Computing Topological Indices of Certain Networks

Vidya S Umadi[1], A M Sangogi[2]

[1]Assistant Professor

Department of Mathematics, Vidya Samvardhak Mandal's

Somashekhar R Kothiwale Institute of Technology, Nipani, Karnataka State, India vidyaumadi@gmail.com

[2]Professor

Department of Mathematics, SGBIT, Belagavi, Karnataka State, India.

amsangogi@gmail.com

Abstract:

In mathematical chemistry, topological indices are molecular descriptors that are calculated on the molecular graph of a chemical compound. The molecular graph is a graph which is obtained from some chemical structures. The degree of every molecular graph cannot exceeds 4. Topological indices are numerical quantities of a graph that describe its topology. An atom represents a vertex and a bond between two atoms represents an edge in a molecular graph. Mainly there are three types of topological indices viz., degree-based, distance based and eigenvalue-based topological indices. The first degree-based topological indices are the first and second Zagreb indices. The first Zagreb index M_1 is defined as the sum of squares of degrees of each vertex in a graph G and the second Zagreb index M_2 is the product of degree of every adjacent vertices. In this case the summation goes on the set of edges of a graph G. The most studied topological indices are degree-based topological indices. Motivated by these topological indices in this paper, we introduce five new degree-based topological indices based on the neighborhood degree of a vertex. Further, we compute the values of various nanostructures like hexagonal parallelogram P(m,n) nanotube, triangular benzenoid G_n, zigzag-edge coronoid fused with starphene nanotubes ZCS(k,l,m), dominating derived networks D_1, D_2, D_3, Porphyrin Dendrimer, Zinc-Porphyrin Dendrimer, Propyl Ether Imine Dendrimer, Poly(Ethylene amido amine Dendrimer, PAMAM dendrimers($PD1, PD2, DS1$), linear polyomino chain L_n, Z_n, B_n^1 (n≥3),B_n^2 (n≥3) and triangular, hourglass, and jagged-rectangle benzenoid systems of these indices. The standard computational techniques are used for the computation of topological indices of nanostructures. For the edge partition of the nanostructures the algebraic techniques are used. Using these techniques computation of topological indices became easy and also helped to get the more accurate results.

Keywords: Molecular Graph, Nanostructures, Dendrimers, Topological indices.

1. Introduction

In the realm of modern chemistry, the quest to understand the intricate structures of molecules and their impact on chemical properties has led researchers to explore various analytical tools and methodologies. Among these, the field of mathematical chemistry stands out for its emphasis on applying mathematical concepts and techniques to unravel the

mysteries of molecular structures. Central to this endeavor is the study of molecular graphs and their characterization through topological indices, which serve as powerful descriptors of molecular topology. Topological indices represent numerical quantities derived from the molecular graph of a chemical compound. The molecular graph itself is a representation of the chemical structure, wherein atoms are depicted as vertices and bonds as edges. By analyzing the connectivity patterns and geometrical arrangements within these graphs, researchers can gain valuable insights into the structural features that influence the behavior of molecules in various chemical contexts[1].

Within the framework of topological indices, three main categories emerge: degree-based, distance-based, and eigenvalue-based indices. Each category offers unique perspectives on molecular topology, with degree-based indices being particularly prominent due to their simplicity and effectiveness in capturing essential structural information. One of the cornerstone degree-based indices is the Zagreb indices, comprising the first and second Zagreb indices. The first Zagreb index, denoted as $M1M1$[2], quantifies the sum of the squares of vertex degrees in the molecular graph, providing a measure of overall connectivity. On the other hand, the second Zagreb index, denoted as $M2M2$, captures the product of degrees of adjacent vertices, thus highlighting local structural motifs within the molecule[3].

Building upon the foundational concepts of degree-based indices, this paper introduces five novel topological indices rooted in the notion of neighborhood degree. The neighborhood degree of a vertex reflects the cumulative degree of its neighboring vertices, offering insights into the local structural environment of each vertex. By incorporating this concept into the design of new indices, the paper aims to enrich the repertoire of tools available for analyzing molecular graphs and uncovering subtle structural variations[4]. Beyond theoretical development, this paper also emphasizes the practical applications of topological indices to a diverse array of nanostructures. Nanostructures, characterized by their unique geometries and properties at the nanoscale, present intriguing challenges and opportunities for topological analysis. Examples of such nanostructures include hexagonal parallelogram nanotubes, benzenoid systems, dendrimers, and polyomino chains, among others. By computing the proposed indices for these nanostructures, the paper seeks to demonstrate their effectiveness in capturing the complex topology inherent in these systems.To facilitate the computation of topological indices for nanostructures, the paper employs a combination of standard computational techniques and algebraic methods for edge partitioning. These techniques not only streamline the calculation process but also enhance the accuracy and reliability of the results obtained. By leveraging computational and algebraic tools, researchers can explore the intricate details of molecular topology with greater efficiency and precision[5].

Introduction of Novel Degree-Based Topological Indices: The primary objective of this paper is to introduce five new degree-based topological indices that are based on the concept of neighborhood degree. These indices are designed to provide a more nuanced characterization of molecular graphs, with a focus on capturing local structural information.

Application to Various Nanostructures: Another objective is to demonstrate the applicability of the proposed indices to a diverse range of nanostructures, including nanotubes, benzenoid systems, dendrimers, and polyomino chains. By computing these indices for different nanostructures, the paper aims to showcase their utility in analyzing complex molecular architectures[6,7]. Utilization of Computational and Algebraic Techniques: The paper aims to leverage standard computational techniques for the computation of topological indices, supplemented by algebraic methods for edge partitioning in nanostructures. This approach is expected to enhance the efficiency and accuracy of the calculations, facilitating more robust analysis and interpretation of the results[8].

Overall, the objectives of the paper encompass both theoretical advancements in topological index theory and practical applications to real-world nanostructures, with a focus on enhancing our understanding of molecular topology in mathematical chemistry[9,10].In this section, we consider chemical structures like hexagonal parallelogram $P(m,n)$ nanotube, triangular benzenoid G_n,zigzag-edge coronoid fused with starphene nanotubes $ZCS(k,l,m)$, dominating derived networks D_1, D_2, D_3, Porphyrin Dendrimer, Zinc-Porphyrin Dendrimer, Propyl Ether Imine Dendrimer, Poly(Ethylene amido amine Dendrimer, PAMAM dendrimers(PD_1, PD_2, DS_1), linear polyomino chain $L_n, Z_n, B_n^1(n \geq 3), B_n^2(n \geq 3)$ and triangular, hourglass, and jagged-rectangle benzenoid systems [2,3,4,5]. For notations and terminology used in this paper are taken from.

