

Research Article

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Calculating the Degree-based Topological Indices of Dendrimers

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Abstract: Topological indices capture the symmetry of molecular structures and provide a mathematical language to predict properties such as boiling points, viscosity, the radius of gyration etc. [1]. We compute some newly developed topological indices of Porphyrin, Propyl Ether Imine, Zinc-Porphyrin and Poly(EThyleneAmidoAmine) Dendrimers. The results are plotted using Maple 2015 software to see the dependence on the involved structural parameters.

Keywords: chemical graph theory; Randić index; Dendrimer.

1 Introduction

In chemical graph theory, a molecular graph is a simple graph having no loops and multiple edges in which atoms and chemical bonds are represented by vertices and edges respectively. A graph $G(V, E)$ with vertex set $V(G)$ and edge set $E(G)$ is connected if there exists a connection between any pair of vertices in G . The degree of a vertex is the number of vertices which are connected to that fixed vertex by the edges. The distance between two vertices u and v is denoted as $d(u, v) = d_G(u, v)$ and is the length of the shortest path between u and v in graph G . The concept of degree is somewhat closely related to the concept of valence in chemistry. For details on the basics of graph theory any standard text such as [2] can be of great help.

Cheminformatics is another emerging field in which quantitative structure-activity (QSAR) and structure-property (QSPR) relationships predict the biological activities and properties of nanomaterials. In these studies, some physico-chemical properties and topological indices are used to predict bioactivity of the chemical compounds for example see [3-6]. Algebraic polynomials have also useful applications in chemistry such as the Hosoya polynomial (also called Wiener polynomial) [7] which play a vital role in determining distance-based topological indices. Among other algebraic polynomials, M-polynomial was introduced by Deutsch and Klavzar [8], plays the same role in determining the closed form of many degree-based topological indices [9-13]. The main advantage of M-polynomial is the wealth of information that it contains about degree-based graph invariants.

Dendrimers are man-made, nanoscale compounds with unique properties that make them useful to the health and pharmaceutical industry as both enhancements to existing products and as entirely new products. Dendrimers are constructed by the successive addition of layers of branching groups. The final generation incorporates the surface molecules that give the dendrimer the desired function for pharmaceutical, life science, chemical, electronic and materials applications. Dendrimers fall under the broad heading of nanotechnology, which covers the manipulation of matter in the size range of 1-100 nanometers (one million nanometers equal one millimeter) to create compounds, structures, and devices with a novel, pre-determined properties.

Dendrimers are repetitively branched molecules. A dendrimer is typically symmetric around the core and often adopts a spherical three-dimensional morphology. The first dendrimers were made by divergent synthesis approaches by Buhleier et al. [14] in 1978. Dendrimers have gained a wide range of applications in chemistry, biology and nanosciences. There are a lot of research papers on the computation of topological indices of dendrimers, for example [9,15,16].

In this report, we discuss degree-based combinatorial facts about four familiar classes of dendrimers,

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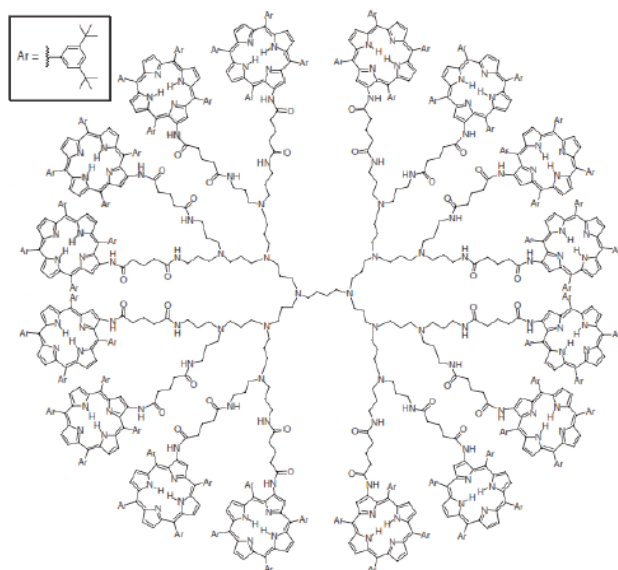


Figure 1: Porphyrin Dendrimer.

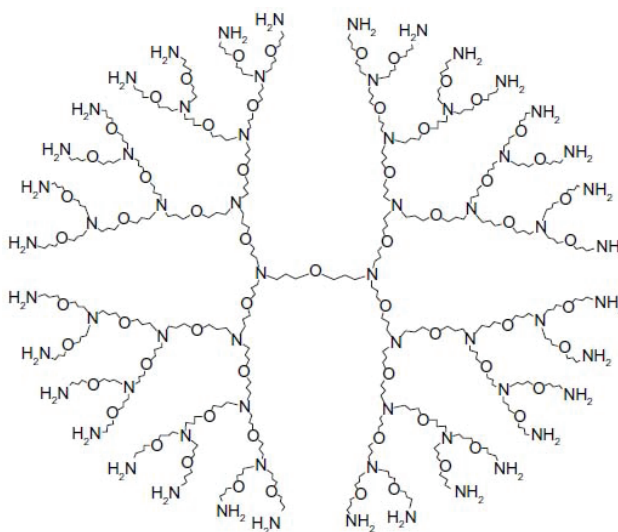


Figure 2: Propyl Ether Imine Dendrimer.

Porphyrin, Propyl Ether Imine, Zinc-Porphyrin and Poly(EThyleneAmidoAmine) Dendrimers. It is important to remark that all dendrimers differ in cores.

2 Basic Definition and Literature Review

Weiner, in 1947, approximated the boiling point of alkanes as $\alpha W(G) + \beta P_3 + \gamma$ where α , β and γ are empirical constants, $W(G)$ is the Wiener index and P_3 is the path of length 3 [17]. Thus Wiener laid the foundation of

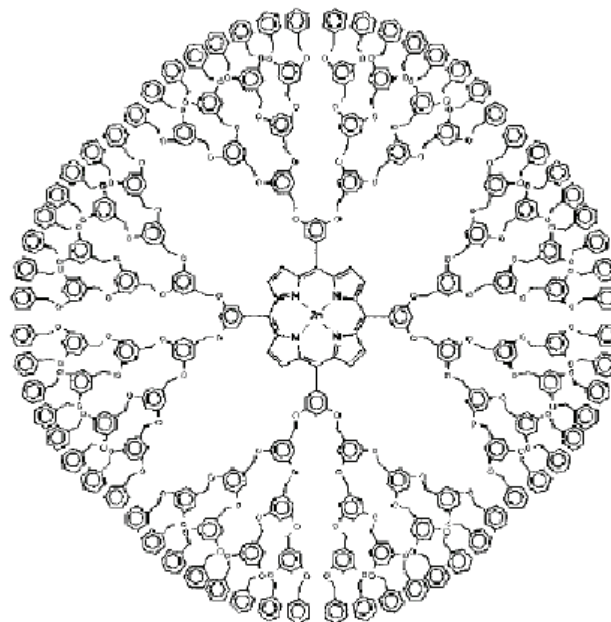


Figure 3: Zinc-Porphyrin Dendrimer.

