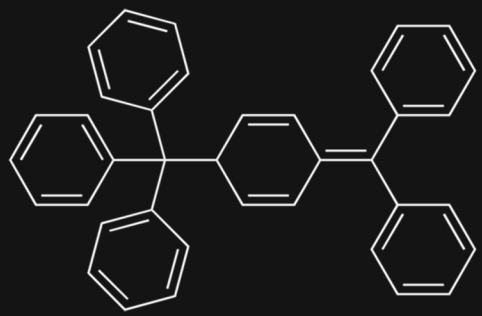
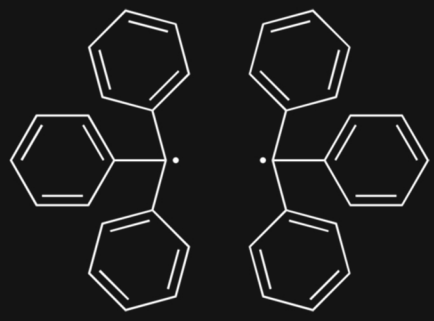
Graph Theory and Its Applications

Topological Indices of Graphs I





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Ayse Dilek Maden
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PREFACE

Editorial on the book series

Graph Theory and Its Applications

Topological Indices of Graphs I

Chemical graph theory, a branch of theoretical chemistry, presents many utilities for the clarification of molecular structures resulting in important applications of graphs. One of these utilities called as topological indices are also known as molecular structure descriptors and have been extensively studied for a long time. Topological indices have attracted the attention of many researchers, particularly in mathematics and chemistry. The literature contains many important results and still-unsolved problems related to topological indices. Obtaining lower and upper bounds for these indices, characterizing graphs in equivalence, and using these indices to analyze the properties of chemical structures, QSAR and QSPR studies are among the primary research topics. Numerous articles have been and are still being studied in this direction in the literature. To provide all researchers working in this field with an opportunity to share their new works, we have attempted to compile a new book series on ***Graph Theory and Its Applications*** and the first volume of this series is titled ***Topological Indices of Graphs I.***

The series will continue with different aspects on Graph Theory and application areas of graphs. We would like to thank all researchers who responded to our invitation and contributed their recent works in this first volume. We hope the increasing continuation of this interest for the forthcoming volumes.

In brief, 20 rigorously selected papers are contributed to this book as follows:

In the first paper "Stress of a Graph - Theory, Algorithms and Applications", R. Yagavi et al. effectively demonstrated some applications of a relatively new notion, stress of a vertex, gave several algorithmic approaches and some applications.

Probably one of the most popular topological graph indices is the first Zagreb index. The second paper in this book is titled "Two New Lower Bounds for the First Zagreb Index and Some Hamiltonian Properties of Graphs" and deals with Hamiltonian problems by means of this index.

Sombor index is a new and very popular topological graph index due to its geometric, algebraic and combinatoric properties widely applied in a short-term literature. The third paper in this volume by Kirgiz and Maden is "Bounds including integrals for Euler-Sombor index" which studied a slight variant of Sombor index with some applications.

Most of the topological graph indices are degree based. Some of these indices are studied in this paper for some algebraic graphs called non-zero component graphs. The next paper "Some Vertex Degree-Based Topological Indices of Non-Zero Component Graphs" by Mathew et al. Deals with relations between algebraic side of graph theory and graph

indices enabling one to obtain new information using these two broad areas.

The fifth paper by Sreeja P. et al. titled "Topological indices of symmetric difference bipartite graph" deals with an interesting family of graphs named as symmetric difference bipartite graphs by calculating several topological graph indices of them.

One of the chemical application areas of graphs is material science. Study of dendrimers is an important application and temperature indices, a very recent class of topological graph indices, is studied in the sixth paper "Computation of temperature indices of Dendrimer structures" by D. S. Kumar and V. Lokesha.

The seventh paper in this book is "Degree-Based Topological Indices on Nanotubes: Analytical Results for ABC and GA Measures" by Masood ur Rehman et al. In this work, authors gave calculations on some degree based topological graph indices for nanotubes.

"QSPR Analysis of Antibiotics via Vertex–Edge Weighted Topological Indices" by Sezer Sorgun dealt with an extensive QSPR analysis for antibiotics by means of weighted topological graph indices.

"Degree Based Indices of Mobius Function Graph of Finite Groups" by Jose and Susha is the nineth paper in this volume, again dealing with algebraic graphs called Mobious function graphs of finite groups interconnecting them with degree based topological graph indices.

"Partial Mycielskian graphs" by Jakkannavar et al. deals with calculation of several topological graph indices of a special and intensively studied type of derived graphs called partial Mycielskian graphs.

The eleventh paper titled "On domination Zagreb indices of monogenic semigroup graphs" by Nacaroglu and Akgunes continues the useful interconnection between Algebra and Graph Theory by studying monogenic semigroup graphs.

"Topological Indices of Order Sum Graphs" by Madhumitha and Naduvath deals with another interesting and new idea of order sum graphs as yet another algebraic graph type and their topological graph indices are calculated.

A very interesting recent graph invariant is the omega invariant defined in 2018 by S. Delen and I. N. Cangul which has close relation with cyclomatic number and Euler characteristic of graphs. It can be used for combinatorial, topological, geometric and graph theoretic calculations related to graphs. "Some New Properties of the Second Omega Coindex" by Nurten Urlu Ozalan introduced and studied a variant of this invariant.

"Interpretation of Fractional Dominating Parameters in Chemical Graphs" by G. Uma et al. is the fourteenth contribution in this volume dealing with fractional dominating parameters of chemical graphs giving several new ideas for application of graphs.

"Predicting Properties of PAHs with Graph Indices and Graph-Based Machine Learning" by Colakoglu and Cenesiz deals with a machine learning approach to PAHs to predict their properties by means of graph parameters.

Another very popular topological graph index is the Wiener index. The next contribution titled "The Wiener Index of Graphs Obtained from the Associate Graph of $\mathbb{Z}_n$" by Barasara and Thakor gave another algebraic graph example named as associate graph and the Wiener index is calculated for these graphs.

Graph products help us to obtain required information on large graphs by means of properties of smaller graphs constituting it. An example of them named as deleted lexicographic product is considered in the next paper "Distance Based Topological Indices of Deleted Lexicographic Product of Graphs" by Caliskan and Aydemir.

The next contribution titled "Reduced first Zagreb index of graphs with added edges" by Hacer Ozden Ayna gives a useful application of some graph transformations adding new edges to a graph and calculating its effect for the reduced first Zagreb index.

"Sombor index for some benzenoids" by Celik and Kaya Gok gave a nice chemical application of Sombor index for benzenoid structures.

The final contribution titled as "Computation of the (a, b) -status indices for line graphs of standard graphs" by Sridhara and Padmanabhan considered status indices another new and useful parameter for graphs.

The 20 papers selected carefully for inclusion in this very first volume of the series all follow the idea of applying mathematical models to the modeling graphs to improve the technological processes. Thus, these papers provide a nice exploration and some applications of graphs for improvization of the technological approaches.

Despite the covered articles have a wide range of subject knowledge, they also contribute to the solution of the existing problems in Chemistry and hence they identify the possible gaps in the literature. We sincerely hope that this special issue will motivate a large number of interdisciplinary research.

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Stress of a Graph - Theory, Algorithms and Applications

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Abstract

A centrality measure assigns a real number to each vertex of a graph and is used for ranking the vertices. It gives the importance or criticality of a vertex from a particular perspective. Degree, betweenness centrality, closeness, eigenvector centrality and stress are some of the vertex centrality measures which are extensively used in analyzing social and biological networks. Stress of a vertex v in a graph G is the number of shortest paths in G having v as an internal vertex. A vertex with high value of stress plays a significant role in keeping together communicating vertices. In this paper we present a brief overview of centrality measures and a detailed study of various aspects of stress. Applications and directions for further research are also given.

Keywords: Centrality measure, Stress, Stress sequence, Stress regular graph
AMS Classification: 05C12, 05C50

1 Introduction

For standard terminology and notations in graph theory, we refer to [2]. All graphs considered in this paper are finite, undirected, connected graphs with neither loops nor multiple edges. Let $G = (V, E)$ be a graph. Its order $|V|$ and size $|E|$ are denoted by n and m, respectively. A $u - v$ path P_k in a graph G is a sequence of vertices $(u = v_1, v_2, \ldots, v_k = v)$ where $(v_i, v_{i+1}) \in E$ and all the v_i's are distinct. The vertex v_1 is called the origin, v_k is called the terminus and the vertices $v_i, 2 \leq i < k$ are called internal vertices of the path P_k. The number of edges in P_k is $k-1$ and is called the length of the path. The path $(v_k, v_{k-1}, \ldots, v_1)$ is called the inverse of P_k and its denoted by P_k^{-1}. Thus, if P_k is a $u-v$ path then P_k^{-1} is a $v-u$ path. In counting the number of $u-v$ paths in a graph, we adopt the convension that P_k and P_k^{-1} are same. The distance $d(u, v)$ between two vertices u and v is the length of a shortest $u-v$ path.

Centrality measure is a core concept for analysing social and biological networks. A vertex centrality measure assigns a real number to each vertex of a graph G and edge centrality measure assigns a real number to every edge of G. It gives the importance or criticality of a vertex or an edge from a particular perspective. A few examples of vertex centrality measures are betweenness, closeness, degree, eigenvector centrality and stress. Such centrality measures are used for ranking the vertices of a graph.

The adjanceny matrix $A = (a_{ij})$ of a graph G with vertex set $\{v_1, v_2, \ldots, v_n\}$ is the $n \times n$ matrix defined by

$$a_{ij} = \begin{cases} 1 & \text{if } v_i v_j \in E \\ 0 & \text{otherwise} \end{cases}.$$

Clearly, A is a $n \times n$ symmetric binary matrix. Hence, its eigenvalues are real.

Theorem 1.1. *Let A be the adjacency matrix of a graph G. Then the ijth entry of A^k is the number of $v_i - v_j$ walks of length k.*

In particular, the ith diagonal entry of A^k is the number of closed walks of length k, starting at v_i.

This paper is organised as follows. In Section 2, we present a brief survey of various centrality measures. A detailed study of the stress of a vertex and its computation are given in Sections 3 and 4. Applications of centrality measures in social and biological networks are dealt with in Section 5. In the concluding section, direction for further research and a few significant unsolved problems are given.

2 A brief overview of Centrality Measures

Centrality measures serve as efficient tools for analyzing large networks. In this section, we present a brief survey of various centrality measures and their significance. Betweenness centrality is a measure of centrality in a graph based on shortest paths and it was introduced by Shaw [8] in 1954.

Definition 2.1. *Let $G = (V, E)$ be a graph of order n and let $v \in V$. The betweenness centrality of v is defined as*

$$C_B(v) = \sum_{s \neq v \neq t} \frac{\sigma_{st}(v)}{\sigma_{st}}, \tag{1}$$

where $\sigma_{st}(v)$ is the number of shortest $s-t$ paths having v as an internal vertex and σ_{st} is the total number of shortest $s-t$ paths.

The summation in (1) has $\binom{n-1}{2}$ terms. Hence, we divide the betweeness centrality by $\binom{n-1}{2}$, so that the betweeness centrality of v lies in the range $[0, 1]$. This enables us to compare betweeness centrality of vertices in two different graphs. For example, to identify a set of significant vertices with respect to betweeness centrality in a large network we can fix a threshold value, say 0.8, and all those vertices for which $C_B \geq 0.8$ can be taken as significant vertices.

Example 2.2. *For the graph G, given in Figure 1 the betweenness centrality of the vertices of G are given in Table 1.*

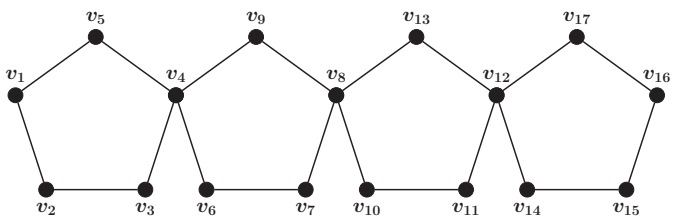


Fig. 1 A graph G with four blocks each isomorphic to C_5

Vertices	v_1	v_2	v_3	v_4	v_5	v_6	v_7	v_8
Betweenness	0.008	0.008	0.108	0.416	0.108	0.041	0.075	0.55

Vertices	v_9	v_{10}	v_{11}	v_{12}	v_{13}	v_{14}	v_{15}	v_{16}	v_{17}
Betweenness	0.375	0.075	0.041	0.416	0.375	0.108	0.008	0.008	0.108

Table 1 Betweenness Centrality of vertices of G

Definition 2.3. *Let $G = (V, E)$ be a graph of order n and let $e \in E$. The edge betweenness centrality of e is defined as*

$$C_B(e) = \sum_{s \neq e \neq t} \frac{\sigma_{st}(e)}{\sigma_{st}}, \tag{2}$$

where $\sigma_{st}(e)$ is the number of shortest $s-t$ paths containing e and σ_{st} is the total number of shortest $s-t$ paths.

The edge betweeness centrality is normalized as in the case of betweeness centrality.

Definition 2.4. *Let $G = (V, E)$ be a graph of order n and let $v \in V$. Closeness centrality of v is defined by*

$$C_C(v) = \frac{n-1}{\sum_{u \in V - \{v\}} d(u, v)}. \tag{3}$$

Hence, the closeness centrality of v is the reciprocal of the average distance of v to all the vertices of $V - \{v\}$. High value of closeness centrality of v indicates that all the vertices are in proximity to v and the low value indicates that all other vertices are distant from v.

Example 2.5. *For the the graph G given in Figure 1, the closeness centrality of the vertices of G are given in Table 2.*

Vertices	v_1	v_2	v_3	v_4	v_5	v_6	v_7	v_8
Closeness	0.22	0.22	0.26	0.33	0.26	0.30	0.33	0.40

Vertices	v_9	v_{10}	v_{11}	v_{12}	v_{13}	v_{14}	v_{15}	v_{16}	v_{17}
Closeness	0.36	0.33	0.30	0.33	0.36	0.26	0.22	0.22	0.26

Table 2 Closeness centrality of the vertices of G

Definition 2.6. *Let $G = (V, E)$ be a graph of order n and let $v \in V$. Then the eccentricity of v is defined by*

$$e(v) = \max\{d(u, v) : u \in V - \{v\}\}. \tag{4}$$

The eccentricity centrality of v is defined by

$$e_C(v) = \frac{1}{e(v)}. \tag{5}$$

The centre of a graph is the set of all vertices with minimum eccentricity. The radius and diameter of a graph are defined as $\text{rad}(G) = \min_{v \in V}\{e(v)\}$ and $\text{diam}(G) = \max_{v \in V}\{e(v)\}$.

Thus, eccentricity measures how close a vertex is to the centre of the graph G. Hence, a vertex with the highest eccentricity centrality is the most central node.

Example 2.7. *For the graph G shown in Fig 1, the eccentricity centrality of the vertices are given in Table 3*

Vertices	v_1	v_2	v_3	v_4	v_5	v_6	v_7	v_8
Eccentricity	8	8	7	6	7	6	5	4

Vertices	v_9	v_{10}	v_{11}	v_{12}	v_{13}	v_{14}	v_{15}	v_{16}	v_{17}
Eccentricity	5	5	6	6	5	7	8	8	7

Table 3 Eccentricity centrality of the vertices of G

Definition 2.8. *Let $G = (V, E)$ be a graph of order n and let $v_i \in V$. The subgraph centrality of v_i, given by,*

$$C_{SG}(v_i) = \sum_{k=0}^{\infty} \frac{A_{ii}^k}{k!}. \tag{6}$$

Since A_{ii}^k is the number of closed walks of length k with v_i as origin and terminus, it follows that shorter closed walks have more influence on the subgraph centrality. To ensure convergence of the series (6), $k!$ is placed in the denominator.

Definition 2.9. *Let $G = (V, E)$ be a graph of order n. Let λ_1 be the largest eigenvalue of the adjacency matrix A, and let $x = (x_1, x_2, \ldots, x_n)$ be an eigenvector corresponding to λ_1 with $\|x\| = 1$. Then, x_i is called the eigenvector centrality of v_i.*

Thus, eigenvector centrality of vertex v_i is the ith coordinate of the eigenvector x corresponding to λ_1 with $\|x\| = 1$.

If a vertex has high eigen vector centrality, then its neighbors also have high eigen vector centrality. Mathematically, the eigen vector centrality of a vertex is proportional to the sum of the eigen vector centralities of its neighbors.

Example 2.10. *For the graph G given in Figure 1, the eigenvector centrality of the vertices of G are given in Table 4.*

Vertices	v_1	v_2	v_3	v_4	v_5	v_6	v_7	v_8
Eigenvector Centrality	0.11	0.11	0.17	0.34	0.17	0.23	0.26	0.43

Vertices	v_9	v_{10}	v_{11}	v_{12}	v_{13}	v_{14}	v_{15}	v_{16}	v_{17}
Eigenvector Centrality	0.30	0.26	0.23	0.34	0.30	0.17	0.11	0.11	0.17

Table 4 Eigenvector centrality of the vertices of G

In the next two sections, we present a complete survey of results on stress of a vertex and its computation. Applications and directions for further research are given in Sections 5 and 6.

3 Stress of a Vertex

The stress of a vertex is an important centrality measure which was introduced by Shimbel [9]. In spite of its applications in biological networks and chemical graph theory, not much theoretical investigation was not carried out. Recently Raksha et al. [5–7] obtained several interesting results on the stress of a graph and its computation. We proceed to present a brief summary of the significant results on stress.

