

## Research Article

# Irregularity Indices of Dendrimer Structures Used as Molecular Disrupter in QSAR Study

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Dendrimers are rising polymeric structures known for their flexibility in medication conveyance and high usefulness, whose properties are same biomolecules. These nanostructured macromolecules have shown potential capacities in capturing as well as conjugating the high subatomic weight hydrophilic/hydrophobic substances by host–visitor collaborations and covalent holding (prodrug approach) individually. In quantitative structure–property relationships (QSPR), topological indices are utilized to gather properties of dendrimers. Topological indices catch symmetry of dendrimer structures and give it a logical reasoning to predict properties, for instance, viscosity, boiling points, the radius of gyration, etc. In this report, we intend to examine dendrimers through irregularity indices that are valuable in QSPR studies. We studied sixteen irregularity indices of diverse dendrimer structures.

## 1. Introduction

Nanoscience and nanotechnology are the study and application of extremely small things and can be used across all the other science fields. It is hard to imagine just how small nanotechnology is. One nanometer is a billionth of a meter ( $10^{-9}$  m). Here are a few illustrative examples. There are 25,400,000 nanometers in an inch. A sheet of newspaper is about 100,000 nanometers thick. Nanotechnology has numerous applications in different fields. The use of nanotechnology in medicine offers some exciting possibilities like drug delivery, diagnostic techniques, antibacterial treatments, wound treatment, etc.

Dendrimers, from a Greek word that means “trees” [1, 2], are monotonously expanded molecules. Dendrimers are commonly symmetrical about the center and for the most part have spherical three-dimensional morphology.

Word dendrites are likewise regularly experienced and usually contain a single chemically addressable group called the focus or core. The first dendrimer was made by Hirsch et al. [3] utilizing distinctive engineered strategies, for example, by Denkewalter et al. [4] and Tomalia et al. [5, 6]. Donald in 1996 [7] presented a combination amalgamation technique. The prevalence of dendrimers has incredibly expanded. By 2005, there were in excess of 5000 logical papers and patents. Employment of dendrimers incorporates conjugating other synthetic species into the dendrimer surface that can fill in as recognizing administrators, for instance, a dye molecule, focusing on parts, fondness ligands, imaging operators, radioligands, or pharmaceutical mixes. Dendrimers have astoundingly strong potential for these applications as their structure can incite multivalent frameworks. All things considered, one dendrimer molecule has a few possible locales to couple to a functioning species. Researchers

expected to utilize the hydrophobic situations of the dendritic media to lead photochemical responses that make the things that are artificially tested. Carboxylic corrosive and phenol-ended water dissolvable dendrimers have been fused to set up their utility in sedative movement, prompting compound reactions in their inner parts. This may empower authorities to associate both centering atoms and medication particles to the equivalent dendrimer, which could diminish negative manifestations of drugs on solid cells. Because of these applications, dendrimers are broadly considered [8–10]. A dendrimer is commonly symmetric around the center and frequently receives a round three-dimensional morphology. The principal dendrimers were made by different union methodologies by Buhleier et al [11] in 1978. Dendrimers have picked up a wide scope of uses in chemistry, physics, and nanosciences. There is a great deal of research papers on the calculation of TIs of dendrimers, e.g., [12–15].

Mathematical chemistry is a zone of research in chemistry in which numerical apparatuses are utilized to take care of issues of chemistry. Chemical graph theory is a significant region of research in mathematical chemistry which we manage with topology of molecular structure, for example, the scientific investigation of isomerism and the improvement of topological descriptors or indices. Contaminate, topological indices (TIs) are real numbers associated with the molecular graph of a chemical compound and have applications in QSPR. TIs remain invariant upto graph isomorphism and help us to foresee numerous properties of synthetic structures without going to lab [16–22]. Other developing field is cheminformatics, in which we use QSAR and QSPR relationship to figure organic action and synthetic properties of molecular structures. In these examinations, a few physicochemical properties and TIs are used to figure out the behaviour of compound structures [23–27]. Like TIs, polynomials also have impressive applications in science, for instance, Hosoya polynomial, which is otherwise called Weiner polynomial, presented in [28] assumes a significant job in calculation of distance-based TIs. M-polynomial [29] was characterized in 2015 and assumes a comparative job in calculation of various degree-based TIs [30, 31]. The M-polynomial contains valuable data about degree-based TIs, and numerous TIs can be calculated from this basic logarithmic polynomial. The primary TI was characterized in 1947 by Weiner when he was studying poiling point of alkanes [32]. This index is currently known as Weiner index. Along these lines, Weiner set up the structure of TIs and the Weiner index is the first and most studied TI [33, 34].

The other oldest TI is the Randić index, given by Milan Randić [35] in 1975. After the success of the Randić index, in the year 1988, the generalized version of Randić index was introduced in [27]. This version attracts both the mathematicians and chemists [36]. Numerous numerical properties of this simple TI are studied in [37].

The Randić index is the most mainstream regularly connected and most concentrated among all other TIs. Numerous research papers and text books, for example [38, 39], are published in different academic journals on this

TI. Surveys on the Randić index were conducted by scientists [40, 41]. The reason behind the success of such a simple TI is as yet a puzzle, although some conceivable clarifications were given.

After the Randić index, the most studied TIs are the first and second Zagreb indices [42–44]. The modified second Zagreb index was defined in [45]. The symmetric division index is one of the 148 important indexes, which is a decent indicator of the aggregate surface area for polychlorobiphenyls [46].

More than one hundred and fifty topological indices are present in literature, which help us to guess properties of compounds to some extent but none of them completely describe the compound. Therefore, there is always room to define new topological indices. In this paper, we defined some degree-based irregularity topological indices for dendrimers and plot our results to see dependence on the involved parameters.

## 2. Topological Indices

Topological index is a numeric quantity associated with a molecular graph. We can classify topological indices into two major types: the first type are degree-based topological indices that depend upon the degree of vertices and the second type are distance-based topological indices that depend upon the distance between vertices.

The first and second Zagreb indices are among the oldest molecular structure descriptors introduced by Gutman in 1975 [47] and their properties are extensively investigated. They are defined as

$$M_1(G) = \sum_{uv \in E(G)} (d_u + d_v), \quad (1)$$

$$M_2(G) = \sum_{uv \in E(G)} (d_u \times d_v). \quad (2)$$

The first genuine degree-based TI was given by Randić in 1975 [35] as

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u \cdot d_v}}. \quad (3)$$

The GRI known as the General Randic Index [48] and is defined as

$$GRI(G) = \sum_{uv \in E(G)} (d_u \cdot d_v)^\alpha, \quad (4)$$

where  $\alpha$  is an arbitrary real number.

The TI is known as irregularity index [49] if TI of graph is greater or equal to zero and TI of graph is equal to zero if and only if graph is regular. The irregularity indices are given below. All these irregularity indices belong to degree-based topological invariants except  $IRM_2(G)$  and are used in QSAR.

$$(i) VAR(G) = \sum_{uv \in V} (d_u - (2m/n))^2 = M_1(G)/n - \frac{(2m/n)^2}{n}$$

$$(ii) AL(G) = \sum_{uv \in E(G)} |d_u - d_v|$$

- (iii)  $\text{IR1}(G) = \sum_{u \in V} (d_u)^3 - (2m/n) \sum_{u \in V} (d_u)^2 = F(G) - (2m/n)M_1(G)$
- (iv)  $\text{IR2}(G) = \sqrt{(\sum_{uv \in E(G)} d_u d_v / m)} - (2m/n) = \sqrt{M_2(G)/m} - (2m/n)$
- (v)  $\text{IRF}(G) = \sum_{uv \in E(G)} (d_u - d_v)^2 = F(G) - 2M_2(G)$
- (vi)  $\text{IRFW}(G) = \text{IRF}(G)/M_2(G)$
- (vii)  $\text{IRA}(G) = \sum_{uv \in E(G)} (d_u^{-1/2} - d_v^{1/2})^2 = n - 2R(G)$
- (viii)  $\text{IRB}(G) = \sum_{uv \in E(G)} (d_u^{1/2} - d_v^{1/2})^2 = M_1(G) - 2\text{RR}(G)$
- (ix)  $\text{IRC}(G) = (\sum_{uv \in E(G)} \sqrt{d_u d_v} / m) - (2m/n) = (\text{RR}(G)/m) - (2m/n)$
- (x)  $\text{IRDIF}(G) = \sum_{uv \in E(G)} |(d_u/d_v) - (d_v/d_u)| = \sum_{i < j} m_{i,j} ((j/i) - (i/j))$
- (xi)  $\text{IRL}(G) = \sum_{uv \in E(G)} |\ln d_u - \ln d_v| = \sum_{i < j} m_{i,j} \ln(j/i)$
- (xii)  $\text{IRLU}(G) = \sum_{uv \in E(G)} |d_u - d_v| / \min(d_u, d_v) = \sum_{i < j} m_{i,j} \ln((j-i)/i)$
- (xiii)  $\text{IRLF}(G) = \sum_{uv \in E(G)} |d_u - d_v| / \sqrt{(d_u d_v)} = \sum_{i < j} m_{i,j} ((j-i)/\sqrt{ij})$
- (xiv)  $\text{IRLA}(G) = 2 \sum_{uv \in E(G)} |d_u - d_v| / (d_u + d_v) = 2 \sum_{i < j} m_{i,j} ((j-i)/(i+j))$
- (xv)  $\text{IRD1}(G) = \sum_{uv \in E(G)} \ln 1 + |d_u - d_v| = \sum_{i < j} m_{i,j} \ln(i+j-1)$
- (xvi)  $\text{IRGA}(G) = \sum_{uv \in E(G)} \ln((d_u + d_v)/2\sqrt{d_u d_v}) \sum_{i < j} m_{i,j} ((i+j)/2\sqrt{ij})$

### 3. Computational Results

This section consists of four subsections. In the first subsection, we will compute irregularity indices for Prophyrin Dendrimer  $D_n P_n$ . The second section consists of the irregularity indices for Propyl Ether Imine Dendrimer (PETIM). Third section is about the irregularity indices for Zinc Prophyrin Dendrimer DPZ<sub>n</sub>. The last subsection contain the results about irregularity indices for Poly(-EThylene Amide Amine) Dendrimer, PETAA.

**3.1. Prophyrin Dendrimer  $D_n P_n$ .** The molecular graph of Prophyrin Dendrimer  $D_n P_n$  is given in Figure 1.

The degree-based edge partition of Prophyrin Dendrimer  $D_n P_n$  is given in Table 1.