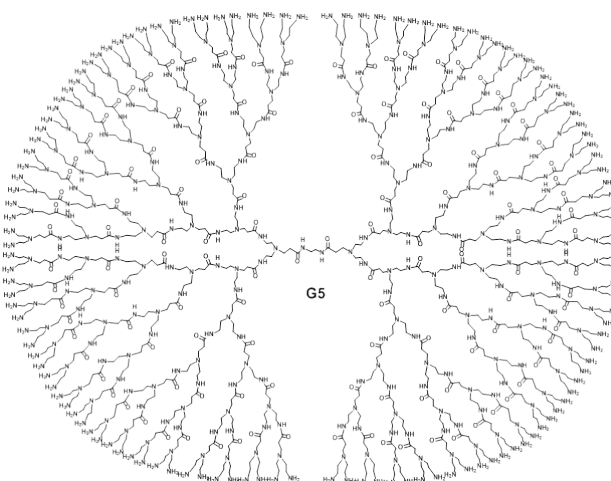


Figure 4: Poly(EThyleneAmidoAmine) Dendrimer.

Topological index which is also known as connectivity index. A lot of chemical experiments require determining the chemical properties of emerging nanotubes and nanomaterials. Chemical-based experiments reveal that out of more than 140 topological indices no single index is strong enough to determine many physico-chemical properties, although, in combination, these topological indices can do this to some extent. The Wiener index is originally the first and most studied topological index, see for details [18,19].

Randić index, [20] denoted by $R_{-1/2}(G)$ and introduced by Milan Randić in 1975 is also one of the oldest

topological indexes. In 1998, working independently, Bollobas and Erdos [21] and Amic *et al.* [22] proposed the generalized Randić index and has been studied extensively by both chemists and mathematicians [23] and many mathematical properties of this index have been discussed in [24]. For a detailed survey we refer the book [25]. The general Randić index is defined as $R_\alpha(G) = \sum_{uv \in E(G)} \frac{1}{(d_u d_v)^\alpha}$, and the inverse Randić index is defined as $RR_\alpha(G) = \sum_{uv \in E(G)} (d_u d_v)^\alpha$. Obviously $R_{-1/2}(G)$ is the particular case of $R_\alpha(G)$ when $\alpha = \frac{1}{2}$, and $R_{-1/2}(G)$ is the particular case of $RR_\alpha(G)$ when $\alpha = -\frac{1}{2}$. The Randić index is the most studied among all other topological indices. Many papers and books such as [26-28] are written on this topological index. Randić himself wrote two reviews on his Randić index [29,30] and there are three more reviews [31-33]. The suitability of the Randić index for drug design was immediately recognized, and eventually, the index was used for this purpose on countless occasions. The physical reason for the success of such a simple graph invariant is still an enigma, although several more-or-less plausible explanations were offered.

Gutman and Trinajstić introduced first Zagreb index and second Zagreb index, which are defined as:

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

and

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

respectively. Further detail about these indices can be found in references [34-47].

The sum connectivity index is defined as

$$\chi(G) = \sum_{uv \in E(G)} \sqrt{d_u d_v}$$

and modified Randić index is defined as

$$R'(G) = \sum_{uv \in E(G)} \frac{1}{\max\{d_u, d_v\}}.$$

Shigehalli and Kanabur [39] introduced following new degree-based topological indices; Arithmetic-Geometric

$$(AG_1) \text{ index } AG_1(G) = \sum_{uv \in E(G)} \frac{d_u + d_v}{2\sqrt{d_u d_v}},$$

Shigehalli & Kanabur indices are defined as:

$$SK(G) = \sum_{uv \in E(G)} \frac{d_u + d_v}{2},$$

$$SK_1(G) = \sum_{uv \in E(G)} \frac{d_u d_v}{2},$$

$$SK_2(G) = \sum_{uv \in E(G)} \left(\frac{d_u + d_v}{2} \right)^2.$$

3 Main Results and Proofs

In this section we give our computational results.

Theorem 1. Let $D_n P_n$ be the Porphyrin Dendrimer.

Then

1. $\chi(D_n P_n) = (6 + \frac{72}{\sqrt{5}} + \frac{13}{\sqrt{6}} + \frac{8}{\sqrt{7}})n - (\frac{5}{2} + \frac{6}{\sqrt{5}}),$
2. $R'(D_n P_n) = 34n - \frac{9}{2},$
3. $AG_1(D_n P_n) = (6\sqrt{3} + 53 + 20\sqrt{6})n - 5 - \frac{5}{2}\sqrt{6},$
4. $SK(D_n P_n) = 271n - 25,$
5. $SK_1(D_n P_n) = \frac{643}{2}n - 28,$
6. $SK_2(D_n P_n) = 713n - \frac{115}{2}.$

Proof: For Porphyrin Dendrimer $D_n P_n$, we have

$$|V(D_n P_n)| = 96n - 10 \text{ and } |E(D_n P_n)| = 105n - 11.$$

There are six types of edges in $E(D_n P_n)$ based on the degree of end vertices. i.e.,

$$E_1(D_n P_n) = \{uv \in E(D_n P_n) : d_u = 1, d_v = 3\};$$

$$E_2(D_n P_n) = \{uv \in E(D_n P_n) : d_u = 1, d_v = 4\};$$

$$E_3(D_n P_n) = \{uv \in E(D_n P_n) : d_u = 2, d_v = 2\};$$

$$E_4(D_n P_n) = \{uv \in E(D_n P_n) : d_u = 2, d_v = 3\};$$

$$E_5(D_n P_n) = \{uv \in E(D_n P_n) : d_u = 3, d_v = 3\};$$

$$E_6(D_n P_n) = \{uv \in E(D_n P_n) : d_u = 3, d_v = 4\}.$$

It can be observed from Figure 1 that $|E_1(D_n P_n)| = 2n$, $|E_2(D_n P_n)| = 24n$, $|E_3(D_n P_n)| = 10n - 5$, $|E_4(D_n P_n)| = 48n - 6$, $|E_5(D_n P_n)| = 13n$ and $|E_6(D_n P_n)| = 8n$.