Definition 3.1 ([6]). *Let G be a graph with vertex set $V(G) = \{v_1, v_2, ..., v_n\}$. Then the stress of a vertex v_i, denoted by $st(v_i)$, is the number of shortest paths in G having v_i as an internal vertex and is denoted by $\mathrm{st}(v_i)$. If $(v_{i_1}, v_{i_2}, \ldots, v_{i_n})$ is an ordering of $V(G)$ such that $st(v_{i_1}) \geq st(v_{i_2}) \geq \ldots \geq st(v_{i_n})$, then $(st(v_{i_1}), st(v_{i_2}), \ldots, st(v_{i_n}))$ is called the stress sequence of G. The stress of a graph G is defined by $\mathrm{st}(G) = \sum_{i=1}^{n} \mathrm{st}(v_i)$.*

Example 3.2. *For the graph G given in Figure 1, the stress of vertices of G are given in Table 5.*

Vertices	v_1	v_2	v_3	v_4	v_5	v_6	v_7	v_8
Stress	1	1	13	50	13	5	9	66

Vertices	v_9	v_{10}	v_{11}	v_{12}	v_{13}	v_{14}	v_{15}	v_{16}	v_{17}
Stress	45	9	5	50	45	13	1	1	13

Table 5 Stress of the vertices of G

Raksha et al. [5] determined the stress of paths and cycles.

Theorem 3.3 ([5]). *Let $P_n = (v_1, v_2, ..., v_n)$ be a path on n vertices. Then*

$$\mathrm{st}(v_i) = (i-1)(n-i).$$

Further, the ranking of the vertices in P_n is given by

$$\mathrm{st}(v_{k+1}) \leq \mathrm{st}(v_{k+2}) \leq \mathrm{st}(v_k) \leq \mathrm{st}(v_{k+3}) \leq \mathrm{st}(v_{k-1}) \leq \ldots \leq \mathrm{st}(v_{k+1}) \leq \mathrm{st}(v_1) \quad \text{if } n = 2k+1,$$

and

$$\mathrm{st}(v_{k+1}) \geq \mathrm{st}(v_k) \geq \mathrm{st}(v_{k+2}) \geq \mathrm{st}(v_{k-1}) \geq \ldots \geq \mathrm{st}(v_{2k}) \geq \mathrm{st}(v_1) \quad \text{if } n = 2k.$$

Corollary 3.4 ([5]). *The stress of P_n is given by,*

$$\mathrm{st}(P_n) = \binom{n}{3}.$$

Observation 3.5 ([5]). *Suppose there exists an automorphism α of G such that $\alpha(v) = w$. Then P is a shortest path with v as an internal vertex if and only if $\alpha(P)$ is a shortest path with w as an internal vertex. Hence $\mathrm{st}(v) = \mathrm{st}(w)$. In particular, if G is vertex transitive, then all the vertices of G have the same stress.*

Theorem 3.6 ([5]). *For the cycle* $C_n = (v_1, v_2, ..., v_n, v_1)$,

$$\mathrm{st}(v_i) = \frac{d(d-1)}{2} \quad \textit{for all } i,$$

where $d = \mathrm{diam}(C_n) = \lfloor \frac{n}{2} \rfloor$. *Further,* $\mathrm{st}(C_n) = n\frac{d(d-1)}{2}$.

Results on the stress of graphs with diameter 2 and 3 are given in [5].

Let $v \in V$ and $\deg v \geq 2$. Let v_1 and v_2 be two nonadjacent vertices in $N(v)$. Then $P = (v_1, v, v_2)$ is a shortest path in G having v as an internal vertex. Thus every pair of nonadjacent vertices in $N(v)$ contributes 1 to the stress of v. Hence if $m(v)$ is the number of edges in the induced subgraph $G[N(v)]$, we have

$$\mathrm{st}(v) \geq \binom{\deg v}{2} - m(v) \tag{7}$$

Now let G be any graph with $\mathrm{diam}\, G = 2$. Then the eccentricity $e(v) = 1$ for any vertex v in the centre of G. Hence $\deg v = n - 1$. In this case

$$\mathrm{st}(v) \geq \binom{\deg v}{2} - m(v)$$

and thus equality holds in

$$\mathrm{st}_G(v) \geq \frac{\deg v}{2} - m(v)$$

.

Also $\mathrm{st}(v) = \binom{\deg v}{2} = \binom{n-1}{2}$ if and only if $m(v) = 0$. In this case $G = K_{1,n-1}$.

Observation 3.7. *A vertex* v *of a graph* G *is called a simplical vertex if the induced subgraph* $G[N(v)]$ *is complete. In this case* $m(v) = \binom{\deg(v)}{2}$. *Thus* $\mathrm{st}(v) = 0$ *if and only if* v *is a simplical vertex.*

Lemma 3.8 ([5]). *Let* G *be a graph of order* n *and size* m *and let* $H = G + K_1$. *Then* $\mathrm{st}(H) = \binom{m}{2} - m + s_2$ *where* s_2 *is the number of shortest paths of length* 2 *in* G.

Proof Let $V(H_1) = \{v\}$. If $u \in V(G)$ and $\deg_G u = 1$, then u is a simplicial vertex both in G and in H. Hence $\mathrm{st}_G(u) = \mathrm{st}_H(v) = 0$.

Now, let $\deg_G u \geq 2$. Since $\mathrm{diam}\, H = 2$, any contribution to $\mathrm{st}_H(u)$ is by a shortest path (v_1, u, v_2) where v_1 and v_2 are two nonadjacent vertices in $N_G(u)$. Each such shortest path contributes 1 to $\mathrm{st}_H(u)$. Hence $\sum_{u \in V(G)} \mathrm{st}_H(u) = s_2$.

Hence $\mathrm{st}(H) = \mathrm{st}_H(v) + s_2 = \binom{n}{2} - m + s_2$.

□

The following theorem is a generalization of the above lemma.

Theorem 3.9 ([5]). *Let* G *be a graph of order* n *and size* m. *Let* $H = G + \overline{K_l}$, *where* $l \geq 2$. *Then*

$$\mathrm{st}(H) = \left[\binom{n}{2} - m\right] l + \binom{l}{2} n + s_2, \tag{8}$$

where s_2 *is the number of shortest paths of length* 2 *in* G.

Using Theorem 3.3, Theorem 3.6 and Lemma 3.8, we obtain the following results.

Theorem 3.10 ([5]). *For the fan graph* $F_{n+1} = P_n + K_1$, *we have* $\mathrm{st}_{F_{n+1}}(v_1) = \mathrm{st}_{F_{n+1}}(v_n) = 0$, $\mathrm{st}_{F_{n+1}}(v_i) = 1$ *for* $2 \leq i \leq n-1$ *and* $\mathrm{st}_{F_{n+1}}(v) = \binom{n-1}{2}$. *Further,*

$$\mathrm{st}(F_{n+1}) = \frac{(n-2)(n+1)}{2}. \tag{9}$$

Corollary 3.11 ([5]). *Let $F_{n+1} = P_n + K_1$. Then the following statements hold.*

(i) $st_{F_{n+1}}(v_i) \leq st_{P_n}(v_i)$, *for all* $v_i \in V(P_n)$.
(ii) $st(F_{n+1}) < st(P_n)$, *for* $n \geq 5$.

Theorem 3.12 ([5]). *For the wheel $W_{n+1} = C_n + K_1$, we have* $\mathrm{st}_{W_{n+1}}(v) = \frac{n(n-3)}{2}$ *and* $\mathrm{st}_{W_{n+1}}(v_i) = 1$ *for all* $1 \leq i \leq n$. *Also*

$$\mathrm{st}(W_{n+1}) = \binom{n}{2}. \tag{10}$$

Corollary 3.13 ([5]). *Let $W_{n+1} = C_n + K_1$. Then the following statements hold.*

(i) $\mathrm{st}_{W_{n+1}}(v_i) \leq \mathrm{st}_{C_n}(v_i)$, *for all* $v_i \in V(C_n)$.
(ii) $\mathrm{st}(W_{n+1}) < \mathrm{st}(C_n)$, *for* $n \geq 6$.

Raksha et al. [6] computed the stress of several families of wheel related graphs. Let $W_{n+1} = C_n + x$ where $C_n = (w_1, w_2, \cdots, w_n, w_1)$ is a cycle of order n. The vertex x is called the central vertex of W_{n+1}.

Definition 3.14. *The graph obtained from W_n by subdividing each edge w_iw_{i+1} of C_n by introducing a new vertex u_i is called the gear graph and is denoted by G_n.*

Definition 3.15. *The helm graph is the graph H_n obtained from the wheel W_n by attaching a pendant vertex u_i adjacent to w_i.*

Definition 3.16. *The friendship graph F_n is a graph obtained from W_{2n} by removing a perfect matching from C_n.*

Definition 3.17. *The flower graph Fl_n is the graph obtained from the wheel W_n, by adding the vertices $\{u_1, u_2, \ldots, u_n\}$ where each u_i is adjacent to w_i and x.*

Definition 3.18. *The sunflower graph SF_n is the graph obtained from the wheel by adding the vertices $\{u_1, u_2, \ldots, u_n\}$ where each u_i is adjacent to w_i and w_{i+1}.*

Theorem 3.19 ([6]). *Let G_n be the gear graph. Then*

$$\mathrm{st}(v) = \begin{cases} \frac{3n}{2}(3n-7) & \text{if } v = x \\ 7 & \text{if } v = w_i \text{ and } n = 3 \\ 3(2n-3) & \text{if } v = w_i \text{ and } n \geq 4 \\ 3 & \text{if } v = u_i \text{ and } n = 3 \\ 4 & \text{if } v = u_i \text{ and } n \geq 4. \end{cases}$$

Corollary 3.20 ([6]). *The stress sequence of the gear graph G_n is given by,* $(7, 7, 7, 7, 3, 3, 3)$ *if* $n = 4$ *and*

$$\left(\frac{3n}{2}(n-1), \underbrace{3(2n-3), \ldots, 3(2n-3)}_{n \text{ times}}, \underbrace{4, 4, 4, \ldots, 4}_{n \text{ times}}\right) \text{ if } n \geq 5.$$

The corresponding ordering of the vertices is $(x, w_1, w_2, \ldots, w_n, u_1, u_2, \ldots, u_n)$.

Corollary 3.21 ([6]). *The stress of the gear graph G_n is given by*

$$\mathrm{st}(G_n) = \begin{cases} 39 & \text{if } n = 3, \\ \frac{n}{2}[21n - 31] & \text{otherwise.} \end{cases}$$

Theorem 3.22 ([6]). *Let H_n be the helm graph. Then*

$$\mathrm{st}(v) = \begin{cases} 2n(n-3) & \text{if } v = x \\ 5 & \text{if } v = w_i \text{ and } n = 3 \\ 2n+7 & \text{if } v = w_i \text{ and } n \geq 4 \\ 0 & \text{if } v = u_i \end{cases}$$

Corollary 3.23 ([6]). *The stress sequence of the Helm graph H_n is given by,*

$$\begin{cases} (18, 5, 5, 5, 0, 0, 0) & \text{if } n = 3 \\ (15, 15, 15, 15, 8, 0, 0, 0, 0) & \text{if } n = 4 \\ (2n(n-4), \underbrace{2n+7, \ldots, 2n+7}_{n \text{ times}}, \underbrace{0, 0, \ldots, 0}_{n \text{ times}}) & \text{if } n \geq 5 \end{cases}$$

The corresponding ordering of the vertices is $(x, w_1, w_2, \ldots, w_n, u_1, u_2, \ldots, u_n)$ if $n \neq 4$ and $(w_1, w_2, w_3, w_4, x, u_1, u_2, u_3, u_4)$ if $n = 4$.

Corollary 3.24 ([6]). *The stress of the helm graph H_n is given by*

$$\mathrm{st}(H_n) = \begin{cases} 15 & \text{if } n = 3, \\ n(4n+1) & \text{otherwise.} \end{cases}$$

Theorem 3.25 ([6]). *Let F_n be the friendship graph. Then*

$$\mathrm{st}(v) = \begin{cases} 2n(n-1) & \text{if } v = x \\ 0 & \text{otherwise} \end{cases}$$

Corollary 3.26 ([6]). *The stress sequence of the friendship graph F_n is given by*

$$(2n(n-1), \underbrace{0, 0, \ldots, 0}_{2n \text{ times}})$$

.

The corresponding ordering of the vertices is $(x, w_1, w_2, \ldots, w_{2n})$.

Corollary 3.27 ([6]). *The stress of the friendship graph F_n is given by*

$$\mathrm{st}(F_n) = 2n(n-1).$$

Theorem 3.28 ([6]). *Let Fl_n be the flower graph. Then*

$$\mathrm{st}(v) = \begin{cases} n(2n-3) & \text{if } v = x \\ 1 & \text{if } v = w_i \text{ and } n = 3 \\ 3 & \text{if } v = w_i \text{ and } n \geq 4 \\ 0 & \text{if } v = u_i \end{cases}$$

Corollary 3.29 ([6]). *The stress sequence of the flower graph Fl_n is given by* $(9,1,1,1,0,0,0)$ *if* $n=3$ *and*

$$\left(n(2n-3),\underbrace{3,3,\ldots,3}_{n\ times},\underbrace{0,0,\ldots,0}_{n\ times}\right) \text{ if } n\geq 4.$$

The corresponding ordering of the vertices is $(x,w_1,w_2,\ldots,w_n,u_1,u_2,\ldots,u_n)$.

Corollary 3.30 ([6]). *The stress of the flower graph Fl_n is given by*

$$\mathrm{st}(Fl_n)=\begin{cases}12 & \text{if } n=3\\ 2n^2 & \text{otherwise.}\end{cases}$$

Theorem 3.31 ([6]). *Let SF_n be the sunflower graph. Then*

$$\mathrm{st}(x)=\begin{cases}0 & \text{if } n=3\\ 2 & \text{if } n=4\\ \frac{n}{2}(9n-39) & \text{otherwise.}\end{cases} \tag{11}$$

$$\mathrm{st}(w_i)=\begin{cases}5 & \text{if } n=3\\ 8 & \text{if } n=4\\ 14 & \text{if } n=5\\ 6n-13 & \text{otherwise.}\end{cases} \tag{12}$$

$$\mathrm{st}(u_i)=0. \tag{13}$$

Corollary 3.32 ([6]). *The stress sequence of the sunflower graph SF_n is given by*

$$\begin{cases}(5,5,5,0,0,0,0) & \text{if } n=3\\ (8,8,8,8,2,0,0,0,0) & \text{if } n=4\\ (15,14,14,14,14,14,0,0,0,0,0,0) & \text{if } n=5\\ \left(\frac{n}{2}(3n-39),\underbrace{6n-13,\ldots,6n-13}_{n\ times},\underbrace{0,\ldots,0}_{n\ times}\right) & \text{if } n\geq 6\end{cases}$$

The corresponding ordering of the vertices is $(x,w_1,w_2,\ldots,w_n,u_1,u_2,\ldots,u_n)$ *if* $n\geq 5$ *and* $(w_1,w_2,\ldots,w_n,x,u_1,u_2,\ldots,u_n)$ *if* $n=3$ *or* 4.

Corollary 3.33 ([6]). *The stress of the sunflower graph SF_n is given by*

$$\mathrm{st}(SF_n)=\begin{cases}15 & \text{for } n=3\\ 34 & \text{for } n=4\\ 85 & \text{for } n=5\\ \frac{3n}{2}(7n-23) & \text{otherwise.}\end{cases} \tag{14}$$

We now proceed to consider graphs G with diameter 3. For any vertex v, let $N_2(v)=\{u\in V : d(u,v)=2\}$.

Let $S(v)=\{xy : xy\in E,\ x\in N_2(v) \text{ and } y\in N(v)\}$.

For any $xy\in S(v)$, let $T(xy)=\{z\in N(v) : d(x,z)=3\}$. Let $k(xy)=|T(xy)|$.

Theorem 3.34 ([5]). *Let G be a graph with diameter 3 and let $v \in V$. Then*

$$\mathrm{st}(v) = \binom{degv}{2} - m(v) + \sum_{xy \in S(v)} k(xy)$$

Example 3.35. *Consider the bistar $G = B_{r,s}$ with $V(G) = \{u, v, u_1, u_2, \ldots, u_r, v_1, v_2, \ldots, v_s\}$, $N(u) = \{v, u_1, \ldots, u_r\}$ and $N(v) = \{u, v_1, \ldots, v_s\}$. Clearly G is a tree with diameter 3. Also $\mathrm{st}(u) = \binom{r+1}{2} + sr$; $\mathrm{st}(v) = \binom{s+1}{2} + sr$ and $\mathrm{st}(w) = 0$ for all $w \neq u, v$. Hence, $\mathrm{st}(G) = \binom{r+1}{2} + \binom{s+1}{2} + 2sr$.*

A connected graph G with at least one cut vertex v is called a separable graph. Since $G - v$ is a disconnected graph, a cut vertex v is an important vertex which holds together several blocks of G. In [5], the authors have determined the stress of a cut vertex of a separable graph with one or two cut vertices.

Theorem 3.36 ([5]). *Let G be a connected graph with a unique cut vertex v. Let $B_1, B_2, \ldots, B_k$ be the blocks of G. Let t_i denote the number of shortest paths in B_i having v as origin. Then*

$$\mathrm{st}_G(v) = \sum_{i=1}^{k} \mathrm{st}_{B_i}(v) + \sum_{\substack{i,j=1 \\ i \neq j}}^{k} t_i t_j.$$

Theorem 3.37 ([5]). *Let G be a connected graph with exactly two cut vertices v and w. Let $B_1, B_2, \ldots, B_r, D_1, D_2, \ldots, D_s$ and H be the blocks in G such that*

(i) $v \in V(B_i)$ *and* $w \notin V(B_i), 1 \leq i \leq r$
(ii) $w \in V(D_j)$ *and* $v \notin V(D_j), 1 \leq j \leq s$
(iii) $v, w \in V(H)$.

