Neighborhood-Based Descriptors for Porphyrin Dendrimers

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Abstract: The symmetry of molecular structures is captured by topological indices, which provide a mathematical vocabulary for predicting features such as boiling temperatures, viscosity, and gyration radius and are also employed in QSAR/QSPR research. Dendrimers are a brand-new type of polymer. It is characterized as a macromolecule due to its highly radiated structure, providing great water solubility and adaptability. Because of these features, dendrimers are a strong alternative for medication delivery. This article investigates some topological indices based on neighborhood degrees such as Modified Randic index, Inverse Sum Index, SK, SK1, and SK2 index for some dendrimers.

Keywords: Neighborhood indices; porphyrin dendrimers; poly(propyl) ether imine dendrimer.

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1. Introduction

An important use of (connected undirected) graphs is representing an atomic structure by a molecular graph where the node represents atoms, and the edges indicate bondings. This is explored in a discipline called chemical graph theory. The overall topological structure of such a network can be captured in a single number known as a chemical index or a topological index [1-3], which is frequently linked to chemical attributes.

G(V,E) is a graph in which V denotes the set of vertices and E denotes the set of edges linking the vertices. The degree of a vertex v in graph G is the number of edges incident with v, symbolized by deg(v). A graph in which each pair of vertices is connected is known as a connected graph. The set of all vertices adjacent to u is denoted by N(u) and defined as a Neighborhood set of u. The sum degree of vertex u is defined as $S(u) = \sum_{v \in N(u)} \deg(v)$[4].

Dendrimers are branching polymeric molecules with a high degree of organization. Dendrimers are symmetric about the core, which have a spherical 3D topology. A core, an inner, and an outer shell are the three major components of dendrimers. To regulate features such as solubility, thermal stability, and chemical attachment for different tasks, a dendrimer can be synthesized with varied functionality in each of these components. It has an ancient legacy of use in targeted, ophthalmic, pulmonary, transdermal, and gene-drug delivery [5-10]. Since it is difficult to synthesize dendrimers, they are difficult to produce and expensive to buy. Analyzing topological indices for dendrimers is an effective way to eliminate the cost and time-consuming laboratory research.

Numerous studies[11-32] have described and determined topological indices of dendrimers like Poly propyl ether imine dendrimer, porphyrin dendrimers, Poly EThylene...
Amido Amine Dendrimer, Phosphorus-Containing Dendrimers, PDI-Cored Dendrimers, Triazine-Based Dendrimers, and Aliphatic Polyamide Dendrimers.

Several research [33-40] have begun to look into Neighborhood-based topological indices. Vignesh Ravi and Kalyani Desikan proposed some Neighborhood-based descriptors, namely SK\textsubscript{N}, SK\textsubscript{1N}, SK\textsubscript{2N}, Modified Randić index(mR\textsubscript{N}), and Inverse Sum Index(ISI\textsubscript{N})[33]. The indices are given below in equations (1) to (5).

\begin{align*}
SK\textsubscript{N}(G) &= \sum_{u,v \in E} \left[ \frac{S(u)+S(v)}{2} \right] \quad (1) \\
SK\textsubscript{1N}(G) &= \sum_{u,v \in E} \left[ \frac{S(u) \times S(v)}{2} \right] \quad (2) \\
SK\textsubscript{2N}(G) &= \sum_{u,v \in E} \left( \frac{S(u)+S(v)}{2} \right)^2 \quad (3) \\
mR\textsubscript{N}(G) &= \sum_{u,v \in E} \left( \frac{1}{\max\{S(u),S(v)\}} \right) \quad (4) \\
ISI\textsubscript{N}(G) &= \sum_{u,v \in E} \left( \frac{S(u) \times S(v)}{S(u)+S(v)} \right) \quad (5)
\end{align*}

In this paper, we evaluate the above-mentioned indices for Poly propyl ether imine (PETIM) dendrimer, Zinc porphyrin (DPZ\textsubscript{g}) dendrimer, and Porphyrin (D\textsubscript{g}P\textsubscript{g}) dendrimer. We also use MATLAB to depict the 2D representations of the indices.