Now,

$$\begin{aligned} \chi(D_n P_n) &= \sum_{uv \in E(D_n P_n)} \frac{1}{\sqrt{d_u d_v}} \\ &= |E_1(D_n P_n)| \frac{1}{\sqrt{1 \cdot 3}} + |E_2(D_n P_n)| \frac{1}{\sqrt{1 \cdot 4}} + |E_3(D_n P_n)| \frac{1}{\sqrt{2 \cdot 2}} \\ &\quad + |E_4(D_n P_n)| \frac{1}{\sqrt{2 \cdot 3}} + |E_5(D_n P_n)| \frac{1}{\sqrt{3 \cdot 3}} + |E_6(D_n P_n)| \frac{1}{\sqrt{3 \cdot 4}} \\ &= \frac{2n}{\sqrt{4}} + \frac{24n}{\sqrt{5}} + \frac{10n-5}{\sqrt{4}} + \frac{48n-6}{\sqrt{5}} + \frac{13n}{\sqrt{6}} + \frac{8n}{\sqrt{7}} \\ &= (6 + \frac{72}{\sqrt{5}} + \frac{13}{\sqrt{6}} + \frac{8}{\sqrt{7}})n - (\frac{5}{2} + \frac{6}{\sqrt{5}}), \end{aligned}$$

$$\begin{aligned} R'(D_n P_n) &= \sum_{uv \in E(D_n P_n)} \frac{1}{\max\{d_u, d_v\}} \\ &= |E_1(D_n P_n)| \frac{1}{\max\{1, 3\}} + |E_2(D_n P_n)| \frac{1}{\max\{1, 4\}} + |E_3(D_n P_n)| \frac{1}{\max\{2, 2\}} \\ &\quad + |E_4(D_n P_n)| \frac{1}{\max\{2, 3\}} + |E_5(D_n P_n)| \frac{1}{\max\{3, 3\}} + |E_6(D_n P_n)| \frac{1}{\max\{3, 4\}} \\ &= \frac{2n}{3} + \frac{24n}{4} + \frac{10n-5}{2} + \frac{48n-6}{3} + \frac{13n}{3} + \frac{8n}{4} \\ &= 34n - \frac{9}{2}, \end{aligned}$$

$$\begin{aligned}
AG_1(D_n P_n) &= \sum_{uv \in E(D_n P_n)} \frac{d_u + d_v}{2\sqrt{d_u \cdot d_v}} \\
&= |E_1(D_n P_n)| \frac{1+3}{2\sqrt{1 \cdot 3}} + |E_2(D_n P_n)| \frac{1+4}{2\sqrt{1 \cdot 4}} + |E_3(D_n P_n)| \frac{2+2}{2\sqrt{2 \cdot 2}} \\
&\quad + |E_4(D_n P_n)| \frac{2+3}{2\sqrt{2 \cdot 3}} + |E_5(D_n P_n)| \frac{3+3}{2\sqrt{3 \cdot 3}} + |E_6(D_n P_n)| \frac{3+4}{2\sqrt{3 \cdot 4}} \\
&= (6\sqrt{3} + 53 + 20\sqrt{6})n - 5 - \frac{5}{2}\sqrt{6},
\end{aligned}$$

$$\begin{aligned}
SK(D_n P_n) &= \sum_{uv \in E(D_n P_n)} \frac{d_u + d_v}{2} \\
&= |E_1(D_n P_n)| \frac{1+3}{2} + |E_2(D_n P_n)| \frac{1+4}{2} + |E_3(D_n P_n)| \frac{2+2}{2} \\
&\quad + |E_4(D_n P_n)| \frac{2+3}{2} + |E_5(D_n P_n)| \frac{3+3}{2} + |E_6(D_n P_n)| \frac{3+4}{2} \\
&= 2n \left(\frac{1+3}{2} \right) + 24n \left(\frac{1+4}{2} \right) + (10n-5) \left(\frac{2+2}{2} \right) + (48n-6) \left(\frac{2+3}{2} \right) + 13n \left(\frac{3+3}{2} \right) + 8n \left(\frac{3+4}{2} \right) \\
&= 271n - 25, \\
SK_1(D_n P_n) &= \sum_{uv \in E(D_n P_n)} \frac{d_u \cdot d_v}{2} \\
&= |E_1(D_n P_n)| \frac{1 \cdot 3}{2} + |E_2(D_n P_n)| \frac{1 \cdot 4}{2} + |E_3(D_n P_n)| \frac{2 \cdot 2}{2} + |E_4(D_n P_n)| \frac{2 \cdot 3}{2} \\
&\quad + |E_5(D_n P_n)| \frac{3 \cdot 3}{2} + |E_6(D_n P_n)| \frac{3 \cdot 4}{2} \\
&= 2n \left(\frac{3}{2} \right) + 24n \left(\frac{4}{2} \right) + (10n-5) \left(\frac{4}{2} \right) + (48n-6) \left(\frac{6}{2} \right) + 13n \left(\frac{9}{2} \right) + 8n \left(\frac{12}{2} \right) \\
&= \frac{643}{2}n - 28,
\end{aligned}$$

$$\begin{aligned}
SK_2(D_n P_n) &= \sum_{uv \in E(D_n P_n)} \left(\frac{d_u + d_v}{2} \right)^2 \\
&= |E_1(D_n P_n)| \left(\frac{1+3}{2} \right)^2 + |E_2(D_n P_n)| \left(\frac{1+4}{2} \right)^2 + |E_3(D_n P_n)| \left(\frac{2+2}{2} \right)^2 \\
&\quad + |E_4(D_n P_n)| \left(\frac{2+3}{2} \right)^2 + |E_5(D_n P_n)| \left(\frac{3+3}{2} \right)^2 + |E_6(D_n P_n)| \left(\frac{3+4}{2} \right)^2 \\
&= 2n \left(\frac{1+3}{2} \right)^2 + 24n \left(\frac{1+4}{2} \right)^2 + (10n-5) \left(\frac{2+2}{2} \right)^2 + (48n-6) \left(\frac{2+3}{2} \right)^2 + 13n \left(\frac{3+3}{2} \right)^2 + 8n \left(\frac{3+4}{2} \right)^2 \\
&= 713n - \frac{115}{2}.
\end{aligned}$$

Hence, the desired results are obtained.

Theorem 2. Let $PETIM$ be the Propyl Ether Imine Dendrimer. Then

1. $\chi(PETIM) = \frac{1}{3}2^{n+1}\sqrt{3} + \frac{1}{2}2^{n+4} - 9 + \frac{1}{5}(6 \cdot 2^n - 6)\sqrt{5}$;
2. $R'(PETIM) = 11 \cdot 2^n - 11$;
3. $AG_1(PETIM) = \frac{3}{2}2^{n+1}\sqrt{2} + 2 \cdot 2^{n+4} - 36 + \frac{5}{6}(6 \cdot 2^n - 6)\sqrt{6}$;
4. $SK(PETIM) = 3 \cdot 2^n + 2^{n+5} + 15 \cdot 2^n - 51$;
5. $SK_1(PETIM) = 2^{n+1} + 2^{n+5} + 18 \cdot 2^n - 54$;
6. $SK_2(PETIM) = 9 \cdot 2^{n-1} + 2^{n+6} + 75 \cdot 2^{n-1} - \frac{219}{2}$.

Proof: For Poly Ether Imine Dendrimer $PETIM$, we infer $|V(PETIM)| = 24 \cdot 2^n - 23$ and $|E(PETIM)| = 24 \cdot 2^n - 24$.

There are three types of edges in $E(PETIM)$ based on the degree of end vertices. i.e.,

$$\begin{aligned}
E_1(PETIM) &= \{uv \in E(PETIM) : d_u = 1, d_v = 2\}; \\
E_2(PETIM) &= \{uv \in E(PETIM) : d_u = 2, d_v = 2\}; \\
E_3(PETIM) &= \{uv \in E(PETIM) : d_u = 2, d_v = 3\}.
\end{aligned}$$

It can be observed from Figure 2 that $|E_1(PETIM)| = 2^{n+1}$, $|E_2(PETIM)| = 2^{n+4} - 18$ and $|E_3(PETIM)| = 6 \cdot 2^n - 6$.

