverse Zagreb indices.

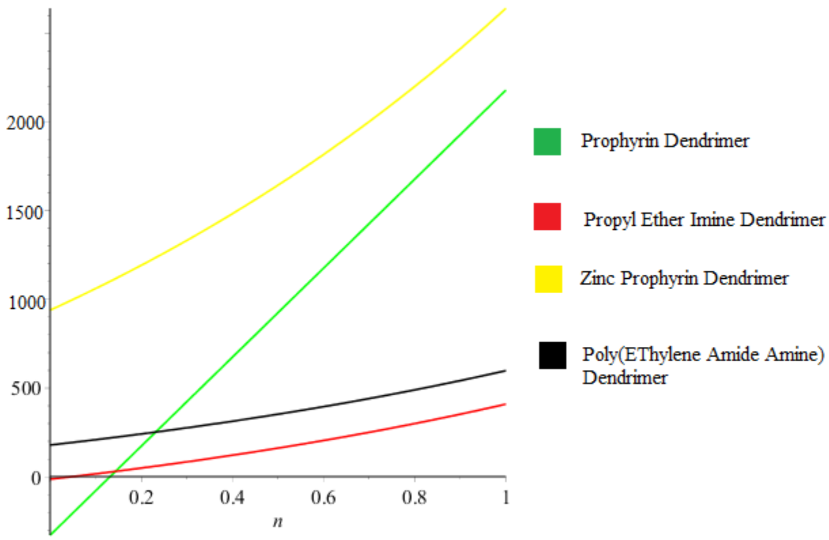

Figure 7. First reverse hyper-Zagreb indices.

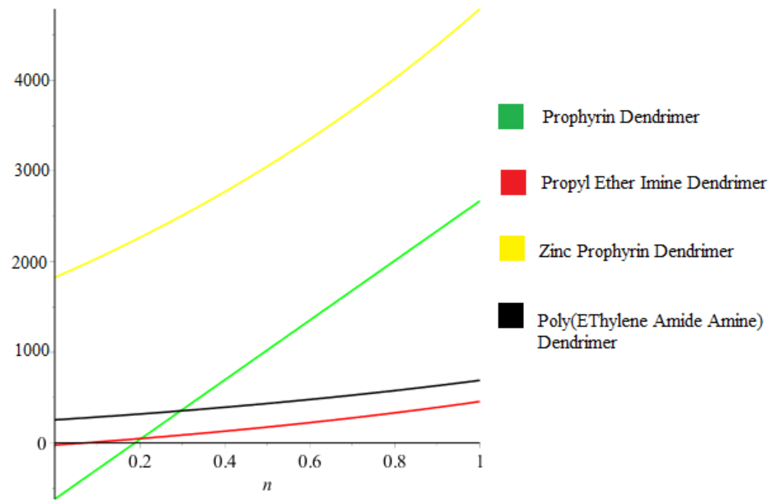

Figure 8. Second reverse hyper-Zagreb indices.

Author Contributions: W.G. designed the problem. M.Y. and A.F. proved the results. A.u.R.V. composed this manuscript and W.N. supervised the work and verify the results.

Funding: This research received no external funding.

Conflicts of Interest: Authors of this paper declare that they have no competing interests.

References

1. Astruc, D.; Boisselier, E.; Ornelas, C. Dendrimers designed for functions: From physical, photophysical, and supramolecular properties to applications in sensing, catalysis, molecular electronics, and nanomedicine. *Chem. Rev.* **2010**, *110*, 1857–1959. [CrossRef] [PubMed]
2. Vogtle, F.; Richardt, G.; Werner, N. *Dendrimer Chemistry Concepts, Syntheses, Properties, Applications*; Wiley: Hoboken, NJ, USA, 2009; ISBN 3-527-32066-0
3. Hirsch, B.E.; Lee, S.; Qiao, B.; Chen, C.; McDonald, K.P.; Tait, S.L.; Flood, A.H. Anion-induced dimerization of 5-fold symmetric cyanostars in 3D crystalline solids and 2D self-assembled crystals. *Chem. Commun.* **2014**, *50*, 9827–9830. [CrossRef] [PubMed]
4. Buhleier, E.; Wehner, W.; Vogtle, F. "Cascade"- and "Nonskid-Chain-like" Syntheses of molecular cavity topologies. *Synthesis* **1978**, *9*, 155–158. [CrossRef]
5. Denkewalter, R.G.; Kolc, J.; Lukasavage, W.J. Macromolecular Highly Branched Homogeneous Compound Based on Lysine Units. U.S. Patent 4,289,872, 6 April 1979.
6. Denkewalter, R.G.; Kolc, J.F.; Lukasavage, W.J. Macromolecular Highly Branched Homogeneous Compound. U.S. Patent 4,410,688, 29 April 1981.
7. Tomalia, A.D.; Dewald, R.J. Dense Star Polymers Having Core, Core Branches, Terminal Groups. U.S. Patent 4,507,466, 7 January 1983.
8. Tomalia, D.A.; Baker, H.; Dewald, J.; Hall, M.; Kallos, G.; Martin, S.; Roeck, J.; Ryder, J.; Smith, P. A new class of polymers: Starburst-dendritic macromolecules. *Polym. J.* **1985**, *17*, 117–132. [CrossRef]
9. Donald, A. Treelike molecules branch out. Tomalia synthesized first dendrimer molecule-chemistry-brief article. *Sci. News* **1996**, *149*, 17–32.
10. Graovac, A.; Ghorbani, M.; Hosseinzadeh, M.A. Computing fifth geometric-arithmetic index for nanostar dendrimers. *J. Math. NanoSci.* **2011**, *1*, 33–42.
11. Ashrafi, A.R.; Mirzargar, M. *PI, Szeged and Edge Szeged Indices of an Infinite Family of Nanostar Dendrimers*; CSIR: New Delhi, India, 2008.
12. Munir, M.; Nazeer, W.; Rafique, S.; Kang, S. M-polynomial and related topological indices of nanostar dendrimers. *Symmetry* **2016**, *8*, 97. [CrossRef]
13. Ghorbani, M.; Hosseinzadeh, M.A. Computing ABC_4 index of nanostar dendrimers. *Optoelectron. Adv. Mater. Rapid Commun.* **2010**, *4*, 1419–1422.