**Theorem 1.** Let  $D_n P_n$  be a Prophyrin Dendrimer, the irregularity indices are

- (1)  $\text{VAR}(D_n P_n) = (1983n^2 - 245n + 4)/(48n - 5)^2$
- (2)  $\text{AL}(D_n P_n) = 124n - 6$
- (3)  $\text{IR1}(D_n P_n) = 2(4329n^2 - 641n + 20)/(48n - 5)$
- (4)  $\text{IR2}(D_n P_n) = ((48n - 5)(\sqrt{547n - 56}) + (11 - 105n)(\sqrt{105n - 11})) / (\sqrt{105n - 11})(48n - 5)$
- (5)  $\text{IRF}(D_n P_n) = 282n - 68$
- (6)  $\text{IRFW}(D_n P_n) = (282/547)n - (17/14)$
- (7)  $\text{IRA}(D_n P_n) = (4/3)(\sqrt{3} - 12\sqrt{6} - 128)n - (2\sqrt{6} + 5)$
- (8)  $\text{IRB}(D_n P_n) = (228 - 96\sqrt{6} - 36\sqrt{3})n - 2(35 - 6\sqrt{6})$
- (9)  $\text{IRC}(D_n P_n) = ((2304\sqrt{6} + 864\sqrt{3} - 58889)n^2 - (240\sqrt{6} + 90\sqrt{3} - 1775)n - 121) / (105n - 11)(96n - 10)$
- (10)  $\text{IRDIF}(D_n P_n) = (434/3)n + 30$
- (11)  $\text{IRL}(D_n P_n) = 56.96n - 2.4$
- (12)  $\text{IRLU}(D_n P_n) = 102.66n - 3$
- (13)  $\text{IRLF}(D_n P_n) = 60.21n - \sqrt{6}$
- (14)  $\text{IRLA}(D_n P_n) = 47.6n - 2.4$
- (15)  $\text{IRD1}(D_n P_n) = 74.1n - 4.14$
- (16)  $\text{IRGA}(D_n P_n) = 13.24n - 0.06$

*Proof*

$$\begin{aligned} \text{VAR}(D_n P_n) &= \sum_{u \in V} \left( d_u - \frac{2m}{n} \right)^2 = \frac{M_1(D_n P_n)}{n} - \left( \frac{2m}{n} \right)^2 \\ &= (542n - 20) - \left( \frac{2(105n - 11)}{96n - 10} \right)^2 \\ &= \frac{1983n^2 - 245n + 4}{(48n - 5)^2}, \end{aligned} \quad (5)$$

$$\begin{aligned} \text{AL}(D_n P_n) &= \sum_{uv \in E(D_n P_n)} |d_u - d_v| \\ &= |1 - 3|(2n) + |1 - 4|(24n) + |2 - 2|(10n - 5) \\ &\quad + |2 - 3|(48n - 6) + |3 - 3|(13n) + |3 - 4|(8n) \\ &= 124n - 6, \end{aligned} \quad (6)$$

$$\begin{aligned}
\text{IR1}(D_n P_n) &= \sum_{u \in V} d_u^3 - \frac{2m}{n} \sum_{u \in V} d_u^2 = F(G) - \left(\frac{2m}{n}\right) M_1(D_n P_n) \\
&= (1366n - 118) - \left(\frac{2(105n - 11)}{96n - 10}\right) (542n - 50) \\
&= \frac{2(4329n^2 - 641n + 20)}{48n - 5},
\end{aligned} \tag{7}$$

$$\begin{aligned}
\text{IR2}(D_n P_n) &= \sqrt{\frac{\sum_{uv \in E(D_n P_n)} d_u d_v}{m}} - \frac{2m}{n} = \sqrt{\frac{M_2(D_n P_n)}{m}} - \frac{2m}{n} \\
&= \sqrt{\frac{547n - 56}{105n - 11}} - \left(\frac{2(105n - 11)}{96n - 10}\right) \\
&= \frac{(48n - 5)(\sqrt{547n - 56}) + (11 - 105n)(\sqrt{105n - 11})}{(\sqrt{105n - 11})(48n - 5)},
\end{aligned} \tag{8}$$

$$\begin{aligned}
\text{IRF}(D_n P_n) &= \sum_{uv \in E(D_n P_n)} (d_u - d_v)^2 \\
&= (1 - 3)^2 (2n) + (1 - 4)^2 (24n) \\
&\quad + (2 - 2)^2 (10n - 5) + (2 - 3)^2 (48n - 6) \\
&= 282n - 68,
\end{aligned} \tag{9}$$

$$\begin{aligned}
\text{IRFW}(D_n P_n) &= \frac{\text{IRF}(D_n P_n)}{M_2(D_n P_n)} \\
&= \frac{282n - 68}{547n - 56},
\end{aligned} \tag{10}$$

$$\begin{aligned}
\text{IRA}(D_n P_n) &= \sum_{uv \in E(D_n P_n)} (d_u^{-1/2} - d_v^{-1/2})^2 = n - 2R(G) \\
&= (96n - 10) - 2\left(\left(\frac{2}{3}(12\sqrt{6 - \sqrt{3}} + 32)\right)n - \frac{1}{2}(5 - 2\sqrt{6})\right) \\
&= \frac{4}{3}((\sqrt{3} - 12\sqrt{6} - 128)n - (2\sqrt{6} + 5)),
\end{aligned} \tag{11}$$

$$\begin{aligned}
\text{IRB}(D_n P_n) &= \sum_{uv \in E(D_n P_n)} (d_u^{1/2} - d_v^{1/2})^2 = M_1(D_n P_n) - 2RR(G) \\
&= (542n - 56) - 2((48\sqrt{6} + 18\sqrt{3} + 107)n - 2(5 - 3\sqrt{6})) \\
&= (228 - 96\sqrt{6} - 36\sqrt{3})n - 2(35 - 6\sqrt{6}),
\end{aligned} \tag{12}$$

$$\begin{aligned}
\text{IRC}(D_n P_n) &= \frac{\sum_{uv \in E(D_n P_n)} \sqrt{d_u d_v}}{m} - \frac{2m}{n} = \frac{RR(D_n P_n)}{m} - \frac{2m}{n} \\
&= \left(\frac{(48\sqrt{6} + 18\sqrt{3} + 107)n - 2(5 - 3\sqrt{6})}{105n - 11}\right) - \left(\frac{2(105n - 11)}{96n - 10}\right) \\
&= \frac{(2304\sqrt{6} + 864\sqrt{3} - 58889)n^2 - (240\sqrt{6} + 90\sqrt{3} - 1775)n - 121}{(105n - 11)(96n - 10)},
\end{aligned} \tag{13}$$

$$\begin{aligned}
\text{IRDIF}(D_n P_n) &= \sum_{uv \in E(D_n P_n)} \left| \frac{d_u}{d_v} - \frac{d_v}{d_u} \right| \\
&= \left| \frac{1}{3} - \frac{3}{1} \right| (2n) + \left| \frac{1}{4} - \frac{4}{1} \right| (24n) + \left| \frac{2}{2} - \frac{2}{2} \right| (10n - 5) \\
&\quad + \left| \frac{2}{3} - \frac{3}{2} \right| (48n - 6) + \left| \frac{3}{3} - \frac{3}{3} \right| (13n) + \left| \frac{3}{4} - \frac{4}{3} \right| (8n) \\
&= \frac{434}{3} n + 30,
\end{aligned} \tag{14}$$

$$\begin{aligned}
\text{IRL}(D_n P_n) &= \sum_{uv \in E(D_n P_n)} |\ln d_u - \ln d_v| \\
&= |\ln 1 - \ln 3| (2n) + |\ln 1 - \ln 4| (24n) + |\ln 2 - \ln 2| (10n - 5) \\
&\quad + |\ln 2 - \ln 3| (48n - 6) + |\ln 3 - \ln 3| (13n) + |\ln 3 - \ln 4| (8n) \\
&= 56.96n - 2.4,
\end{aligned} \tag{15}$$

$$\begin{aligned}
\text{IRLU}(D_n P_n) &= \sum_{uv \in E(D_n P_n)} \frac{|d_u - d_v|}{\min(d_u, d_v)} \\
&= \left( \frac{|1 - 3|}{1} \right) (2n) + \left( \frac{|1 - 4|}{1} \right) (24n) + \left( \frac{|2 - 2|}{2} \right) (10n - 5) \\
&\quad + \left( \frac{|2 - 3|}{2} \right) (105n - 11) + \left( \frac{|3 - 3|}{2} \right) (13n) + \left( \frac{|3 - 4|}{2} \right) (8n) \\
&= 102.66n - 3,
\end{aligned} \tag{16}$$

$$\begin{aligned}
\text{IRLF}(D_n P_n) &= \sum_{uv \in E(D_n P_n)} \frac{|d_u - d_v|}{\sqrt{d_u \cdot d_v}} \\
&= \left( \frac{|1 - 3|}{\sqrt{3}} \right) (2n) + \left( \frac{|1 - 4|}{\sqrt{4}} \right) (24n) + \left( \frac{|2 - 2|}{\sqrt{4}} \right) (10n - 5) \\
&\quad + \left( \frac{|2 - 3|}{\sqrt{6}} \right) (48n - 6) + \left( \frac{|3 - 3|}{\sqrt{9}} \right) (13n) \left( \frac{|3 - 4|}{\sqrt{12}} \right) (8n) \\
&= 60.21n - \sqrt{6},
\end{aligned} \tag{17}$$

$$\begin{aligned}
\text{IRLA}(D_n P_n) &= \sum_{uv \in E(D_n P_n)} 2 \frac{|d_u - d_v|}{(d_u + d_v)} \\
&= 2 \left( \frac{|1 - 3|}{1 + 3} \right) (2n) + 2 \left( \frac{|1 - 4|}{1 + 4} \right) (24n) + \left( 2 \frac{|2 - 2|}{2 + 2} \right) (10n - 5) \\
&\quad + 2 \left( \frac{|2 - 3|}{2 + 3} \right) (48n - 6) + 2 \left( \frac{|3 - 3|}{3 + 3} \right) (13n) + 2 \left( \frac{|3 - 4|}{3 + 4} \right) (8n) \\
&= 47.6n - 2.4,
\end{aligned} \tag{18}$$

$$\begin{aligned}
\text{IRD1}(D_n P_n) &= \sum_{uv \in E(D_n P_n)} \ln \{ 1 + |d_u - d_v| \} \\
&= \ln \{ 1 + |1 - 3| \} (2n) + \ln \{ 1 + |1 - 4| \} (24n) + \ln \{ 1 + |2 - 2| \} (10n - 5) \\
&\quad + \ln \{ 1 + |2 - 3| \} (48n - 6) + \ln \{ 1 + |3 - 3| \} (13n) + \ln \{ 1 + |3 - 4| \} (8n) \\
&= 74.1n - 4.14,
\end{aligned} \tag{19}$$

$$\begin{aligned}
\text{IRGA}(D_n P_n) &= \sum_{uv \in E(D_n P_n)} \ln \left( \frac{d_u + d_v}{2\sqrt{d_u d_v}} \right) \\
&= \ln \left( \frac{1+3}{2} \sqrt{1 \times 3} \right) (2) + \ln \left( \frac{1+4}{2\sqrt{1 \times 4}} \right) (24n) + \ln \left( \frac{2+2}{2\sqrt{2 \times 2}} \right) (10n - 5) \\
&\quad + \ln \left( \frac{2+3}{2\sqrt{2 \times 3}} \right) (48n - 6) + \ln \left( \frac{3+3}{2\sqrt{3 \times 3}} \right) (13n) + \ln \left( \frac{3+4}{2\sqrt{3 \times 4}} \right) (8n) \\
&= 13.24n - 0.06.
\end{aligned} \tag{20}$$

□

**3.2. Propyl Ether Imine Dendrimer (PETIM).** The molecular graph of Propyl Ether Imine Dendrimer (PETIM) is given in Figure 2.