Thus,

$$\begin{aligned}
\chi(PETIM) &= |E_1(PETIM)| \frac{1}{\sqrt{1+2}} + |E_2(PETIM)| \frac{1}{\sqrt{2+2}} + |E_3(PETIM)| \frac{1}{\sqrt{2+3}} \\
&= \frac{1}{3}2^{n+1}\sqrt{3} + \frac{1}{2}2^{n+4} - 4 + \frac{1}{5}(6 \cdot 2^n - 6)\sqrt{5},
\end{aligned}$$

$$\begin{aligned}
R'(PETIM) &= |E_1(PETIM)| \frac{1}{\max\{1,2\}} + |E_2(PETIM)| \frac{1}{\max\{2,2\}} + |E_3(PETIM)| \frac{1}{\max\{2,3\}} \\
&= 11 \cdot 2^n - 11,
\end{aligned}$$

$$\begin{aligned}
AG_1(PETIM) &= |E_1(PETIM)| \frac{1+2}{2\sqrt{1 \cdot 2}} + |E_2(PETIM)| \frac{2+2}{2\sqrt{2 \cdot 2}} + |E_3(PETIM)| \frac{2+3}{2\sqrt{2 \cdot 3}} \\
&= 2^{n+1} \left(\frac{1+2}{2\sqrt{1 \cdot 2}} \right) + (2^{n+4} - 18) \left(\frac{2+2}{2\sqrt{2 \cdot 2}} \right) + (6 \cdot 2^n - 6) \left(\frac{2+3}{2\sqrt{2 \cdot 3}} \right) \\
&= \frac{1}{3}2^{n+1}\sqrt{3} + \frac{1}{2}2^{n+4} - 9 + \frac{1}{5}(6 \cdot 2^n - 6)\sqrt{5},
\end{aligned}$$

$$\begin{aligned}
SK(PETIM) &= |E_1(PETIM)| \frac{1+2}{2} + |E_2(PETIM)| \frac{2+2}{2} + |E_3(PETIM)| \frac{2+3}{2} \\
&= 2^{n+1} \left(\frac{1+2}{2} \right) + (2^{n+4} - 18) \left(\frac{2+2}{2} \right) + (6 \cdot 2^n - 6) \left(\frac{2+3}{2} \right) \\
&= 3 \cdot 2^n + 2^{n+5} + 15 \cdot 2^n - 51,
\end{aligned}$$

$$\begin{aligned}
SK_1(PETIM) &= |E_1(PETIM)| \frac{1 \cdot 2}{2} + |E_2(PETIM)| \frac{2 \cdot 2}{2} + |E_3(PETIM)| \frac{2 \cdot 3}{2} \\
&= 2^{n+1} \left(\frac{1 \cdot 2}{2} \right) + (2^{n+4} - 18) \left(\frac{2 \cdot 2}{2} \right) + (6 \cdot 2^n - 6) \left(\frac{2 \cdot 3}{2} \right) \\
&= 2^{n+1} + 2^{n+5} + 18 \cdot 2^n - 54,
\end{aligned}$$

$$\begin{aligned}
SK_2(PETIM) &= |E_1(PETIM)| \left(\frac{1+2}{2} \right)^2 + |E_2(PETIM)| \left(\frac{2+2}{2} \right)^2 + |E_3(PETIM)| \left(\frac{2+3}{2} \right)^2 \\
&= 2^{n+1} \left(\frac{1+2}{2} \right)^2 + (2^{n+4} - 18) \left(\frac{2+2}{2} \right)^2 + (6 \cdot 2^n - 6) \left(\frac{2+3}{2} \right)^2 \\
&= 9 \cdot 2^{n-1} + 2^{n+6} + 75 \cdot 2^{n-1} - \frac{219}{2}.
\end{aligned}$$

Therefore, we finish the proof.

Theorem 3. Let DPZ_n be the Zinc-Porphyrin Dendrimer. Then

1. $\chi(DPZ_n) = 8 \cdot 2^n - 2 + \frac{1}{5}(40 \cdot 2^n - 16)\sqrt{5} + \frac{1}{6}(8 \cdot 2^n - 16)\sqrt{6} + \frac{4}{7}\sqrt{7}$;
2. $R'(DPZ_n) = 24 \cdot 2^n - \frac{35}{3}$;
3. $AG_1(DPZ_n) = 24 \cdot 2^n - 20 + \frac{5}{12}(40 \cdot 2^n - 16)\sqrt{6} + \frac{7}{3}\sqrt{3}$;
4. $SK(DPZ_n) = 156 \cdot 2^n - 82$;
5. $SK_1(DPZ_n) = 188 \cdot 2^n - 104$;
6. $SK_2(DPZ_n) = 386 \cdot 2^n - 211$.

Proof: For Zinc-Porphyrin Dendrimer DPZ_n , we deduce $|V(DPZ_n)| = 96n - 10$ and $|E(DPZ_n)| = 105n - 11$.

There are four types of edges in $E(DPZ_n)$ based on the degree of end vertices. i.e.,

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

$$E_2(DPZ_n) = \{uv \in E(DPZ_n) : d_u = 2, d_v = 3\};$$

$$E_3(DPZ_n) = \{uv \in E(DPZ_n) : d_u = 3, d_v = 3\};$$

$$E_4(DPZ_n) = \{uv \in E(DPZ_n) : d_u = 3, d_v = 4\}.$$

It can be observed from Figure 3 that $|E_1(DPZ_n)| = 16 \cdot 2^n - 4$, $|E_2(DPZ_n)| = 40 \cdot 2^n - 16$, $|E_3(DPZ_n)| = 8 \cdot 2^n - 16$ and $|E_4(DPZ_n)| = 4$.

Therefore, in terms of the index definitions, we get

$$\begin{aligned} \chi(DPZ_n) &= |E_1(DPZ_n)| \frac{1}{\sqrt{2+2}} + |E_2(DPZ_n)| \frac{1}{\sqrt{2+3}} + |E_3(DPZ_n)| \frac{1}{\sqrt{3+3}} + |E_4(DPZ_n)| \frac{1}{\sqrt{3+4}} \\ &= (16 \cdot 2^n - 4) \left(\frac{1}{\sqrt{2+2}} \right) + (40 \cdot 2^n - 16) \left(\frac{1}{\sqrt{2+3}} \right) + (8 \cdot 2^n - 16) \left(\frac{1}{\sqrt{3+3}} \right) + 4 \left(\frac{1}{\sqrt{3+4}} \right) \\ &= 8 \cdot 2^n - 2 + \frac{1}{5} (40 \cdot 2^n - 16) \sqrt{5} + \frac{1}{6} (8 \cdot 2^n - 16) \sqrt{6} + \frac{4}{7} \sqrt{7}, \end{aligned}$$

$$R'(DPZ_n) = |E_1(DPZ_n)| \frac{1}{\max\{2, 2\}} + |E_2(DPZ_n)| \frac{1}{\max\{2, 3\}}$$