Let l_i and l denote respectively the number of shortest paths in B_i and in H having v as origin. Let k_i and k denote respectively the number of shortest paths in D_j and in H having w as origin. Let t denote the number of shortest v-w paths in H. Then

$$\mathrm{st}_G(v) = \mathrm{st}_H(v) + \sum_{i=1}^{r} \mathrm{st}_{B_i}(v) + \sum_{\substack{i,j=1 \\ i \neq j}}^{r} l_i l_j + l \sum_{i=1}^{r} l_i + t \sum_{i=1}^{r} \sum_{j=1}^{s} l_i k_j$$

and

$$\mathrm{st}_G(w) = \mathrm{st}_H(w) + \sum_{j=1}^{s} \mathrm{st}_{D_j}(w) + \sum_{\substack{i,j=1 \\ i \neq j}}^{s} k_i k_j + k \sum_{j=1}^{s} k_i + t \sum_{i=1}^{r} \sum_{j=1}^{s} l_i k_j.$$

The friendship graph G_n has one cut vertex v and having n blocks, where each block is a K_3. Clearly $\mathrm{st}(v) > 0$ and $\mathrm{st}(w) = 0$ for all $w \neq v$. The star graph $K_{1,n}$ also has this property. The following theorem characterizes all connected graphs which contains a unique vertex with nonzero stress

Theorem 3.38 ([5]). *Let G be a connected graph of order n. Then there exists a vertex $v \in V$ such that $\mathrm{st}(v) > 0$ and $\mathrm{st}(w) = 0$ for all $w \in V - \{v\}$ if and only if G is a block graph with v as its unique cut vertex.*

Definition 3.39. *A graph G is called a vertex transitive graph if for any two vertices u and v there exists an automorphism α of G such that $\alpha(u) = v$.*

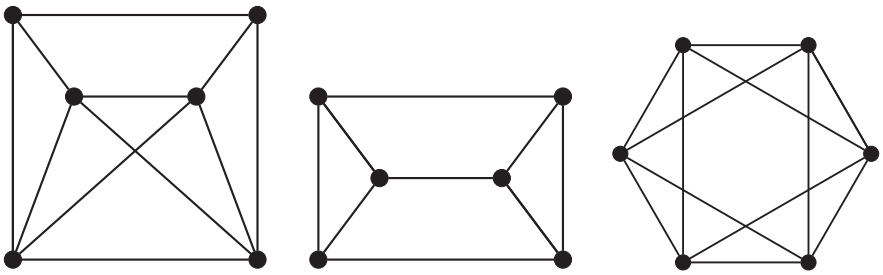
Clearly, P is a shortest path in G having u as an internal vertex if and only if $\alpha(P)$ is a shortest path having v as an internal vertex. Hence it follows that $\mathrm{st}(u) = \mathrm{st}(v)$. Thus in a vertex transitive graph G, all the vertices of G have the same stress.

Definition 3.40. *A graph G is called $k-$stress regular if $\mathrm{st}(v) = k$ for all $v \in V$.*

Clearly a graph G is $0-$stress regular if and only if $G = K_n$. Bhargava et al. [1] obtained a characterization of $1-$stress regular and $2-$stress regular graphs.

Theorem 3.41 ([1])**.** *A graph G is $1-$stress regular if and only if $G = C_4$ or C_5.*

Theorem 3.42 ([1])**.** *A graph G is $2-$stress regular if and only if G is isomorphic to one of the graphs G_1, G_2, G_3 given in Fig 2.*



G_1 G_2 G_3

Fig. 2 $2-$ stress regular graphs

Problem 3.43. *Characterize $k-$stress regular graphs for $k \geq 3$.*

Entriger et al [3] have proved that among all trees of order n, the star $K_{1,n-1}$, has minimum Weiner index and the path P_n has maximum Weiner index. In general, given a family $\mathcal{F}$ of graphs of order n and a graph theoretic parameter η, it is natural to investigate which graphs in $\mathcal{F}$ have minimum value of η and which graphs in $\mathcal{F}$ have maximum value of η. Raksha et al [5] investigated this problem for stress.

Let $\mathcal{F}$ be a family of graphs of order n and let η be a graph theoretic parameter. Let $G_{\min}(\mathcal{F})$ and $G_{\max}(\mathcal{F})$ be the subfamilies of $\mathcal{F}$ for which η is minimum and maximum respectively.

Theorem 3.44. *Let $\mathcal{F}$ be the family of all trees of order $n \geq 4$. For the parameter $\mathrm{st}(G)$ we have*

(i) $G_{\max}(\mathcal{F}) = \{P_n\}$
(ii) $G_{\min}(\mathcal{F}) = \{K_{1,n-1}\}$.

Theorem 3.45. *Let $\mathcal{F}$ be the family of all complete bipartite graphs of order n. For the parameter $\mathrm{st}(G)$, we have*

(i) $G_{\max}(\mathcal{F}) = \{K_{r,s} : |r - s| = 1 \text{ or } 0\}$
(ii) $G_{\min}(\mathcal{F}) = \{K_{1,n-1}\}$.

Problem 3.46. *For the parameter stress and for families $\mathcal{F}$ of graphs of order n such as complete multipartite graphs, chordal graphs, unicyclic graphs and split graphs, determine $G_{\max}(\mathcal{F})$ and $G_{\min}(\mathcal{F})$.*

4 Computation of Stress

In [7] the authors have used the adjacency matrix of a graph as an effective tool to compute the stress of a vertex and presented an algorithm for the same. Let $P(u,v)$ denote the set of all shortest $u-v$ paths and $P_w(u,v)$ denote the set of all shortest $u-v$ paths, having w as an internal vertex. Let $G=(V,E)$ be a connected graph of order n and let $V=\{v_1,v_2,\ldots,v_n\}$. The adjacency matrix $A(G)=(a_{ij})$ is the $n\times n$ matrix defined by

$$a_{ij}=\begin{cases}1 & \text{if } v_i \text{ and } v_j \text{ adjacent}\\ 0 & \text{otherwise.}\end{cases} \tag{15}$$

It follows Theorem 1.1 that the $(i,j)^{th}$ entry of A^k is the number of v_i-v_j walks of length k in G.

The distance matrix $D=(d_{ij})$ is the $n\times n$ matrix where $d_{ij}=d(v_i,v_j)$.

The shortest path matrix $N=(\eta_{ij})$ is the $n\times n$ matrix where η_{ij} is the number of shortest v_i-v_j paths. We adopt the convention that $\eta_{ii}=1$. Thus $\eta_{ij}=|P(v_i,v_j)|$.

The following lemma gives the stress of any vertex in terms of the entries of N.

Lemma 4.1 ([7]). *If G is a connected graph with $N(G)=(\eta_{ij})$, then for any vertex $v_k\in V(G)=\{v_1,v_2,\ldots,v_n\}$,*

$$\mathrm{st}_G(v_k)=\sum_{\substack{1\le i,j\le n\\ i<j,i,j\neq k\\ d(v_i,v_k)+d(v_k,v_j)=d(v_i,v_j)}}\eta_{ik}\eta_{kj}. \tag{16}$$

It follows Theorem 1.1 that the $(i,j)^{th}$ entry of A^k is the number of v_i-v_j walks of length k. In particular, if p is the least positive integer such that $(i,j)^{th}$ entry of A^p is nonzero, then $d(v_i,v_j)=p$ and $(A^p)_{ij}=\eta_{ij}$. Hence the shortest path matrix $N=(\eta_{ij})$ is given by

$$\eta_{ij}=\begin{cases}1 & \text{if } i=j\\ (A^p)_{ij} & \text{otherwise}\end{cases} \tag{17}$$

where p is the least positive integer for which the $(i,j)^{th}$ entry of A^p is nonzero. Now, the following theorem is immediate.

Theorem 4.2 ([7]). *If G is a graph with adjacency matrix A, then for any vertex $v_k\in V(G)=\{v_1,v_2,\ldots,v_n\}$,*

$$\mathrm{st}_G(v_k)=\sum_{\substack{i,j=1\\ i<j,i,j\neq k\\ d(v_i,v_k)+d(v_k,v_j)=d(v_i,v_j)}}^{n}\eta_{ik}\eta_{kj}, \tag{18}$$

where

$$\eta_{ij}=\begin{cases}1 & \textit{for } i=j\\ (A^p)_{ij} & \textit{otherwise}\end{cases}$$

and p is the least integer for which the ijth entry of A^p is nonzero.

Also from the definition of betweenness centrality and Lemma 4.1, we have the following theorem which gives an expression to compute the betweenness centrality of a vertex.

Theorem 4.3 ([7]). *If G is a graph with adjacency matrix A, then for any vertex $v_k \in V(G) = \{v_1, v_2, \ldots, v_n\}$, the betweenness centrality of v_k is given by*

$$C_B(v_k) = \sum_{\substack{i,j=1 \\ i<j, i,j\neq k \\ d(v_i,v_k)+d(v_k,v_j)=d(v_i,v_j)}}^{n} \frac{\eta_{ik}\eta_{kj}}{\eta_{ij}}, \tag{19}$$

where

$$\eta_{ij} = \begin{cases} 1 & \text{for } i = j \\ (A^p)_{ij} & \text{otherwise} \end{cases}$$

and p is the least integer for which the ijth entry of A^p is nonzero.

It follows from Theorem 4.2 and Theorem 4.3 the stress $\mathrm{st}(v)$ and betweenness centrality $C_B(v)$ of any vertex v can be computed using the entries of the powers of the adjacency matrix A. Exploiting this idea, in [7], the authors have presented algorithms for computing $\mathrm{st}(v)$ and $C_B(v)$ in any connected graph and the time complexity of the algorithm is $\mathcal{O}(m^4)$ where $m = |E(G)|$. For further details interested readers may refer to [7].

In [7], the authors have used Theorem 4.2 for computing the stress of vertices in the Cartesian product and corona of two graphs.

Definition 4.4. *The Cartesian product of two graphs G and H, denoted by $G\Box H$, is a graph with vertex set $V(G) \times V(H)$, where two vertices (u_1, v_1) and (u_2, v_2) are adjacent if $u_1 = u_2$ and $v_1v_2 \in E(H)$ or $v_1 = v_2$ and $u_1u_2 \in E(G)$.*

Theorem 4.5 ([7]). *For any connected graphs G and H, the stress of a vertex (u_i, v_j) in $G\Box H$ is given by*

$$\begin{aligned} \mathrm{st}_{G\Box H}(u_i, v_j) = \frac{1}{2} \sum & \left[\binom{d_G(u_i, u_{i1}) + d_H(v_j, v_{j1})}{d_G(u_i, u_{i1})} \eta^G_{ii_1} \eta^H_{jj_1} \right] \\ & \times \left[\binom{d_G(u_i, u_{i2}) + d_H(v_j, v_{j2})}{d_G(u_i, u_{i2})} \eta^G_{ii_2} \eta^H_{jj_2} \right] \end{aligned} \tag{20}$$

where the summation is taken over all pairs of vertices (u_{i1}, v_{j1}) and (u_{i2}, v_{j2}) different from (u_i, v_j) in $G\Box H$ satisfying $d_G(u_{i1}, u_i) + d_G(u_i, u_{i2}) = d_G(u_{i1}, u_{i2})$ and $d_H(v_{j1}, v_j) + d_H(v_j, v_{j2}) = d_H(v_{j1}, v_{j2})$

Theorem 4.6 ([7]). *If $P_2 = (u_1, u_2)$ and $P_n = (v_1, v_2, \ldots, v_n)$ are paths of length 1 and $n-1$, respectively, then the stress of any vertex (u_i, v_j) in the ladder graph $L_n = P_2\Box P_n$ is given by,*

$$\begin{aligned} \mathrm{st}_{P_2\Box P_n}(u_i, v_j) = (j-1)(n-j) + \frac{(j-1)(n-j+1)(n-j+2)}{2} + \\ \frac{(n-j)j(j+1)}{2} \end{aligned} \tag{21}$$

Definition 4.7. *The corona $G \circ H$ of two graphs G and H is defined as the graph obtained by taking one copy of G and $|V(G)|$ copies of H, and joining by an edge each vertex of ith copy of H with the ith vertex of G.*

Theorem 4.8 ([7]). *Let G be a graph with vertices $v_1, v_2, \ldots, v_m$ and let $w^i_1, w^i_2, \ldots, w^i_n$ be the vertices in the ith copy of the graph H in $G \circ H$. Then*

$$\mathrm{st}_{G\circ H}(w^i_j) = \mathrm{st}_{u+H}(w_j); \quad 1 \le i \le m, 1 \le j \le m \tag{22}$$

$$\mathrm{st}_{G\circ H}(v_i) = (n^2+n+1)\,\mathrm{st}_G(v_i) + \mathrm{st}_{v_i+H}(v_i) + (n^2+n)\sum_{\substack{j=1\\ j\neq i}}^{m}\eta_{ij}^G. \tag{23}$$

where η_{ij} is the ijth entry of the shortest path matrix $N(G)$ of G and $u+H$ is the join graph obtained by adding a vertex u adjacent to all the vertices of H.

5 Applications

Understanding the significance of each vertex of a graph from different perspectives plays an important role in analyzing biological and social networks. In this context centrality measures are extensively used for ranking the vertices and those vertices with centrality measure greater than a prefixed threshold value are taken as important vertices. For instance, suppose the vertices of a graph are ranked independently using eight centrality measures cm_i, $1 \leq i \leq 8$. Let S_i be the set of all important vertices with respect to cm_i. Then $S = \bigcap_{i=1}^{8} S_i$ is the set of vertices which are important with respect to all the eight centrality measures. The authors in [10] and [11] adopted this approach for production of drug target varicella zoster on human host and for identification of the role of potassium transporter in Barley respectively. For a detailed account of biological network analysis using the software Cytoscape, we refer to [12] and [13]. Patota et al.[4] introduced DAFNES, a distributed algorithm that leverages stress to optimize energy use in communication networks.

6 Conclusion and Scope

A centrality measure assigns a real number to each vertex of a graph and it quantifies the importance or criticality of a vertex from a particular perspective. Different centrality measures describe the importance of a vertex from different perspectives. Betweenness centrality and closeness indicate the efficiency of a vertex in information flow within a network. The stress indicates the relevance of a vertex in holding together communicating vertices. Centrality measures are used to rank the vertices of a graph. In this paper we have presented a survey of significant results on stress of a vertex. The following are challenging problems for further investigation.

Problem 6.1. *Let $\Pi = (a_1 \geq a_2 \geq \ldots a_n)$ be a sequence of non-negative integers. Then Π is called a stress sequence if there exists a graph G of order n such that $a_i = \mathrm{st}(v_i)$, $1 \leq i \leq n$. Obtain necessary or sufficient condition for Π to be a stress sequence.*

Problem 6.2. *Let Π be a stress sequence. A graph G whose stress sequence is Π is called a realization of Π. Characterize stress sequences having a unique realization.*

Stress regular graphs are significant in the context of networks since all vertices are equally important in the communication process within the network.

Problem 6.3. *Characterize k- stress regular graphs for $k \geq 3$.*

In [5], the authors have investigated computation of stress in graphs with diameter 2 or 3.

Problem 6.4. *Compute the stress sequence of a graph G with diameter at least 4.*

Determining graphs with minimum or maximum stress in a given family of graphs of order n is an interestig problem. This problem has been investigated for the family of all trees of order n and for the family of complete bipartite graphs of oder n.

Problem 6.5. *Determine graphs with minimum or maximum stress in other families of graphs of order n such as unicyclic graphs, split graphs, complete multipartite graphs and chordal graphs.*

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Two New Lower Bounds for the First Zagreb Index and Some Hamiltonian Properties of Graphs

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Abstract

The first Zagreb index of a graph G is defined as $\sum_{u\in V} d_G^2(u)$, where $d_G(u)$ is the degree of vertex u in G. Using Wagner's inequality, we first obtain two new lower bounds for the first Zagreb index of a graph. We further present sufficient conditions for some Hamiltonian properties of graphs via utilizing the ideas of obtaining one of the two lower bounds.

Keywords: First Zagreb index, Hamiltonian graph, Traceable graph
AMS Classification: 05C45, 05C09

1 Introduction

We consider only finite undirected graphs without loops or multiple edges. Notation and terminology not defined in this paper follow those in [2]. Let $G = (V(G), E(G))$ be a graph. We use n and e to denote the number of vertices and the number of edges in G, respectively. The degree of a vertex u in G is represented by $d_G(u)$. We use $\delta = d_1 \leq d_2 \leq \cdots \leq d_n = \Delta$ to denote the degree sequence of a graph G. A subset of $V(G)$ in a graph G is an independent set if any two vertices in the subset are not adjacent. An independent set in a graph G is called a maximum independent set if its size is as large as possible. The independence number, denoted $\beta(G)$, of a graph G is defined as the size of a maximum independent set in G. For two disjoint vertex subsets A and B of $V(G)$, we define $E(A, B)$ as the set of all the edges in $E(G)$ such that one end vertex of each edge is in A and another end vertex of the edge is in B. Namely, $E(A, B) := \{\, e : e = ab \in E, a \in A, b \in B \,\}$. We also use $K_{p,\,q}$ to denote a complete bipartite graph with two partition sets X and Y such that $|X| = p$ and $|Y| = q$. A cycle C in a graph G is a Hamilton cycle of G if all the vertices of G are on C. A graph G is called Hamiltonian if G contains a Hamilton cycle. A path P in a graph G is a Hamilton path of G if all the vertices of G are on P. A graph G is called traceable if G contains a Hamilton path.

The first Zagreb index of a graph was introduced by Gutman and Trinajstić in [7]. See also [6]. For a graph G, its first Zagreb index, denoted $Z_1(G)$, is defined as $\sum_{u\in V(G)} d_G^2(u)$. As one of the most important topological indices of a graph, the first Zagreb index has been intensively investigated since its introduction. Many results on the first Zagreb index of a graph have been obtained. The survey paper [3] and the references therein are good resources for the results. Using Wagner's inequality, we in this paper obtain two new lower bounds for the first Zagreb index of a graph.

Recently, a lot of sufficient conditions based on the first Zagreb index for some Hamiltonian properties have been obtained. Some of them can be found in [1], [9], [10], [11], [12], [13], [14], and [15]. Using the ideas of obtaining one of the two lower bounds for the first Zagreb index of a graph, we further present sufficient conditions for Hamiltonian graphs and traceable graphs. Below are the results of this paper.