2. Related Works

Topological indices have got importance due to its applications in chemistry as well as in life science. Recently, Hosamani et al. [11], have put forward the following new degree-based topological indices:

$$S_1(G) = \sum_{v_i \in V} d(v_i)^{|d(v_i)|} \tag{1}$$

$$S_2(G) = \sum_{v_i v_j \in E}(d(v_i)^{|d(v_i)|} + d(v_j)^{|d(v_j)|}) \tag{2}$$

$$S_3(G) = \sum_{v_i v_j \in E}(d(v_i)^{|d(v_j)|} + d(v_j)^{|d(v_i)|}) \tag{3}$$

$$S_4(G) = \sum_{v_i v_j \in E}(d(v_i)^{|d(v_i)|} + d(v_j)^{|d(v_j)|}) \tag{4}$$

$$S_5(G) = \sum_{v_i v_j \in E}(d(v_i)^{|d(v_j)|} + d(v_j)^{|d(v_i)|}) \tag{5}$$

3. Methodology

Motivated by the inverse degree of a vertex and the above-mentioned topological indices, here we introduced the following topological indices in the field of chemical graph theory.

$$RS_1(G) = \sum_{v_i \in V} \frac{1}{d(v_i)^{|d(v_i)|}} \tag{6}$$

$$RS_2(G) = \sum_{uv \in E} \frac{1}{d(u)^{|d(u)|} + d(v)^{|d(v)|}} \tag{7}$$

$$RS_3(G) = \sum_{uv \in E} \frac{1}{d(u)^{|d(v)|} + d(v)^{|d(u)|}} \tag{8}$$

$$RS_4(G) = \sum_{uv \in E} \frac{1}{d(u)^{|d(u)|} d(v)^{|d(v)|}} \tag{9}$$

$$RS_5(G) = \sum_{uv \in E} \frac{1}{d(u)^{|d(v)|} d(v)^{|d(u)|}} \tag{10}$$

In this paper, we consider their chemical structures like hexagonal parallelogram $P(m, n)$ nanotube, triangular benzenoid G_n, zigzag-edge coronoid fused with starphene nanotubes $ZCS(k, l, m)$, dominating derived networks D_1, D_2, D_3, Porphyrin Dendrimer, Zinc-Porphyrin Dendrimer, Propyl Ether Imine Dendrimer, Poly(Ethylene amido amine Dendrimer, PAMAM dendrimers(PD_1, PD_2, DS_1), linear polyomino chain $L_n, Z_n, B_n^1(n \geq 3), B_n^2(n \geq 3)$ and triangular, hourglass, and jagged-rectangle benzenoid systems which are depicted in the following figures 2.1, 2.2, 2.3, 2.4, 2.5 and 2.6 respectively:
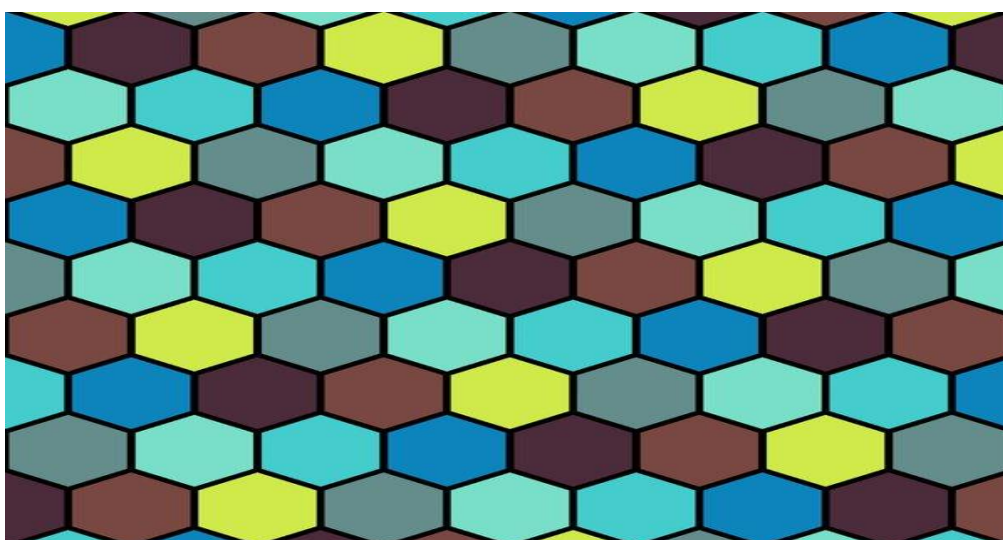

Figure 2.1: hexagonal parallelogram .
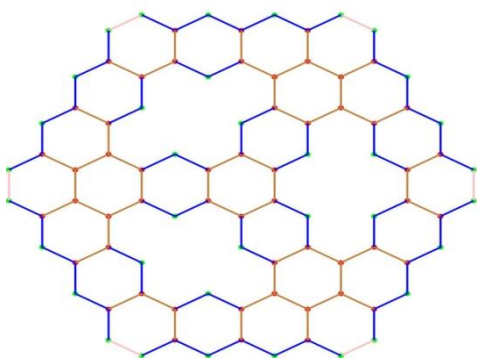

Figure 2.2: Triangular benzenoid .

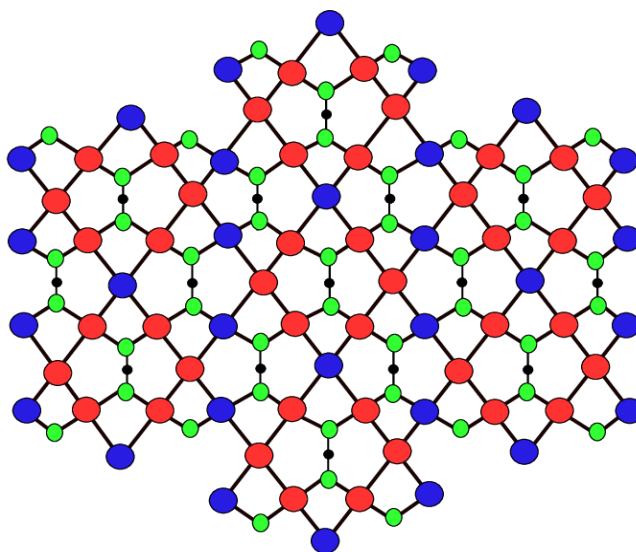Figure 2.3: The zigzag-edge coronoid fused with starphene.