The degree-based edge partition of Propyl Ether Imine Dendrimer (PETIM) is given in Table 2

**Theorem 2.** Let (PETIM) be the Propyl Ether Imine Dendrimer. The irregularity indices are

- (1)  $\text{VAR}(\text{PETIM}) = (24.9^{2n} \cdot 2^n - 48.2^{2n} - 23.9^{2n} - 2.2^n - 42) / (24.2^n - 23)^2$
- (2)  $\text{AL}(\text{PETIM}) = 2^{n+1} + 6.2^n - 6$
- (3)  $\text{IR1}(\text{PETIM}) = 6(64.4^n - 100.2^n + 35) / (24.2^n - 23)$
- (4)  $\text{IR2}(\text{PETIM}) = ((24.2^n - 23) / (\sqrt{2.2^{n+1} + 4.2^{n+4} + 36.2^n - 108}) - 2(24.2^n - 24) / (\sqrt{24.2^n - 23})) / (24.2^n - 23)^{3/2}$
- (5)  $\text{IRF}(\text{PETIM}) = 2^{n+1} + 6.2^n - 6$
- (6)  $\text{IRFW}(\text{PETIM}) = (4.2^n - 3) / 2(26.2^n - 27)$

- (7)  $\text{IRA}(\text{PETIM}) = 24.2^n - 5 - \sqrt{2}2^{n+1} - 2^{n+4} - (1/3)(6.2^n - 6)$
- (8)  $\text{IRB}(\text{PETIM}) = 30.2^n + (3 - 2\sqrt{2})2^{n+1} - 30 - 2\sqrt{6}(6.2^n - 6)$
- (9)  $\text{IRC}(\text{PETIM}) = (352.2^n + (72\sqrt{6} - 24\sqrt{2} - 192)2^{2n} - (141\sqrt{3} + 23)2^{1/2+n} + (69\sqrt{6} - 162)) / 12(24.2^n - 23)(2^n - 1)$
- (10)  $\text{IRDIF}(\text{PETIM}) = (1/2)(26.2^n - 3.2^{n+1} - 26)$
- (11)  $\text{IRL}(\text{PETIM}) = (2.4)2^n + (0.69)2^{n+1} - 2.4$
- (12)  $\text{IRLU}(\text{PETIM}) = 3.2^n + 2^{n+1} - 3$
- (13)  $\text{IRLF}(\text{PETIM}) = (1/\sqrt{2})[(1 + \sqrt{3})2^{n+1} - 2\sqrt{3}]$
- (14)  $\text{IRLA}(\text{PETIM}) = (1/15)(10.2^{n+1} + 36.2^n - 36)$
- (15)  $\text{IRD1}(\text{PETIM}) = (0.69)2^{n+1} + (1.38)2^n - 1.38$
- (16)  $\text{IRGA}(\text{PETIM}) = (0.05)2^{n+1} + (0.12)2^n - 0.12$

*Proof*

$$\begin{aligned}
\text{VAR}(\text{PETIM}) &= \sum_{u \in V} \left( d_u - \frac{2m}{n} \right)^2 = \frac{M_1(\text{PETIM})}{n} - \left( \frac{2m}{n} \right)^2 \\
&= 3.2^{n+1} + 4.2^{n+4} + 30.2^n - 102 \left( \frac{2(24.2^n - 24)}{24.2^n - 23} \right)^2 \\
&= \frac{24.9^{2n} \cdot 2^n - 48.2^{2n} - 23.9^{2n} - 2.2^n - 42}{(24.2^n - 23)^2},
\end{aligned} \tag{21}$$

$$\begin{aligned}
\text{AL}(\text{PETIM}) &= \sum_{uv \in E(\text{PETIM})} |d_u - d_v| \\
&= |1 - 2|(2^{n+1}) + |2 - 2|(2^{n+4} - 18) + |2 - 3|(6^{2n} - 6) \\
&= 2^{n+1} + 6.2^n - 6,
\end{aligned} \tag{22}$$

$$\begin{aligned}
\text{IR1}(\text{PETIM}) &= \sum_{u \in V} d_u^3 - \frac{2m}{n} \sum_{u \in V} d_u^2 = F(G) - \frac{2m}{n} M_1(\text{PETIM}) \\
&= (5.2^{n+1} + 8.2^{n+4} + 78.2^n - 222) \\
&\quad - \left( \frac{2(24.2^n - 24)}{24.2^n - 23} \right) (3.2^{n+1} + 4.2^{n+4} + 30.2^n - 102) \\
&= \frac{6(64.4^n - 100.2^n + 35)}{24.2^n - 23},
\end{aligned} \tag{23}$$

$$\begin{aligned}
\text{IR2(PETIM)} &= \sqrt{\frac{\sum_{uv \in E(\text{PETIM})} d_u d_v}{m}} - \frac{2m}{n} = \sqrt{\frac{M_2(\text{PETIM})}{m}} - \frac{2m}{n} \\
&= \sqrt{\frac{2.2^{n+1} + 4.2^{n+4} + 36.2^n - 108}{24.2^n - 24}} - \left( \frac{2(24.2^n - 24)}{24.2^n - 23} \right) \\
&= \frac{(24.2^n - 23)(\sqrt{2.2^{n+1} + 4.2^{n+4} + 36.2^n - 108}) - 2(24.2^n - 24)(\sqrt{24.2^n - 23})}{(24.2^n - 23)^{3/2}},
\end{aligned} \tag{24}$$

$$\begin{aligned}
\text{IRF(PETIM)} &= \sum_{uv \in E(\text{PETIM})} (d_u - d_v)^2 \\
&= (1-2)^2(2^{n+1}) + (2-2)^2(2^{n+4} - 18) + (2-3)^2(6.2^n - 6) \\
&= 2^{n+1} + 6.2^n - 6,
\end{aligned} \tag{25}$$

$$\begin{aligned}
\text{IRFW(PETIM)} &= \frac{\text{IRF(PETIM)}}{M_2(\text{PETIM})} \\
&= \frac{2^{n+1} + 6.2^n - 6}{2.2^{n+1} + 4.2^{n+4} + 36.2^n - 108},
\end{aligned} \tag{26}$$

$$\begin{aligned}
\text{IRA(PETIM)} &= \sum_{uv \in E(\text{PETIM})} (d_u^{-1/2} - d_v^{-1/2})^2 = n - 2R(\text{PETIM}) \\
&= (24.2^n - 23) - 2\left(\frac{1}{2}\sqrt{2}.2^{n+1} + \frac{1}{2}2^{n+4} - 36 + \sqrt{6}(6.2^n - 6)\right) \\
&= 24.2^n - 5 - \sqrt{2}2^{n+1} - 2^{n+4} - \frac{1}{3}(6.2^n - 6),
\end{aligned} \tag{27}$$

$$\begin{aligned}
\text{IRB(PETIM)} &= \sum_{uv \in E(\text{PETIM})} (d_u^{1/2} - d_v^{1/2})^2 = M_1(D_n P_n) - 2RR(\text{PETIM}) \\
&= (3.2^{n+1} + 4.2^{n+4} + 30.2^n - 102) - 2(\sqrt{2}.2^{n+1} + 2.2^{n+4} - 36 + \sqrt{6}(6.2^n - 6)) \\
&= 30.2^n + (3 - 2\sqrt{2})2^{n+1} - 30 - 2\sqrt{6}(6.2^n - 6),
\end{aligned} \tag{28}$$

$$\begin{aligned}
\text{IRC(PETIM)} &= \frac{\sum_{uv \in E(\text{PETIM})} \sqrt{d_u d_v}}{m} - \frac{2m}{n} = \frac{RR(\text{PETIM})}{m} - \frac{2m}{n} \\
&= \frac{\sqrt{2}.2^{n+1} + 2.2^{n+4} - 36 + \sqrt{6}(6.2^n - 6)}{24.2^n - 24} - \frac{2(24.2^n - 24)}{24.2^n - 23} \\
&= \frac{352.2^n + (72\sqrt{6} - 24\sqrt{2} - 192)2^{2n} - (141\sqrt{3} + 23)2^{1/2+n} + (69\sqrt{6} - 162)}{12(24.2^n - 23)(2^n - 1)},
\end{aligned} \tag{29}$$

$$\begin{aligned}
\text{IRDIF(PETIM)} &= \sum_{uv \in E(\text{PETIM})} \left| \frac{d_u}{d_v} - \frac{d_v}{d_u} \right| \\
&= \left| \frac{1}{2} - \frac{2}{1} \right| (2^{n+1}) + \left| \frac{2}{2} - \frac{2}{2} \right| (2^{n+4} - 18) + \left| \frac{2}{3} - \frac{3}{2} \right| (6.2^n - 6) \\
&= \frac{1}{2} (26.2^n - 3.2^{n+1} - 26),
\end{aligned} \tag{30}$$

$$\begin{aligned}
\text{IRL(PETIM)} &= \sum_{uv \in E(\text{PETIM})} |\ln d_u - \ln d_v| \\
&= |\ln 1 - \ln 2|(2^{n+1}) + |\ln 2 - \ln 2|(2^{n+4} - 18) \\
&\quad + |\ln 2 - \ln 3|(6.2^n - 6) \\
&= (2.4)2^n + (0.69)2^{n+1} - 2.4,
\end{aligned} \tag{31}$$

$$\begin{aligned}
\text{IRLU(PETIM)} &= \sum_{uv \in E(\text{PETIM})} \frac{|d_u - d_v|}{\min(d_u, d_v)} \\
&= \left( \frac{|1-2|}{1} \right) (2^{n+1}) + \left( \frac{|2-2|}{2} \right) (2^{n+4} - 18) \\
&\quad + \left( \frac{|2-3|}{2} \right) (6 \cdot 2^n - 6) \\
&= 3 \cdot 2^n + 2^{n+1} - 3,
\end{aligned} \tag{32}$$

$$\begin{aligned}
\text{IRLF(PETIM)} &= \sum_{uv \in E(\text{PETIM})} \frac{|d_u - d_v|}{\sqrt{d_u \cdot d_v}} \\
&= \left( \frac{|1-2|}{\sqrt{2}} \right) (2^{n+1}) + \left( \frac{|2-2|}{\sqrt{4}} \right) (2^{n+4} - 18) \\
&\quad + \left( \frac{|2-3|}{\sqrt{6}} \right) (6 \cdot 2^n - 6) \\
&= \frac{1}{\sqrt{2}} [(1 + \sqrt{3}) 2^{n+1} - 2\sqrt{3}],
\end{aligned} \tag{33}$$

$$\begin{aligned}
\text{IRLA(PETIM)} &= \sum_{uv \in E(\text{PETIM})} 2 \frac{|d_u - d_v|}{(d_u + d_v)} \\
&= 2 \left( \frac{|1-2|}{1+2} \right) (2^{n+1}) + 2 \left( \frac{|2-2|}{2+2} \right) (2^{n+4} - 18) \\
&\quad + 2 \left( \frac{|2-3|}{2+3} \right) (6 \cdot 2^n - 6) \\
&= \frac{1}{15} (10 \cdot 2^{n+1} + 36 \cdot 2^n - 36),
\end{aligned} \tag{34}$$

$$\begin{aligned}
\text{IRD1(PETIM)} &= \sum_{uv \in E(\text{PETIM})} \ln \{ 1 + |d_u - d_v| \} \\
&= \ln \{ 1 + |1-2| \} (2^{n+1}) + \ln \{ 1 + |2-2| \} (2^{n+4} - 18) \\
&\quad + \ln \{ 1 + |2-3| \} (6 \cdot 2^n - 6) \\
&= (0.69) 2^{n+1} + (1.38) 2^n - 1.38,
\end{aligned} \tag{35}$$

$$\begin{aligned}
\text{IRGA(PETIM)} &= \sum_{uv \in E(\text{PETIM})} \ln \left( \frac{d_u + d_v}{2\sqrt{d_u d_v}} \right) \\
&= \ln \left( \frac{1+2}{2\sqrt{1 \times 2}} \right) (2^{n+1}) + \ln \left( \frac{2+2}{2\sqrt{2 \times 2}} \right) (2^{n+4} - 18) \\
&\quad + \ln \left( \frac{2+3}{2\sqrt{2 \times 3}} \right) (6 \cdot 2^n - 6) \\
&= (0.05) 2^{n+1} + (0.12) 2^n - 0.12.
\end{aligned} \tag{36}$$

□

**3.3. Zinc Prophyrin Dendrimer  $\text{DPZ}_n$ .** The molecular graph of Zinc Prophyrin Dendrimer,  $\text{DPZ}_n$ , is given in Figure 3.