Theorem 1. Let G be a graph with n vertices and e edges. Suppose θ is real number with $0 \leq \theta \leq 1$. Then

$$Z_1(G) \geq \frac{4e^2(1+\theta(n-1))}{n} - \theta n(n-1)\Delta^2$$

with equality if and only if G is a regular graph.

Theorem 2. Let G be a connected graph with $n \geq 2$ vertices and e edges. Suppose β is the independence number of G and θ is real number with $0 \leq \theta \leq 1$. Then

$$Z_1(G) \geq \beta\delta^2 + \frac{e^2(1+\theta(n-\beta-1))}{n-\beta} - \theta(n-\beta)(n-\beta-1)\Delta^2$$

with equality if and only if G is in $\{ H : H$ is a bipartite graph with partition sets of A and $V-A$ such that $|A| = \beta$, $d(u) = \delta$ for each vertex $u \in A$ and $d(v) = \Delta$ for each vertex $v \in V - A \}$.

Theorem 3. Let G be a k-connected ($k \geq 2$) graph with $n \geq 3$ vertices and e edges. Suppose θ is real number with $0 \leq \theta \leq 1$.
If

$$Z_1(G) \leq (k+1)\delta^2 + \frac{e^2(1+\theta(n-k-2))}{n-k-1} - \theta(n-k-1)(n-k-2)\Delta^2,$$

then G is Hamiltonian or G is $K_{k,\,k+1}$.

Theorem 4. Let G be a k-connected ($k \geq 1$) with $n \geq 9$ vertices and e edges. Suppose θ is real number with $0 \leq \theta \leq 1$.
If

$$Z_1(G) \leq (k+2)\delta^2 + \frac{e^2(1+\theta(n-k-3))}{n-k-2} - \theta(n-k-2)(n-k-3)\Delta^2,$$

then G is traceable or G is $K_{k,\,k+2}$.

2 Lemmas

We will use some existing results as our lemmas. Lemma 1 below is Wagner's inequality [17] (see also Theorem 2.56 on Page 22 in [5]).

Lemma 1 [17] [5]. Let a_k and b_k $(k = 1, 2, \cdots, s)$ be real numbers. Suppose θ is a real number with $0 \leq \theta \leq 1$. Then

$$\left(\sum_{k=1}^{s} a_k b_k + \theta \sum_{i \neq j} a_i b_j\right)^2 \leq \left(\sum_{k=1}^{s} a_k^2 + 2\theta \sum_{i<j} a_i a_j\right)\left(\sum_{k=1}^{s} b_k^2 + 2\theta \sum_{i<j} b_i b_j\right).$$

The next two results are from [4].

Lemma 2 [4]. Let G be a k-connected graph of order $n \geq 3$. If $\beta \leq k$, then G is Hamiltonian.

Lemma 3 [4]. Let G be a k-connected graph of order n. If $\beta \leq k+1$, then G is traceable.

Lemma 4 below is from [16].

Lemma 4 [16]. Let G be a balanced bipartite graph of order $2n$ with bipartition (A, B). If $d(x) + d(y) \geq n + 1$ for any $x \in A$ and any $y \in B$ with $xy \notin E$, then G is Hamiltonian.

Lemma 5 below is from [8].

Lemma 5 [8] Let G be a 2-connected bipartite graph with bipartition (A, B), where $|A| \geq |B|$. If each vertex in A has degree at least s and each vertex in B has degree at least t, then G contains a cycle of length at least $2\min(|B|, s + t - 1, 2s - 2)$.

3 Proofs

Proof of Theorem 1. Let $G = (V, E)$ be a graph with n vertices and e edges, where $V := \{ v_1, v_2, ..., v_n \}$. Suppose θ is real number with $0 \leq \theta \leq 1$. Applying Lemma 1 with $s = n$, $a_i = d(v_i)$ and $b_i = 1$ for each $i = 1, 2, ..., n$, we have that

$$\left(\sum_{i=1}^{n} d(v_i) * 1 + \theta \sum_{1 \leq i \neq j \leq n} d(v_i) * 1 \right)^2$$

$$\leq \left(\sum_{i=1}^{n} d^2(v_i) + 2\theta \sum_{1 \leq i < j \leq n} d(v_i) * d(v_j) \right) \left(\sum_{i=1}^{n} 1^2 + 2\theta \sum_{1 \leq i < j \leq n} 1 * 1 \right)$$

$$\leq \left(\sum_{i=1}^{n} d^2(v_i) + 2\theta \sum_{1 \leq i < j \leq n} \Delta * \Delta \right) (n + \theta n(n-1))$$

$$= (Z_1(G) + \theta n(n-1)\Delta^2)(n + \theta n(n-1)).$$

Thus

$$4e^2 \left(1 + \theta(n-1)\right)^2$$

$$= \left(\sum_{i=1}^{n} d(v_i) \right)^2 \left(1 + \theta(n-1)\right)^2$$

$$= \left(\sum_{i=1}^{n} d(v_i) * 1 + \theta \sum_{1 \leq i \neq j \leq n} d(v_i) * 1 \right)^2$$

$$\leq (Z_1(G) + \theta n(n-1)\Delta^2)(n + \theta n(n-1)).$$

Therefore

$$Z_1(G) \geq \frac{4e^2(1 + \theta(n-1))}{n} - \theta n(n-1)\Delta^2.$$

Suppose

$$Z_1(G) = \frac{4e^2(1 + \theta(n-1))}{n} - \theta n(n-1)\Delta^2.$$

In reviewing of the proofs above, we have that $d(v) = \Delta$ for each $v \in V$. Thus G is a regular graph.

If G is a regular graph, a simple computation shows that

$$Z_1(G) = \frac{4e^2(1 + \theta(n-1))}{n} - \theta n(n-1)\Delta^2.$$

This completes the proof of Theorem 1.

Notice that if $\theta = 0$ in Theorem 1 then we have that $Z_1(G) \geq \frac{4e^2}{n}$, a well-known lower bound for $Z_1(G)$.

Proof of Theorem 2. Let G be a connected graph with $n \geq 2$ vertices and e edges. Suppose $I := \{ u_1, u_2, ..., u_\beta \}$ is a maximum independent set in G. Since $n \geq 2$ and G is connected, we have that $\beta < n$. Set $V - I = \{ v_1, v_2, ..., v_{n-\beta} \}$. Clearly,

$$\sum_{u \in I} d(u) = |E(I, V - I)| \leq \sum_{v \in V - I} d(v).$$

Since $\sum_{u \in I} d(u) + \sum_{v \in V - I} d(v) = 2e$, we have that

$$\sum_{u \in I} d(u) \leq e \leq \sum_{v \in V - I} d(v).$$

Applying Lemma 1 with $s = (n-\beta)$, $a_i = d(v_i)$ and $b_i = 1$ for each $i = 1, 2, ..., (n-\beta)$, we have that

$$\left(\sum_{i=1}^{n-\beta} d(v_i) * 1 + \theta \sum_{1 \leq i \neq j \leq (n-\beta)} d(v_i) * 1 \right)^2$$

$$\leq \left(\sum_{i=1}^{n-\beta} d^2(v_i) + 2\theta \sum_{1 \leq i < j \leq (n-\beta)} d(v_i) * d(v_j) \right) \left(\sum_{i=1}^{n-\beta} 1^2 + 2\theta \sum_{1 \leq i < j \leq (n-\beta)} 1 * 1 \right)$$

$$\leq \left(\sum_{i=1}^{n-\beta} d^2(v_i) + 2\theta \sum_{1 \leq i < j \leq (n-\beta)} \Delta * \Delta \right) ((n-\beta) + \theta(n-\beta)(n-\beta-1))$$

$$\leq \left(\sum_{i=1}^{n-\beta} d^2(v_i) + \theta(n-\beta)(n-\beta-1)\Delta^2 \right) ((n-\beta) + \theta(n-\beta)(n-\beta-1)).$$

Thus

$$e^2 \left(1 + \theta(n-\beta-1)\right)^2$$

$$\leq \left(\sum_{i=1}^{n-\beta} d(v_i) \right)^2 \left(1 + \theta(n-\beta-1)\right)^2$$

$$= \left(\sum_{i=1}^{n-\beta} d(v_i) * 1 + \theta \sum_{1 \leq i \neq j \leq (n-\beta)} d(v_i) * 1 \right)^2$$

$$\leq \left(\sum_{i=1}^{n-\beta} d^2(v_i) + \theta(n-\beta)(n-\beta-1)\Delta^2 \right) ((n-\beta) + \theta(n-\beta)(n-\beta-1)).$$

Therefore

$$\sum_{i=1}^{n-\beta} d^2(v_i) \geq \frac{e^2(1 + \theta(n-\beta-1))}{n-\beta} - \theta(n-\beta)(n-\beta-1)\Delta^2.$$

Hence

$$Z_1(G) = \sum_{i=1}^{\beta} d^2(u_i) + \sum_{i=1}^{n-\beta} d^2(v_i)$$

$$\geq \beta\delta^2 + \frac{e^2(1 + \theta(n-\beta-1))}{n-\beta} - \theta(n-\beta)(n-\beta-1)\Delta^2.$$

Suppose

$$Z_1(G) = \sum_{i=1}^{\beta} d^2(u_i) + \sum_{i=1}^{n-\beta} d^2(v_i)$$

$$= \beta\delta^2 + \frac{e^2(1+\theta(n-\beta-1))}{n-\beta} - \theta(n-\beta)(n-\beta-1)\Delta^2.$$

In reviewing of the proofs above, we have that $\sum_{i=1}^{n-\beta} d(v_i) = e$ which implies $\sum_{u\in I} d(u) = e$ and G is a bipartite graph with partition sets of I and $V-I$ such that $|I| = \beta$. We further have that $d(u) = \delta$ for each vertex $u \in I$ and $d(v) = \Delta$ for each vertex $v \in V - I$. Thus $G \in \{ H : H$ is a bipartite graph with partition sets of A and $V - A$ such that $|A| = \beta$, $d(u) = \delta$ for each vertex $u \in A$ and $d(v) = \Delta$ for each vertex $v \in V - A \}$.

If $G \in \{ H : H$ is a bipartite graph with partition sets of A and $V - A$ such that $|A| = \beta$, $d(u) = \delta$ for each vertex $u \in A$ and $d(v) = \Delta$ for each vertex $v \in V - A \}$, then $e = (n-\beta)\Delta$. A simple computation shows that

$$Z_1(G) = \beta\delta^2 + \frac{e^2(1+\theta(n-\beta-1))}{n-\beta} - \theta(n-\beta)(n-\beta-1)\Delta^2.$$

This completes the proof of Theorem 2.

Proof of Theorem 3. Let G be a k-connected ($k \geq 2$) graph with $n \geq 3$ vertices and e edges satisfying the conditions in Theorem 3. Suppose G is not Hamiltonian. Then Lemma 2 implies that $\beta \geq k+1$. Also, we have that $n \geq 2\delta + 1 \geq 2k + 1$ otherwise $\delta \geq k \geq n/2$ and G is Hamiltonian. Let $I_1 := \{ u_1, u_2, ..., u_\beta \}$ be a maximum independent set in G. Then $I := \{ u_1, u_2, ..., u_{k+1} \}$ is an independent set in G. Set $V - I = \{ v_1, v_2, ..., v_{n-k-1} \}$. Following the proof of in Theorem 2, we have that

$$\sum_{u\in I} d(u) \leq e \leq \sum_{v\in V-I} d(v).$$

Let $s = n-(k+1)$, $a_i = d(v_i)$ and $b_i = 1$ for each $i = 1, 2, ..., n-(k+1)$ in Lemma 1. Following the proof of in Theorem 2 again, we have that

$$Z_1(G) \geq (k+1)\delta^2 + \frac{e^2(1+\theta(n-k-2))}{n-k-1} - \theta(n-k-1)(n-k-2)\Delta^2.$$

From the given conditions in Theorem 3, we have that

$$Z_1(G) = (k+1)\delta^2 + \frac{e^2(1+\theta(n-k-2))}{n-k-1} - \theta(n-k-1)(n-k-2)\Delta^2.$$

Following the proof of Theorem 2, we have that G is a bipartite graph with partition sets of I and $V - I$ such that $|I| = (k+1)$, $d(u) = \delta$ for each vertex $u \in I$ and $d(v) = \Delta$ for each vertex $v \in V - I \}$. Since $\delta(k+1) = e = \Delta(n-k-1) \geq \delta(n-k-1)$, we have that $n \leq 2n + 2$. Notice that $n \geq 2k + 1$, we have that $n = 2k + 1$ or $n = 2k + 2$. If $n = 2k + 1$, then G is $K_{k,\,k+1}$. If $n = 2k + 2$, then Lemma 4 implies that G is Hamiltonian, a contradiction.

This completes the proof of Theorem 3.

Proof of Theorem 4. Let G be a k-connected ($k \geq 1$) graph with $n \geq 9$ vertices and e edges satisfying the conditions in Theorem 4. Suppose G is not traceable. Then Lemma 3 implies that $\beta \geq k+2$. Also, we have that $n \geq 2\delta + 2 \geq 2k + 2$ otherwise $\delta \geq k \geq (n-1)/2$ and G is traceable. Let $I_1 := \{ u_1, u_2, ..., u_\beta \}$ be a maximum independent set in G. Then $I := \{ u_1, u_2, ..., u_{k+2} \}$ is an independent set in G. Set $V - I = \{ v_1, v_2, ..., v_{n-k-2} \}$. Following the proof of in Theorem 2, we have that

$$\sum_{u\in I} d(u) \leq e \leq \sum_{v\in V-I} d(v).$$

Let $s = n - (k+2)$, $a_i = d(v_i)$ and $b_i = 1$ for each $i = 1, 2, ..., n-(k+2)$ in Lemma 1. Following the proof of in Theorem 2 again, we have that

$$Z_1(G) \geq (k+2)\delta^2 + \frac{e^2(1+\theta(n-k-3))}{n-k-2} - \theta(n-k-2)(n-k-3)\Delta^2.$$

From the given conditions in Theorem 4, we have that

$$Z_1(G) = (k+2)\delta^2 + \frac{e^2(1+\theta(n-k-3))}{n-k-3} - \theta(n-k-3)(n-k-3)\Delta^2.$$

Following the proof of Theorem 1, we have that G is a bipartite graph with partition sets of I and $V - I$ such that $|I| = (k+2)$, $d(u) = \delta$ for each vertex $u \in I$ and $d(v) = \Delta$ for each vertex $v \in V - I$ }. Since $\delta(k+2) = e = \Delta(n-k-2) \geq \delta(n-k-2)$, we have that $n \leq 2n+4$. Notice that $n \geq 2k+2$, we have that $n = 2k+2$, $n = 2k+3$, or $n = 2k+4$. If $n = 2k+2$, then G is $K_{k,\,k+2}$. If $n = 2k+3$, then $k \geq 3$ since $n \geq 9$. Thus Lemma 5 implies that G has a cycle of length at least $(n-1)$ and thereby G is traceable, a contradiction. If $n = 2k+4$, then $k \geq 3$ since $n \geq 9$. Thus Lemma 4 implies that G is Hamiltonian and thereby G is traceable, a contradiction.

This completes the proof of Theorem 4.

4 Conclusion

In this paper, we, utilizing Wagner's inequality, obtain two lower bounds for the first Zagreb index of a graph. We further present new sufficient conditions based on the first Zagreb index for the Hamiltonian graphs and traceable graphs. In future, we will explore to use the ideas in this paper to obtain new bounds for the variants of the first Zagreb index of a graph.

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Bounds Including Integrals for Euler-Sombor Index

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Abstract

In this work, using an integral-based approach outlined in Kirgiz and Maden (2022), new lower and upper bounds are established for the the Euler–Sombor index (ES) of graphs. The edge set is divided into pendent, high-low degree, and non-pendent blocks by interpreting the degree-dependent kernels underlying these indices as monotone functions. Each block is then subjected to unit-interval integral estimates. Sharp inequalities are produced by this framework with respect to basic graph parameters, such as the number of edges, pendent vertices, maximum degree, and minimum non-pendent degree. The precise distribution of pendent edges is incorporated into the integral method, which not only unifies and extends a number of previous results but also yields tighter bounds. Consequently, our findings show the efficacy of integral-based methods for bounding a wide class of degree-based molecular descriptions and improve upon previous estimates for both indications.

Keywords: Topological indices, Integral-based method, Lower bounds, Upper bounds
AMS Classification: 05C35, 05C09

1 Introduction

Let G be a simple, connected graph with $V(G)$ and $E(G)$, i.e. vertex set and edge set, respectively. m denotes the size of G and p denotes pendent vertices. The number of a vertex's neighbors, represented by d_v, is its degree in G. If u and v are adjacent vertices, then $e = uv$ is the label for the edge that connects them.

Two essential definitions are required: $\Delta = max\{d_v|v \in G\}$ and $\delta = min\{d_v|v \in G\}$ are the definitions of a graph G's maximum and minimum degrees, represented by Δ and δ, respectively. δ_n denotes minimum non-pendent degree.

Topological indices are numerical graph invariants that encode structural properties of molecules and complex networks, and they play a central role in mathematical chemistry and network science [5, 6, 8, 9, 14]. Many of the most studied indices are degree–based, since vertex degrees represent the connectivity of atoms or nodes and provide natural descriptors for a variety of physical and chemical phenomena [10–12].

Gutman introduced the Sombor index, gave the geometric motivation and basic properties [12]:

$$S(G) = \sum_{uv \in E(G)} \sqrt{d_u^2 + d_v^2}$$

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Using the Euclidean norm of the degree pair (d_u, d_v) as the starting point, researchers developed a number of geometric refinements, including the reduced Sombor index, the elliptic Sombor index, and most recently, the Euler Sombor index. Tang et al. (2024) gave the definition of Euler-Sombor index $ES(G)$ as following [13]:

$$ES(G) = \sum_{uv \in E(G)} \sqrt{d_u^2 + d_v^2 + d_u d_v}.$$

In [13], sharp bounds were obtained in terms of basic parameters like the number of edges, minimum degree, and maximum degree; equality in these bounds is characterized by regular graphs. Further, extremal values of the Euler–Sombor index were determined for trees, together with explicit identification of the structures that achieve those extrema.