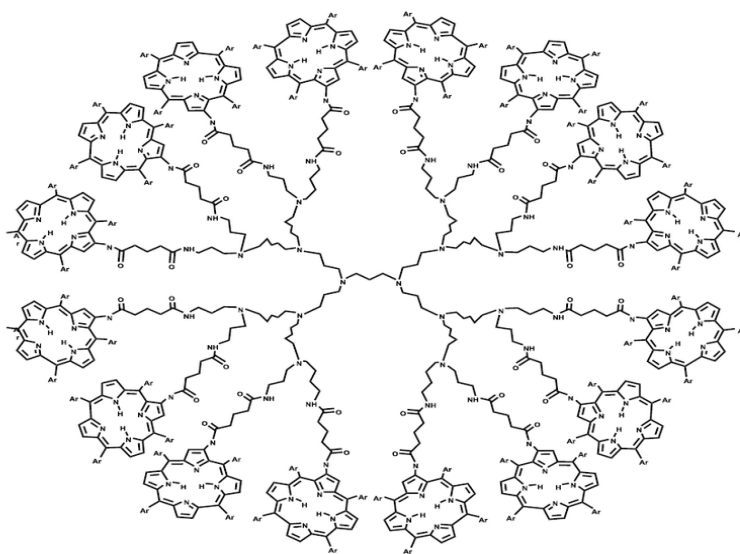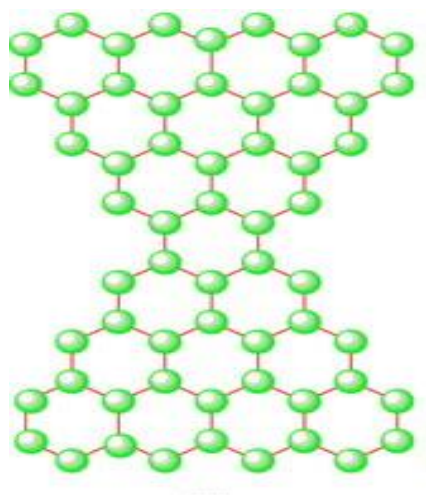Figure 2.4: Dominating derived network.

Figure 2.5: Porphyrin dendrimer.

Figure 2.6: Benzoid hourglass system.

4. Results and Discussion

Theorem 1. *Let G denotes the line graph* of *subdivision graph* of *the hexagonal parallelogram, then*

$$RS_2(G) = \frac{1}{2}mn + \frac{1145}{3348}(m+n) + \frac{1087}{1674} \tag{11}$$

$$RS_3(G) = \frac{1}{6}mn + \frac{823}{1836}(m+n) + \frac{401}{918} \tag{12}$$

$$RS_4(G) = \frac{1}{81}mn + \frac{929}{5832}(m+n) + \frac{611}{1458} \tag{13}$$

$$RS_5(G) = \frac{1}{81}mn + \frac{1037}{5832}(m+n) + \frac{557}{1458} \tag{14}$$

Proof. Let $(m,)$; $\in \mathbb{Z}^+$ be a hexagonal parallelogram of order $2(m+n+mn$i and size $(3mn+2m+2n+1)$ respectively. Let $G= L(S(P(m,n)))$ denotes the line graph of subdivision graph of $P(m,n)$; $m,n \in \mathbb{Z}^+$ then clearly, the order and size of G are $2(3mn+2m+2n+1)$ and

$9mn+4m+4n+5$ respectively. The edge set of G can be partitioned into three disjoint sets $\varepsilon_{2,2}, \varepsilon_{2,3}$ andi $\varepsilon_{3,3}$, where $\varepsilon(L(S(P(m,n)))) = \varepsilon_{2,2} \cup \varepsilon_{2,3} \cup \varepsilon_{3,3}$. Further, $|\varepsilon_{2,2}| = 2(m+n+4)$, $|\varepsilon_{2,3}| = 4(m+n-2)$, $|\varepsilon_{3,3}| = 9mn-2m-2n-5$. Such that $|\varepsilon(L(S(P(m,n))))| = |\varepsilon_{2,2}|+|\varepsilon_{2,3}|+|\varepsilon_{3,3}| = 9mn+4m+4n+5$. Thus, with this background by employing equations (1)-(5) and (6)-(10), we get the required results.

Theorem 2. *Let $((G_n))$ denotes the*ir *line graph*ic of *subdivision graph* of *the hexagonal parallelogram, then*

$$RS_2(L(S(G_n))) = \frac{83}{1000}n^2 + \frac{3}{5}n + \frac{41}{50} \tag{15}$$

$$RS_3(L(S(G_n))) = \frac{9}{108}n^2 + \frac{19}{25}n - \frac{9}{100} \tag{16}$$

$$RS_4(L(S(G_n))) = \frac{9}{1458}n^2 + \frac{1}{4}n + \frac{3}{25} \tag{17}$$

$$RS_5(L(S(G_n))) = \frac{9}{1458}n^2 + \frac{27}{100}n + \frac{47}{100} \tag{18}$$

Proof. Let $G_n; \in \mathbb{Z}^+$ be a triangular benzenoid of order $n^2 + 4n + 1$ and size $\frac{3}{2}n(n + 3)$ respectively. Let $(S(G_n))$ denotes the line graph of subdivision graph of G_n then clearly, the order and size of $L(S(G_n))$ are $3n(n + 3)$ and $\frac{3(3n^2 + 7n + 2)}{2}$ respectively. The edge set of $(S(G_n))$ can be partitioned into three disjoint sets $\varepsilon_{2,2}, \varepsilon_{2,3}$ and $\varepsilon_{3,3}$, where

$(L(S(G_n))) = \varepsilon_{2,2} \cup \varepsilon_{2,3} \cup \varepsilon_{3,3}$. Further, $|\varepsilon_{2,2}| = 3(n + 3)$, $|\varepsilon_{2,3}| = 6(n - 1)$, $|\varepsilon_{3,3}| = \frac{3(3n^2 + n - 4)}{2}$. Such that

$$\left| \varepsilon\left(L\big(S(G_n)\big)\right) \right| = \left| \varepsilon_{2,2} \right| + \left| \varepsilon_{2,3} \right| + \left| \varepsilon_{3,3} \right| = \frac{3(3n^2 + 7n + 2)}{2}.$$

Thus, with this background by employing equations (1)-(5) and (6)-(10), we get the required results.