The degree-based edge partition of Zinc Prophyrin Dendrimer,  $\text{DPZ}_n$ , is given in Table 3

**Theorem 3.** Let  $\text{DPZ}_n$  be a Zinc Prophyrin Dendrimer, the irregularity indices are

$$(1) \text{VAR}(\text{DPZ}_n) = (7488.2^n n - 11025.n^2 - 782.2^n - 1626.n + 289)/(48n - 5)^2$$

- $$(2) AL(DPZ_n) = 40.2^n - 12$$
- $$(3) IR1(DPZ_n) = 12(438.2^n n - 44.2^n - 277n + 28)/(48n - 5)$$
- $$(4) IR2(DPZ_n) = ((96n - 10)(\sqrt{367.2^n - 208}) - 2(\sqrt{105n - 11})(105n - 11))/(\sqrt{105n - 11})(96n - 10)$$
- $$(5) IRF(DPZ_n) = 40.2^n - 12$$
- $$(6) IRFW(DPZ_n) = (10.2^n - 3)/2(47.2^n - 26)$$
- $$(7) IRA(DPZ_n) = 96n - (40/3)\sqrt{6}2^n - (94/3) - (1/9)(6\sqrt{2} - 22\sqrt{6} - 48)\sqrt{6}$$
- $$(8) IRB(DPZ_n) = 312.2^n - 2(56 + 40\sqrt{6})2^n - 52 - 16\sqrt{3} + 32\sqrt{6}$$

- $$(9) IRC(DPZ_n) = (1/(105n - 11)(48n - 5))[(1920\sqrt{3}n - 200\sqrt{3})2^{(1/2)+n} - (768\sqrt{6} - 384)\sqrt{3} + 658] + 2688.2^n n - 11025n^2 + (80\sqrt{6} + 159)]$$
- $$(10) IRDIF(DPZ_n) = (1/3)(100.2^n - 33)$$
- $$(11) IRL(DPZ_n) = 16.2^n - 5.28$$
- $$(12) IRLU(DPZ_n) = (1/3)(60.2^n - 20)$$
- $$(13) IRLF(DPZ_n) = (1/\sqrt{6})40.2^n - (1/3)(8\sqrt{6} - 2\sqrt{3})$$
- $$(14) IRLA(DPZ_n) = (1/35)(560.2^n - 184)$$
- $$(15) IRD1(DPZ_n) = (27.60)2^{n+1} - 8.28$$
- $$(16) IRGA(DPZ_n) = (0.40)2^n - 0.124$$

*Proof*

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$$\begin{aligned} \text{VAR}(DPZ_n) &= \sum_{u \in V} \left( d_u - \frac{2m}{n} \right)^2 = \frac{M_1(DPZ_n)}{n} - \left( \frac{2m}{n} \right)^2 \\ &= (312.2^n - 164) \left( \frac{2(105n - 11)}{96n - 10} \right)^2 \\ &= \frac{7488.2^n n - 11025.n^2 - 782.2^n - 1626.n + 289}{(48n - 5)^2}, \end{aligned} \quad (37)$$

$$\begin{aligned} \text{AL}(DPZ_n) &= \sum_{uv \in E(DPZ_n)} |d_u - d_v| \\ &= |2 - 2|(16.2^n - 4) + |2 - 3|(40.2^n - 16) \\ &\quad + |3 - 3|(8.2^n - 16) + |3 - 4|(4) \\ &= 40.2^n - 12, \end{aligned} \quad (38)$$

$$\begin{aligned} \text{IR1}(DPZ_n) &= \sum_{u \in V} d_u^3 - \frac{2m}{n} \sum_{u \in V} d_u^2 = F(G) - \left( \frac{2m}{n} \right) M_1(DPZ_n) \\ &= (792.2^n - 428) - \left( \frac{2(105n - 11)}{96n - 10} \right) (312.2^n - 164) \\ &= \frac{12(438.2^n n - 44.2^n - 277n + 28)}{48n - 5}, \end{aligned} \quad (39)$$

$$\begin{aligned} \text{IR2}(DPZ_n) &= \sqrt{\frac{\sum_{uv \in E(DPZ_n)} d_u d_v}{m}} - \frac{2m}{n} = \sqrt{\frac{M_2(DPZ_n)}{m}} - \frac{2m}{n} \\ &= \sqrt{\frac{376.2^n - 208}{105n - 11}} - \frac{2(105n - 11)}{96n - 10} \\ &= \frac{(96n - 10)(\sqrt{367.2^n - 208}) - 2(\sqrt{105n - 11})(105n - 11)}{(\sqrt{105n - 11})(96n - 10)}, \end{aligned} \quad (40)$$

$$\begin{aligned} \text{IRF}(DPZ_n) &= \sum_{uv \in E(DPZ_n)} (d_u - d_v)^2 \\ &= (2 - 2)^2(16.2^n - 4) + (2 - 3)^2(40.2^n - 16) \\ &\quad + (3 - 3)^2(8.2^n - 16) + (3 - 4)^2(4) \\ &= 40.2^n - 12, \end{aligned} \quad (41)$$

$$\text{IRFW}(\text{DPZ}_n) = \frac{\text{IRF}(D_n P_n)}{M_2(\text{DPZ}_n)} = \frac{40.2^n - 12}{376.2^n - 208}, \quad (42)$$

$$\begin{aligned} \text{IRA}(\text{DPZ}_n) &= \sum_{uv \in E(\text{DPZ}_n)} (d_u^{-1/2} - d_v^{-1/2})^2 = n - 2R(\text{DPZ}_n) \\ &= (96n - 10) - 2\left(\frac{1}{3}(20\sqrt{6+32})2^n - \frac{1}{3\sqrt{3}}(6\sqrt{2} - 22\sqrt{6} - 48)\right) \\ &= 96n - \frac{40}{3}\sqrt{6}2^n - \frac{94}{3} - \frac{1}{9}(6\sqrt{2} - 22\sqrt{6} - 48)\sqrt{6}, \end{aligned} \quad (43)$$

$$\begin{aligned} \text{IRB}(\text{DPZ}_n) &= \sum_{uv \in E(\text{DPZ}_n)} (d_u^{1/2} - d_v^{1/2})^2 = M_1(D_n P_n) - 2RR(\text{DPZ}_n) \\ &= (312.2^n - 164) - 2[(56 + 40\sqrt{6})2^n + (8\sqrt{3} - 16\sqrt{6} - 56)] \\ &= 312.2^n - 2(56 + 40\sqrt{6})2^n - 52 - 16\sqrt{3} + 32\sqrt{6}, \end{aligned} \quad (44)$$

$$\begin{aligned} \text{IRC}(\text{DPZ}_n) &= \frac{\sum_{uv \in E(\text{DPZ}_n)} \sqrt{d_u d_v}}{m} - \frac{2m}{n} = \frac{RR(\text{DPZ}_n)}{m} - \frac{2m}{n} \\ &= \frac{(56 + 40\sqrt{6})2^n + (8\sqrt{3} - 16\sqrt{6} - 56)}{105n - 11} - \frac{2(105n - 11)}{96n - 10} \\ &= \frac{1}{(105n - 11)(48n - 5)} \\ &\quad ((1920\sqrt{3}n - 200\sqrt{3})2^{(1/2)+n} - (768\sqrt{6} - 384\sqrt{3} + 658) + 2688.2^n n - 11025n^2 + (80\sqrt{6} + 159)), \end{aligned} \quad (45)$$

$$\begin{aligned} \text{IRDIF}(\text{DPZ}_n) &= \sum_{uv \in E(\text{DPZ}_n)} \left| \frac{d_u}{d_v} - \frac{d_v}{d_u} \right| \\ &= \left| \frac{2}{2} - \frac{2}{2} \right| (16.2^n - 4) + \left| \frac{2}{3} - \frac{3}{2} \right| (40.2^n - 16) \\ &\quad + \left| \frac{3}{3} - \frac{3}{3} \right| (8.2^n - 16) + \left| \frac{3}{4} - \frac{4}{3} \right| (4) \\ &= \frac{1}{3} (100.2^n - 33), \end{aligned} \quad (46)$$

$$\begin{aligned} \text{IRL}(\text{DPZ}_n) &= \sum_{uv \in E(\text{DPZ}_n)} |\ln d_u - \ln d_v| \\ &= |\ln 2 - \ln 2| (16.2^n - 4) + |\ln 2 - \ln 3| (40.2^n - 16) \\ &\quad + |\ln 3 - \ln 3| (8.2^n - 16) + |\ln 3 - \ln 4| (4) \\ &= 16.2^n - 5.28, \end{aligned} \quad (47)$$

$$\begin{aligned} \text{IRLU}(\text{DPZ}_n) &= \sum_{uv \in E(\text{DPZ}_n)} \frac{|d_u - d_v|}{\min(d_u, d_v)} \\ &= \left( \frac{|2 - 2|}{2} \right) (16.2^n - 4) + \left( \frac{|2 - 3|}{2} \right) (40.2^n - 16) \\ &\quad + \left( \frac{|3 - 3|}{3} \right) (8.2^n - 16) + \left( \frac{|3 - 4|}{3} \right) (4) \\ &= \frac{1}{3} (60.2^n - 20), \end{aligned} \quad (48)$$

$$\begin{aligned}
\text{IRLF}(\text{DPZ}_n) &= \sum_{uv \in E(\text{DPZ}_n)} \frac{|d_u - d_v|}{\sqrt{d_u d_v}} \\
&= \left( \frac{|2-2|}{\sqrt{4}} \right) (16.2^n - 4) + \left( \frac{|2-3|}{\sqrt{6}} \right) (40.2^n - 16) \\
&\quad + \left( \frac{|3-3|}{\sqrt{9}} \right) (8.2^n - 16) + \left( \frac{|3-4|}{\sqrt{12}} \right) (4) \\
&= \frac{1}{\sqrt{6}} 40.2^n - \frac{1}{3} (8\sqrt{6} - 2\sqrt{3}),
\end{aligned} \tag{49}$$

$$\begin{aligned}
\text{IRLA}(\text{DPZ}_n) &= \sum_{uv \in E(\text{DPZ}_n)} 2 \frac{|d_u - d_v|}{(d_u + d_v)} \\
&= 2 \left( \frac{|2-2|}{2+2} \right) (16.2^n - 4) + 2 \left( \frac{|2-3|}{2+3} \right) (4.2^n - 16) \\
&\quad + 2 \left( \frac{|3-3|}{3+3} \right) (8.2^n - 16) + 2 \left( \frac{|3-4|}{3+4} \right) (4) \\
&= \frac{1}{35} (560.2^n - 184),
\end{aligned} \tag{50}$$

$$\begin{aligned}
\text{IRD1}(\text{DPZ}_n) &= \sum_{uv \in E(\text{DPZ}_n)} \ln \{ 1 + |d_u - d_v| \} \\
&= \ln \{ 1 + |2-2| \} (16.2^n - 4) + \ln \{ 1 + |2-3| \} (40.2^n - 16) \\
&\quad + \ln \{ 1 + |3-3| \} (8.2^n - 16) + \ln \{ 1 + |3-4| \} (4) \\
&= (27.60)2^{n+1} - 8.28,
\end{aligned} \tag{51}$$

$$\begin{aligned}
\text{IRGA}(\text{DPZ}_n) &= \sum_{uv \in E(\text{DPZ}_n)} \ln \left( \frac{d_u + d_v}{2\sqrt{d_u d_v}} \right) \\
&= \ln \left( \frac{2+2}{2\sqrt{2 \times 2}} \right) (16.2^n - 4) + \ln \left( \frac{2+3}{2\sqrt{2 \times 3}} \right) (40.2^n - 16) \\
&\quad + \ln \left( \frac{3+3}{2\sqrt{3 \times 3}} \right) (8.2^n - 16) + \ln \left( \frac{3+4}{2\sqrt{3 \times 4}} \right) (4) \\
&= (0.40)2^n - 0.124,
\end{aligned} \tag{52}$$

□

**3.4. Poly(EThylene Amide Amine) Dendrimer PETAA.** The molecular graph of Poly(EThylene Amide Amine) Dendrimer, PETAA, is given in Figure 4.