The Euler Sombor index is introduced with both geometric and chemical motivations. The geometric basis for the index is the interpretation of each edge uv as contributing a term that resembles an ellipse-perimeter approximation built from the pair of degrees (d_u, d_v), in contrast to the classical Sombor index, where the term $\sqrt{d_u^2 + d_v^2}$ is tied to Euclidean distance from the origin [16, 17]. The Euler-Sombor index has been proposed as a molecular descriptor with demonstrated strong correlation to experimentally relevant properties on a chemical level [18].

In [21], the minimum and maximum Euler–Sombor index is determined for fixed order and fixed girth, and the extremal graphs are explicitly characterized for unicyclic graphs. Also, the Euler–Sombor index is computed for benzenoid hydrocarbons and selected drug molecules.

A significant area of investigation has been dedicated to establishing bounds for the Euler-Sombor index using fundamental graph characteristics, followed by pinpointing specific graphs that attain these bounds. For a connected simple graph G on n vertices and m edges with minimum degree δ and maximum degree Δ, it is known that

$$\sqrt{3}(n-1) \leq ES(G) \leq \frac{\sqrt{3}}{2} n(n-1)$$

where the lower bound is attained exactly by the single edge K_2 and the upper bound is attained exactly by the complete graph K_n. Among all trees on n vertices, the path P_n uniquely gives the minimum Euler Sombor index, while the star S_n uniquely gives the maximum [14].

For unicyclic graphs, recent work has determined, for each order ($n \geq 5$), which unicyclic graphs minimize and maximize the Euler Sombor index, and has even ranked the first, second, and third extremal structures [15]. Another study analyzes unicyclic graphs along with trees and general chemical graphs ($\Delta \leq 4$), again identifying which members of these families are extremal for the Euler Sombor index [14]. Such classifications hold significance in chemical graph theory due to the fact that unicyclic and low-degree graphs serve as representations of prevalent ring-containing organic structures.

In [16], the bounds of the Euler Sombor index determined for maximal outerplanar graphs. An outerplanar graph with the maximum number of edges on n points contains precisely $2n - 3$ connecting lines and a minimum of one point with a degree of 2. For such graphs, lower and upper bounds on the Euler Sombor index are obtained as functions of n, and the extremal graphs attaining these bounds are fully characterized.

There is also a dedicated line of work on molecular trees and related constrained families. A molecular graph is defined as a graph of maximum degree at most 4, reflecting typical valence constraints in organic chemistry. For molecular trees with fixed order n and a fixed number of pendent vertices, sharp extremal upper bounds on the Euler Sombor index have been established [18].

In [19], for graphs with higher cyclomatic number, the author studied on tricyclic graphs. A specific methodology involves starting from a base tricyclic graph and prove that certain local edge relocations strictly lower the Euler Sombor index. In particular,

if two pendent-like paths meet a vertex of degree at least 3, then rerouting one path to attach further from that high-degree core can only decrease the index.

In [17], the Euler-Sombor index is studied via the function $\Psi(x_1, x_2) = \sqrt{x_1^2 + x_2^2 + x_1 x_2}$. By showing that Ψ is monotone in each argument, the authors apply general extremal principles for graphs with fixed cyclomatic number. For k-cyclic graphs with $n + k - 1$ edges, and specifically for tricyclic graphs ($k = 3$), the unique minimizers have only degrees 2 and 3 and a very controlled pattern of edges between them; for large n, this same structure also minimizes the index among molecular tricyclic graphs.

A more recent work involves treating the Euler–Sombor index as one instance in a broader parametric family. The variable Euler–Sombor index is defined by

$$ES(\lambda, G) = \sum_{uv \in E(G)} \sqrt{d_u^2 + d_v^2 + \lambda d_u d_v}$$

with $\lambda \in \mathbb{R}$. This perspective facilitates the establishment of general constraints regarding the minimum and maximum degree associated with graph products, offers approximation formulas for $ES(\lambda)$ in relation to established indices, and further proposes methodologies for adjusting λ to optimize the predictive capacity of the resultant descriptor concerning a specific molecular property [22].

In this paper, we give new lower and upper bounds for Euler-Sombor index. Also, we provide some corollaries and examples related to these bounds.

2 Preliminaries

In this section, we state the lemmas that will lead to our main results. We first define the function $f : [1, \infty) \to \mathbb{R}$ where $y \geq 1$ is constant. It is known that for two integrable functions g_1 and g_2 which are defined on $[a, b]$ such that $g_1(x) \leq g_2(x)$, we have $\int_a^b g_1(x)\, dx \leq \int_a^b g_2(x)\, dx$, $x \in [a, b]$.

Lemma 2.1. *[3] Let the function $f_y(x)$ is increasing where y is a constant. If we take $y \geq 1$ and $x_0 \geq 2$. Then we have*

$$\int_{x_0-1}^{x_0} f_y(x)\, dx \;\leq\; f_y(x_0) \;\leq\; \int_{x_0}^{x_0+1} f_y(x)\, dx.$$

Lemma 2.2. *[3] Let the function $f_y(x)$ be as defined above and $\delta_n \leq y \leq \Delta$, $\delta_{n+1} \leq x_0 \leq \Delta$, then*

$$f_y(x_0) \geq \int_{\delta_n}^{\delta_{n+1}} f_{\delta_n}(x)dx \geq f_{\delta_n}(\delta_n), \tag{1}$$

and for $\delta_n \leq y \leq \Delta$, $\delta_n \leq x_0 \leq \Delta - 1$, we get

$$f_y(x_0) \leq \int_{\Delta-1}^{\Delta} f_\Delta(x)dx \leq f_\Delta(\Delta). \tag{2}$$

For $\delta_n \leq x_0 \leq \Delta - 1$ and $y = 1$, we have

$$f_1(x_0) \leq \int_{\Delta-1}^{\Delta} f_1(x)dx \leq f_1(\Delta). \tag{3}$$

For $\delta_{n+1} \leq x_0 \leq \Delta$ and $y = 1$,

$$f_1(x_0) \geq \int_{\delta_n}^{\delta_{n+1}} f_1(x)dx \geq f_1(\delta_n). \tag{4}$$

3 Main Results

For fixed y, $f_y(x) = \sqrt{x^2+xy+y^2}$ where $x, y \geq 1$. f_y is increasing in x for $y \geq 1$. For the quadratic $Q(x) = x^2 + yx + y^2$, one primitive is

$$\int \sqrt{Q(x)}\,dx = \frac{2x+y}{4}\sqrt{Q(x)} \;+\; \frac{3y^2}{8}\ln\Big(2\sqrt{Q(x)} + 2x + y\Big) \;+\; C,$$

i.e.

$$\int \sqrt{x^2+xy+y^2}\,dx = \tfrac{2x+y}{4}\sqrt{x^2+xy+y^2} \;+\; \tfrac{3y^2}{8}\ln\left(2\sqrt{x^2+xy+y^2}+2x+y\right)+C.$$

The number of edges connecting a degree-1 and a degree-x vertex denotes $C_{1,x}$. The number of edges with endpoints (Δ,Δ) denotes w_Δ, and the number of edges with endpoints (δ_n,δ_n) denotes w_{δ_n}, where $\delta_n \neq 1$.

Throughout this article, edges will be divided into 4 partition: X (edges of type $(1,\Delta)$ or $(1,\delta_n)$), Y (other pendent edges), T (edges with (Δ,Δ) or (δ_n,δ_n)) and Z (remaining edges). We denote $S_\beta = \sum_{ij\in\beta} f_{d_j}(d_i)$ where $\beta \in \{X,Y,T,Z\}$.

Theorem 3.1. *Let G be a simple connected graph with m edges, p pendent vertices, maximum degree Δ, and minimum non-pendent degree δ_n. Let $C_{1,x}$ be as defined in introduction section. Then the following pair of inequalities hold:*

$$\begin{aligned}
ES(G) \;&\leq\; (m-p-w_\Delta)\int_{\Delta-1}^{\Delta} f_\Delta(x)\,dx \;+\; (p-C_{1,\Delta})\int_{\Delta-1}^{\Delta} f_1(x)\,dx \\
&+\; C_{1,\Delta}\sqrt{1+\Delta^2+\Delta} + w_\Delta\sqrt{3}\Delta, \\
ES(G) \;&\geq\; (m-p-w_{\delta_n})\int_{\delta_n}^{\delta_n+1} f_{\delta_n}(x)\,dx \;+\; (p-C_{1,\delta_n})\int_{\delta_n}^{\delta_n+1} f_1(x)\,dx \\
&+\; C_{1,\delta_n}\sqrt{1+\delta_n^2+\delta_n} + w_{\delta_n}\sqrt{3}\delta_n
\end{aligned}$$

with equality if and only if G is a regular graph or $G \cong K_{1,n-1}$.

Proof Partition edges into X, Y, Z, T and write $ES(G) = S_X + S_Y + S_Z + S_T$ with each partial sum over the corresponding set.

Every edge in X contributes $f_1(\Delta) = \sqrt{1+\Delta+\Delta^2}$. Hence

$$S_X = C_{1,\Delta}\sqrt{1+\Delta+\Delta^2}.$$

Every edge in T contributes $f_\Delta(\Delta) = \sqrt{\Delta^2+\Delta^2+\Delta^2}$. Hence

$$S_T = w_\Delta\sqrt{3}\Delta.$$

For $uv \in Z$ both ends are non-pendent, so by monotonicity in each argument

$$f_{d_v}(d_u) \leq f_\Delta(d_u) \leq \int_{\Delta-1}^{\Delta} f_\Delta(x)dx$$

and by summing

$$S_Z \leq |Z|\int_{\Delta-1}^{\Delta} f_\Delta(x)dx = (m-p-w_\Delta)\int_{\Delta-1}^{\Delta} f_\Delta(x)dx.$$

Each edge in Y has type $(1,y)$ with $y < \Delta$. Then

$$f_1(x_0) \leq f_1(\Delta-1) \leq \int_{\Delta-1}^{\Delta} f_1(x)dx$$

so

$$S_Y \leq |Y|\int_{\Delta-1}^{\Delta} f_1(x)dx = (p-C_{1,\Delta})\int_{\Delta-1}^{\Delta} f_1(x)dx.$$

Collecting S_X, S_Y, S_T, S_Z gives the upper inequality.

Every edge in X contributes $f_1(\delta_n) = \sqrt{1+\delta_n+\delta_n^2}$. Hence

$$S_X = C_{1,\delta_n}\sqrt{1+\delta_n+\delta_n^2}.$$

For $uv \in Z$ we have $d_u, d_v \geq \delta_n$. Monotonicity yields

$$f_{d_v}(d_u) \geq f_{\delta_n}(d_u) \geq \int_{\delta_n}^{\delta_n+1} f_{\delta_n}(x)dx$$

hence

$$S_Z \geq (m-p-w_{\delta_n})\int_{\delta_n}^{\delta_n+1} f_{\delta_n}(x)dx.$$

Each edge is $(1,y)$ with $y > \delta_n$. Then

$$f_1(y) \geq f_1(\delta_{n+1}) \geq \int_{\delta_n}^{\delta_n+1} f_1(x)dx$$

so

$$S_Y \geq (p-C_{1,\delta_n})\int_{\delta_n}^{\delta_n+1} f_1(x)dx$$

and the exact $(1,\delta_n)$ edges there are (C_{1,δ_n}) of them contribute

$$S_Y = C_{1,\delta_n} f_1(\delta_n) = C_{1,\delta_n}\sqrt{1+\delta_n+\delta_n^2}.$$

Every edge in T contributes $f_{\delta_n}(\delta_n) = \sqrt{\delta_n^2+\delta_n^2+\delta_n^2}$. Hence

$$S_T = w_{\delta_n}\sqrt{3}\delta_n.$$

Summing all partitions proves the lower inequality.

If $d_u = \Delta$ or $d_u = \delta_n$, there are no degree-1 vertices. So, $p = 0$ and $C_{1,\Delta} = 0$ or $C_{1,\delta_n} = 0$. Since every edge belong to w_Δ or w_{δ_n}, they take the value m. We have $m-p-w_\Delta = m-0-m = 0$ and $m-p-w_{\delta_n} = m-0-m = 0$. So, the integral terms equals to 0. Equality holds when G is regular or $G \cong K_{1,n-1}$.

□

Remark 3.2. *Since* $f_y(x) = \sqrt{x^2+xy+y^2}$ *and*

$$\Phi_y(x) = \tfrac{1}{2}\left[(x+\tfrac{y}{2})\sqrt{x^2+xy+y^2} + \tfrac{3y^2}{4}\ln\left(x+\tfrac{y}{2}+\sqrt{x^2+xy+y^2}\right)\right] \quad (\Phi_y' = f_y)$$

we obtain

$$\begin{aligned} ES(G) &\leq (m-p-w_\Delta)\big[\Phi_\Delta(\Delta)-\Phi_\Delta(\Delta-1)\big] + (p-C_{1,\Delta})\big[\Phi_1(\Delta)-\Phi_1(\Delta-1)\big] \\ &\quad + C_{1,\Delta}\sqrt{1+\Delta+\Delta^2} + w_\Delta\sqrt{3}\Delta, \\ ES(G) &\geq (m-p-w_{\delta_n})\big[\Phi_{\delta_n}(\delta_n+1)-\Phi_{\delta_n}(\delta_n)\big] + (p-C_{1,\delta_n})\big[\Phi_1(\delta_n+1)-\Phi_1(\delta_n)\big] \\ &\quad + C_{1,\delta_n}\sqrt{1+\delta_n+\delta_n^2} + w_{\delta_n}\sqrt{3}\delta_n. \end{aligned}$$

In particular, we can provide the following corollary if $w_\Delta = 0$, $w_{\delta_n} = 0$, and $C_{1,x} = 0$.

Corollary 3.3. *Let* G *be a graph as in Theorem 3.1. Then we get:*

$$(m-p)\sqrt{3}\delta_n + p\sqrt{1+\delta_n+\delta_n^2} \leq ES(G) \leq (m-p)\sqrt{3}\Delta + p\sqrt{1+\Delta+\Delta^2}.$$

One can derive the following corollary from Corollary 3.3 if G contains no pendent edges ($p = 0$). The following theorem also appears in [13]-Theorem 3.1.

Corollary 3.4. *Consider a simple connected graph* G *with* m *edges, a maximum vertex degree of* Δ*, and a minimum vertex degree of* δ*. Then*

$$m\sqrt{3}\delta \leq ES(G) \leq m\sqrt{3}\Delta$$

with equality if and only if G *is regular.*

Example 3.5. *Let G be a tricyclic graph as in Figure 1. Clearly, $ES(G) = 45,6206$. Then, the lower bound in Theorem 3.1 can be computed as $ES(G) \geq 41,5638$. In [19], the author gave the following lower bound for Euler-Sombor index of tricyclic graphs:*

$$ES(G) \geq 2\sqrt{3}n + 5\sqrt{3} + 2\sqrt{19} \tag{5}$$

which is equal to $38,1626$ for the tricyclic graph shown in Figure 1. Consequently, we have seen that the lower bound in Theorem 3.1 is better than (5) for the above mentioned graph.

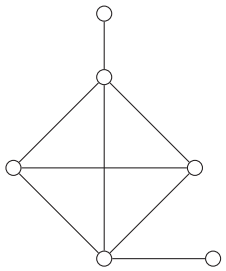

Fig. 1 A tricyclic graph G.

Example 3.6. *Let H be a unicyclic graph as in Figure 2. Clearly, $ES(G) = 35,2068$. Then, the lower bound in Theorem 3.1 can be computed as $35,2068$. In [20], the following lower bounds are given for Euler-Sombor index of unicyclic graphs:*

$$ES(G) \geq 2\sqrt{3}(n-3) + 2\sqrt{19} + \sqrt{13} \tag{6}$$

$$ES(G) \geq 3\sqrt{19} + \sqrt{7} + 2\sqrt{3}(n-4) \tag{7}$$

which is equal to $29,6438$ and $29,5788$, respectively for the graph shown in Figure 2. Consequently, we have seen that the lower bound in Theorem 3.1 is better than (6) and also (7) for the above mentioned graph.

Example 3.7. *Let Γ be a unicyclic graph as in Figure 3. Clearly, $ES(G) = 15,787$. Then, the lower bound in Theorem 3.1 can be computed as $14,402$. In [20], the author gave the following lower bounds for Euler-Sombor index of unicyclic graphs:*

$$ES(G) \geq 4\sqrt{3}d \tag{8}$$

which is equal to $13,856$ for the graph shown in Figure 3. Consequently, we have seen that the lower bound in Theorem 3.1 is better than (8) for the above mentioned graph.

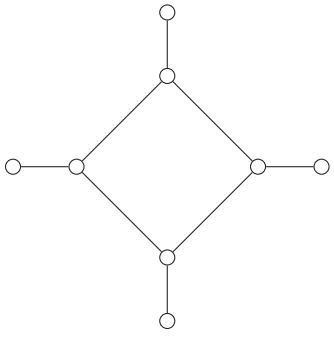

Fig. 2 A unicyclic graph H.

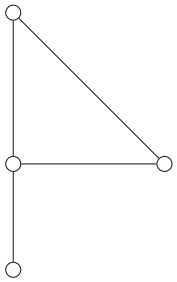

Fig. 3 A unicyclic graph Γ.

4 Conclusion

This work used integral-based methods to obtain sharp upper and lower bounds for Euler–Sombor index, using short-interval integral averages of the relevant functions in place of the traditional coarse per-edge extremal estimates.

For the Euler–Sombor index, the bounds reveal an improvement over earlier algebraic estimates, especially in irregular graphs where the Euler term $\sqrt{d(u)^2 + d(v)^2 - d(u)d(v)}$ is highly sensitive to degree variation. The integral approach captures these variations more accurately by exploiting monotonicity and averaging over unit intervals.