Theorem 3. *Let $(L(S(I)))$ be the line graph of the subdivision graph of zigzag-edges coronoid fused with starphene nanotubes $ZCS(k, l, m)$ for $k = l = m = 4$. Then*

$$RS_2(L(S(I))) = \frac{3}{2}(k + l + m) - \frac{355}{1116} \qquad (19)$$

$$RS_3(L(S(I))) = \frac{1129}{612}(k + l + m) - \frac{941}{100} \qquad (20)$$

$$RS_4(L(S(I))) = \frac{103}{200}(k + l + m) - \frac{271}{100} \qquad (21)$$

$$RS_5(L(S(I))) = \frac{57}{100}(k + l + m) - \frac{31}{10} \qquad (22)$$

Proof. Let be zizag-edge coronoid fused with starphene nanotubes $(k,)$ for $k = l = m = 4$ of order $36k + 54$ and size $15(k + l + m) - 63$ respectively. Let $(L(S(I)))$ be the line graphic of the subdivision graph of zigzag-edge coronoid fused with starphene nanotubes (k, m) for $k = l = m = 4$. Then clearly, the order and size of $(L(S(I)))$ are $30(k + l + m126)$ and $39(k + l + m) + 153$ respectively. The edge set of $L(S(I))$ can be partitioned into three disjoint sets $\varepsilon_{2,2}, \varepsilon_{2,3}$ and $\varepsilon_{3,3}$, where $\varepsilon(L(S(I))) = \varepsilon_{2,2i} \cup \varepsilon_{2,3} \cup \varepsilon_{3,3}$. Further, $|\varepsilon_{2,2}| = 6(k + l + m - 5)$, $|\varepsilon_{2,3}| = 12(k + l + m - 7)$, $|\varepsilon_{3,3}| = 21(k + l + m) - 39$. Such that $|(L(S(I)))| = |\varepsilon_{2,2}| + |\varepsilon_{2,3}| + |\varepsilon_{3,3}| = 39(k + l + m) + 153$. Thus, with this background by employing equations (1)-(5) and (6)-(10), we get the required results.

Theorem 4. *Let $D_1(n)$ be the dominating derived network of 1st type. Then*

$$RS_2(D_1(n)) = \frac{9}{25}n^2 + \frac{1}{5}n + \frac{3}{100} \qquad (23)$$

$$RS_3(D_1(n)) = \frac{49}{100}n^2 + \frac{19}{25}n - \frac{8}{25} \qquad (24)$$

$$RS_4(D_1(n)) = \frac{9}{500}n^2 + \frac{29}{100}n - \frac{21}{500} \qquad (25)$$

$$RS_5(D_1(n)) = \frac{1}{50}n^2 + \frac{39}{10}n - \frac{11}{100} \qquad (26)$$

Proof. Let $D_1(n)$ be the dominating derived network of 1st type. The edge set of $D_1(n)$ can be partitioned into six disjoint sets $\varepsilon_{2,2}, \varepsilon_{2,3}, \varepsilon_{2,4}, \varepsilon_{3,3}, \varepsilon_{3,4}$ and $\varepsilon_{4,4}$, where $\varepsilon(D_1(n)) =$

$\mathcal{E}_{2,2} \cup \mathcal{E}_{2,3} \cup \mathcal{E}_{2,4} \cup \mathcal{E}_{3,3} \cup \mathcal{E}_{3,4} \cup \mathcal{E}_{4,4}$. Further, $|\mathcal{E}_{2,2}| = 4n$, $|\mathcal{E}_{2,3}| = 4n-4$, $|\mathcal{E}_{2,4}| = 28n\ 16\ |\mathcal{E}_{3,3}| = 9n^2 - 13n + 5$, $|\mathcal{E}_{3,4}| = 36n^2 - 56n + 24$ and $|\mathcal{E}_{4,4}| = 36n^2 - 52n + 20$. Such that

$|\mathcal{E}(D_1(n))| = |\mathcal{E}_{2,2}||\mathcal{E}_{2,3}| + |\mathcal{E}_{2,4}| + |\mathcal{E}_{3,3}| + i\ |\mathcal{E}_{3,4}| + |\mathcal{E}_{4,4}|$. Thus, with this background by employing equations (1)-(5) and (6)-(10), we get the required results.

Theorem 5. *Let $D_2(n)$ be the dominating derived network of 2nd type. Then*

$$RS_2\big(D_2(n)\big) = \frac{79}{100}n^2 - \frac{2}{5}n + \frac{13}{50} \tag{27}$$

$$RS_3\big(D_2(n)\big) = \frac{69}{50}n^2 - \frac{41}{100}n + \frac{3}{50} \tag{28}$$

$$RS_4\big(D_2(n)\big) = \frac{17}{100}n^2 + \frac{13}{200}n + \frac{11}{250} \tag{29}$$

$$RS_5\big(D_2(n)\big) = \frac{13}{50}n^2 + \frac{21}{500}n + \frac{13}{500} \tag{30}$$

Proof. Let $D_2(n)$ be the dominating derived network of 2nd type. The edge set of $D_1(n)$ can be partitioned into five disjoint sets $\mathcal{E}_{2,2}, \mathcal{E}_{2,3}, \mathcal{E}_{2,4}, \mathcal{E}_{3,4}$ and $\mathcal{E}_{4,4}$, where

$(D_2(n)) = \mathcal{E}_{2,2} \cup \mathcal{E}_{2,3} \cup \mathcal{E}_{2,4} \cup \mathcal{E}_{3,4} \cup \mathcal{E}_{4,4}$. Further, $|\mathcal{E}_{2,2}| = 4n$, $|\mathcal{E}_{2,3}| = 18n^2 - 22n + 6$, i $|\mathcal{E}_{2,4}| = 28n - 16$,

$|\mathcal{E}_{3,4}| = 36n^2 - 56n + 24$ and $|\mathcal{E}_{4,4}| = 36n^2 - 52n + 20$. Such that $|(D_2(n))| = |\mathcal{E}_{2,2}| + |\mathcal{E}_{2,3}| + |\mathcal{E}_{2,4}| + |\mathcal{E}_{3,4}| + |\mathcal{E}_{4,4}|$.

Thus, with this background by employing equations(1)-(5) and (6)-(10), we get the required results.

Theorem 6. *Let $D_3(n)$ be the dominating derived network* of *3rd type. Then*

$$RS_2\big(D_3(n)\big) = \frac{7}{25}n^2 + \frac{21}{100}n + \frac{17}{200} \tag{31}$$

$$RS_3\big(D_3(n)\big) = \frac{127}{100}n^2 - \frac{17}{50}n + \frac{43}{500} \tag{32}$$

$$RS_4\big(D_3(n)\big) = \frac{9}{250}n^2 + \frac{23}{100}n + \frac{7}{1000} \tag{33}$$

$$RS_5\big(D_3(n)\big) = \frac{141}{1000}n^2 + \frac{17}{100}n + \frac{7}{1000} \tag{34}$$

Proof. Let $D_3(n)$ be the dominating derived network of 3rd type. The edge set of $D_1(n)$ can be partitioned into three disjoint sets $\mathcal{E}_{2,2}, \mathcal{E}_{2,4}$ and $\mathcal{E}_{4,4}$, where $\mathcal{E}(D_3(n)) = \mathcal{E}_{2,2} \cup \mathcal{E}_{2,4} \cup$

$\mathcal{E}_{4,4}$. Further, $|\mathcal{E}_{2,2}| = 4n$, $|\mathcal{E}_{2,4}| = 36n^2 - 20n$ and $|\mathcal{E}_{4,4}| = 72n^2 - 108n + 44$. Such that $|(D_3(n))| = |\mathcal{E}_{2,2}| + |\mathcal{E}_{2,4}| + |\mathcal{E}_{4,4}|$. Thus, with this background by employing equations

(1)-(5) and (6)-(10), we get the required results.