The degree-based edge partition of Poly(EThylene Amide Amine) Dendrimer, PETAA, is given in Table 4

**Theorem 4.** Let PETAA be a Poly(EThylene Amide Amine) Dendrimer, The irregularity indices are

$$(1) \text{VAR}(\text{PETAA}) = (352.4^n - 254.2^n + 43)/2(22.2^n - 9)^2$$

$$(2) \text{AL}(\text{PETAA}) = 32.2^n - 13$$

$$(3) \text{IR1}(\text{PETAA}) = 2(37404^n - 12852^n - 97)/(222^n - 9)$$

$$\begin{aligned}
(4) \text{IR2}(\text{PETAA}) &= ((44.2^n - 18)(\sqrt{204.2^n - 92}) - 2 \\
&\quad (\sqrt{44.2^n - 19})(44.2^n - 19))/(44.2^n - 18) \\
&\quad (\sqrt{44.2^n - 19})
\end{aligned}$$

$$(5) \text{IRF}(\text{PETAA}) = 40.2^n - 17$$

$$(6) \text{IRFW}(\text{PETAA}) = (40.2^n - 17)/4(51.2^n - 23)$$

$$\begin{aligned}
(7) \text{IRA}(\text{PETAA}) &= 28.2^n - 10 - 4\sqrt{2}.2^n - (2/3)\sqrt{3} \\
&\quad (4.2^n - 2) - (1/3)\sqrt{6}(26.2^n - 9)
\end{aligned}$$

$$\begin{aligned}
(8) \text{IRB}(\text{PETAA}) &= 128.2^n - 53 - 8\sqrt{2}2^n - 2\sqrt{2}(4.2^n - 2) - 2\sqrt{6}(20.2^n - 9)
\end{aligned}$$

$$\begin{aligned}
(9) \text{IRC}(\text{PETAA}) &= (1/(44.2^n - 19)(22.2^n - 9))[(44\sqrt{6} \\
&\quad + 88\sqrt{3} - 88\sqrt{2} - 1232)4^n - (378\sqrt{6} + 36\sqrt{2} + 80\sqrt{3} - 1032)2^n + (81\sqrt{6} + 18\sqrt{3} - 217)]
\end{aligned}$$

$$(10) \text{IRDIF}(\text{PETAA}) = (1/6)(200.2^n - 77)$$

$$(11) \text{IRL}(\text{PETAA}) = (15.12)2^n - 5.78$$

$$(12) \text{IRLU}(\text{PETAA}) = (1/2)(44.2^n - 17)$$

$$(13) \text{IRLF}(\text{PETAA}) = 2\sqrt{2}2^n + (2/3)\sqrt{3}(4.2^n - 2) + (1/6)\sqrt{6}(20.2^n - 9)$$

$$(14) \text{IRLA}(\text{PETAA}) = (1/15)(220.2^n - 84)$$

$$(15) \text{IRD1}(\text{PETAA}) = (20.92)2^{n+1} - 8.39$$

$$(16) \text{IRGA}(\text{PETAA}) = (1.16)2^n - 0.46$$

*Proof*

$$\begin{aligned} \text{VAR}(\text{PETAA}) &= \sum_{u \in V} \left( d_u - \frac{2m}{n} \right)^2 = \frac{M_1(\text{PETAA})}{n} - \left( \frac{2m}{n} \right)^2 \\ &= (192.2^n - 85) \left( \frac{2(44.2^n - 19)}{44.2^n - 19} \right)^2 \\ &= \frac{352.4^n - 254.2^n + 43}{2(22.2^n - 9)^2}, \end{aligned} \quad (53)$$

$$\begin{aligned} \text{AL}(\text{PETAA}) &= \sum_{uv \in E(\text{PETAA})} |d_u - d_v| \\ &= |1 - 2|(4.2^n) + |1 - 3|(4.2^n - 2) \\ &\quad + |2 - 2|(16.2^n - 8) + |2 - 3|(20.2^n - 9) \\ &= 32.2^n - 13, \end{aligned} \quad (54)$$

$$\begin{aligned} \text{IR1}(\text{PETAA}) &= \sum_{u \in V} d_u^3 - \frac{2m}{n} \sum_{u \in V} d_u^2 = F(G) - \left( \frac{2m}{n} \right) M_1(\text{PETAA}) \\ &= (448.2^n - 201) - \frac{2(44.2^n - 19)}{44.2^n - 18} (192.2^n - 85) \\ &= \frac{-2(37404^n - 12852^n - 97)}{222^n - 9}, \end{aligned} \quad (55)$$

$$\begin{aligned} \text{IR2}(\text{PETAA}) &= \sqrt{\frac{\sum_{uv \in E(\text{PETAA})} d_u d_v}{m}} - \frac{2m}{n} = \sqrt{\frac{M_2(\text{PETAA})}{m}} - \frac{2m}{n} \\ &= \sqrt{\frac{204.2^n - 92}{44.2^n - 19}} - \frac{2(44.2^n - 19)}{44.2^n - 19} \\ &= \frac{(44.2^n - 18)(\sqrt{204.2^n - 92}) - 2(\sqrt{44.2^n - 19})(44.2^n - 19)}{(44.2^n - 18)(\sqrt{44.2^n - 19})}, \end{aligned} \quad (56)$$

$$\begin{aligned} \text{IRF}(\text{PETAA}) &= \sum_{uv \in E(\text{PETAA})} (d_u - d_v)^2 \\ &= (1 - 2)^2(4.2^n) + (1 - 3)^2(4.2^n - 2) \\ &\quad + (2 - 2)^2(16.2^n - 8) + (2 - 3)^2(20.2^n - 9) \\ &= 40.2^n - 17, \end{aligned} \quad (57)$$

$$\begin{aligned} \text{IRFW}(\text{PETAA}) &= \frac{\text{IRF}(D_n P_n)}{M_2(\text{PETAA})} \\ &= \frac{40.2^n - 17}{204.2^n - 92}, \end{aligned} \quad (58)$$

$$\begin{aligned}
\text{IRA(PETAA)} &= \sum_{uv \in E(\text{PETAA})} (d_u^{-1/2} - d_v^{-1/2})^2 = n - 2R(\text{PETAA}) \\
&= (44.2^n - 18) - 2 \left( 2\sqrt{2} \cdot 2^n + \frac{1}{3}\sqrt{3}(4.2^n - 2) + 8.2^n - 4 + \frac{1}{6}\sqrt{6}(20.2^n - 9) \right) \\
&= 28.2^n - 10 - 4\sqrt{2} \cdot 2^n - \frac{2}{3}\sqrt{3}(4.2^n - 2) - \frac{1}{3}\sqrt{6}(26.2^n - 9),
\end{aligned} \tag{59}$$

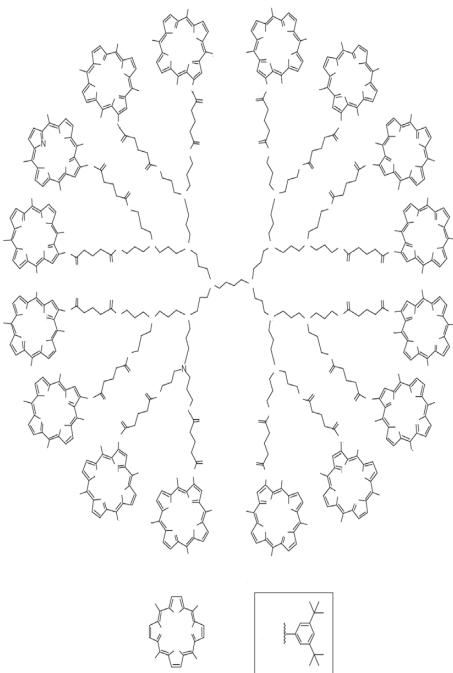
$$\begin{aligned}
\text{IRB(PETAA)} &= \sum_{uv \in E(\text{PETAA})} (d_u^{1/2} - d_v^{1/2})^2 = M_1(D_n P_n) - 2RR(\text{PETAA}) \\
&= (192.2^n - 85) - 2(4\sqrt{2} \cdot 2^n + \sqrt{3}(4.2^n - 2) + 32.2^n - 16 + \sqrt{6}(20.2^n - 9)) \\
&= 128.2^n - 53 - 8\sqrt{2} \cdot 2^n - 2\sqrt{2}(4.2^n - 2) - 2\sqrt{6}(20.2^n - 9),
\end{aligned} \tag{60}$$

$$\begin{aligned}
\text{IRC(PETAA)} &= \frac{\sum_{uv \in E(\text{PETAA})} \sqrt{d_u d_v}}{m} - \frac{2m}{n} = \frac{RR(\text{PETAA})}{m} - \frac{2m}{n} \\
&= \frac{4\sqrt{2} \cdot 2^n + \sqrt{3}(4.2^n - 2) + 32.2^n - 16 + \sqrt{6}(20.2^n - 9)}{44.2^n - 19} - \frac{2(44.2^n - 19)}{44.2^n - 18} \\
&= \frac{1}{(44.2^n - 19)(22.2^n - 9)} \\
&\quad ((44\sqrt{6} + 88\sqrt{3} - 88\sqrt{2} - 1232)4^n - (378\sqrt{6} + 36\sqrt{2} + 80\sqrt{3} - 1032)2^n + (81\sqrt{6} + 18\sqrt{3} - 217)),
\end{aligned} \tag{61}$$

$$\begin{aligned}
\text{IRDIF(PETAA)} &= \sum_{uv \in E(\text{PETAA})} \left| \frac{d_u}{d_v} - \frac{d_v}{d_u} \right| \\
&= \left| \frac{1}{2} - \frac{2}{1} \right|(4.2^n) + \left| \frac{1}{3} - \frac{3}{1} \right|(4.2^n - 2) \\
&\quad + \left| \frac{2}{2} - \frac{2}{2} \right|(16.2^n - 8) + \left| \frac{2}{3} - \frac{3}{2} \right|(20.2^n - 9) \\
&= \frac{1}{6}(200.2^n - 77),
\end{aligned} \tag{62}$$

$$\begin{aligned}
\text{IRL(PETAA)} &= \sum_{uv \in E(\text{PETAA})} |\ln d_u - \ln d_v| \\
&= |\ln 1 - \ln 2|(4.2^n) + |\ln 1 - \ln 3|(4.2^n - 2) \\
&\quad + |\ln 2 - \ln 2|(16.2^n - 8) + |\ln 2 - \ln 3|(20.2^n - 9) \\
&= (15.12).2^n - 5.78,
\end{aligned} \tag{63}$$

$$\begin{aligned}
\text{IRLU(PETAA)} &= \sum_{uv \in E(\text{PETAA})} \frac{|d_u - d_v|}{\min(d_u, d_v)} \\
&= \left( \frac{|1 - 2|}{1} \right)(4.2^n) + \left( \frac{|1 - 3|}{1} \right)(4.2^n - 2) \\
&\quad + \left( \frac{|2 - 2|}{2} \right)(16.2^n - 8) + \left( \frac{|2 - 3|}{2} \right)(20.2^n - 9) \\
&= \frac{1}{2}(44.2^n - 17).
\end{aligned} \tag{64}$$

FIGURE 1: Prophyrin Dendrimer  $D_n P_n$ .TABLE 1: Degree-based edge partition of  $D_n P_n$ , of end vertices of each edge.