14. Madanshekaf, A.; Ghaneeei, M. Computing two topological indices of nanostars dendrimer. *Optoelectron. Adv. Mater. Rapid Commun.* **2010**, *4*, 2200–2202.
15. Dorosti, N.; Iranmanesh, A.; Diudea, M.V. Computing the cluj index of dendrimer nanostars. *Match* **2009**, *62*, 389–395.
16. Aslam, A.; Bashir, Y.; Rafiq, M.; Haider, F.; Muhammad, N.; Bibi, N. Three new/old vertex-degree-based topological indices of some dendrimers structure. *Electron. J. Biol.* **2017**, *13*, 94–99.
17. Gao, W.; Iqbal, Z.; Ishaq, M.; Sarfraz, R.; Aamir, M.; Aslam, A. On eccentricity-based topological indices study of a class of porphyrin-cored dendrimers. *Biomolecules* **2018**, *8*, 71. [CrossRef] [PubMed]
18. 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. [CrossRef]
19. Kang, S.M.; Zahid, M.A.; Nazeer, W.; Gao, W. Calculating the degree-based topological indices of dendrimers. *Open Chem.* **2018**, *16*, 681–688. [CrossRef]
20. Kulli, V.R. Reverse Zagreb and reverse hyper-Zagreb indices and their polynomials of rhombus silicate networks. *Ann. Pure Appl. Math.* **2018**, *16*, 47–51. [CrossRef]
21. West, D.B. *Introduction to Graph Theory*; Prentice Hall: Upper Saddle River, NJ, USA, 2001; Volume 2.
22. Hosoya, H. On some counting polynomials in chemistry. *Discret. Appl. Math.* **1988**, *19*, 239–257. [CrossRef]
23. Siddiqui, M.K.; Imran, M.; Ahmad, A. On Zagreb indices, Zagreb polynomials of some nanostar dendrimers. *Appl. Math. Comput.* **2016**, *280*, 132–139. [CrossRef]
24. Deutsch, E.; Klavzar, S. M-polynomial and degree-based topological indices. *arXiv* **2014**, arXiv:1407.1592.
25. Munir, M.; Nazeer, W.; Rafique, S.; Kang, S.M. M-polynomial and degree-based topological indices of polyhex nanotubes. *Symmetry* **2016**, *8*, 149. [CrossRef]
26. Fath-Tabar, G. Zagreb polynomial and PI indices of some nano structures. *Digest J. Nanomater. Biostructures* **2009**, *4*, 189–191.
27. Iranmanesh, M.; Saheli, M. On the harmonic index and harmonic polynomial of caterpillars with diameter four. *Iran. J. Math. Chem.* **2015**, *6*, 41–49.
28. Devillers, J.; Balaban, A.T. (Eds.) *Topological Indices and Related Descriptors in QSAR and QSPAR*; CRC Press: Boca Raton, FL, USA, 2000.
29. Karelson, M. *Molecular Descriptors in QSAR/QSPR*; Wiley-Interscience: Hoboken, NJ, USA, 2000.
30. Karelson, M.; Lobanov, V.S.; Katritzky, A.R. Quantum-chemical descriptors in QSAR/QSPR studies. *Chem. Rev.* **1996**, *96*, 1027–1044. [CrossRef] [PubMed]
31. Bashir, Y.; Aslam, A.; Kamran, M.; Qureshi, M.I.; Jahangir, A.; Rafiq, M.; Muhammad, N. On forgotten topological indices of some dendrimers structure. *Molecules* **2017**, *22*, 867. [CrossRef] [PubMed]
32. Aslam, A.; Guirao, J.L.G.; Ahmad, S.; Gao, W. Topological indices of the line graph of subdivision graph of complete bipartite graphs. *Appl. Math.* **2017**, *11*, 1631–1636. [CrossRef]
33. Aslam, A.; Ahmad, S.; Gao, W. On certain topological indices of boron triangular nanotubes. *Z. Naturforsch. A* **2017**, *72*, 711–716. [CrossRef]
34. Gao, W.; Wang, W.F.; Dimitrov, D.; Wang, Y.Q. Nano properties analysis via fourth multiplicative ABC indicator calculating. *Arabian J. Chem.* **2018**, *11*, 793–801. [CrossRef]
35. Wiener, H. Structural determination of paraffin boiling points. *J. Am. Chem. Soc.* **1947**, *69*, 17–20. [CrossRef] [PubMed]
36. Randić, M. Characterization of molecular branching. *J. Am. Chem. Soc.* **1975**, *97*, 6609–6615. [CrossRef]
37. Li, X.; Shi, Y. A survey on the Randić index. *MATCH Commun. Math. Comput. Chem.* **2008**, *59*, 127–156.
38. Hu, Y.; Li, X.; Shi, Y.; Xu, T.; Gutman, I. On molecular graphs with smallest and greatest zeroth-order general Randić index. *MATCH Commun. Math. Comput. Chem.* **2005**, *54*, 425–434.
39. Li, X.; Yang, Y. Sharp bounds for the general Randić index. *MATCH Commun. Math. Comput. Chem.* **2004**, *51*, 155–166.
40. Clark, L.H.; Moon, J.W. On the general Randić index for certain families of trees. *Ars Comb.* **2000**, *54*, 223–235.
41. Hu, Y.; Li, X.; Yuan, Y. Trees with minimum general Randić index. *MATCH Commun. Math. Comput. Chem.* **2004**, *52*, 119–128.
42. Gutman, I.; Das, K.C. The first Zagreb index 30 years after. *MATCH Commun. Math. Comput. Chem.* **2004**, *50*, 83–92.
43. Gutman, I. An exceptional property of first Zagreb index. *MATCH Commun. Math. Comput. Chem.* **2014**, *72*, 733–740.