Theorem 7. *Let D_nP_n be the prophyrin dendrimer. Then*

$$RS_2(D_nP_n) = \frac{323}{100}n - \frac{41}{50} \tag{35}$$

$$RS_3(D_nP_n) = \frac{967}{100}n - \frac{49}{50} \tag{36}$$

$$RS_4(D_nP_n) = \frac{63}{50}n - \frac{37}{100} \tag{37}$$

$$RS_5(D_nP_n) = \frac{399}{50}n - \frac{79}{200} \tag{38}$$

Proof. Let D_nP_n be the prophyrin dendrimer of order $96n-10$ and size $105n-11$ respectively. The edge set of D_nP_n can be partitioned into six disjoint sets $\varepsilon_{1,3}, \varepsilon_{1,4}, \varepsilon_{2,2}, \varepsilon_{2,3}, \varepsilon_{3,3}$ and $\varepsilon_{3,4}$, where $\varepsilon(D_nP_n) = \varepsilon_{1,3} \cup \varepsilon_{1,4} \cup \varepsilon_{2,2} \cup \varepsilon_{2,3} \cup \varepsilon_{3,3} \cup \varepsilon_{3,4}$. Further, $|\varepsilon_{1,3}| = 2n$, $|\varepsilon_{1,4}| = 24n$, $|\varepsilon_{2,2}| = 10n-5$, $|\varepsilon_{2,3}| = 48n-6$, $|\varepsilon_{3,3}| = 13n$ and $|\varepsilon_{3,4}| = 8n$. Such that $|(D_nP_n)| = |\varepsilon_{1,3}| + |\varepsilon_{1,4}| + |\varepsilon_{2,2}| |\varepsilon_{2,3}| + |\varepsilon_{3,3}| + |\varepsilon_{3,4}| = 105n-11$. Thus, with this background by employing equations (1)-(5) and (6)-(10), we get the required results.

Theorem 8. *Let DPZ_n be the Zinc-Porphyrin dendrimer. Then*

$$RS_2(DPZ_n) = \frac{343}{100}2^n - \frac{13}{10} \tag{39}$$

$$RS_3(DPZ_n) = \frac{9}{2}2^n - \frac{171}{100} \tag{40}$$

$$RS_4(DPZ_n) = \frac{69}{50}2^n - \frac{21}{50} \tag{41}$$

$$RS_5(DPZ_n) = \frac{8}{5}2^n - \frac{1}{2} \tag{42}$$

Proof. Let DPZ_n be the Zinc-Porphyrin dendrimer. of order $96n-10$ and size $105n-11$ respectively. The edge set of DPZ_n can be partitioned into four disjoint sets $\varepsilon_{2,2}, \varepsilon_{2,3}, \varepsilon_{3,3}$ and $\varepsilon_{3,4}$, where $\varepsilon(DPZ_n) = \varepsilon_{2,2} \cup \varepsilon_{2,3} \cup \varepsilon_{3,3} \cup \varepsilon_{3,4}$. Further, $|\varepsilon_{2,2}| = 16 \cdot 2^n - 4$, $|\varepsilon_{2,3}| = 40 \cdot 2^n - 16$, $|\varepsilon_{3,3}| = 8 \cdot 2^n - 16i$ and $|\varepsilon_{3,4}| = 4$. Such that $|(DPZ_n)| = |\varepsilon_{2,2}| + |\varepsilon_{2,3}| + |\varepsilon_{3,3}| + |\varepsilon_{3,4}| = 105n-11$. Thus, with this background by employing equations (1)-(5) and (6)-(10), we get the required results.

Theorem 9. *For the PAMAM dendrimers PD_1, we have*

$$RS_2(PD_1) = \frac{37}{10}2^n - \frac{81}{50} \tag{43}$$

$$RS_3(PD_1) = \frac{599}{100}2^n - \frac{13}{5} \tag{44}$$

$$RS_4(PD_1) = \frac{23}{10}2^n - \frac{39}{50} \tag{45}$$

$$RS_5(PD_1) = \frac{59}{12}2^n - \frac{173}{100} \tag{46}$$

Proof. Let PD_1 denote PAMAM dendrimers with trifunctional core unit generated by G_n with n growth stages. The edge set of PD_1 can be partitioned into four disjoint sets

$\varepsilon_{1,2}, \varepsilon_{1,3}, \varepsilon_{2,2}$ and $\varepsilon_{2,3}$, where $\varepsilon(PD_1) = \varepsilon_{1,2} \cup \varepsilon_{1,3} \cup \varepsilon_{2,2} \cup \varepsilon_{2,3}$. Further, $|\varepsilon_{1,2}| = 3 \cdot 2^n$, $|\varepsilon_3| = 6 \cdot 2^n - 3$, $|\varepsilon_{2,2}| = 18 \cdot 2^n - 9$ and $|\varepsilon_{2,3}| = 21 \cdot 2^n - 12$. Such that $|(PD_1)| = |\varepsilon_{1,2}| + |\varepsilon_{1,3}| + |\varepsilon_{2,2}| + |\varepsilon_{2,3}|$. Thus, with this background by employing equations (1)-(5) and (6)-(10), we get the required results.

Theorem 10. *For their PAMAM dendrimers PD_2, we have*

$$RS_2(PD_2) = \frac{499}{100}2^n - \frac{49}{25} \tag{47}$$

$$RS_3(PD_2) = \frac{399}{50}2^n - \frac{16}{5} \tag{48}$$

$$RS_4(PD_2) = \frac{61}{20}2^n - \frac{24}{25} \tag{49}$$

$$RS_5(PD_2) = \frac{59}{9}2^n - \frac{11}{5} \tag{50}$$

Proof. Let PD_{2i} denote PAMAM dendrimers with different core unit generated by dendrimer G_n with n growth stages. The edge set of PD_{2i} can be partitioned into four disjoint sets $\varepsilon_{1,2}, \varepsilon_{1,3}, \varepsilon_{2,2}$ and $\varepsilon_{2,3}$, where $\varepsilon(PD2) = \varepsilon_{1,2i} \cup \varepsilon_{1,3} \cup \varepsilon_{2,2} \cup \varepsilon_{2,3}$. Further, $|\varepsilon_{1,2}| = 4 \cdot 2^n$, $|\varepsilon_{1,3}| = i8 \cdot 2^n - 4$, $|\varepsilon_{2,2}| = 24 \cdot 2^n - 11$ and $|\varepsilon_{2,3}| = 28 \cdot 2^n - 14$. Such that $|(PD_2)| = |\varepsilon_{1,2}| + |\varepsilon_{1,3}| + |\varepsilon_{2,2}| + |\varepsilon_{2,3}|$. Thus, with this background by employing equations (1)-(5) and (6)-(10), we get the required results.