2. Materials and Methods

The Neighborhood degree-based topological indices of dendrimers are our most important computational results. The results were analyzed using the edge partition method and graph-theoretical ideas. In Figures 5–14, the outcomes are visually depicted using MATLAB R2020a.

3. Results and Discussion

3.1. PETIM dendrimer.

The polynomial of PETIM dendrimer expands from the oxygen as the base and sprouts out at each tertiary nitrogen, which is separated by an eight-bond spacer in every iteration of the dendrimer. Figure 1 shows growth stages for the molecular graph G of PETIM dendrimer with generation G\textsubscript{g}. The PETIM dendrimer graph is composed of four wings and an eight-edged central core. In each branch, we have \(8 + 2 \times 8 + 2^2 \times 8 + \ldots + 2^8 \times 8 + 4 \times 2^6 = 6 \times 2^8 - 8 \) edges. Also, the total number of bonds in G is \(24 \times 2^8 \) – 24. By this, the number of atoms in G can be given directly as \(24 \times 2^8 \) – 23 since it is a tree [11].

The total number of vertices with degree 1 in \(G\textsubscript{g}\) is \(2^{g+1}\), which is the number of leaves in the tree. The vertices of degree 3 and degree 2 are \(2^{g+1} - 2 \) and \(20 \times 2^g - 21\), respectively. For the pair \((S(u),S(v))\) where \(u,v \in E(G)\) the edges are partitioned as \(2 \times 2^g\) for the pairs (2,3) and (3,4); \(8 \times 2^g - 12\) for the pair (4,4) and \(6 \times 2^g - 6\) for the pairs (4,5) and (5,6).

3.1.1. Theorem: SK\textsubscript{N} (PETIM) = 104 \times 2^g – 108.

Proof:

\[SK\textsubscript{N} (PETIM) = \sum_{u,v \in E} \frac{S(u)+S(v)}{2} = 2 \times 2^g \left( \frac{2^3 + 3}{2} \right) + 2 \times 2^g \left( \frac{3^4 + 4}{2} \right) + (8 \times 2^g - 12) \left( \frac{4^4 + 4}{2} \right) + (6 \times 2^g - 6) \left( \frac{4^5 + 5}{2} \right) + (6 \times 2^g - 6) \left( \frac{5^5 + 6}{2} \right)\]

\[= (5 \times 2^g) + (7 \times 2^g) + 4(8 \times 2^g - 12) + (9 \times 3)(2^g - 1) + (11 \times 3)(2^g - 1)\]
= 104 × 2^\varepsilon − 108.

3.1.2. Theorem SK1_N (PETIM) = 232 × 2^\varepsilon − 246.

Proof:

SK1_N (PETIM) = \sum_{u,v \in E} \frac{S(u) \times S(v)}{2} \\
= 2 \times 2^\varepsilon \left( \frac{2 \times 3}{2} \right) + 2 \times 2^\varepsilon \left( \frac{3 \times 4}{2} \right) + (8 \times 2^\varepsilon - 12) \left( \frac{4 \times 4}{2} \right) + (6 \times 2^\varepsilon - 6) \left( \frac{4 \times 5}{2} \right) \\
+ (6 \times 2^\varepsilon - 6) \left( \frac{5 \times 6}{2} \right) \\
= (2 \times 2^\varepsilon \times 3) + (2 \times 2^\varepsilon \times 6) + 8(8 \times 2^\varepsilon - 12) + 10(6 \times 2^\varepsilon - 6) + 15(6 \times 2^\varepsilon - 6) \\
= 232 \times 2^\varepsilon - 246.