44. Hosamani, S.M.; Basavanagoud, B. New upper bounds for the first Zagreb index. *MATCH Commun. Math. Comput. Chem.* **2015**, *74*, 97–101.
45. Das, K.C.; Gutman, I. Some properties of the second Zagreb index. *MATCH Commun. Math. Comput. Chem.* **2004**, *52*, 3.
46. Zhou, B.; Gutman, I. Further properties of Zagreb indices. *MATCH Commun. Math. Comput. Chem.* **2005**, *54*, 233–239.
47. Gao, W.; Wu, H.L.; Siddiqui, M.K.; Baig, A.Q. Study of biological networks using graph theory. *Saudi J. Biol. Sci.* **2018**, *25*, 1212–1219. [CrossRef] [PubMed]
48. Gao, W.; Younas, M.; Farooq, A.; Mahboob, A.; Nazeer, W. M-polynomials and degree-based topological indices of crystallographic structure of molecules. *Biomolecules.* **2018**, *8*, 107. [CrossRef] [PubMed]
49. Zhou, B. Zagreb indices. *MATCH-Commun. Math. Comput. Chem.* **2004**, *52*, 113–118.
50. Milicevic, A.; Nikolic, S.; Trinajstic, N. On reformulated Zagreb indices. *Mol. Divers.* **2004**, *8*, 393–399. [CrossRef] [PubMed]
51. Eliasi, M.; Iranmanesh, A.; Gutman, I. Multiplicative versions of first Zagreb index. *Match-Commun. Math. Comput. Chem.* **2012**, *68*, 217.
52. Hao, J. Theorems about Zagreb indices and modified Zagreb indices. *MATCH Commun. Math. Comput. Chem.* **2011**, *65*, 659–670.
53. Kulli, V.R. Multiplicative hyper-zagreb indices and coindices of graphs: computing these indices of some nanostructures. *Int. Res. J. Pure Algebra* **2016**, *6*, 7.
54. Kwun, Y.C.; Virk, A.R.; Nazeer, W.; Kang, S.M. On the multiplicative degree-based topological indices of silicon-carbon $Si2C3-I[p,q]$ and $Si2C3-II[p,q]$. *Symmetry* **2018**, *10*, 320. [CrossRef]
55. Shirdel, G.H.; Ezapour, H.; Sayadi, A.M. The hyper-Zagreb index of graph operations. *Iran. J. Math. Chem.* **2013**, *4*, 213–220.
56. Soleimani, N.; Bahnamiri, S.B.; Nikmehr, M.J. Study of dendrimers by topological indices. *Acta Chem. Iasi* **2017**, *25*, 145–162. [CrossRef]
57. Omolara, O.A. The mechanisms, kinetics and thermodynamics of the gas-phase pyrolysis of sec-butyl bromide: A computational approach. *Int. Res. J. Pure Appl. Chem.* **2018**, *16*, 1–10.