Theorem 11. *For their PAMAM dendrimers DS_1, we have*

$$RS_2(DS_1) = \frac{32}{25} 3^n - \frac{253}{200} \qquad (51)$$

$$RS_3(DS_1) = \frac{87}{40} 3^n - \frac{11}{8} \qquad (52)$$

$$RS_3(DS_1) = \frac{165}{256} 3^n - \frac{161}{256} \qquad (53)$$

$$RS_2(DS_1) = \frac{105}{64} 3^n - \frac{16}{25} \qquad (54)$$

Proof. Let DS_{1i} denote PAMAM dendrimers with different core unit generated by dendrimer G_n with n growth stages. The edge set of DS_1 can be partitioned into three

disjoint sets $\varepsilon_{1,4}, \varepsilon_{2,2}$ and $\varepsilon_{2,4}$, where $\varepsilon(DS_1) = \varepsilon_{1,4i} \cup \varepsilon_{2,2} \cup \varepsilon_{2,4}$. Further, $|\varepsilon_{1,4}| = 4 \cdot 3^n$, $|\varepsilon_{2,2}| = 10 \cdot 3^n - 10$, and $|\varepsilon_{2,4}| = 4 \cdot 3^n - 4$. Such that $|(DS_1)| = |\varepsilon_{1,4}| + |\varepsilon_{2,2}| + |\varepsilon_{2,4}|$. Thus,

with this background by employing equations (1)-(5) and (6)-(10), we get the required results.

Theorem 12. *For a linear polyomino chain L_n we have*

$$RS_2(L_n) = \frac{1}{18} n + \frac{143}{500} \qquad (55)$$

$$RS_3(L_n) = \frac{1}{18} n + \frac{393}{1000} \qquad (56)$$

$$RS_4(L_n) = \frac{1}{243} n + \frac{31}{200} \qquad (57)$$

$$RS_5(L_n) = \frac{1}{243} n + \frac{873}{500} \qquad (58)$$

Proof. Let L_n be their polyomino chain with n squares where $l_1 = I$ n and $m = 1$. The edge set of L_n can be partitioned into three disjoint sets $\varepsilon_{2,2}, \varepsilon_{2,3}$ and $\varepsilon_{3,3}$, I where $\varepsilon(L_n) = \varepsilon_{2,2i} \cup \varepsilon_{2,3} \cup \varepsilon_{3,3}$. Further, $|\varepsilon_{2,2}| = 2, i |\varepsilon_{2,3}| = 4$, and $|\varepsilon_{3,3}| = 3n - 5$. Such that $|(L_n)| = |\varepsilon_{2,2}| + |\varepsilon_{2,3}| + |\varepsilon_{3,3}|$. Thus, with this background by employing equations (1)-(5) and (6)-(10), we get the required results.

Theorem 13. *Let Z_n be zigzag polyomino chain with n squares such that $l = 2$ and $m = n - 1$. Then*

$$RS_2(Z_n) = \frac{63}{16640} m + \frac{3}{512} n + \frac{37}{100} \qquad (59)$$

$$RS_3(Z_n) = \frac{15}{256} m + \frac{3}{512} n + \frac{43}{100} \qquad (60)$$

$$RS_4(Z_n) = \frac{63}{32768} m + \frac{3}{65536} n + \frac{4}{25} \qquad (61)$$

$$RS_5(Z_n) = \frac{255}{32768}m + \frac{3}{65536}n + \frac{17}{100} \qquad (62)$$

Proof Let Z_n be zigzag polyomino chain with n squares such that $l = 2$ and $m = n-1$. Polyomino chain consists of a sequence of segments $S_{1,2},\cdots,S_m$ and $l(S) = l$ where $m \geq 1$ and $\in \{1,2,\cdots,m\}$. The edge set of Z_n can be partitioned into five disjoint sets $\mathcal{E}_{2,2}, \mathcal{E}_{2,3}, \mathcal{E}_{2,4}, \mathcal{E}_{3,4}$ and $\mathcal{E}_{4,4}$, where $\mathcal{E}(Z_n) = \mathcal{E}_{2,2i} \cup \mathcal{E}_{2,3} \cup \mathcal{E}_{2,4} \cup \mathcal{E}_{3,4} \cup \mathcal{E}_{4,4}$. Further, $|\mathcal{E}_{2,2}| = 2$, $|\mathcal{E}_{2,3}| = 4$, $|\mathcal{E}_{2,4}| = 2(m-1)$, $|\mathcal{E}_{3,4}| = 2$ and $|\mathcal{E}_{4,4}| = 3n - 2m - 5$. Such that $|(Z_n)| = |\mathcal{E}_{2,2}| + |\mathcal{E}_{2,3}| + |\mathcal{E}_{2,4}| + |\mathcal{E}_{3,4}| + i |\mathcal{E}_{4,4}|$. Thus, with this background by employing equations (1)-(5) and (6)-(10), we get the required results.

Theorem 14. *For the polyomino chain with n squares and of m segments S_1 and S_{2i} satisfying $l_1 = 2$ and $l_2 = n-1$, $B_n^1(n \geq 3)$ we have the following:*

$$RS_2(B_n^1) = \frac{1}{18}n + \frac{6}{25} \qquad (63)$$

$$RS_3(B_n^1) = \frac{1}{18}n + \frac{41}{100} \qquad (64)$$

$$RS_4(B_n^1) = \frac{1}{243}n + \frac{4}{25} \qquad (65)$$

$$RS_5(B_n^1) = \frac{1}{243}n + \frac{9}{50} \qquad (66)$$

Proof. Let $B_n^1(n \geq 3)$ be the polyomino chain with n squares and m segments S_{1i} and S_{2i} satisfying $l_1 = 2$ and $l_2 = n-1$. The edge set of $B_n^1(n \geq 3)$ can be partitioned into five disjoint sets $\varepsilon_{2,2}, \mathcal{E}_{2,3}, \mathcal{E}_{2,4}, \mathcal{E}_{3,3i}$ and $\mathcal{E}_{3,4}$, where $\varepsilon(B_n^1(n \geq 3)) = \varepsilon_{22} \cup \varepsilon_{23} \cup \varepsilon_{24} \cup \varepsilon_{33} \cup \varepsilon_{34}$. Further, $|\mathcal{E}_{2,2}| = 2$, $|\mathcal{E}_{2,3}| = 5$, $|\mathcal{E}_{2,4}| = 1$, $|\mathcal{E}_{3,3}| = 3n - 10$ and $|\mathcal{E}_{3,4}| = 3$. Such that $|(B_n^1(n \geq 3))| |\mathcal{E}_{2,2}| + |\mathcal{E}_{2,3}| + |\mathcal{E}_{2,4}| + |\mathcal{E}_{3,3}| + |\mathcal{E}_{3,4}|$. Thus, with this background by employing equations (1)-(5) and (6)-(10), we get the required results.