$(d_u, d_v)$	Frequency
(1, 3)	$2n$
(1, 4)	$124n$
(2, 2)	$10n - 5$
(2, 3)	$48n - 6$
(3, 3)	$13n$
(3, 4)	$8n$

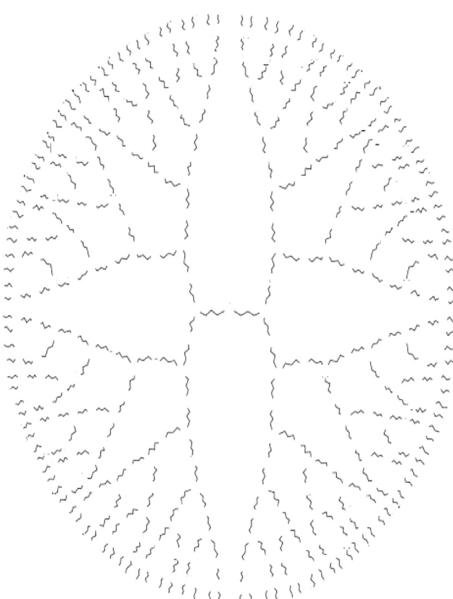
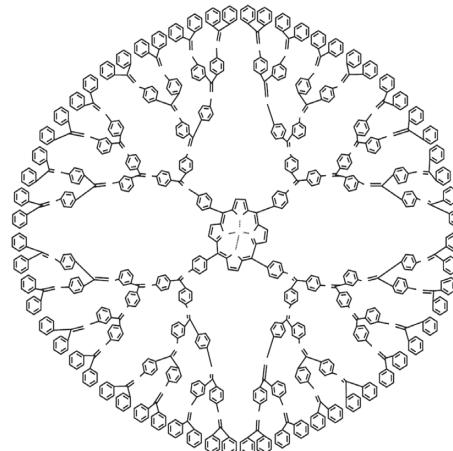


FIGURE 2: Propyl Ether Imine Dendrimer (PETIM).

TABLE 2: Degree-based edge partition of PETIM, of end vertices of each edge.

$(d_u, d_v)$	Frequency
(1, 2)	$2^{n+1}$
(2, 2)	$2^{n+4} - 18$
(2, 3)	$6.2^n - 6$

FIGURE 3: Zinc Prophyrin Dendrimer  $DPZ_n$ .TABLE 3: Degree-based edge partition of  $DPZ_n$ , of end vertices of each edge.

$(d_u, d_v)$	Frequency
(2, 2)	$16.2^n - 4$
(2, 3)	$40.2^n - 16$
(3, 3)	$8.2^n - 16$
(3, 4)	4

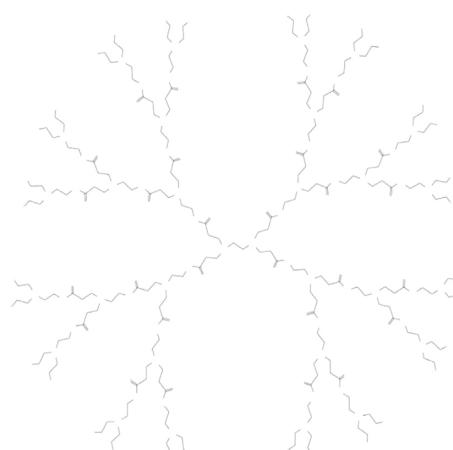
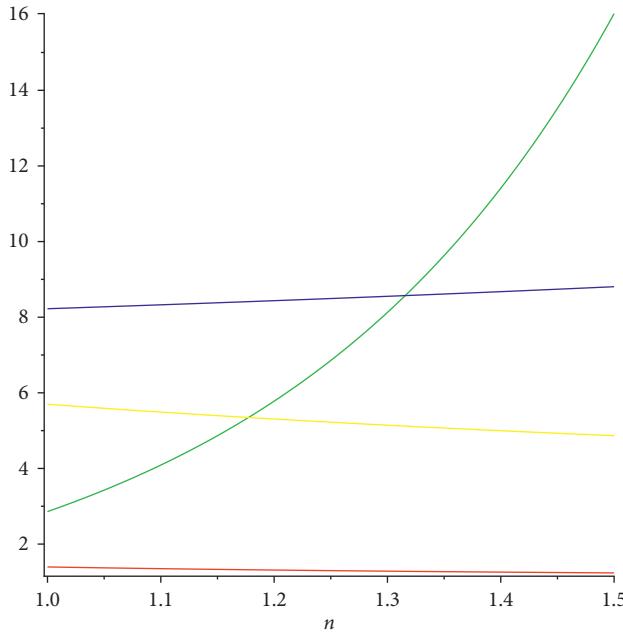


FIGURE 4: Poly(EThylene Amide Amine) Dendrimer.

TABLE 4: Degree-based edge partition of PETAA, of end vertices of each edge.

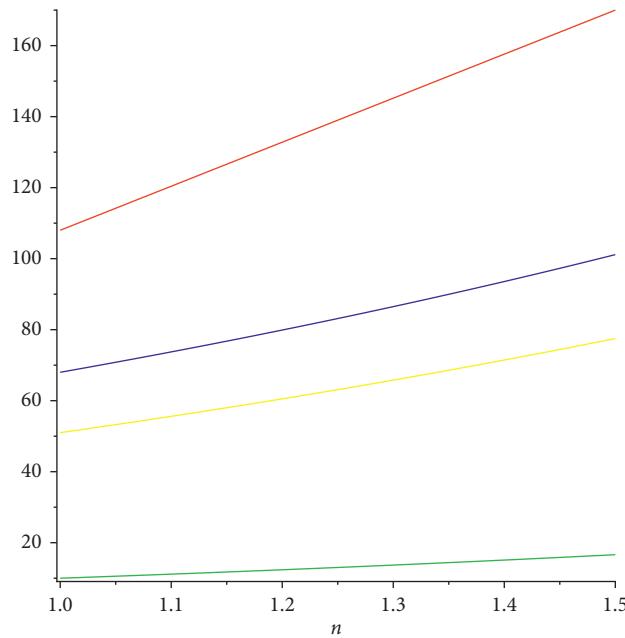
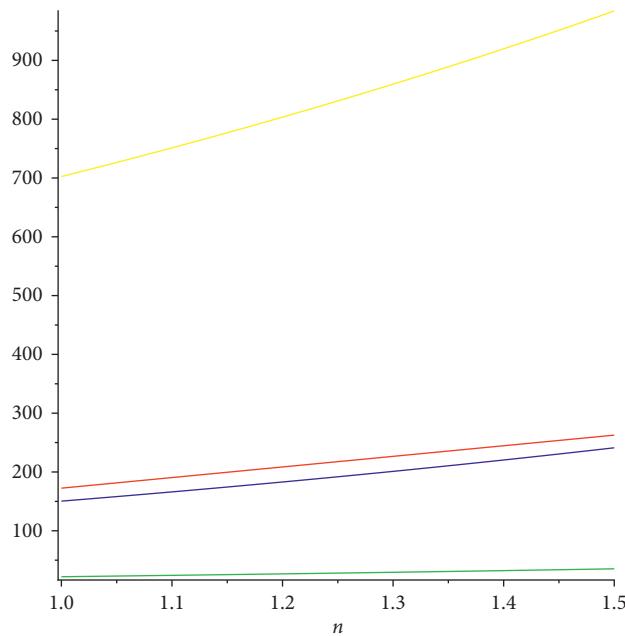
$(d_u, d_v)$	Frequency
(1, 2)	$4.2^n$
(1, 3)	$4.2^n - 2$
(2, 2)	$16.2^n - 8$
(2, 3)	$20.2^n - 9$

FIGURE 5: VAR of  $D_n P_n$ , PETIM, DPZ<sub>n</sub>, and PETAA.

$$\begin{aligned}
 \text{IRLF(PETAA)} &= \sum_{uv \in E(\text{PETAA})} \frac{|d_u - d_v|}{\sqrt{d_u \cdot d_v}} \\
 &= \left( \frac{|1-2|}{\sqrt{2}} \right) (4.2^n) + \left( \frac{|1-3|}{\sqrt{3}} \right) (4.2^n - 2) \\
 &\quad + \left( \frac{|2-2|}{\sqrt{4}} \right) (16.2^n - 8) + \left( \frac{|2-3|}{\sqrt{6}} \right) (20.2^n - 9) \\
 &= 2\sqrt{2} \cdot 2^n + \frac{2}{3}\sqrt{3}(4.2^n - 2) + \frac{1}{6}\sqrt{6}(20.2^n - 9),
 \end{aligned} \tag{65}$$