$$+ |E_3(DPZ_n)| \frac{1}{\max\{3, 3\}} + |E_4(DPZ_n)| \frac{1}{\max\{3, 4\}}$$

$$= (16 \cdot 2^n - 4) \left(\frac{1}{2} \right) + (40 \cdot 2^n - 16) \left(\frac{1}{3} \right) + (8 \cdot 2^n - 16) \left(\frac{1}{3} \right) + 4 \left(\frac{1}{4} \right)$$

$$= 24 \cdot 2^n - \frac{35}{3}.$$

$$AG_1(DPZ_n) = |E_1(DPZ_n)| \frac{2+2}{2\sqrt{2 \cdot 2}} + |E_2(DPZ_n)| \frac{2+3}{2\sqrt{2 \cdot 3}} + |E_3(DPZ_n)| \frac{3+3}{2\sqrt{3 \cdot 3}} + |E_4(DPZ_n)| \frac{3+4}{2\sqrt{3 \cdot 4}}$$

$$= (16 \cdot 2^n - 4) \left(\frac{2+2}{2\sqrt{2 \cdot 2}} \right) + (40 \cdot 2^n - 16) \left(\frac{2+3}{2\sqrt{2 \cdot 3}} \right) + (8 \cdot 2^n - 16) \left(\frac{3+3}{2\sqrt{3 \cdot 3}} \right) + 4 \left(\frac{3+4}{2\sqrt{3 \cdot 4}} \right)$$

$$= 24 \cdot 2^n - 20 + \frac{5}{12} (40 \cdot 2^n - 16) \sqrt{6} + \frac{7}{3} \sqrt{3},$$

$$SK(DPZ_n) = |E_1(DPZ_n)| \frac{2+2}{2} + |E_2(DPZ_n)| \frac{2+3}{2} + |E_3(DPZ_n)| \frac{3+3}{2} + |E_4(DPZ_n)| \frac{3+4}{2}$$

$$= (16 \cdot 2^n - 4) \left(\frac{2+2}{2} \right) + (40 \cdot 2^n - 16) \left(\frac{2+3}{2} \right) + (8 \cdot 2^n - 16) \left(\frac{3+3}{2} \right) + 4 \left(\frac{3+4}{2} \right)$$

$$= 156 \cdot 2^n - 82,$$

$$SK_1(DPZ_n) = |E_1(DPZ_n)| \frac{2 \cdot 2}{2} + |E_2(DPZ_n)| \frac{2 \cdot 3}{2} + |E_3(DPZ_n)| \frac{3 \cdot 3}{2} + |E_4(DPZ_n)| \frac{3 \cdot 4}{2}$$

$$= (16 \cdot 2^n - 4) \left(\frac{2 \cdot 2}{2} \right) + (40 \cdot 2^n - 16) \left(\frac{2 \cdot 3}{2} \right) + (8 \cdot 2^n - 16) \left(\frac{3 \cdot 3}{2} \right) + 4 \left(\frac{3 \cdot 4}{2} \right)$$

$$= 188 \cdot 2^n - 104,$$

$$SK_2(DPZ_n) = |E_1(DPZ_n)| \left(\frac{2+2}{2} \right)^2 + |E_2(DPZ_n)| \left(\frac{2+3}{2} \right)^2$$

$$+ |E_3(DPZ_n)| \left(\frac{3+3}{2} \right)^2 + |E_4(DPZ_n)| \left(\frac{3+4}{2} \right)^2$$

$$= (16 \cdot 2^n - 4) \left(\frac{2+2}{2} \right)^2 + (40 \cdot 2^n - 16) \left(\frac{2+3}{2} \right)^2 + (8 \cdot 2^n - 16) \left(\frac{3+3}{2} \right)^2 + 4 \left(\frac{3+4}{2} \right)^2$$

$$= 386 \cdot 2^n - 211.$$

Theorem 4. Let $PETAA$ be the Poly(EThyleneAmidoAmine) Dendrimer. Then

$$1. \quad \chi(PETAA) = \frac{4}{\sqrt{3}} 2^n + 10 \cdot 2^n - 5 + \frac{1}{\sqrt{5}} (20 \cdot 2^n - 9);$$

$$2. \quad R'(PETAA) = \frac{46}{3} 2^n - \frac{19}{3};$$

$$3. \quad AG_1(PETAA) = 3 \cdot 2^n \sqrt{2} + \frac{2}{\sqrt{3}} (4 \cdot 2^n - 2) + 16 \cdot 2^n - 8 + \frac{5}{12} (20 \cdot 2^n - 9) \sqrt{6};$$

$$4. \quad SK(PETAA) = 96 \cdot 2^n - \frac{85}{2};$$

$$5. \quad SK_1(PETAA) = 102 \cdot 2^n - 46;$$

$$6. \quad SK_2(PETAA) = 214 \cdot 2^n - \frac{385}{4}.$$

Proof: For $PETAA$ Dendrimer, we derive that $|V(PETAA)| = 44 \cdot 2^n - 18$ and $|E(PETAA)| = 44 \cdot 2^n - 19$.

There are four type of edges in $E(PETAA)$ based on the degree of end vertices. i.e.,

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

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

$$E_3(PETAA) = \{uv \in E(PETAA) : d_u = 2, d_v = 2\};$$

$$E_4(PETAA) = \{uv \in E(PETAA) : d_u = 2, d_v = 3\}.$$

It can be observed from Figure 4 that $|E_1(PETAA)| = 4 \cdot 2^n$,

$$|E_2(PETAA)| = 4 \cdot 2^n - 2, \quad |E_3(PETAA)| = 16 \cdot 2^n - 8 \text{ and}$$

$$|E_4(PETAA)| = 20 \cdot 2^n - 9.$$

In light of the definition of indices, we have

$$\chi(PETAA) = |E_1(PETAA)| \frac{1}{\sqrt{1+2}} + |E_2(PETAA)| \frac{1}{\sqrt{1+3}} + |E_3(PETAA)| \frac{1}{\sqrt{2+2}} + |E_4(PETAA)| \frac{1}{\sqrt{2+3}}$$

$$= (4 \cdot 2^n) \left(\frac{1}{\sqrt{1+2}} \right) + (4 \cdot 2^n - 2) \left(\frac{1}{\sqrt{1+3}} \right) + (16 \cdot 2^n - 8) \left(\frac{1}{\sqrt{2+2}} \right) + (20 \cdot 2^n - 9) \left(\frac{1}{\sqrt{2+3}} \right)$$

$$= \frac{4}{\sqrt{3}} 2^n + 10 \cdot 2^n - 5 + \frac{1}{\sqrt{5}} (20 \cdot 2^n - 9),$$

$$R'(PETAA) = |E_1(PETAA)| \frac{1}{\max\{2, 2\}} + |E_2(PETAA)| \frac{1}{\max\{2, 3\}}$$

$$+ |E_3(PETAA)| \frac{1}{\max\{3, 3\}} + |E_4(PETAA)| \frac{1}{\max\{3, 4\}}$$

$$= (4 \cdot 2^n) \left(\frac{1}{2} \right) + (4 \cdot 2^n - 2) \left(\frac{1}{3} \right) + (16 \cdot 2^n - 8) \left(\frac{1}{2} \right) + (20 \cdot 2^n - 9) \left(\frac{1}{3} \right)$$