Theorem 15. *For their polyomino chain with n squares and of m segments $S_{1,2},\cdots s_m$ satisfying $l_1 = l_m = 2$ and $l_2, l_3, \cdots, \geq 3$ $B_n^2(n \geq 4)$ we have the following:*

$$RS_2(B_n^2) = -\frac{2543}{78957}m + \frac{1}{18}n + \frac{29}{100} \qquad (67)$$

$$RS_3(B_n^2) = \frac{17}{500}m + \frac{1}{18}n + \frac{33}{100} \qquad (68)$$

$$RS_4(B_n^2) = \frac{1}{100}m + \frac{1}{243}n + \frac{13}{100} \qquad (69)$$

$$RS_5(B_n^2) = \frac{1}{50}m + \frac{1}{243}n + \frac{13}{100} \qquad (70)$$

Proof. Let $B_n^2(n \geq 4)$ be the polyomino chain with n squares and m segments m segments $S_1, S_2, \cdots s_m$ satisfying $l_1 = l_m = 2$ and $l_2, l_3, \cdots, \geq 3$. The edge set of $B_n^2(n \geq 4)$ can be partitioned into five disjoint sets $\mathcal{E}_{2,2}, \mathcal{E}_{2,3}, \mathcal{E}_{2,4}, \mathcal{E}_{3,3}$ and $\mathcal{E}_{3,4}$ where $\varepsilon(B_n^2(n \geq 3)) = \varepsilon_{22} \cup \varepsilon_{23} \cup \varepsilon_{24} \cup \varepsilon_{33} \cup \varepsilon_{34}$. Further, $|\mathcal{E}_{2,2}| = 2$, $|\mathcal{E}_{2,3}| = 2m$, $|\mathcal{E}_{2,4}| = 2$, $|\mathcal{E}_{3,3}| = 3n - 6m + 3$ and $|\mathcal{E}_{3,4}| = 4m - 6$. Such that $|(B_n^2(n \geq 3))| = |\mathcal{E}_{2,2}| + |\mathcal{E}_{2,3}| + |\mathcal{E}_{2,4}| + |\mathcal{E}_{3,3}| + |\mathcal{E}_{3,4}|$. Thus, with this background by employing equations (1)-(5) and (6)-(10), we get the required results.

Theorem 16. *Let T_p be a triangular benzenoid where p i shows the number of hexagons in the base graph ic and total number of hexagons in T_p is $\frac{p(p+1)}{2}$. Then*

$$RS_2\big(T_p\big) = \frac{1}{36}p^2 + \frac{185}{1116}p + \frac{69}{124} \tag{71}$$

$$RS_3\big(T_p\big) = \frac{1}{36}p^2 + \frac{199}{612}p + \frac{27}{68} \tag{72}$$

$$RS_4\big(T_p\big) = \frac{1}{486}p^2 + \frac{13}{243}p + \frac{23}{72} \tag{73}$$

$$RS_5\big(T_p\big) = \frac{1}{486}p^2 + \frac{79}{972}p + \frac{7}{24} \tag{74}$$

Proof. Let T_p be a triangular benzenoid where p shows the number of hexagons in the base graphic and total number of hexagons in T_p is $\frac{p(p+1)}{2}$. The edge set of T_p can be partitioned into three disjoint sets $\mathcal{E}_{2,2}, \mathcal{E}_{2,3i}$ and $\mathcal{E}_{3,3}$ where $\mathcal{E}(T_p) = \mathcal{E}_{2,2} \cup \mathcal{E}_{2,3} \cup \mathcal{E}_{3,3}$. Further, $|\mathcal{E}_{2,2}| = 6$, $|\mathcal{E}_{2,3}| = 6(p-1)$ and $|\varepsilon_{33}| = \frac{3p(p-1)}{2}$. Such that $|(T_p)| = |\mathcal{E}_{2,2}| + |\mathcal{E}_{2,3}| + |\mathcal{E}_{3,3}|$. Thus, with this background by employing equations (1)-(5) and (6)-(10), we get the required results.

Theorem 17. *Let X_p be a benzenoid hourglass. Then*

$$RS_2\big(X_p\big) = \frac{1}{18}p^2 + \frac{185}{558}p + \frac{467}{837} \tag{75}$$

$$RS_3\big(X_p\big) = \frac{1}{18}p^2 + \frac{199}{306}p + \frac{61}{459} \tag{76}$$

$$RS_4\big(X_p\big) = \frac{1}{243}p^2 + \frac{26}{243}p + \frac{521}{1458} \tag{77}$$

$$RS_5\big(X_p\big) = \frac{1}{243}p^2 + \frac{79}{486}p + \frac{413}{1458} \tag{78}$$

Proof. Let X_p be a benzenoid hourglass. The edge set of X_p can be partitioned into three disjoint sets $\mathcal{E}_{2,2}, \mathcal{E}_{2,3i}$ and $\mathcal{E}_{3,3i}$ where $\mathcal{E}(X_p) = \mathcal{E}_{2,2} \cup \mathcal{E}_{2,3i} \cup \mathcal{E}_{3,3}$. Further, $|\mathcal{E}_{2,2}| = 8$, $|\mathcal{E}_{2,3}| = 4(3p-4)$ and $|\mathcal{E}_{3,3}| = 3p^2-3p+4$. Such that $|(X_p)| = |\mathcal{E}_{2,2}|+|\mathcal{E}_{2,3}|+|\mathcal{E}_{3,3}|$. Thus, with this background by employing equations (1)-(5) and (6)-(10), we get the required results.