3.1.3. Theorem SK2_N (PETIM) = 468 \times 2^\varepsilon - 495.

Proof:

SK2_N (PETIM) = \sum_{u,v \in E} \left( \frac{S(u) + S(v)}{2} \right)^2 \\
= 2 \times 2^\varepsilon \left( \frac{2^3 + 3}{2} \right)^2 + 2 \times 2^\varepsilon \left( \frac{3^4 + 4}{2} \right)^2 + (8 \times 2^\varepsilon - 12) \left( \frac{4^4 + 4}{2} \right)^2 + (6 \times 2^\varepsilon - 6) \left( \frac{4^5 + 5}{2} \right)^2 \\
+ (6 \times 2^\varepsilon - 6) \left( \frac{5^6 + 6}{2} \right)^2 \\
= \left( \frac{2^5}{2} \times 2^\varepsilon \right) + \left( \frac{4^9}{2} \times 2^\varepsilon \right) + \frac{64}{2} \times (4 \times 2^\varepsilon - 6) + \frac{81}{2} \times (3 \times 2^\varepsilon - 3) + \frac{121}{2} \times (3 \times 2^\varepsilon - 3) \\
= 468 \times 2^\varepsilon - 495.

3.1.4. Theorem: mR_N (PETIM) = \frac{161}{30} \times 2^\varepsilon - \frac{26}{5}.
Proof:

\[ m_{RN} (PETIM) = \sum_{uv \in E} \left( \frac{1}{\max (S(u), S(v))} \right) \]

\[ = (2 \times 2^5) \left( \frac{1}{\max (2,3)} \right) + (2 \times 2^5) \left( \frac{1}{\max (3,4)} \right) + (8 \times 2^{8-12}) \left( \frac{1}{\max (4,4)} \right) \]

\[ + (6 \times 2^{8-6}) \left( \frac{1}{\max (4,5)} \right) + (6 \times 2^{8-6}) \left( \frac{1}{\max (5,6)} \right) \]

\[ = (2 \times 2^8 \times \frac{1}{3}) + (2 \times 2^8 \times \frac{1}{4}) + (8 \times 2^{8-12}) + \frac{1}{5} (6 \times 2^{8-6}) + \frac{1}{6} (6 \times 2^{8-6}) \]

\[ = \frac{161}{30} \times 2^8 - \frac{26}{5}. \]

3.1.5. Theorem ISI\(_N\) (PETIM) = \( \frac{59512}{1155} \times 2^8 = \frac{14176}{264} \).

Proof:

\[ ISI_N (PETIM) = \sum_{uv \in E} \left( \frac{S(u) \times S(v)}{S(u) + S(v)} \right) \]

\[ = (2 \times 2^8) \left( \frac{2 \times 3^3}{2^3} \right) + (2 \times 2^8) \left( \frac{3 \times 4^4}{3^4 + 4} \right) + (8 \times 2^{8-12}) \left( \frac{4 \times 4^4}{4^4 + 4} \right) + (6 \times 2^{8-6}) \left( \frac{4 \times 5}{4^4 + 5} \right) \]

\[ + (6 \times 2^{8-6}) \left( \frac{5 \times 6}{5^4 + 6} \right) \]

\[ = (2 \times 2^8 \times \frac{6}{5}) + (2 \times 2^8 \times \frac{12}{7}) + \frac{16}{6} (8 \times 2^{8-12}) + \frac{20}{9} (6 \times 2^{8-6}) + \frac{30}{11} (6 \times 2^{8-6}) \]

\[ = \frac{59512}{1155} \times 2^8 - \frac{14176}{264}. \]

3.2. DPZ\(_6\) dendrimer.

DPZ\(_6\) has four identical branches and a central core in its molecular graph. DPZ\(_6\) has 96g-10 atoms and 105g-11 bonds in its molecular graph. The edge-set partition of DPZ\(_6\) are shown [11] as 8 x 2\(^8\) for the pair (4,4), 8 for the pairs (4,5), (5,8), (8,9) and (8,10), 16 x 2\(^8\) - 12 for the pairs (5,5) and (5,7), 8 x 2\(^8\) - 12 for the pairs (5,6), 8 x 2\(^8\) - 12 for the pair (7,8), 4 x 2\(^8\) for the pair (6,6), 4 for the pairs (6,7), (7,9) and (10,12), 4 x 2\(^8\) - 4 for the pair (6,8). Figure 2 depicts the chemical structure of the zinc porphyrin dendrimer DPZ\(_6\).