$$= \frac{46}{3} 2^n - \frac{19}{3},$$

$$AG_1(PETAA) = \sum_{uv \in E_1(PETAA)} \frac{d_u + d_v}{2\sqrt{d_u \cdot d_v}} + \sum_{uv \in E_2(PETAA)} \frac{d_u + d_v}{2\sqrt{d_u \cdot d_v}} + \sum_{uv \in E_3(PETAA)} \frac{d_u + d_v}{2\sqrt{d_u \cdot d_v}} + \sum_{uv \in E_4(PETAA)} \frac{d_u + d_v}{2\sqrt{d_u \cdot d_v}}$$

$$= |E_1(PETAA)| \frac{1+2}{2\sqrt{1 \cdot 2}} + |E_2(PETAA)| \frac{1+3}{2\sqrt{1 \cdot 3}} + |E_3(PETAA)| \frac{2+2}{2\sqrt{2 \cdot 2}} + |E_4(PETAA)| \frac{2+3}{2\sqrt{2 \cdot 3}}$$

$$= (4 \cdot 2^n) \left(\frac{1+2}{2\sqrt{1 \cdot 2}} \right) + (4 \cdot 2^n - 2) \left(\frac{1+3}{2\sqrt{1 \cdot 3}} \right) + (16 \cdot 2^n - 8) \left(\frac{2+2}{2\sqrt{2 \cdot 2}} \right) + (20 \cdot 2^n - 9) \left(\frac{2+3}{2\sqrt{2 \cdot 3}} \right)$$

$$= 3 \cdot 2^n \sqrt{2} + \frac{2}{\sqrt{3}} (4 \cdot 2^n - 2) + 16 \cdot 2^n - 8 + \frac{5}{12} (20 \cdot 2^n - 9) \sqrt{6}.$$

$$SK(PETAA) = \sum_{uv \in E_1(PETAA)} \frac{d_u + d_v}{2} + \sum_{uv \in E_2(PETAA)} \frac{d_u + d_v}{2} + \sum_{uv \in E_3(PETAA)} \frac{d_u + d_v}{2} + \sum_{uv \in E_4(PETAA)} \frac{d_u + d_v}{2}$$

$$= |E_1(PETAA)| \frac{1+2}{2} + |E_2(PETAA)| \frac{1+3}{2} + |E_3(PETAA)| \frac{2+2}{2} + |E_4(PETAA)| \frac{2+3}{2}$$

$$= (4 \cdot 2^n) \left(\frac{1+2}{2} \right) + (4 \cdot 2^n - 2) \left(\frac{1+3}{2} \right) + (16 \cdot 2^n - 8) \left(\frac{2+2}{2} \right) + (20 \cdot 2^n - 9) \left(\frac{2+3}{2} \right)$$

$$= 96 \cdot 2^n - \frac{85}{2}.$$

$$\begin{aligned} SK_1(PETAA) &= |E_1(PETAA)| \frac{1 \cdot 2}{2} + |E_2(PETAA)| \frac{1 \cdot 3}{2} + |E_3(PETAA)| \frac{2 \cdot 2}{2} + \\ &+ |E_4(PETAA)| \frac{2 \cdot 3}{2} = (4 \cdot 2^n) \left(\frac{1 \cdot 2}{2} \right) + (4 \cdot 2^n - 2) \left(\frac{1 \cdot 3}{2} \right) + \\ &+ (16 \cdot 2^n - 8) \left(\frac{2 \cdot 2}{2} \right) + (20 \cdot 2^n - 9) \left(\frac{2 \cdot 3}{2} \right) = 102 \cdot 2^n - 46. \\ SK_2(PETAA) &= |E_1(PETAA)| \left(\frac{1+2}{2} \right)^2 + |E_2(PETAA)| \left(\frac{1+3}{2} \right)^2 \\ &+ |E_3(PETAA)| \left(\frac{2+2}{2} \right)^2 + |E_4(PETAA)| \left(\frac{2+3}{2} \right)^2 \\ &= (4 \cdot 2^n) \left(\frac{2+2}{2} \right)^2 + (4 \cdot 2^n - 2) \left(\frac{2+3}{2} \right)^2 + (16 \cdot 2^n - 8) \left(\frac{3+3}{2} \right)^2 + \\ &+ (20 \cdot 2^n - 9) \left(\frac{3+4}{2} \right)^2 = 214 \cdot 2^n - \frac{385}{4}. \end{aligned}$$

In all, we get the conclusions.

4 Graphical Comparison and Conclusions

Graph theory as a tool has been widely applied to molecular topology theory of chemical computation. The results are of guiding significance to the engineering application. In this paper, several important chemical structures are considered, and by means of edge set dividing trick and molecular graph structure analysis, the accurate formulas of some important degree-based indices are calculated. Our calculated results, for example the Randic index is useful for determining physio-chemical properties of alkanes as noticed by chemist Melan Randic in 1975. He noticed the correlation between the Randic index R and several physico-chemical properties of alkanes, for examples enthalpies of formation, boiling points, chromatographic retention times, vapor pressure and surface areas. An example is shown in Figure 5, adapted from [20], relating the boiling point of some alkanes and their correlation with Randic index.

Now we give geometric comparison of the results. In figures 4-9, red, blue, lime and aqua colors are for Porphyrin, Propyl Ether Imine, Zinc-Porphyrin and Poly(EThyleneAmidoAmine) dendrimers respectively. Figures 6, 7 and 9 illustrate that the Poly(EThyleneAmidoAmine) dendrimer has greatest value of sum connectivity, Modify Randic and SK indices while the Porphyrin dendrimers have the lowest value of sum connectivity, Modify Randic and SK indices. From figure 8 and 11 we can observe that the Porphyrin dendrimers have the largest value of AG_1 and SK_2 indices while Propyl Ether Imine dendrimers have the lowest s least

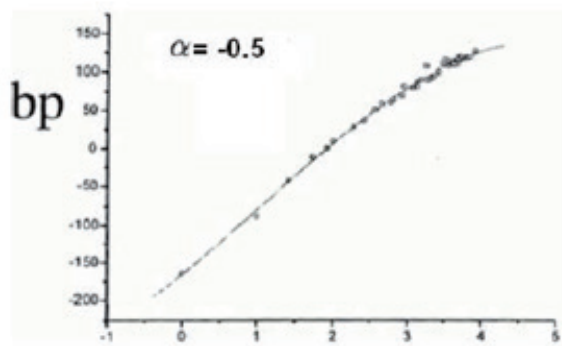


Figure 5: Correlation of Randic index with the boiling point of a selected set of alkanes.