In summary, these integral bounds explicitly account for pendent edges and the concentration of degrees near extremes. So, these bounds are usually sharper than classical bounds in many cases.

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Some Vertex Degree-Based Topological Indices of Non-Zero Component Graphs

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Abstract

As a new example in Algebraic Graph Theory, the non-zero component graph $\Gamma(\mathbb{V})$ of a finite $n-$ dimensional vector space $\mathbb{V}$ over a finite field $\mathbb{F}$ has recently been defined as the graph $\Gamma(\mathbb{V}) = (V(\Gamma(\mathbb{V})), E(\Gamma(\mathbb{V})))$ where the vertices of $\Gamma(\mathbb{V})$ are the non-zero vectors in $\mathbb{V}$ such that two of which are adjacent if they share at least one basis vector with non-zero coefficients in their basic representation. The vertex degrees of the elements of this graph is known. Here we obtain the vertex and edge partitions and calculate several degree based topological indices of these graphs for the first time. The edge partition given here can be used for calculating many other vertex degree based topological graph indices.

Keywords: Non-zero component graph, Topological index, Vertex partition
AMS Classification: 05C07, 05C09, 05C25, 05C30

1 Significance of the work

Graph theory is getting more popular each day because of its numerous applications and techniques in many areas including some industrial applications. Therefore, graph theory is getting more importance and new methods are introduced. In this paper, we studied some topological graph indices based on vertex degrees for a new class of graphs named as non-zero component graphs. This work used linear algebraic methods which are apperently new in spectral graph theory. The methods introduced and used here can be applied to many other cases as this ideas and methods are quite new.

2 Introduction

There are several graph types which are defined by means of some algebraic properties or over some algebraic structures. Some examples are zero-divisor graphs, annihilator graphs, middle graphs, power graphs, undirected power graphs and intersection graphs. The non-zero component graph is recently introduced and studied in a few papers already. There are many possible problems related to this graph. We introduce the vertex and edge partition of this graph and calculate some degree based topological

*Corresponding Author

graph indices of them to give the idea. The list of topological indices can be extended easily.

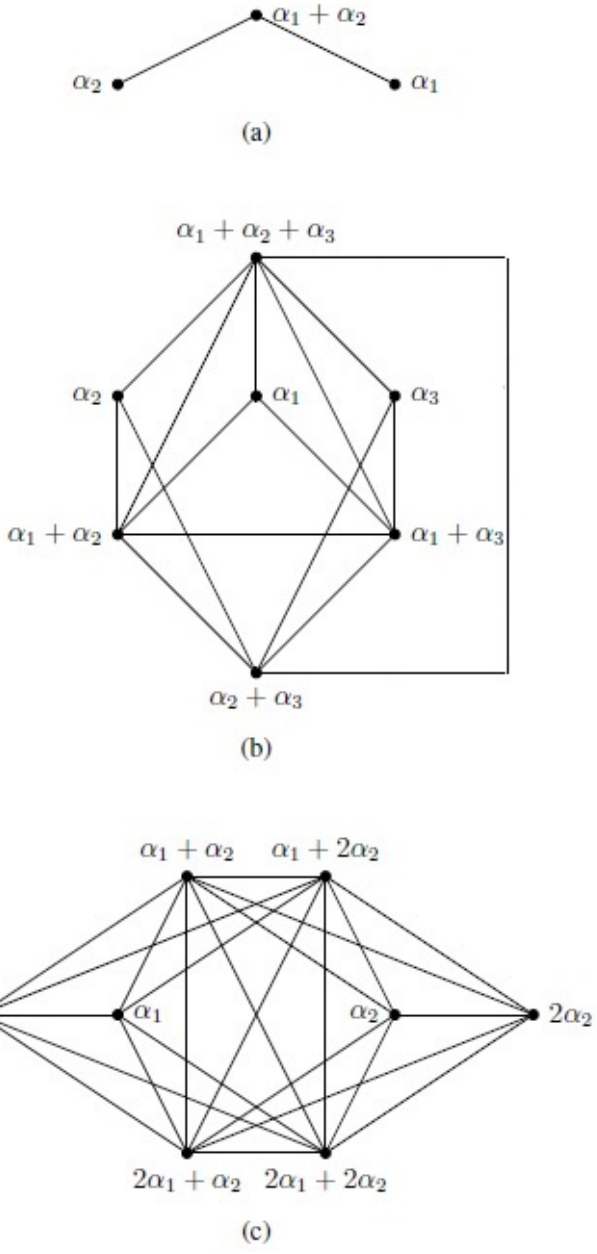

Fig. 1 Non-zero component graphs with (n,q) = (2,2), (3,2) and (2,3)

Let $\{\alpha_1, \alpha_2, \cdots, \alpha_n\}$ be a basis of the vector space $\mathbb{V}$ of dimension n over a finite field $\mathbb{F}$ with q elements. Let Θ be the null vector. Let $\mathbb{V}' = \mathbb{V} - \{\Theta\}$. Any vector $v \in \mathbb{V}$ can be expressed uniquely as a linear combination of the form $v = a_1\alpha_1 + a_2\alpha_2 + \cdots + a_n\alpha_n$. This is the basic representation of v with respect to $\{\alpha_1, \alpha_2, \cdots, \alpha_n\}$.

The non-zero component graph of a finite dimensional vector space over a finite field $\mathbb{F}$ is the graph $\Gamma(\mathbb{V}) = (V(\Gamma(\mathbb{V})), E(\Gamma(\mathbb{V})))$ where the vertices of $\Gamma(\mathbb{V})$ are the non-zero vectors in $\mathbb{V}$ such that two of which are adjacent if they share at least one basis vector with non-zero coefficients in their basic representation. That is, if $v_1, v_2 \in \mathbb{V}'$, $v_1 \sim v_2$ if and only if v_1 and v_2 shares at least one α_i with non-zero coefficient in their basic representations. It is well-known that $\Gamma(\mathbb{V})$ is always connected and has

diameter 2. Also $\Gamma(\mathbb{V})$ is complete if and only if $\mathbb{V}$ is one dimensional. We shall denote the order and size of $\Gamma(\mathbb{V})$ by c and d, respectively. In [5], it is shown that $c = q^n - 1$ and $d = \frac{q^{2n}-q^n+1-(2q-1)^n}{2}$. See [4, 5] for definition and further fundamental properties.

We illustrate the non-zero component graphs with (n,q) = (2,2), (3,2) and (2,3) in Figure 1. The vertex partition tables for these three non-zero component graphs are given in Table 1.

k	d_{v_i}	$\sharp\ v_i$		k	d_{v_i}	$\sharp\ v_i$		k	d_{v_i}	$\sharp\ v_i$
1	1	2		1	3	3		1	5	4
2	2	1		2	5	3		2	7	4
				3	6	1				

Table 1 The vertex partition tables of non-zero component graphs with (n,q) = (2,2), (3,2) and (2,3), respectively

In 1947, chemist Harold Wiener introduced a new concept which proved to be incredibly useful not only for mathematicians but also for chemists, pharmacologists, physicians, biologists, social scientists, etc. The concept he defined is today known as the Wiener index. It is the first topological index and more than 3000 followed it for several physical, chemical applications or at least for some nice mathematical properties. Most of the existing topological indices are defined in terms of vertex degrees and others are defined by means of edge degrees, eccentricity, distance, etc. There is a large number of papers in the literature on topological indices and applications, see e.g. [9, 13–18] for some recent applications of degree based indices.

Topological graph indices of many graph types and classes have already been intensively studied in literature. But interestingly enough, they have not been studied for algebraic graphs. The possible reason for that seems to be the complicated structure of the vertex and edge partitions of these graphs compared to the classical ones. Here we calculate some vertex based topological graph indices of non-zero component graphs by first determining their vertex partition.

3 Vertex partition of non-zero component graphs

The vertex partition of a graph G is the table giving the number of vertices of several possible degrees in G. It is useful in calculating degree-based topological graph indices such as the family of Zagreb indices, Randić index, ABC index, GA and AG indices, harmonic index, forgotten index etc. together with their reduced, inverse, modified, etc. versions. They are also useful in finding several graph polynomials related to such indices.

Let $\mathbb{V}$ be an $n-$dimensional vector space over a field $\mathbb{F}$ with q elements. Then any vector in $\mathbb{V}$ can be represented as $\sum_{i=1}^{k} c_i\alpha_i$, where $1 \leq k \leq n$. The degree of a vertex in $\Gamma(\mathbb{V})$ corresponding to any such vector was obtained as $(q^k-1)q^{n-k}-1$ in [4]. Our aim is to determine the number of vertices corresponding to each possible degree. In the following result, we calculate this number:

Theorem 3.1. *Let $v = \sum_{i=1}^{k} c_i\alpha_i$ be any vertex in $\Gamma(\mathbb{V})$ with degree $(q^k-1)q^{n-k}-1$. Then the number of vertices having the same degree with v is*

$$\binom{n}{k}(q-1)^k. \tag{1}$$

Proof In a non-zero component graph $\Gamma(\mathbb{V})$, there are n possible degrees for the vertices. The set of vertices having the same degree corresponds to those vertices having same number of basis vectors in the linear combinations. In particular, when $k = n$, the vectors corresponding to the vertices will be of the form $\sum_{i=1}^{n} c_i\alpha_i, \forall c_i \neq 0$. There are $q-1$ possibilities for each c_i and hence in turn there are $(q-1)^n$ vectors which are expressed in terms of all basis vectors.

When $k = n-1$, the vectors corresponding to the vertices of $\Gamma(\mathbb{V})$ will be of the form $\sum_{i=1}^{n} c_i\alpha_i$ where exactly one scalar $c_i = 0$. There are $(q-1)^{n-1}$ possibilities for each scalar and there are $\binom{n}{1}$ ways for choosing the particular basis vector which has to be missing from the linear combination. Hence in total, there are $\binom{n}{1}(q-1)^{n-1}$. Proceeding further we get, the number of vectors having exactly k basis vectors in the linear combinations is given by $\binom{n}{n-k}(q-1)^k$. Hence the number of vertices having same degree follows as mentioned in Equation (1). □

If the set of all vertex degrees of a graph G is $D = \{1^{(a_1)}, 2^{(a_2)}, 3^{(a_3)}, \cdots, \Delta^{(a_\Delta)}\}$ where a_i's are non-negative integers, then D is called the degree sequence of G. Here Δ is the maximum vertex degree. Similarly, δ denotes the minimum vertex degree. For every graph G, there is a degree sequence. But for a degree sequence, there may or may not exist a graph. If there is a graph, then D is said to be realisable. For every realisable degree sequence, there is at least one graph; usually there are many.

In [7], a new graph invariant called Ω invariant was defined by

$$\Omega(D) = \sum_{i=1}^{\Delta}(i-2)a_i.$$

Several properties of Ω invariant were obtained in [7] and [8]. One of its most important properties were given in [7] for the number of faces of all realizations of the given degree sequence as follows: The number of faces of all realizations of a given degree sequence $D = \{1^{(a_1)}, 2^{(a_2)}, 3^{(a_3)}, \cdots, \Delta^{(a_\Delta)}\}$ is

$$r(G) = \frac{\Omega(G)}{2} + c(G) \tag{2}$$

where $c(G)$ is the number of components of G. Now we shall form the degree sequence of a non-zero component graph and calculate its omega invariant and the number of faces. As all non-zero component graphs are connected, $c(G) = 1$.

The degree sequence of a non-zero component graph is obtained as

$$DS(\Gamma(\mathbb{V})) = \left\{\left(q^{n-1}(q^1-1)-1\right)^{\binom{n}{1}(q-1)}, \left(q^{n-2}(q^2-1)-1\right)^{\binom{n}{2}(q-1)^2}, \ldots, \left(q^{n-n}(q^n-1)-1\right)^{\binom{n}{n}(q-1)^n}\right\}.$$

We now can obtain the omega invariant of a non-zero component graph:

Theorem 3.2. *The omega invariant of a non-zero component graph $\Gamma(\mathbb{V})$ is*

$$\Omega(\Gamma(\mathbb{V})) = q^{2n} - 3q^n + 3 - (2q-1)^n.$$

Proof

$$\begin{aligned}
\Omega(\Gamma(\mathbb{V})) &= \textstyle\sum_{k=1}^{n}\binom{n}{k}(q-1)^k\left[q^{n-k}(q^k-1)-1-2\right] \\
&= \textstyle\sum_{k=1}^{n}\binom{n}{k}(q-1)^k\left[q^n - q^{n-k} - 3\right] \\
&= (q^n-3)\textstyle\sum_{k=1}^{n}\binom{n}{k}(q-1)^k 1^{n-k} - \sum_{k=1}^{n}\binom{n}{k}(q-1)^k q^{n-k} \\
&= (q^n-3)\left[\textstyle\sum_{k=0}^{n}\binom{n}{k}(q-1)^k 1^{n-k} - 1\right] - \left[\sum_{k=0}^{n}\binom{n}{k}(q-1)^k q^{n-k} - q^n\right] \\
&= (q^n-3)\left[(q-1+1)^n - 1\right] - \left[(q-1+q)^n - q^n\right] \\
&= q^{2n} - 3q^n + 3 - (2q-1)^n.
\end{aligned}$$

□

By the size formula for the non-zero component graph, we can write $(2q-1)^n = q^{2n} - q^n + 1 - 2d$ which gives us the following result:

Corollary 3.3.

$$\Omega(\Gamma(\mathbb{V})) = 2d + 2 - 2q^n.$$

As $c = q^n - 1$, we deduce the following:

Corollary 3.4.

$$\Omega(\Gamma(\mathbb{V})) = 2(d - c).$$

Note that this coincides with Theorem 2.1 of [7]. So the number of faces of $\Gamma(\mathbb{V})$ is obtained as follows:

Theorem 3.5. *The number of faces of a non-zero component graph* $\Gamma(\mathbb{V})$ *is*

$$r(\Gamma(\mathbb{V})) = d + 2 - q^n.$$

4 Edge partition of non-zero component graphs

The edge partition of a graph is the table giving possible pairs of vertex degrees at the ends of all edges of the graph together with their numbers. Some of the degree based topological indices can be calculated by means of edge partition.

Theorem 4.1. *Let* $M = \binom{n}{k}(q-1)^k$. *Assuming w.l.o.g. that* $t \leq k$, *the number of pairs of vertices in a non-zero component graph forming an edge with vertex degrees* $(q^t-1)q^{n-t}-1$ *and* $(q^k-1)q^{n-k}-1$ *is*

$$\begin{cases} \binom{n}{t}(q-1)^{t+k}\sum_{i=1}^{t}(-1)^{i+1}\binom{t}{i}\binom{n-i}{k-i}, & \text{if } t < k; \\ \binom{M}{2}, & \text{if } t = k > \lfloor \frac{n}{2} \rfloor; \\ \binom{n}{k}(q-1)^{2k}\sum_{i=1}^{k-1}(-1)^{i+1}\binom{k}{i}\binom{n-i}{k-i}, & \text{if } t = k < \lceil \frac{n}{2} \rceil; \\ \frac{1}{2}\binom{M}{2}, & \text{if } n \text{ is even and } t = k = \frac{n}{2}; \end{cases}$$

where $\binom{1}{2}$ *is taken as zero.*

Proof Any two vertices with the degree $(q^t-1)q^{n-t}-1$ and $(q^k-1)q^{n-k}-1$ will be of the form $u = \sum_{i=1}^{t} c_i\alpha_i$ and $v = \sum_{i=1}^{k} c_i\alpha_i$. The number of edges having corresponding pair of vertex degrees on their edges can be found out by considering the following cases.

Case 1. When $t < k$. To find the edge partition in this case, we need to determine the number of vertices adjacent to u and are expressed in terms of k basis vectors. The presence of at least one of the t basis vectors in u make another vector v adjacent to it. Thus there are $\binom{t}{1}\binom{n-1}{k-1}(q-1)^k - \binom{t}{2}\binom{n-2}{k-2}(q-1)^k + \ldots + (-1)^t\binom{t}{t}\binom{n-t}{k-t}(q-1)^k$ vectors adjacent to u and having same degree. Also there are $\binom{n}{t}(q-1)^t$ vertices having same degree as that of u. Thus there are $\binom{n}{t}(q-1)^{t+k}\sum_{i=1}^{t}(-1)^{i+1}\binom{t}{i}\binom{n-i}{k-i}$ number of edges with the end vertices having respective degrees $(q^t-1)q^{n-t}-1$ and $(q^k-1)q^{n-k}-1$, where $t < k$.

Case 2. Let $t = k > \lfloor \frac{n}{2} \rfloor$, each of the vertices will be adjacent to each other and there are $M = \binom{n}{k}(q-1)^k$ such vertices. Choosing any two vertices out of these would give the pair of vertices having the same degree i.e., there are $\binom{M}{2}$ number of possibilities for the same.

Case 3. When $t = k < \lceil \frac{n}{2} \rceil$, the corresponding vertices contain less than half of the basis vectors in their linear combination. For each vertex u, the number vertices adjacent to u and having same vertex degree will be one less than that of the number obtained for each u in case 1. Hence the number of edges in this particular case will be $\binom{n}{t}(q-1)^{2k}\sum_{i=1}^{t-1}(-1)^{i+1}\binom{t}{i}\binom{n-i}{k-i}$.