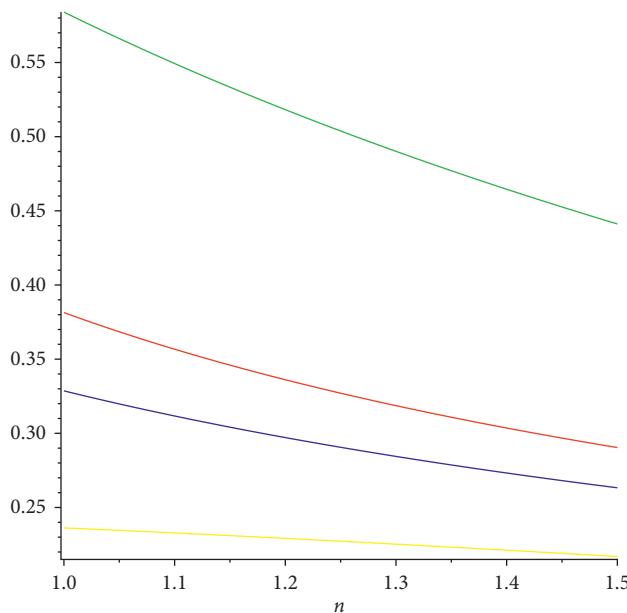
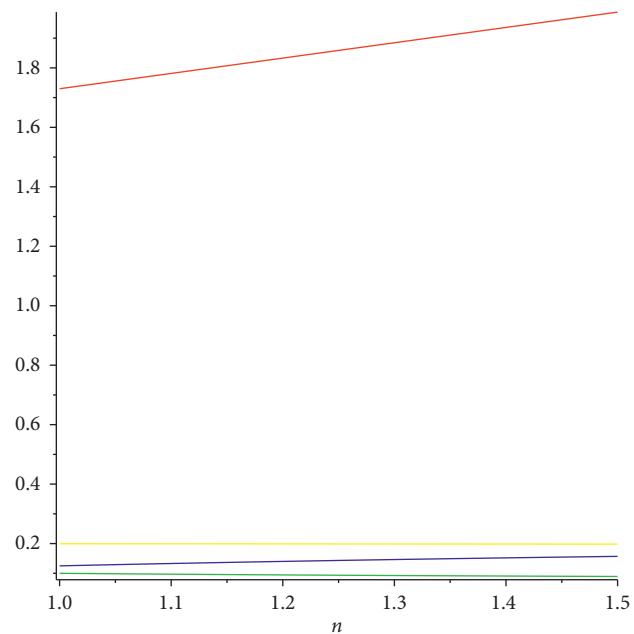
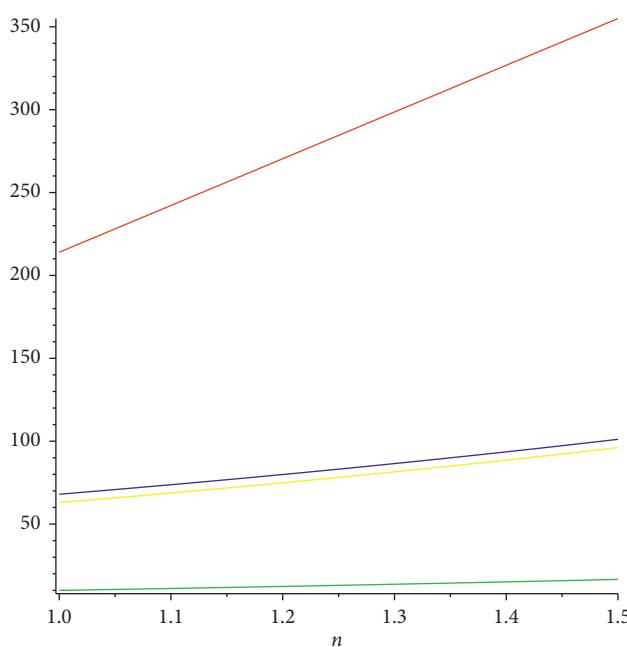
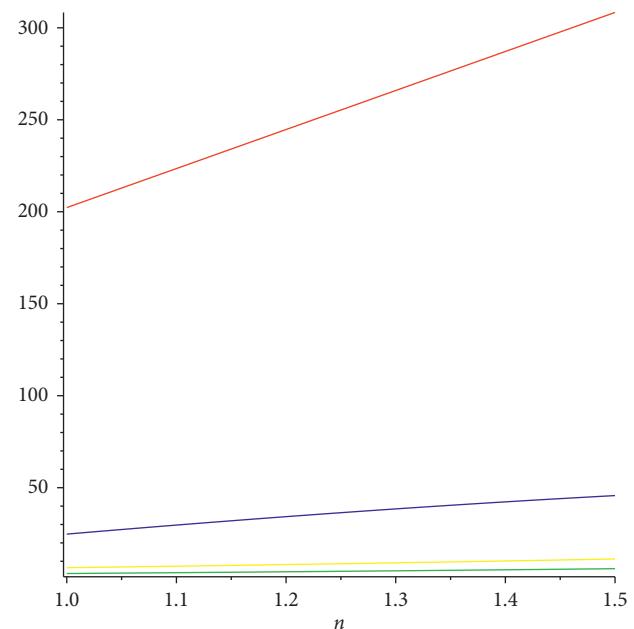
$$\begin{aligned}
 \text{IRLA(PETAA)} &= \sum_{uv \in E(\text{PETAA})} 2 \frac{|d_u - d_v|}{(d_u + d_v)} \\
 &= 2 \left( \frac{|1-2|}{1+2} \right) (4.2^n) + 2 \left( \frac{|1-3|}{1+3} \right) (4.2^n - 2) \\
 &\quad + 2 \left( \frac{|2-2|}{2+2} \right) (16.2^n - 8) + 2 \left( \frac{|2-3|}{2+3} \right) (20.2^n - 9) \\
 &= \frac{1}{15} (220.2^n - 84),
 \end{aligned} \tag{66}$$

$$\begin{aligned}
 \text{IRD1(PETAA)} &= \sum_{uv \in E(\text{PETAA})} \ln \{1 + |d_u - d_v|\} \\
 &= \ln \{1 + |1-2|\} (4.2^n) + \ln \{1 + |1-3|\} (4.2^n - 2) \\
 &\quad + \ln \{1 + |2-2|\} (16.2^n - 8) + \ln \{1 + |2-3|\} (20.2^n - 9) \\
 &= (20.92)2^{n+1} - 8.39,
 \end{aligned} \tag{67}$$

FIGURE 6: AL of  $D_n P_n$ , PETIM, DPZ<sub>n</sub>, and PETAA.FIGURE 7: IR1 of  $D_n P_n$ , PETIM, DPZ<sub>n</sub>, and PETAA.

$$\begin{aligned}
 \text{IRGA(PETAA)} &= \sum_{uv \in E(\text{PETAA})} \ln\left(\frac{d_u + d_v}{2\sqrt{d_u d_v}}\right) \\
 &= \ln\left(\frac{1+2}{2\sqrt{1 \times 2}}\right)(4.2^n) + \ln\left(\frac{1+3}{2\sqrt{1 \times 3}}\right)(4.2^n - 2) \\
 &\quad + \ln\left(\frac{2+2}{2\sqrt{2 \times 2}}\right)(16.2^n - 8) + \ln\left(\frac{2+3}{2\sqrt{2 \times 3}}\right)(20.2^n - 9) \\
 &= (1.16)2^n - 0.46.
 \end{aligned} \tag{68}$$

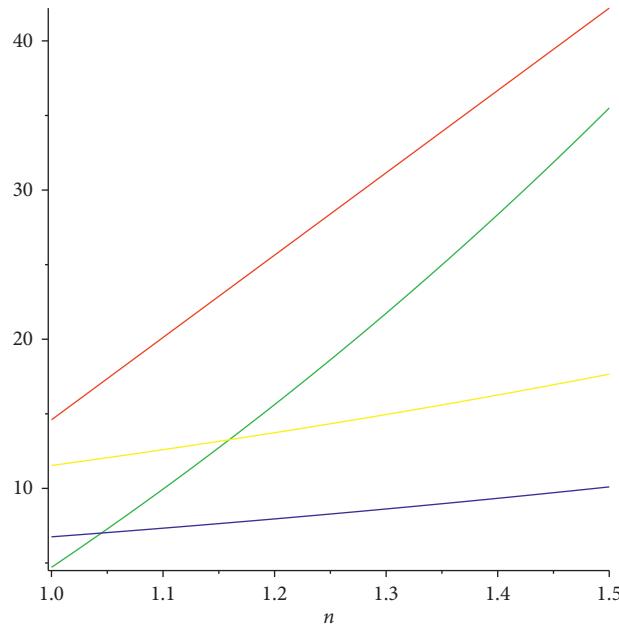
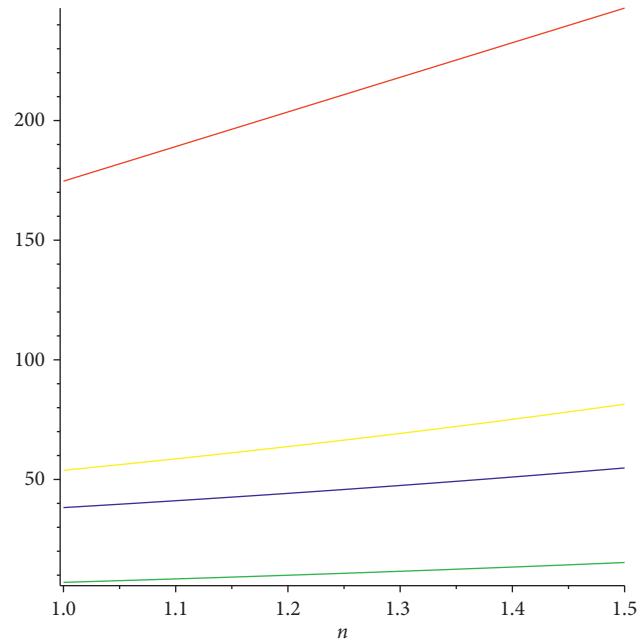
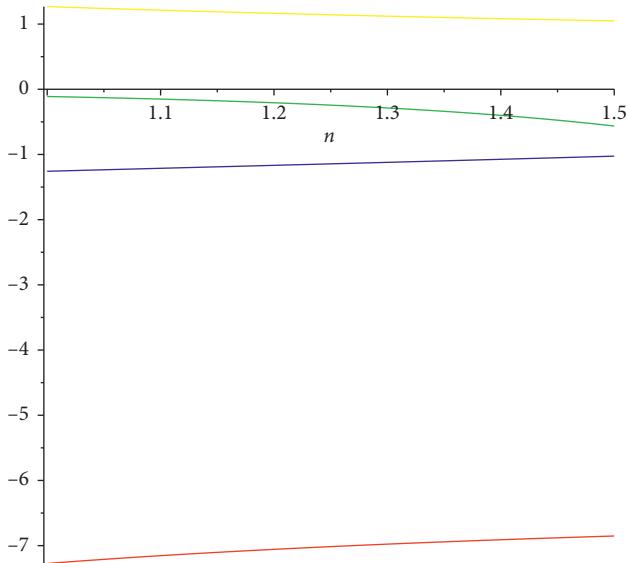
□

FIGURE 8: IR2 of  $D_nP_n$ , PETIM, DPZ<sub>n</sub>, and PETAA.FIGURE 10: IRFW of  $D_nP_n$ , PETIM, DPZ<sub>n</sub>, and PETAA.FIGURE 9: IRF of  $D_nP_n$ , PETIM, DPZ<sub>n</sub>, and PETAA.FIGURE 11: IRA of  $D_nP_n$ , PETI, DPZ<sub>n</sub>, and PETAA.

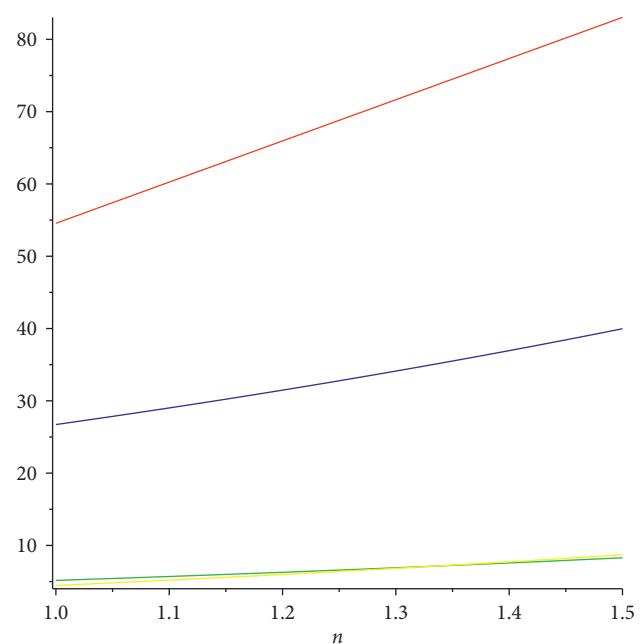
#### 4. Graphical Comparison

Figures 5–20 show the graphical representation of irregularity indices for dendrimers. The colors red, green, blue, and yellow are fixed for Prophyrin Dendrimer  $D_nP_n$ , Propyl Ether Imine Dendrimer (PETIM), Zinc Prophyrin Dendrimer DPZ<sub>n</sub>, and Poly(ETHylene Amide Amine) Dendrimer PETAA, respectively. Figure 5 shows the graphical

comparison of VAR irregularity index for dendrimers. It can be observed that  $D_nP_n$  gives the greatest value for VAR irregularity index while PETAA gives the least value for VAR irregularity index. Figure 6 shows the graphical comparison of AL irregularity index for dendrimers. It can be observed that DPZ<sub>n</sub> gives the greatest value for AL irregularity index while  $D_nP_n$  gives the least value for AL irregularity index. Figure 7 shows the graphical comparison of IR1 irregularity index for dendrimers. It can be observed that  $D_nP_n$  gives the

FIGURE 12: IRB of  $D_nP_n$ , PETIM, DPZ<sub>n</sub>, and PETAA.FIGURE 14: IRDIF of  $D_nP_n$ , PETIM, DPZ<sub>n</sub>, and PETAA.FIGURE 13: IRC of  $D_nP_n$ , PETIM, DPZ<sub>n</sub>, and PETAA.

greatest value for IR1 irregularity index while PETIM gives the least value for IR1 irregularity index. Figure 8 shows the graphical comparison of IR2 irregularity index for dendrimers. It can be observed that PETIM gives the greatest value for IR2 irregularity index while PETAA gives the least value for IR2 irregularity index. Figure 9 shows the graphical comparison of IRF irregularity index for dendrimers. It can be observed that  $D_nP_n$  gives the greatest value for IRF irregularity index while PETIM gives the least value for IRF irregularity index. Figure 10 shows the graphical comparison

FIGURE 15: IRL of  $D_nP_n$ , PETIM, DPZ<sub>n</sub>, and PETAA.

of IRFW irregularity index for dendrimers. It can be observed that PETAA gives the greatest value for IRFW irregularity index while  $D_nP_n$  gives the least value for IRFW irregularity index. Figure 11 shows the graphical comparison of IRA irregularity index for dendrimers. It can be observed that DPZ<sub>n</sub> gives the greatest value for IRA irregularity index while  $D_nP_n$  gives the least value for IRA irregularity index.