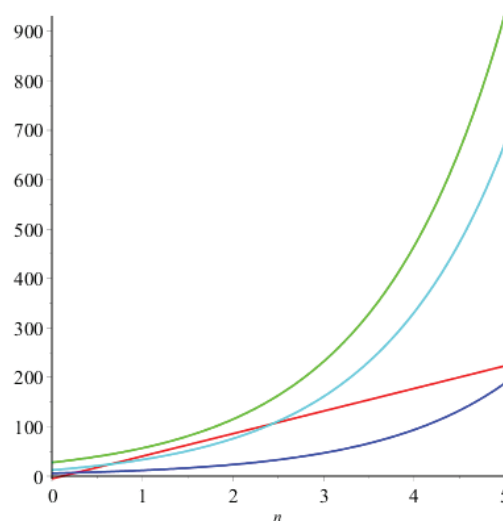


Figure 6: Sum Connectivity Index.

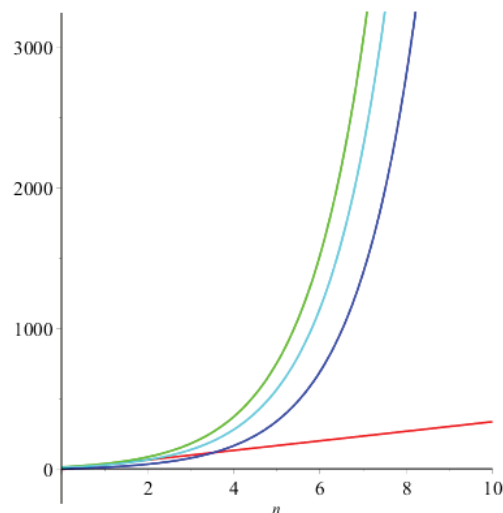
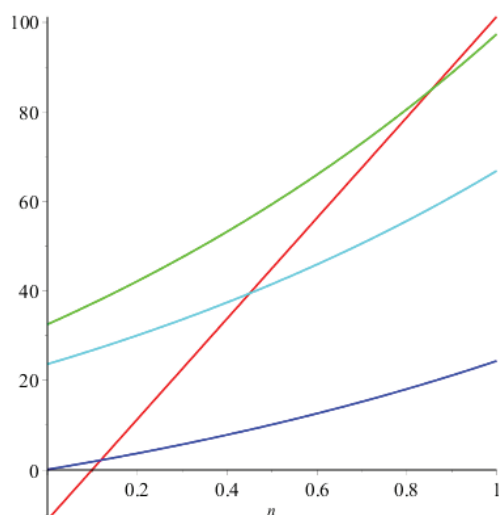
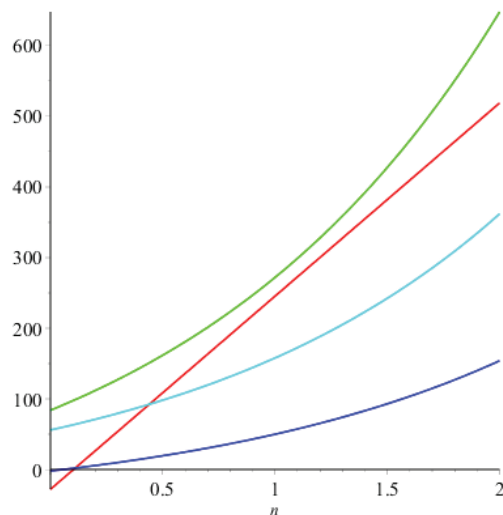
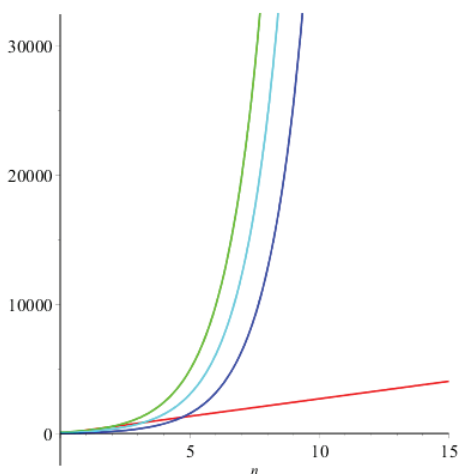
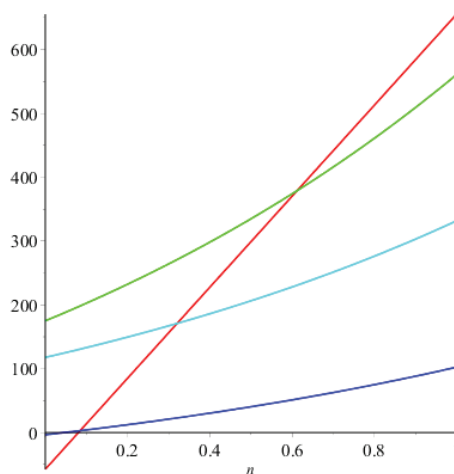


Figure 7: Modify Randic Index.

Figure 8: AG Index.Figure 10: SK_1 Index.Figure 9: SK Index.Figure 11: SK_2 Index.

value of AG_1 and SK_2 indices. From Figure 10 one can make observation that the SK_1 index has largest value for Poly(EThyleneAmidoAmine) Dendrimers and least value for Propyl Ether Imine dendrimers.

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References

- [1] Rucker G., Rucker C., On topological indices, boiling points, and cycloalkanes, *J. Chem. Inf. Comput. Sci.*, 1999, 39, 788–802.
- [2] West D. B., *An Introduction to Graph Theory.*, Prentice-Hall, 1996.
- [3] Klavžar S., Gutman I., A Comparison of the Schultz molecular topological index with the Wiener index., *J. Chem. Inf. Comput. Sci.*, 1996, 36, 1001–1003.
- [4] Brückler F. M., Došlić T., Graovac A., Gutman I., On a class of distance-based molecular structure descriptors., *Chem. Phys. Lett.*, 2011, 503, 336–338.
- [5] Gao W., Wang Y.Q., Wang W.F., Shi, L., The first multiplication atom-bond connectivity index of molecular structures in drugs., *Saudi Pharmaceutical Journal.*, 2017, 25(4), 548–555.