Theorem 3.2.1: SK\(_N\)(DPZ\(_6\)) = 324 x 2\(^8\) + 44.

Proof:

\[ SK_N (DPZ_6) = (8 \times 2^8) \left( \frac{4^4}{2} \right) + 8 \left( \frac{4^4 + 5}{2} \right) + (16 \times 2^{8-12}) \left( \frac{5^5 + 5}{2} \right) + (8 \times 2^{8-12}) \left( \frac{5^5 + 6}{2} \right) \]

\[ + (16 \times 2^{8-12}) \left( \frac{5^5 + 7}{2} \right) + 8 \left( \frac{5^5 + 8}{2} \right) + (4 \times 2^5) \left( \frac{6^6 + 6}{2} \right) + 4 \left( \frac{6^7 + 7}{2} \right) + (4 \times 2^5 - 4) \left( \frac{6^8 + 8}{2} \right) \]

\[ + (8 \times 2^{8-8}) \left( \frac{7^9 + 8}{2} \right) + 4 \left( \frac{7^9 + 9}{2} \right) + 8 \left( \frac{8^9 + 10}{2} \right) + 4 \left( \frac{10^{10 + 12}}{2} \right) \]

\[ = (32 \times 2^8) + 36 + (80 \times 2^6) - 60 + (4 \times 2^8) - 60 + (96 \times 2^8) - 72 + 52 + (24 \times 2^8) + 26 \]

\[ + (28 \times 2^8) - 28 + (60 \times 2^8) - 60 + 32 + 68 + 72 + 44 \]

\[ = 324 \times 2^8 + 44. \]

3.2.2. Theorem SK\(_1N\)(DPZ\(_6\)) = 1056 x 2\(^8\) + 438.

Proof:

\[ SK_1N (DPZ_6) = (8 \times 2^8) \left( \frac{4 \times 4}{2} \right) + 8 \left( \frac{5 \times 4}{2} \right) + (16 \times 2^{8-12}) \left( \frac{5 \times 5}{2} \right) + (8 \times 2^{8-12}) \left( \frac{5 \times 6}{2} \right) \]

\[ + (16 \times 2^{8-12}) \left( \frac{5 \times 7}{2} \right) + 8 \left( \frac{5 \times 8}{2} \right) + (4 \times 2^6) \left( \frac{6 \times 6}{2} \right) + 4 \left( \frac{6 \times 7}{2} \right) + (4 \times 2^{8-4}) \left( \frac{6 \times 8}{2} \right) \]
+ (8 x 2⁸- 8)\left(\frac{7 x 8}{2}\right) + 4\left(\frac{7 x 9}{2}\right) + 8 \left(\frac{8 x 9}{2}\right) + 8 \left(\frac{8 x 10}{2}\right) + 4 \left(\frac{10 x 12}{2}\right)

= (8 x 2⁸x 8) + 80 + \frac{25}{2} (16 x 2⁸- 12) + 15(8 x 2⁸ -12) + \frac{35}{2} (16 x2⁸- 12) + 160 + (18 x 4 x 2⁸) 

+ 84 + 24(4 x 2⁸ - 4) + 28(8 x 2⁸ - 8) + 126 + 288 + 320 + 240

= 1056 x 2⁸ + 438.

**Figure 2.** Zinc porphyrin dendrimer DPZgmolecular structure.

3.2.3. Theorem SK2N (DPZg) = 2136 x 2⁸ + 894.

Proof:

\[
\text{SK2}_N (\text{DPZ}_g) = (8 x 2^8) \left(\frac{4+4}{2}\right)^2 + 8\left(\frac{5+4}{2}\right)^2 + (16 x 2^8-12) \left(\frac{5+5}{2}\right)^2 + (8 x 2^8- 12)\left(\frac{5+6}{2}\right)^2
\]