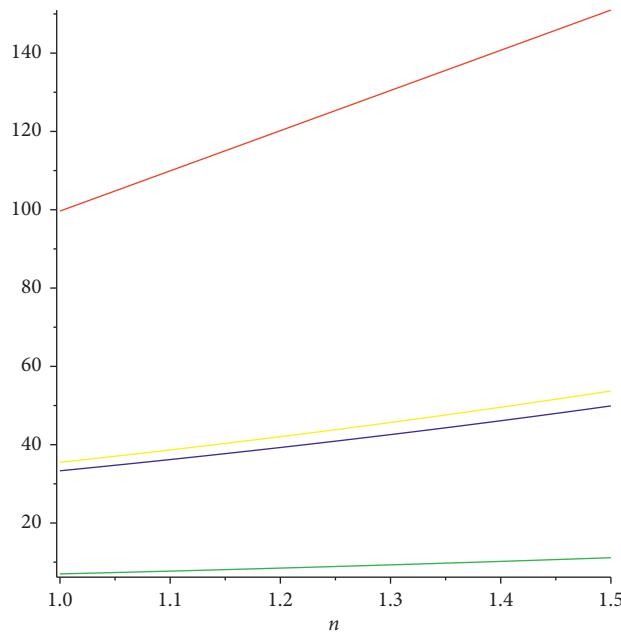
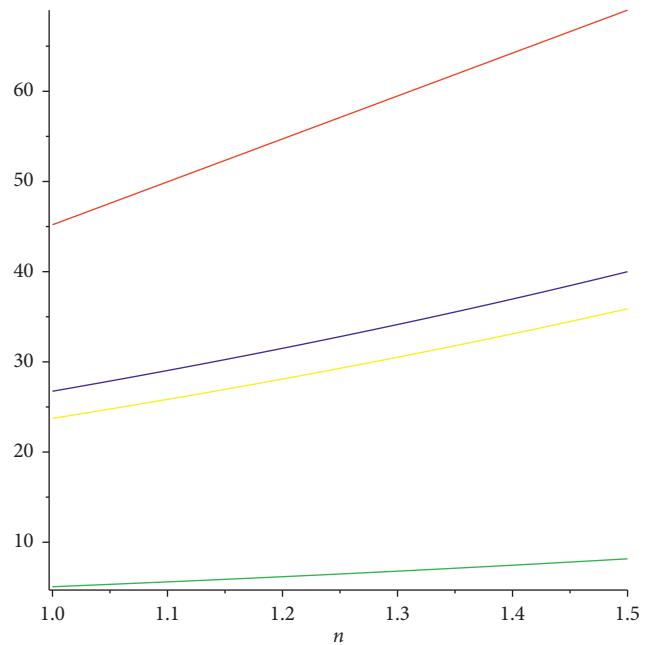
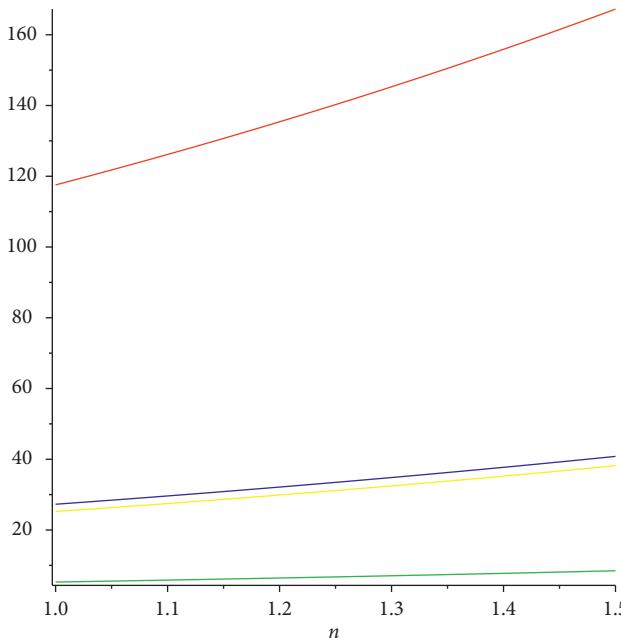
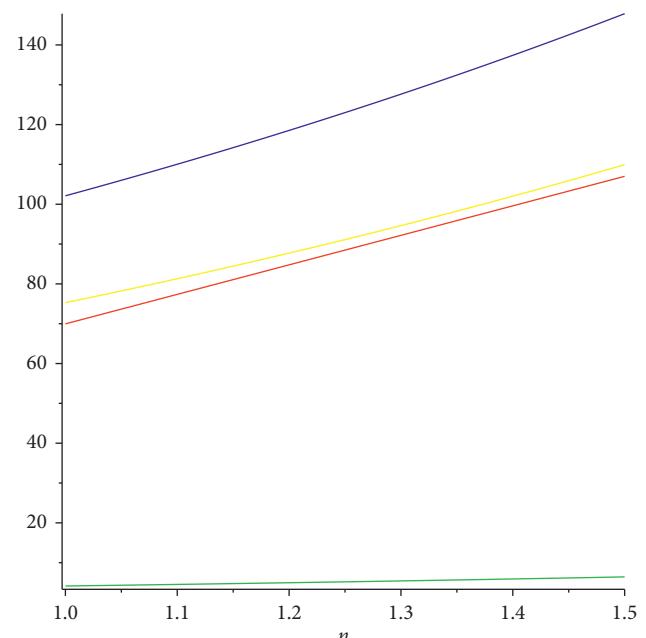
FIGURE 16: IRLU of  $D_nP_n$ , PETIM, DPZ<sub>n</sub>, and PETAA.FIGURE 18: IRLA of  $D_nP_n$ , PETIM, DPZ<sub>n</sub>, and PETAA.FIGURE 17: IRLF of  $D_nP_n$ , PETIM, DPZ<sub>n</sub>, and PETAA.FIGURE 19: IRD1 of  $D_nP_n$ , PETIM, DPZ<sub>n</sub>, and PETAA.

Figure 12 shows the graphical comparison of IRB irregularity index for dendrimers. It can be observed that PETAA gives the greatest value for IRB irregularity index while  $D_nP_n$  gives the least value for IRB irregularity index. Figure 13 shows the graphical comparison of IRC irregularity index for dendrimers. It can be observed that  $D_nP_n$  gives the greatest value for IRC irregularity index while DPZ<sub>n</sub> gives the least value for IRC irregularity index. Figure 14 shows the graphical comparison of IRDIF irregularity index for dendrimers. It can be observed that  $D_nP_n$  gives the greatest value

for IRDIF irregularity index while PETIM gives the least value for IRDIF irregularity index. Figure 15 shows the graphical comparison of IRL irregularity index for dendrimers. It can be observed that  $D_nP_n$  gives the greatest value for IRL irregularity index while PETAA gives the least value for IRL irregularity index. Figure 16 shows the graphical comparison of IRLU irregularity index for dendrimers. It can be observed that  $D_nP_n$  gives the greatest value for IRLU irregularity index while PETIM gives the least value for IRLU irregularity index. Figure 17 shows the graphical

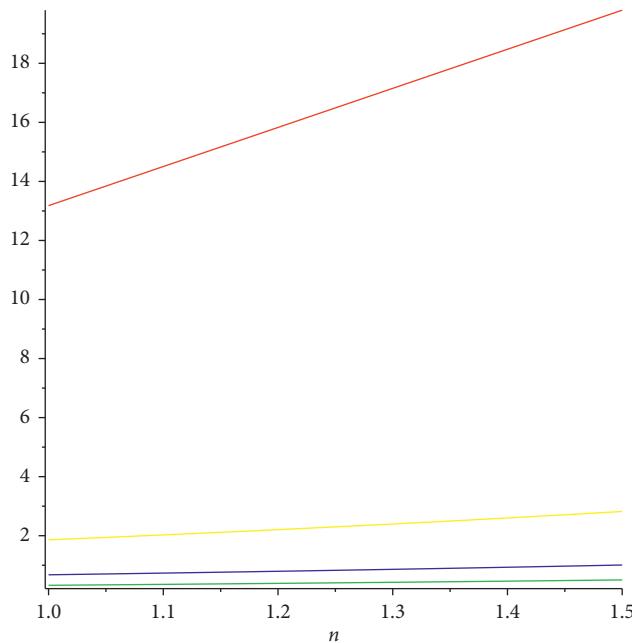


FIGURE 20: IRGA of  $D_nP_n$ , PETIM,  $DPZ_n$ , and PETAA.

comparison of IRLF irregularity index for dendrimers. It can be observed that  $D_nP_n$  gives the greatest value for IRLF irregularity index while PETIM gives the least value for IRLF irregularity index. Figure 18 shows the graphical comparison of IRLA irregularity index for dendrimers. It can be observed that  $D_nP_n$  gives the greatest value for IRLA irregularity index while PETIM gives the least value for IRLA irregularity index. Figure 19 shows the graphical comparison of IRD1 irregularity index for dendrimers. It can be observed that  $DPZ_n$  gives the greatest value for IRD1 irregularity index while PETIM gives the least value for IRD1 irregularity index. Figure 20 shows the graphical comparison of IRGA irregularity index for dendrimers. It can be observed that  $D_nP_n$  gives the greatest value for IRGA irregularity index while PETIM gives the least value for IRGA irregularity index.

## 5. Conclusion

In this paper, we have computed several degree-based irregularity indices of Dendrimers. Our results are applicable in chemistry, physics, and other applied sciences. It is a proven fact that topological indices help to predict many properties without going to the wet lab. For example, the first and second Zagreb indices were found to happen for the calculation of the  $\pi$ -electron energy of dendrimers, the Randić index corresponds with the boiling point, the atomic bond connectivity (ABC) index gives an exceptionally decent relationship to figuring the strain energy of dendrimers and augmented Zagreb index is a good tool to guess heat of formation of dendrimers, etc. There are more than around 148 topological indices, but none of them can completely describe all properties of a chemical compound. Therefore, there is always room to define and study new topological indices. Redefined Zagreb indices are one step in this

direction and are very close to Zagreb indices. Zagreb indices are very well studied by chemists and mathematicians due to their huge applications in chemistry.

## Data Availability

All data used for this research are included within this paper.

## Conflicts of Interest

The authors declare that they have no conflicts of interest.

## Authors' Contributions

All authors contributed equally to the paper.

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