Case 4. When $t = k = \frac{n}{2}$, then there are $\binom{n}{\frac{n}{2}}(q-1)^{\frac{n}{2}}$ vertices containing exactly half number of vertices. Thus, there are $\binom{M}{2}$ pair of vertices which contains half of the basis vectors. Out of these half of them are not adjacent as the remaining half of the vertices contribute to the clique number. Hence there are $\frac{1}{2}\binom{M}{2}$ pairs of vertices having same degree at the ends of the edges. This completes the proof. □

5 Vertex degree based topological indices of non-zero component graphs

Most of the topological graph indices are defined in terms of vertex degrees. Each such vertex degree based index consists of some mathematical formula in terms of either vertex degrees or the pairs of the degrees of adjacent vertices in the given graph. For this reason, we need to determine the vertex and edge partition of the graph under consideration. Such an index formula frequently contains a sum or product over the vertices or edges of the graph. In this section, we calculate some additive topological indices of the non-zero component graphs to give a feel of calculation methods of these indices. We first recall the four indices, namely the first and second Zagreb indices, the forgotten index, and the sigma index, that we calculated. Two of them, the first Zagreb index and the forgotten index, are defined in terms of only vertex degrees and the other two, the second Zagreb index and the sigma index are defined in terms of pairs of vertex degrees at the end of edges. Although there are a few papers on the topological indices of non-zero component graphs, see e.g. [2, 12], they are all about the ones of the first type, that is, they are formulated by means of a sum over vertices of the graph. So this work is the first paper, up to the authors' knowledge, that a topological graph index containing a sum over the edges is calculated for the non-zero component graphs. Other vertex based topological graph indices can be calculated similarly.

The first and second Zagreb indices are

$$M_1(G) = \sum_{v\in V(G)} d_G(v)^2 \text{ and } M_2(G) = \sum_{uv\in E(G)} d_G(u)d_G(v),$$

respectively. They were defined nearly five decades ago by Gutman and Trinajstić, [11]. Some properties of these indices are studied in [1, 3, 6]. The forgotten index is defined as

$$F(G) = \sum_{v\in V(G)} d_G(v)^3$$

as a modification of the $M_1(G)$. Its name comes from the fact that it has not been mentioned for some time after its release and used for the first time until Furtula and Gutman used it and named it as a forgotten index in [10].

Next we recall the sigma index. It is an important irregularity measure defined by

$$\sigma(G) = \sum_{uv\in E(G)} (du - dv)^2 .$$

By calculating sigma index, we shall be able to have some idea about the irregularity degree of non-zero component graphs.

Let $\Gamma(\mathbb{V})$ be a non-zero component graph on a finite dimensional vector space of dimension n over a finite field $\mathbb{F}$ with q elements.

Theorem 5.1. *The first Zagreb index of* $\Gamma(\mathbb{V})$ *is*

$$M_1(\Gamma(\mathbb{V})) = (q^2+q-1)^n - c(c^2+c+2-2nd) - 1.$$

Proof By the definition of the first Zagreb index and by the vertex partition of the non-zero component graphs, we can write

$$\begin{aligned}
M_1(\Gamma(\mathbb{V})) &= \sum_{v\in V(\Gamma(\mathbb{V}))} d_{\Gamma(\mathbb{V})}(v)^2 \\
&= \sum_{k=1}^{n} \binom{n}{k}(q-1)^k \left(q^{n-k}(q^k-1)-1\right)^2 \\
&= \sum_{k=0}^{n} \binom{n}{k}(q-1)^k \left(q^{n-k}(q^k-1)-1\right)^2 - 1 \\
&= \sum_{k=0}^{n} \binom{n}{k}(q-1)^k \left[q^{2n-2k}\left(q^{2k}-2q^k+1\right)+2q^{n-k}-2q^n+1\right] - 1 \\
&= \sum_{k=0}^{n} \binom{n}{k}(q-1)^k \left[(q^n-1)^2-2q^{2n-k}+(q^2)^{n-k}+2q^{n-k}\right] - 1 \\
&= (q^n-1)^2q^n - 2q^n(2q-1)^n + (q^2+q-1)^n + 2(2q-1)^n - 1 \\
&= (q^2+q-1)^n - c(c^2+c+2-2nd) - 1.
\end{aligned}$$

□

The statement in Theorem 5.1 can be restated as below:

Corollary 5.2. *The first Zagreb index of the non-zero component graph* $\Gamma(\mathbb{V})$ *is*

$$M_1(\Gamma(\mathbb{V})) = c\left[(c(c+1)-2(q^{2n}-q^n+1-nd))\right] + (q^2+q-1)^n - 1.$$

The proof follows by the definitions of c and d after some calculations.

Theorem 5.3. *The forgotten index of* $\Gamma(\mathbb{V})$ *is*

$$F(\Gamma(\mathbb{V})) = 3c(q^2+q-1)^n - (q^3+q-1)^n - 2c^4 - 3c^2(c-2d+1).$$

Proof By the definition, we have

$$\begin{aligned}
F(\Gamma(\mathbb{V})) &= \sum_{v\in V(\Gamma(\mathbb{V}))} d_{\Gamma(\mathbb{V})}(v)^3 \\
&= \sum_{k=1}^{n} \binom{n}{k}(q-1)^k \left(q^{n-k}(q^k-1)-1\right)^3 \\
&= \sum_{k=0}^{n} \binom{n}{k}(q-1)^k \left(q^{n-k}(q^k-1)-1\right)^3 + 1 \\
&= \sum_{k=0}^{n} \binom{n}{k}(q-1)^k \Big[q^{3n-3k}(q^{3k}-3q^{2k}+3q^k-1) \\
&\qquad -3q^{2n-2k}(q^{2k}-2q^k+1)+3q^n-3q^{n-k}-1\Big] + 1 \\
&= (q^n-1)^3q^n - 3q^{2n}(2q-1)^n + 3q^n(q^2+q-1)^n \\
&\qquad -(q^3+q-1)^n + 6q^n(2q-1)^n - 3(q^2+q-1)^n \\
&\qquad -3(2q-1)^n - q^n + 1 \\
&= 3c(q^2+q-1)^n - (q^3+q-1)^n - 2c^4 - 3c^2(c-2d+1).
\end{aligned}$$

□

Theorem 5.4. *The second Zagreb index of* $\Gamma(\mathbb{V})$ *is*

$$\begin{aligned} M_2(\Gamma(\mathbb{V})) &= \textstyle\sum_{1\le t<k\le n}\binom{n}{t}(q-1)^{t+k}\sum_{i=1}^{t}(-1)^{i+1}\binom{t}{i}\binom{n-i}{k-i} \\ &\cdot(c-q^{n-t})(c-q^{n-k}) + \textstyle\sum_{\lfloor n/2\rfloor<t=k\le n}\binom{M}{2}(c-q^{n-k})^2 \\ &+ \textstyle\sum_{1\le t=k\le\lceil n/2\rceil}\binom{n}{k}(q-1)^{2k}\sum_{i=1}^{k-1}(-1)^{i+1}\binom{k}{i}\binom{n-i}{k-i}(c-q^{n-k})^2 \\ &+ \textstyle\sum_{t=k=n/2}\frac{1}{2}\binom{M}{2}(c-q^{n/2})^2. \end{aligned}$$

Proof By the definition, the second Zagreb index is the sum of the products of the vertex degrees of the end vertices of all edges in the graph. So we have to use the edge partition of the graph $\Gamma(\mathbb{V})$. By Theorem 4.1, first, when $t<k$, there are $\binom{n}{t}(q-1)^{t+k}\sum_{i=1}^{t}(-1)^{i+1}\binom{t}{i}\binom{n-i}{k-i}$ edges having end vertex degrees $(q^t-1)q^{n-t}-1$ and $(q^k-1)q^{n-k}-1$ which all contribute to the second Zagreb index as much as

$$\sum_{1\le t<k\le n}\binom{n}{t}(q-1)^{t+k}\sum_{i=1}^{t}(-1)^{i+1}\binom{t}{i}\binom{n-i}{k-i}(c-q^{n-t})(c-q^{n-k}).$$

Secondly, when $t=k>\lfloor\frac{n}{2}\rfloor$, there are $\binom{M}{2}$ edges having both end vertex degrees equal to $(q^k-1)q^{n-k}-1$ which altogether contribute to the second Zagreb index as much as

$$\sum_{\lfloor n/2\rfloor<t=k\le n}\binom{M}{2}(c-q^{n-k})^2.$$

Thirdly, when $t=k<\lceil\frac{n}{2}\rceil$, there are $\binom{n}{k}(q-1)^{2k}\sum_{i=1}^{k-1}(-1)^{i+1}\binom{k}{i}\binom{n-i}{k-i}$ edges having both end vertex degrees equal to $(q^k-1)q^{n-k}-1$ which altogether contribute to the second Zagreb index as much as

$$\sum_{1\le t=k<\lceil n/2\rceil}\binom{n}{k}(q-1)^{2k}\sum_{i=1}^{k-1}(-1)^{i+1}\binom{k}{i}\binom{n-i}{k-i}(c-q^{n-k})^2.$$

Finally, when $t=k=\frac{n}{2}$, there are $\frac{1}{2}\binom{M}{2}$ edges having both end vertex degrees equal to $(q^k-1)q^{n-k}-1$ which altogether contribute to the second Zagreb index as much as

$$\sum_{t=k=n/2}\frac{1}{2}\binom{M}{2}(c-q^{n/2})^2.$$

Hence, considering the contributions in all four possible cases and applying some algebraic calculations, we obtain the result. □

Next, we calculate second Zagreb index of the first three non-zero component graphs without proof:

Theorem 5.5. *The second Zagreb index of* $\Gamma(\mathbb{V})$ *is*

$$\begin{cases} 4, & \text{if } q=2,\ n=2; \\ 549, & \text{if } q=2,\ n=3; \\ 1004, & \text{if } q=3,\ n=2. \end{cases}$$

Theorem 5.6. *The sigma index of* $\Gamma(\mathbb{V})$ *is*

$$\sigma(\Gamma(\mathbb{V})) = \sum_{1\le t<k\le n}\binom{n}{t}(q-1)^{t+k}\sum_{i=1}^{t}(-1)^{i+1}\binom{t}{i}\binom{n-i}{k-i}q^{2(n-tk)}(q^t-q^k)^2.$$

Proof As in the second Zagreb index, we again need the edge partition of $\Gamma(\mathbb{V})$. In Theorem 4.1, we see that second, third and fourth type edges have the same end vertex degrees so that they do not contribute to sigma index. So only the first type of edges must be considered. When $1 \leq t < k \leq n$, there are $\sum_{1\leq t<k\leq n} \binom{n}{t}(q-1)^{t+k} \sum_{i=1}^{t}(-1)^{i+1}\binom{t}{i}\binom{n-i}{k-i}$ edges with vertex degrees $(q^t-1)q^{n-t}-1$ and $(q^k-1)q^{n-k}-1$ which altogether contribute to the sigma index as much as

$$\sum_{1\leq t<k\leq n} \binom{n}{t}(q-1)^{t+k} \sum_{i=1}^{t}(-1)^{i+1}\binom{t}{i}\binom{n-i}{k-i}\left[(c-q^{n-t})-(c-q^{n-k})\right]^2.$$

After some algebraic operations, we get the required result. □

Next we calculate the sigma index of the first three non-zero component graphs without proof:

Theorem 5.7. *The sigma index of* $\Gamma(\mathbb{V})$ *is*

$$\begin{cases} 8, & \text{if } q=2,\ n=2; \\ 2055, & \text{if } q=2,\ n=3; \\ 576, & \text{if } q=3,\ n=2. \end{cases}$$

6 Conclusion

In this paper, we studied some topological graph indices based on vertex degrees for a relatively new class of graphs called non-zero component graphs. This work used linear algebraic methods which are apperently new in spectral graph theory. The methods introduced and used here can be applied to many other cases as this idea is quite new.

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Topological Indices of Symmetric Difference Bipartite Graph

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Abstract

Symmetric difference bipartite graph, $SDB(n, k, i)$, is a class of bipartite irregular graphs with two disjoint vertex partitions V_1 and V_2, such that V_1 contains k-element subsets, and V_2 contains subsets of sizes $k - i$ and $k + i$ elements of $\{1, 2, \ldots, n\}$, for $1 \leq k \leq n - 1$ and $1 \leq i \leq \min\{n - k, k - 1\}$. An edge between a vertex $U \in V_1$ and a vertex $W \in V_2$ exists if their symmetric difference has exactly i elements. We determined various graph theoretic properties and established certain topological indices of symmetric difference bipartite graphs.

Keywords: Symmetric difference bipartite graphs, Zagreb index, General Randic index, General sum connectivity index, Sombor index, Wiener index, Minimum degree Wiener index
AMS Classification: 05C09, 05C12, 05C40

1 Introduction

In the fields of chemical sciences and pharmaceuticals, graph theory serves as a crucial tool for understanding various algebraic structures and molecular properties. Topological indices, [9, 18], are graph-theoretic invariants derived from molecular graphs that characterize a graph's topology and are widely utilized to explore quantitative structure-activity relationships (QSAR), linking chemical structures to their biological activity. There are various types of topological indices, including degree-based indices, distance-based indices, and eccentricity-based indices [5, 6, 15, 21]. Degree-based indices [2] hold significant relevance

in chemical graph theory, and in [17], certain degree-based topological indices of Boron B_{12} were discussed.

The Wiener index $W(G)$ of a graph G, introduced by Harold Wiener in 1947, is a well-known topological index in mathematical chemistry, [7], which calculates average distance and is used in chemistry, crystallography, communication theory, and facility location. The index has been studied in pure mathematics under various names, including gross status and graph transmission. Wiener also introduced the Wiener polarity index $W_p(G)$ as the count of unordered pairs of vertices at distance 3 in G, [1]. In [10, 12], the terminal Wiener index was introduced in relation to the terminal distance matrix, which finds applications in genetic codes and the mathematical modeling of proteins, [13, 16]. Additionally, in [4], authors introduced the entire Wiener index of a graph and calculated exact values of this index for trees and certain graph families, while establishing several properties and bounds.

Using the idea of terminal Wiener index, the authors in [19] introduced a new topological index named minimum degree Wiener index together with minimum δ-distance matrix. The properties of this matrix as well as the index are analysed for various class of graphs including molecular graphs. While considering different graphs, the interest in hypercube graphs [3, 14] has led to the introduction of new family of graphs called symmetric difference bipartite graphs[20].

In this paper, we compute various topological indices of symmetric difference bipartite graphs.

2 Preliminaries

Let $G = (V, E)$ be a graph with vertex set V and edge set E. For a vertex $u \in V(G)$, let $d(u)$ denotes the degree of the vertex u in G. The minimum and maximum degree of a graph G are $\delta(G) = \min_{u \in V(G)} \{d(u)\}$, and $\Delta(G) = \max_{u \in V(G)} \{d(u)\}$, respectively. The distance between any two vertices u and w in a connected graph G is the length of the shortest path between them and is denoted by $d(u, w)$. The *diameter* is given by $diam(G) = \max_{u,w \in V(G)} \{d(u, w)\}$. For a connected graph G that is not complete, a *vertex-cut* is a set S of vertices of G such that $G - S$ is disconnected. The cardinality of a minimum vertex-cut is the *vertex connectivity* of G, denoted by $\kappa(G)$. The cardinality of the minimum number of edges whose removal disconnect the graph is the *edge connectivity*, $\lambda(G)$.

Graph invariants are properties or characteristics of a graph that remain unchanged under graph isomorphisms. These parameters play a fundamental role in advancing various fields within science and engineering, including information technology. Below are some examples of such graph invariants based on [11, 17].

Lemma 2.1. *For a simple graph G, let α be any real number. Then,*

1. *the general Randic index is* $R_\alpha(G) = \sum_{uw\in E(G)} \big[d(u)d(w)\big]^\alpha$. *In particular,* $R_1(G)$ *is the second Zagreb index,* $R_{\frac{-1}{2}}(G)$ *is the Randic connectivity index, and* $R_{-1}(G)$ *is the modified Zagreb index which is usually denoted as* $M_2^*(G)$.

2. *the first general Zagreb index is* $M_\alpha(G) = \sum_{u\in V(G)} \big[d(u)\big]^\alpha$. *When* $\alpha = 3$, *it is the forgotten index.*

3. *the general sum connectivity index is* $\chi_\alpha(G) = \sum_{uw\in E(G)} \Big[d(u)+d(w)\Big]^\alpha$. *The first Zagreb index is* $\chi_1(G)$ *and when* $\alpha = -\frac{1}{2}$, *it is called as sum connectivity index.*

4. *the ABC index or atom-bond connectivity index is* $ABC(G) = \sum_{uw\in E(G)} \left[\sqrt{\frac{d(u)+d(w)-2}{d(u)d(w)}}\right]$.

5. *the augmented Zagreb index is* $AZI(G) = \sum_{uw\in E(G)} \left[\frac{d(u)d(w)}{d(u)+d(w)-2}\right]^3$.

6. *the geometric-arithmetic index is* $GA(G) = \sum_{uw\in E(G)} \left[\frac{2\sqrt{d(u)d(w)}}{d(u)+d(w)}\right]$.

7. *the harmonic index is* $H(G) = \sum_{uw\in E(G)} \left[\frac{2}{d(u)+d(w)}\right]$.

8. *the Narumi-Katayama index is* $NK(G) = \prod_{u\in V(G)} d(u)$.

9. *the first multiplicative Zagreb index is* $\prod_1(G) = \prod_{u\in V(G)} d(u)^2$.

10. *the Sombor index is* $SO(G) = \sum_{uw\in E(G)} \sqrt{d(u)^2+d(w)^2}$.

Definition 2.2. The *Wiener index*, $W(G)$ is defined as the sum of distances between all unordered pairs of vertices of the graph G. That is, $W(G) = \sum_{u,w\in V(G)} d(u,w)$.

Milan Randic first introduced the *hyper Wiener index* in 1993. The hyper-Wiener index of a graph G, $WW(G) = \frac{1}{2}\sum_{u,w\in V(G)} [d^2(u,w)+d(u,w)]$, was given by Klein, Lukovits and Gutman in 1995, [8]. The *Wiener Polarity index* [1], $W_p(G)$ is defined to be the number of unordered pairs of vertices at distance 3 in G.

Let n be a positive integer and $[n] = \{1,2,3,\ldots,n\}$. Then the symmetric difference bipartite graph is defined as follows:.