\[
+ (16 x 2^8- 12)\left(\frac{5+7}{2}\right)^2 + 8\left(\frac{5+8}{2}\right)^2 + (4 x 2^8) \left(\frac{6+6}{2}\right)^2 + 4 \left(\frac{6+7}{2}\right)^2 + (4 x 2^8- 4)\left(\frac{6+8}{2}\right)^2
\]

\[
+ (8 x 2^8-8) \left(\frac{7+8}{2}\right)^2 + 4\left(\frac{7+9}{2}\right)^2 + 8\left(\frac{8+9}{2}\right)^2 + 8\left(\frac{8+10}{2}\right)^2 + 4 \left(\frac{10+12}{2}\right)^2
\]

\[
= (8 x 16 x 2^8) + (2 x 81) + (16 x 25 x 2^8) - (12 x 25) + (121 x 2 x 2^8) - (121 x 3) + (36 x 16 x 2^8) - (36 x 12) + (2 x 169) + (361 x 4 x 2^8) + 169 + (49 x 4 x 2^8) 

- (49 x 4) + (225 x 2 x 2^8) - (225 x 2) + (4 x 64) + (2 x 289) + (8 x 81) + 484

= 2136 x 2^8 + 894.

3.2.4. Theorem mRN (DPZg) = \frac{2307}{210} x 2^8 - \frac{41}{42}.

Proof:
mRN(DPZ_d) = (8 × 2^8) \left(\frac{1}{\max(4,4)}\right) + 8 \left(\frac{1}{\max(5,5)}\right) + (16 × 2^8– 12) \left(\frac{1}{\max(5,5)}\right) 
+ (8 × 2^8– 16) \left(\frac{1}{\max(5,5)}\right) + (16 × 2^8– 12) \left(\frac{1}{\max(5,7)}\right) + 8 \left(\frac{1}{\max(5,8)}\right) + (4 × 2^8) \left(\frac{1}{\max(6,6)}\right) 
+ 4 \left(\frac{1}{\max(6,7)}\right) + (4 × 2^8) \left(\frac{1}{\max(6,8)}\right) + (8 × 2^8– 8) \left(\frac{1}{\max(7,8)}\right) + 4 \left(\frac{1}{\max(7,9)}\right) 
+ 8 \left(\frac{1}{\max(8,9)}\right) + 8 \left(\frac{1}{\max(8,10)}\right) + 4 \left(\frac{1}{\max(10,12)}\right) 
= \frac{1}{4} (8 × 2^8) + 8 \left(\frac{1}{5}\right) + \frac{1}{5} (16 × 2^8– 12) + \frac{1}{6} (8 × 2^8– 12) + \frac{1}{7} (16 × 2^8– 12) + 8 \left(\frac{1}{6}\right) 
+ \frac{1}{6} (4 × 2^8) + 4 \left(\frac{1}{7}\right) + \frac{1}{8} (4 × 2^8– 4) + \frac{1}{8} (8 × 2^8– 8) + 4 \left(\frac{1}{9}\right) + 8 \left(\frac{1}{10}\right) + 4 \left(\frac{1}{12}\right) 
= \frac{2307}{210} × 2^8 \approx 41.42.

3.2.5. Theorem ISI_N(DPZ_d) = \frac{215522}{1155} × 2^8 - 64367463 \frac{3063060}{306060}.

Proof:

ISI_N(DPZ_d) = (8 × 2^8) \left(\frac{4 × 4}{4+4+4}\right) + 8 \left(\frac{5 × 4}{5+4}\right) + (16 × 2^8– 12) \left(\frac{5 × 5}{5+5}\right) + (8 × 2^8– 12) \left(\frac{5 × 6}{5+6}\right) 
+ (16 × 2^8– 12) \left(\frac{5 × 7}{5+7}\right) + 8 \left(\frac{5 × 8}{5+8}\right) + (4 × 2^8) \left(\frac{6 × 6}{6+6}\right) + 4 \left(\frac{6 × 7}{6+7}\right) + (4 × 2^8– 4) \left(\frac{6 × 8}{6+8}\right) 
+ (8 × 2^8– 8) \left(\frac{7 × 8}{7+8}\right) + 4 \left(\frac{7 × 9}{7+9}\right) + 8 \left(\frac{8 × 9}{8+9}\right) + 8 \left(\frac{8 × 10}{8+10}\right) + 4 \left(\frac{10 × 12}{10+12}\right) 
= \frac{215522}{1155} × 2^8 - 64367463 \frac{3063060}{306060}.