- [6] Zhao B., Wu H.L., Pharmacological characteristics analysis of two molecular structures., *Applied Mathematics and Nonlinear Sciences*, 2017, 2(1), 93-110.
- [7] Gao W., Wang Y.Q., Basavanagoud B., Jamil, M.K., Characteristics studies of molecular structures in drugs., *Saudi Pharmaceutical Journal*, 2017, 25(4), 580-586.
- [8] Deutsch E., Klavzar S., M-Polynomial, and degree-based topological indices., *Iran. J. Math. Chem.*, 2015, 6, 93-102.
- [9] Munir M., Nazeer W., Rafique S., Kang S. M., M-polynomial and related topological indices of Nanostar dendrimers., *Symmetry*, 2016, 8(9), 97, 10.3390/sym8090097.
- [10] Munir M., Nazeer W., Rafique S., Nizami A. R., Kang S. M., M-polynomial and degree-based topological indices of titania nanotubes., *Symmetry*, 2016, 8(11), 117, 10.3390/sym8110117.
- [11] Munir M., Nazeer W., Rafique S., Kang, S. M., M-polynomial and degree-based topological indices of polyhex nanotubes., *Symmetry*, 2016, 8(12), 149, 10.3390/sym8120149.
- [12] Ajmal M., Nazeer W., Munir M., Kang S. M., Kwun Y. C., Some Algebraic Polynomials and Topological Indices of Generalized Prism and Toroidal Polyhex Networks, *Symmetry*, 2017, 9(1), 5, 10.3390/sym9010005.
- [13] Munir M., Nazeer W., Shahzadi S., Kang S. M., Some invariants of circulant graphs., *Symmetry*, 2016, 8(11), 134; 10.3390/sym8110134.
- [14] Buhleier E., Wehner W., Vgtle F., "Cascade"- and "Nonskid-Chainlike" Syntheses of Molecular Cavity Topologies., *Synthesis*, 1978, 2 (1978)155158, doi:10.1055/s-1978-24702.
- [15] Alikhani S., Hasni R., Arif H., On the atom-bond connectivity index of some families of dendrimers., *J. Comput. Theor. Nanosci.*, 2014, 11, 1802-1805.
- [16] Ashrafi A. R., Mirzargar M., Pi, Szeged and edge Szeged indices of an infinite family of nanostars dendrimers., *Indian J. Chem.*, 2008, 47A, 538-541.
- [17] Wiener H., Structural determination of paraffin boiling points., *J. Am. Chem. Soc.*, 1947, 69, 17-20.
- [18] Dobrynin A. A., Entringer R., Gutman I., Wiener index of trees: theory and applications., *Acta Appl. Math.*, 2001, 66, 211-249.
- [19] Gutman I., Polansky O. E., *Mathematical Concepts in Organic Chemistry*, Springer-Verlag New York, USA, 1986.
- [20] Randic M., On the characterization of molecular branching., *J. Am. Chem. Soc.*, 1975, 97, 6609- 6615.
- [21] Bollobas B., Erdos P., Graphs of extremal weights., *Ars. Combin.*, 1998, 50, 225-233.
- [22] Amic D., Beslo D., Lucic B., Nikolic S., Trinajstić N., The vertex-connectivity index revisited., *J. Chem. Inf. Comput. Sci*, 1998, 38, 819-822.
- [23] Hu Y., Li X., Shi Y., Xu T., Gutman I., On molecular graphs with smallest and greatest zeroth-Corder general randic index., *MATCH Commun. Math. Comput. Chem.*, 2005, 54, 425-434.
- [24] Caporossi G., Gutman I., Hansen P., Pavlovic L., Graphs with maximum connectivity index., *Comput. Biol. Chem.*, 2003, 27, 85-90.
- [25] Li X., Gutman I., *Mathematical Chemistry Monographs*, No 1., Kragujevac, 2006.
- [26] Gao W., Wang W. F., The eccentric connectivity polynomial of two classes of nanotubes., *Chaos, Solitons and Fractals*, 2016, 89, 290-294.
- [27] Gao W., Wang W. F., The fifth geometric arithmetic index of bridge graph and carbon nanocones., *Journal of Difference Equations and Applications*, 2017, 23(1-2), 100-109.
- [28] Li X., Gutman I., Mathematical aspects of Randić-type molecular structure descriptors., *Univ. Kragujevac, Kragujevac*, 2006.
- [29] Randić M., On history of the Randić index and emerging hostility toward chemical graph theory., *MATCH Commun. Math. Comput. Chem.*, 2008, 59, 5-124.
- [30] Randić M., The connectivity index 25 years after., *J. Mol. Graphics Modell.*, 2001, 20, 19-35.
- [31] Gutman I., Furtula B., Recent Results in the Theory of Randić Index., *Univ. Kragujevac, Kragujevac*, 2008.
- [32] Li X., Shi Y., A survey on the Randić index., *MATCH Commun. Math. Comput. Chem.*, 2008, 59, 127-156.
- [33] Li X., Shi Y., Wang L., in: Recent Results in the Theory of Randić Index, I. Gutman and B. Furtula (Eds.) 9-47, *Univ. Kragujevac, Kragujevac*, 2008.
- [34] Gao W., Yan L., Shi L., Generalized zagreb index of polyomino chains and nanotubes., *Optoelectronics and Advanced Materials--Rapid Communications*, 2017, 11(1-2), 119-124.
- [35] Basavanagoud B., Desai V. R., Patil S., (β, α) -Connectivity index of graphs., *Applied Mathematics and Nonlinear Sciences*, 2017, 2(1), 21-30.
- [36] Sunilkumar M. H., Bhagyashri B. K., Ratnamma G. B., Vijay M. G., QSPR analysis of certain graph theoretical matrices and their corresponding energy., *Applied Mathematics and Nonlinear Sciences*, 2017, 2(1), 131-150.
- [37] Trinajstić N., Nikolic S., Milicevic, A., Gutman I., On Zagreb indices., *Kem. Ind.*, 2010, 59, 577-589.
- [38] Gao W., Siddiqui M. K., Molecular descriptors of nanotube, oxide, silicate, and triangulene networks., *Journal of Chemistry*, 2017, (2017), 6540754, <https://doi.org/10.1155/2017/6540754>.
- [39] Shigehalli V. S., Kanabur R., Computation of new degree-based topological indices of graphene., *Journal of Nanomaterials*, 2016, (2016), 4341919.
- [40] Sardar M. S., Pan X. F., Gao W., Farahani M. R., Computing Sanskruti Index of Titania Nanotubes., *Open J. Math. Sci.*, 2017, 1(1), 126-131, <http://dx.doi.org/10.30538/oms2017.0012>
- [41] De N., Hyper Zagreb Index of Bridge and Chain Graphs., *Open J. Math. Sci.*, 2018, 2(1), 01-17, <http://dx.doi.org/10.30538/oms2018.0013>
- [42] Riaz M., Gao M., Baig A. Q., M-Polynomials and degree-based Topological Indices of Some Families of Convex Polytopes., *Open J. Math. Sci.*, 2018, 2(1), 18-28, <http://dx.doi.org/10.30538/oms2018.0014>
- [43] Gao W., Muzaffar B., Nazeer W., K-Banhatti and K-Hyper Banhatti Indices of Dominating David Derived Network., *Open J. Math. Anal.*, 2017, 1(1), 13-24.
- [44] Siddiqui H., Farahani M. R., Forgotten Polynomial and Forgotten Index of Certain Interconnection Networks., *Open J. Math. Anal.*, 2017, 1(1), 45-60.
- [45] Tang Z., Liang L., Gao W., Wiener polarity index of quasi-tree molecular structures., *Open J. Math. Sci.*, 2018, 2(1), 73-83, <http://dx.doi.org/10.30538/oms2018.0018>
- [46] Sardar M. S., Zafar S., Farahani M. R., The Generalized Zagreb Index of Capra-Designed Planar Benzenoid Series Cak(C6), *Open J. Math. Sci.*, 2017, 1(1), 44-51, <http://dx.doi.org/10.30538/oms2017.0005>
- [47] Mutee ur Rehman H., Sardar R., Raza A., Computing topological indices of Hex Board and its line graph., *Open J. Math. Sci.*, 2017, 1(1), 62-71, <http://dx.doi.org/10.30538/oms2017.0007>