Theorem 18. *Let $B_{p,q}$ be denote a jagged rectangle benzenoid system for all $p, q \in N-1$. Then*

$$RS_2\big(B_{p,q}\big) = \frac{1}{9}pq + \frac{247}{1674}p + \frac{959}{3348}q + \frac{497}{1674} \tag{79}$$

$$RS_3\big(B_{p,q}\big) = \frac{1}{9}pq + \frac{233}{918}p + \frac{721}{1836}q + \frac{175}{918} \tag{80}$$

$$RS_4\big(B_{p,q}\big) = \frac{2}{243}pq + \frac{26}{729}p + \frac{905}{5832}q + \frac{605}{2916} \tag{81}$$

$$RS_5\big(B_{p,q}\big) = \frac{2}{243}pq + \frac{79}{1458}p + \frac{1013}{5832}q + \frac{551}{2916} \tag{82}$$

Proof. Let $B_{p,q}$ be denotes a jagged rectangle benzenoid system for all $p, q \in N-1$. The edge set of $B_{p,q}$ can be partitioned into three disjoint sets $\mathcal{E}_{2,2}, \mathcal{E}_{2,3}$ and $\mathcal{E}_{3,3}$ where $\mathcal{E}(B_{p,q}) = \mathcal{E}_{2,2} \cup \mathcal{E}_{2,3} \cup \mathcal{E}_{3,3}$. Further, $|\mathcal{E}_{2,2}| = 2q+4$, $|\mathcal{E}_{2,3}| = 4p+4q-4$ and $|\mathcal{E}_{3,3}| = 6pq+p-5q-4$. Such that $|(B_{p,q})| = |\mathcal{E}_{2,2}| + |\mathcal{E}_{2,3}| + |\mathcal{E}_{3,3}|$. Thus, with this background by employing equations (1)-(5) and (6)-(10), we get the required results. $\overline{}$

Conclusion

In this paper, we have computed the topological index values of chemical structures like hexagonal parallelogram $P(m,n)$ nanotube, triangular benzenoid G_n, zigzag-edge coronoid fused with starphene nanotubes $ZCS(k,l,m)$, dominating derived networks D_1, D_2, D_3 , Porphyrin Dendrimer, Zinc-Porphyrin Dendrimer, Propyl Ether Imine Dendrimer, Poly(Ethylene amido amine Dendrimer, PAMAM dendrimers(PD_1, PD_2, DS_1), linear polyomino chain $L_n, Z_n, B_n^1(n \geq 3), B_n^2(n \geq 3)$ and triangular, hourglass, and jagged-rectangle benzenoid systems.

References

[1]   M.S. Ahmad, W. Nazeer, S.M. Kang, M. Imran, and W. Gao, "Calculating degree-based topological indices of dominating David derived networks", *Open Physics*, vol. 15, no. 1, pp. 1015-1021, 2017.

[2]   W. Gao, M.K. Jamil, A. Javed, M.R. Farahani, and M. Imran, "Inverse sum indeg index of the line graphs of subdivision graphs of some chemical structures", *UPB Sci. Bulletin B*, vol. 80, no. 3, pp. 97-104, 2018.

[3]   S.M. Hosamani, "Computing Sanskruti index of certain nanostructures", *Journal of Applied Mathematics and Computing*, vol. 54, pp. 425-433, 2017.

[4]   Y.C. Kwun, A. Farooq, W. Nazeer, Z. Zahid, S. Noreen, and S.M. Kang, "Computations of the M-polynomials and degree-based topological indices for dendrimers and polyomino chains", *International Journal of Analytical Chemistry*, vol. 2018, 2018.

[5]   Y.C. Kwun, A. Ali, W. Nazeer, M. Ahmad Chaudhary, and S.M. Kang, M-polynomials and degree-based topological indices of triangular, hourglass, and jagged-rectangle benzenoid systems. *Journal of chemistry*, *2018*, 2018.

[6]   F. Harary, Graph Theory *(Addison-Weslay Publ. Comp. Reading Massachusets)*, 1969.

[7]   A.R. Ashrafi, T. Došlić, and A. Hamzeh, "The Zagreb coindices of graph operations", *Discrete applied mathematics*, vol. 158, no. 15, pp. 1571-1578, 2010.

[8]   B. Basavanagoud, I. Gutman, and C.S. Gali, "On second Zagreb index and coindex of some derived graphs", *Kragujevac J. Sci*, vol. 37, pp.113-121, 2015.

[9]   Furtula, B. and Gutman, I., 2015. A forgotten topological index. *Journal of mathematical chemistry*, *53*(4), pp.1184-1190.

[10]   Gutman, I. and Trinajstić, N., 1972. Graph theory and molecular orbitals. Total φ-electron energy of alternant hydrocarbons. *Chemical physics letters*, *17*(4), pp.535-538.

[11]   S. M. Hosamani, V. B. Awati and R. S. Honamore, "Estimation of numerical invariants associated with nanostructures and dendrimers via degree based descriptors", Researchgate https://www.researchgate.net/publication/337151723

[12]   S.M. Hosamani, and I. Gutman, "Zagreb indices of transformation graphs and total transformation graphs", *Applied Mathematics and Computation*, vol. 247, pp.1156-1160, 2014.

[13]   S.M. Hosamani, and B. Basavanagoud, "New upper bounds for the first Zagreb index", *MATCH Commun. Math. Comput. Chem*, vol. 74, no. 1, pp. 97-101, 2015.

[14]   S.M. Hosamani, S.H. Malghan, and I.N. Cangul, "The first geometric-arithmetic index of graph operations", *Advances and Applications in Mathematical Sciences*, vol. 14, no. 6, p.155, 2015.

[15]   S.M. Kang, M.A. Zahid, A.U.R. Virk, W. Nazeer, and W. Gao, "Calculating the degree-based topological indices of dendrimers", *Open Chemistry*, vol. 16, no. 1, pp. 681-688, 2018.

[16]   X. Li, and J. Zheng, "A unified approach to the extremal trees for different indices", *MATCH Commun. Math. Comput. Chem*, vol. 54, no. 1, pp. 195-208, 2005.

[17]   M.F. Nadeem, S. Zafar and Z. Zahid, "On certain topological indices of the line graph of subdivision graphs", *Applied mathematics and computation*, vol. 271, pp. 790-794, 2015.

[18]   P.S. Ranjini, V. Lokesha and I.N. Cangül, "On the Zagreb indices of the line graphs of the subdivision graphs", *Applied Mathematics and Computation*, vol. 218, no. 3, pp. 699-702, 2011.

[19]   G. Su, and L. Xu, "Topological indices of the line graph of subdivision graphs and their Schur-bounds. *Applied mathematics and computation*, vol. 253, pp. 395-401, 2015.

[20]   H. Timmerman, R. Todeschini, V. Consonni, R. Mannhold, and H. Kubinyi, "Handbook of molecular descriptors", 2002.

[21]   R. Todeschini, D. Ballabio, and V. Consonni, "Novel molecular descriptors based on functions of new vertex degrees", *Mathematical Chemistry Monographs*, pp. 73-100, 2010.

[22]   R. Todeschini, and V. Consonni, New local vertex invariants and molecular descriptors based on functions of the vertex degrees. *MATCH Commun. Math. Comput. Chem*, vol. 64, no. 2, pp.359-372, 2010.