3.3. D_2P_8 dendrimer.

D_2P_8 molecular graph comprises four comparable wings and a center core with five more edges (Figures 3 and 4). The total number of atoms in porphyrin dendrimer [11] is 96g– 10, and the number of bonds in D_2P_8 is 105g- 11. Note that g = 2^i, where i ≥ 2. The edge-set partition of D_2P_8 are given as 2g, g+1, 8g-6, 24g, 4g, 4g-6, 6g, 18g, 25g, 11g for the pairs (3,5), (4,4), (4,5), (4,6), (5,5), (5,6), (5,7), (6,7), (6,8) and (7,9) respectively and g for the pairs (7,8) and (8,9).

3.3.1. Theorem SK_N(D_2P_8) = 642g - 56.

Proof:

SK_N(D_2P_8) = 2g \left(\frac{3 + 5}{2}\right) + (g + 1) \left(\frac{4 + 4}{2}\right) + (8g - 6) \left(\frac{4 + 5}{2}\right) + 24g \left(\frac{4 + 6}{2}\right) + 4g \left(\frac{5 + 5}{2}\right) 
+ (4g - 6) \left(\frac{5 + 6}{2}\right) + 6g \left(\frac{5 + 7}{2}\right) + 18g \left(\frac{6 + 7}{2}\right) + 25g \left(\frac{6 + 8}{2}\right) + g \left(\frac{7 + 8}{2}\right) + 11g \left(\frac{7 + 9}{2}\right) + g \left(\frac{8 + 9}{2}\right) 
= 8g + 4g + 4 + 36g - 27 + 120g + 20g + 22g - 33 + 36g + 117g + 175g 
+ 15g + 8g + 8g + 80g - 60 + 288g + 50g + 60g - 90 + 105g + 378g + 600g 
= 642g - 56.

3.3.2. Theorem SK_1_N(D_2P_8) = 1994.5g - 142.

Proof:

SK_1_N(D_2P_8) = 2g \left(\frac{3 + 5}{2}\right) + (g + 1) \left(\frac{4 + 4}{2}\right) + (8g - 6) \left(\frac{4 + 5}{2}\right) + 24g \left(\frac{4 + 6}{2}\right) + 4g \left(\frac{5 + 5}{2}\right) 
+ (4g - 6) \left(\frac{5 + 6}{2}\right) + 6g \left(\frac{5 + 7}{2}\right) + 18g \left(\frac{6 + 7}{2}\right) + 25g \left(\frac{6 + 8}{2}\right) + g \left(\frac{7 + 8}{2}\right) + 11g \left(\frac{7 + 9}{2}\right) + g \left(\frac{8 + 9}{2}\right) 
= 15g + 8g + 8 + 80g - 60 + 288g + 50g + 60g - 90 + 105g + 378g + 600g.
+ 28g + \frac{693g}{2} + 36g \\
= 1994.5g - 142.

**Figure 3.** Porphyrin Dendrimer $D_4P_4$ molecular graph.

**Figure 4.** Porphyrin Dendrimer $D_{16}P_{16}$ molecular graph.
3.3.3. Theorem SK2_N (D_2P_e) is 4065g - 287.

Proof:
SK2_N (D_2P_e) = 2g \left( \frac{3+5}{2} \right)^2 + (g+1) \left( \frac{4+4}{2} \right)^2 + (8g-6) \left( \frac{4+5}{2} \right)^2 + 24g \left( \frac{4+6}{2} \right)^2 + 4g \left( \frac{5+5}{2} \right)^2 + (4g-6) \left( \frac{5+6}{2} \right)^2 + 6g \left( \frac{5+7}{2} \right)^2 + 18g \left( \frac{6+7}{2} \right)^2 + 25g \left( \frac{6+8}{2} \right)^2 + g \left( \frac{7+9}{2} \right)^2 + g \left( \frac{8+9}{2} \right)^2
= 4065g - 287.

3.3.4. Theorem mR_N (D_2P_e) = \frac{1101g}{70} - \frac{39}{20}.

Proof:
mR_N (D_2P_e) = 2g \left( \frac{1}{\text{max}(3,5)} \right) + (g+1) \left( \frac{1}{\text{max}(4,4)} \right) + (8g-6) \left( \frac{1}{\text{max}(4,5)} \right) + 24g \left( \frac{1}{\max(4,6)} \right) + 4g \left( \frac{1}{\text{max}(5,5)} \right) + (4g-6) \left( \frac{1}{\text{max}(5,6)} \right) + 6g \left( \frac{1}{\text{max}(5,7)} \right) + 18g \left( \frac{1}{\text{max}(5,8)} \right) + g \left( \frac{1}{\text{max}(6,7)} \right) + 11g \left( \frac{1}{\max(6,8)} \right) + 6g \left( \frac{1}{7,9} \right) + 25g \left( \frac{1}{8,9} \right) + 4g \left( \frac{1}{8,10} \right) \frac{1}{1}\right) + (4g-6) \left( \frac{1}{9} \right) + 6g \left( \frac{1}{9} \right)
= \frac{1101g}{70} - \frac{39}{20}.

3.3.5. Theorem ISI_N (D_2P_e) = \frac{771121993g}{2450448} - \frac{914}{33}.

Proof:
ISI_N (D_2P_e) = 2g \left( \frac{5 \times 5}{3+5} \right) + (g+1) \left( \frac{5 \times 4}{4+4} \right) + (8g-6) \left( \frac{4 \times 5}{4+5} \right) + 24g \left( \frac{4 \times 6}{4+6} \right) + 4g \left( \frac{5 \times 5}{5+5} \right) + (4g-6) \left( \frac{5 \times 6}{5+6} \right) + 6g \left( \frac{5 \times 5}{5+7} \right) + 18g \left( \frac{6 \times 7}{6+7} \right) + 25g \left( \frac{6 \times 8}{6+8} \right) + g \left( \frac{7 \times 8}{7+8} \right) + 11g \left( \frac{7 \times 9}{7+9} \right) + g \left( \frac{8 \times 9}{8+9} \right)
= \frac{771121993g}{2450448} - \frac{914}{33}.

Figure 5. SK_N index of PETIM, DPZ_e and D_2P_e dendrimers.

Figure 6. SK1_N index of PETIM, DPZ_e and D_2P_e.
3.4. Graphical representation.

The graphical representation of $SK_N$, $SK1_N$, $SK2_N$, $mR_N$, and $ISI_N$ for the dendrimers PETIM, $DPZ_g$, and $D_gP_g$ are given in Figure 5-9. In the following figures, the $x$-axis represents the number of growth-stage $g$, and the $y$-axis represents the corresponding index. PETIM, $DPZ_g$, and $D_gP_g$ dendrimers are plotted by red, blue, and green colors, respectively. It is observed from the figures that $DPZ_g$ has a higher value for Neighborhood-based indices than PETIM and $D_gP_g$.

4. Conclusions

The molecular study and the research of relation between indices and molecular attributes are made possible by computing numerous topological indices of graphs connected with chemical graphs. In this study, we proposed several Neighborhood-based topological indices for dendrimers, namely PETIM, $DPZ_g$, and $D_gP_g$. Chemistry, physics, and other practical disciplines can benefit from our findings. Topological indices have been shown to aid in predicting various properties without the need for a wet lab. MATLAB was also used to
illustrate the 2D representations of these indices. We plan to establish the link between these descriptors and various chemical features of dendrimers in the future.

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Conflicts of Interest

The authors declare no conflict of interest.

References