Definition 2.3. [20] For a fixed positive integer n, $1 \le k \le n-1$, and for a fixed i, $1 \le i \le \min\{n-k, k-1\}$, define a simple bipartite graph G with vertex set $V = W_1 \cup W_2$, where W_1

contains all k-element subsets of $[n]$, and W_2 contains $(k-i)$ or $(k+i)$-element subsets of $[n]$, and a vertex in W_1 is adjacent with a vertex in W_2 if and only if their symmetric difference is an i-element subset of $[n]$. This graph is called as symmetric difference bipartite graph or SDB-type k graph and is denoted as $SDB(n,k,i)$.

The graph $SDB(n,k,i)$ is connected. When $k=1$, W_2 contains only $(k+1)$-element subsets of $[n]$.

If we consider all other subsets except the k-element subsets of $[n]$ in the partite set V_2, then the graph becomes disconnected. Let us consider the following examples.

Example 2.4. *See $SDB-$type k graph for $n=4$ and $k=1$.*

Here $V_1 = \{\{1\},\{2\},\{3\},\{4\}\}$ *and* $V_2 = \{\{1,2\},\{1,3\},\{1,4\},\{2,3\},\{2,4\},\{3,4\}\}$

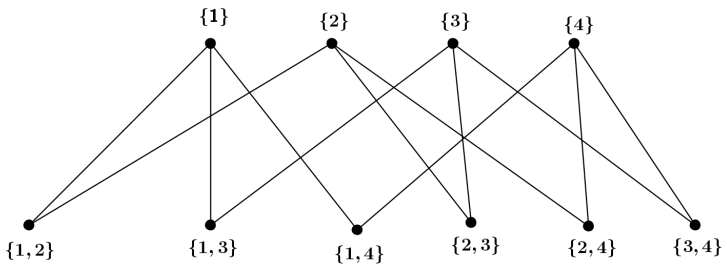

Figure 1: The graph $SDB(4,1,1)$

Example 2.5. *Consider the graph $SDB(4,2,1)$.*

$V_1 = \{\{1,2\},\{1,3\},\{1,4\},\{2,3\},\{2,4\},\{3,4\}\}$ *and*

$V_2 = \{\{1\},\{2\},\{3\},\{4\},\{1,2,3\},\{1,2,4\},\{1,3,4\},\{2,3,4\}\}$

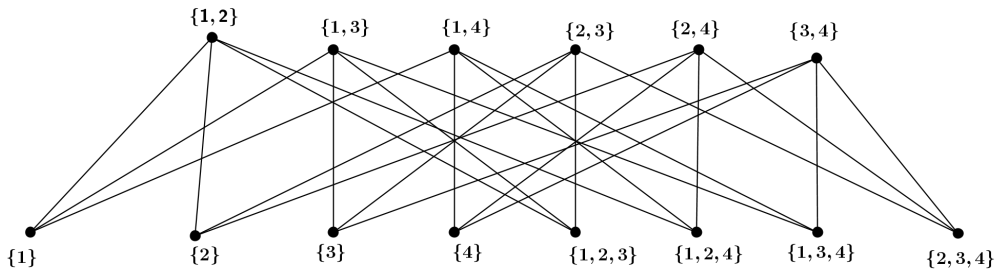

Figure 2: The graph $SDB(4,2,1)$

Also, the symmetric difference bipartite graphs $SDB(4,1,1)$ and $SDB(4,2,1)$ are planar.

Proposition 2.6. *[20] The order and size of the graph $SDB(n,k,i)$, when $k \neq 1$ are $\binom{n}{k} + \binom{n}{k-i} + \binom{n}{k+i}$ and $\binom{n}{k}\left[\binom{k}{k-i} + \binom{n-k}{i}\right]$, respectively.*

In particular, when $k = 1$ and $i = 1$ $V_2 = \{W \subseteq \mathcal{S}_n : |W| = 2\}$. Thus order and size of the corresponding graph $SDB(n,1,1)$ are $\dfrac{n(n+1)}{2}$ and $n(n-1)$ respectively.

The degree sequence of $SDB(n,k,1)$ is given by the following lemma:

Lemma 2.7. *[20]*

1. *For $SDB(n,1,1)$ graph, n vertices have degree $n-1$ and $\dfrac{n(n-1)}{2}$ vertices have degree 2.*
2. *The graph $SDB(n,n-1,1)$ have $n+1$ vertices with degree n and $\dfrac{n(n-1)}{2}$ vertices with degree 2.*
3. *For the graph $SDB(n,k,1)$, $k = \frac{n}{2}$, there are $\binom{n}{k}$ vertices with degree n and $\binom{n}{k-1}+\binom{n}{k+1}$ vertices with degree $k+1$.*
4. *In all other instances, when $k > 1$, the number of vertices having degrees $n-k+1, n,$ and $k+1$ are $\binom{n}{k-1}, \binom{n}{k}$, and $\binom{n}{k+1}$, respectively.*

Above lemma shows, the maximum degree of the graph $SDB(n,k,1)$ is n and the minimum degree for $1 \leq k \leq \left\lfloor \frac{n}{2} \right\rfloor$ is $k+1$. Also, the graph is not regular and not vertex transitive.

Theorem 2.8. *[20] The vertex connectivity and edge connectivity of the graph $SDB(n,k,1)$ is $k+1$ for $1 \leq k \leq \left\lfloor \frac{n}{2} \right\rfloor$.*

Theorem 2.9. *[20] The diameter of the graphs $SDB(n,n-1,1)$, and $SDB(n,1,1), n \geq 4$ is 4.*

For bipartite Kneser type graphs, a novel neighbourhood is defined as follows:

Definition 2.10. [20] Let G be a bipartite Kneser type graph with parts W_1 and W_2 such that $V = W_1 \cup W_2$. Let $W \in V$ and U be any subset or superset of W with $|U \triangle W| = i$. Let $|W| = l$ and $j \in \{l-i, l+i\}$. Then *Sym-i-nbd* of W, denoted by $N^i_{sym}(W)$, is defined to be $N^i_{sym}(W) = \{U^{(j)} \subset V\}$, where $U^{(j)} = \{U : |U| = j\}$.

The sum of the distances between all unordered pairs of pendant vertices on a graph G is the *terminal Wiener index* of that graph [12]. Motivated from the concept of terminal Wiener index, the authors in [19] introduce a new distance related topological index called minimum degree Wiener index. Let G be a simple connected graph. Then the minimum degree Wiener index of G denoted as $MDW(G)$ and is defined as follows:

Definition 2.11. [19] Let $V_{min} \subseteq V(G)$ denote the set of all vertices with minimum degree in G. That is, $V_{min} = \{U_i \in V(G) : d(U_i) = \delta\}$. Define the minimum degree Wiener index, $MDW(G)$ of G as $MDW(G) = \sum_{U_i, U_j \in V_{min}} d(U_i, U_j)$, where $d(U_i, U_j)$ is the distance between all unordered pairs of distinct vertices U_i and U_j in V_{min}.

A *restricted distance matrix* of a graph G is defined as $MDM(G) = [U_{ij}]$,

where $U_{ij} = \begin{cases} d(U_i, U_j) & if \quad U_i, U_j \in V_{min} \\ 0 & \text{otherwise.} \end{cases}$

This matrix is a real symmetric matrix with 0 as diagonal elements. Order of the matrix is $|V(G)|$.

By indexing the rows and columns with the vertex subset V_{min} of G, minimum δ-distance matrix of a graph G is defined as follows:

Definition 2.12. [19] Let G be a graph with $|V(G)| = n$. If G has m vertices with minimum degree, and these m vertices are labeled as $U_1, U_2, \ldots, U_m$, then its minimum δ-distance matrix denoted by $M_\delta DM(G)$ is the square matrix of order m whose $(i, j)^{th}$- entry is $d(U_i, U_j)$. That is, $M_\delta DM(G) = [U_{ij}]$, where $U_{ij} = d(U_i, U_j)$, $U_i, U_j \in V_{min}$. This is also a real symmetric matrix with all diagonal entries 0.

3 Main results

This section presents the principal findings of our study concerning the *symmetric difference bipartite graph*, denoted by $SDB(n, k, i)$. The analysis focuses on the derivation and characterization of several *degree-based* and *distance-based topological indices*, which play a crucial role in understanding the structural properties of complex networks modeled by such graphs. These indices provide quantitative measures that capture both the *local connectivity patterns* and the *global transmission characteristics* of the graph.

In the first part, we develop explicit expressions for various *degree-based topological indices* of $SDB(n, k, i)$, including those that depend on vertex degrees and their mutual interactions. These indices highlight how vertex connectivity and bipartite irregularity contribute to the overall graph structure.

3.1 Degree based indices for the graph $SDB(n, k, i)$

First of all, using the properties of the graphs $SDB(n, k, i)$, degree-based indices are given in the following theorem:

Theorem 3.1. *Let α be any real number. Then, for the graphs $SDB(n, k, i)$, for any positive integer n with $1 \leq k \leq n-1$, and $1 \leq i \leq min\{n-k, k-1\}$,*

1. *the general Randic index is given by*

$$R_\alpha(SDB(n,k,i)) = \begin{cases} \binom{n}{k}\left[\binom{k}{k-i}+\binom{n-k}{i}\right]^\alpha \left\{\binom{k}{k-i}\binom{n-k+i}{i}^\alpha + \binom{n-k}{i}\binom{k+i}{k}^\alpha\right\} & if\ \ k\neq 1, \\ 2n(n-1)^{\alpha+1} & if\ \ k=1. \end{cases}$$

2. *the general sum connectivity index is*

$$\chi_\alpha(SDB(n,k,i)) = \begin{cases} \binom{n}{k}\binom{k}{i}\left\{\binom{k}{i}+\binom{n-k}{i}+\binom{n-k+i}{i}\right\}^\alpha + \binom{n}{k}\binom{n-k}{i}\left\{\binom{k}{i}+\binom{n-k}{i}+\binom{k+i}{i}\right\}^\alpha & if\ k\neq 1, \\ n(n-1)(n+1)^\alpha & if\ k=1. \end{cases}$$

3. *the first general Zagreb index is given by*

$$M_\alpha(SDB(n,k,i)) = \begin{cases} \binom{n}{k}\left[\binom{k}{k-i}+\binom{n-k}{i}\right]^\alpha + \binom{n}{k-i}\binom{n-k+i}{i}^\alpha + \binom{n}{k+i}\binom{k+i}{k}^\alpha & if\ \ k\neq 1, \\ n(n-1)^\alpha + \dfrac{n(n-1)}{2}\,2^\alpha & if\ \ k=1. \end{cases}$$

4. *the atom-bond connectivity index is*

$$ABC(SDB(n,k,i)) = \begin{cases} \begin{cases} \binom{n}{k}\binom{k}{i}\sqrt{\dfrac{\binom{k}{i}+\binom{n-k}{i}+\binom{n-k+i}{i}-2}{\left(\binom{k}{i}+\binom{n-k}{i}\right)\binom{n-k+i}{i}}} + \\ \binom{n}{k}\binom{n-k}{i}\sqrt{\dfrac{\binom{k}{i}+\binom{n-k}{i}+\binom{k+i}{i}-2}{\left(\binom{k}{i}+\binom{n-k}{i}\right)\binom{k+i}{i}}} \end{cases} & if\ \ k\neq 1, \\ \sqrt{2}\,\binom{n}{2} & if\ \ k=1. \end{cases}$$

5. *the augmented Zagreb index is*

$$AZI(SDB(n,k,i)) = \begin{cases} \begin{cases} \binom{n}{k}\binom{k}{i}\left[\dfrac{\left(\binom{k}{i}+\binom{n-k}{i}\right)\binom{n-k+i}{i}}{\binom{k}{i}+\binom{n-k}{i}+\binom{n-k+i}{i}-2}\right]^3 + \\ \binom{n}{k}\binom{n-k}{i}\left[\dfrac{\left(\binom{k}{i}+\binom{n-k}{i}\right)\binom{k+i}{i}}{\binom{k}{i}+\binom{n-k}{i}+\binom{k+i}{i}-2}\right]^3 \end{cases} & if\ \ k\neq 1, \\ \dfrac{n(n-1)}{8} & if\ \ k=1. \end{cases}$$

6. *the geometric-arithmetic index is*

$$GA(SDB(n,k,i)) = \begin{cases} \begin{cases} \binom{n}{k}\binom{k}{i}\left[2\dfrac{\sqrt{\left(\binom{k}{i}+\binom{n-k}{i}\right)\binom{n-k+i}{i}}}{\binom{k}{i}+\binom{n-k}{i}+\binom{n-k+i}{i}}\right] + \\ \binom{n}{k}\binom{n-k}{i}\left[2\dfrac{\sqrt{\left(\binom{k}{i}+\binom{n-k}{i}\right)\binom{k+i}{i}}}{\binom{k}{i}+\binom{n-k}{i}+\binom{k+i}{i}}\right] \end{cases} & if\ \ k\neq 1, \\ 2\sqrt{2}\,\dfrac{n(n-1)^{\frac{3}{2}}}{n+1} & if\ \ k=1. \end{cases}$$

7. *the harmonic index is*

$$H(SDB(n,k,i)) = \begin{cases} \begin{cases} \binom{n}{k}\binom{k}{i}\left[\frac{2}{\binom{k}{i}+\binom{n-k}{i}+\binom{n-k+i}{i}}\right]+ \\ \binom{n}{k}\binom{n-k}{i}\left[\frac{2}{\binom{k}{i}+\binom{n-k}{i}+\binom{k+i}{i}}\right] \end{cases} & if\ \ k \neq 1, \\ \frac{2n(n-1)}{n+1} & if\ k = 1. \end{cases}$$

8. *the Narumi-Katayama index is*

$$NK(SDB(n,k,i)) = \begin{cases} \left[\binom{k}{i}+\binom{n-k}{i}\right]^{\binom{n}{k}} \ \binom{n-k+i}{i}^{\binom{n}{k-i}} \ \binom{k+i}{i}^{\binom{n}{k+i}} & if\ \ k \neq 1, \\ (n-1)^n 2^{\binom{n}{2}} & if\ k = 1. \end{cases}$$

9. *the first multiplicative Zagreb index is*

$$\prod_{U \in V(SDB(n,k,i))} (d(U))^2 = \begin{cases} \left[\binom{k}{i}+\binom{n-k}{i}\right]^{2\binom{n}{k}} \ \binom{n-k+i}{i}^{2\binom{n}{k-i}} \ \binom{k+i}{i}^{2\binom{n}{k+i}} & if\ \ k \neq 1, \\ (n-1)^{2n}\ 2^{n(n-1)} & if\ k = 1. \end{cases}$$

10. *the Sombor index is*

$$SO(SDB(n,k,i)) = \begin{cases} \begin{cases} \binom{n}{k}\binom{k}{i}\left[\sqrt{\left(\binom{k}{i}+\binom{n-k}{i}\right)^2+\binom{n-k+i}{i}^2}\right]+ \\ \binom{n}{k}\binom{n-k}{i}\left[\sqrt{\left(\binom{k}{i}+\binom{n-k}{i}\right)^2+\binom{k+i}{i}^2}\right] \end{cases} & if\ \ k \neq 1, \\ n(n-1)\sqrt{n^2-2n+5} & if\ k = 1. \end{cases}$$

Proof. Using the Proposition 2.6 and the Lemma 2.7, partition the edge set of $SDB(n,k,i),\ k \neq 1$ into two disjoint sets in which one contains all the edges of the graph having end vertices with degrees $\binom{k}{k-i}+\binom{n-k}{i}$ and $\binom{n-k+i}{i}$, and the other contains all the edges of the graph with end vertices having degrees $\binom{k}{k-i}+\binom{n-k}{i}$ and $\binom{k+i}{k}$.
For $k = 1$, there are $n(n-1)$ edges having end vertices with degrees $n-1$ and 2.

Table 1: Table showing edge partition in the graph $SDB(n,k,i)$

Number of edges	$(d(U), d(W))$
$\binom{n}{k}\binom{k}{k-i}$	$\left(\binom{k}{k-i}+\binom{n-k}{i}, \binom{n-k+i}{i}\right)$
$\binom{n}{k}\binom{n-k}{i}$	$\left(\binom{k}{k-i}+\binom{n-k}{i}, \binom{k+i}{k}\right)$

By substituting these in the Lemma 2.1, and using combinatorics relations such as $\binom{k}{k-i} = \binom{k}{i}$ and $\binom{k+i}{k} = \binom{k+i}{i}$, we obtain the desired result.

1. $R_\alpha(SDB(n,k,i)) = \begin{cases} \binom{n}{k}\binom{k}{k-i}\left[\left(\binom{k}{k-i}+\binom{n-k}{i}\right)\binom{n-k+i}{i}\right]^\alpha + \\ \binom{n}{k}\binom{n-k}{i}\left[\left(\binom{k}{k-i}+\binom{n-k}{i}\right)\binom{k+i}{k}\right]^\alpha \end{cases}$

   Hence,

$$R_\alpha(SDB(n,k,i)) = \binom{n}{k}\left[\binom{k}{k-i}+\binom{n-k}{i}\right]^\alpha\left\{\binom{k}{k-i}\binom{n-k+i}{i}^\alpha+\binom{n-k}{i}\binom{k+i}{k}^\alpha\right\}.$$

2. $\chi_\alpha(SDB(n,k,i)) = \begin{cases} \binom{n}{k}\binom{k}{k-i}\left[\left(\binom{k}{k-i}+\binom{n-k}{i}\right)+\binom{n-k+i}{i}\right]^\alpha + \\ \binom{n}{k}\binom{n-k}{i}\left[\left(\binom{k}{k-i}+\binom{n-k}{i}\right)+\binom{k+i}{k}\right]^\alpha \end{cases}$

   So, $\chi_\alpha(SDB(n,k,i)) = \begin{cases} \binom{n}{k}\binom{k}{i}\left\{\binom{k}{i}+\binom{n-k}{i}+\binom{n-k+i}{i}\right\}^\alpha + \\ \binom{n}{k}\binom{n-k}{i}\left\{\binom{k}{i}+\binom{n-k}{i}+\binom{k+i}{i}\right\}^\alpha. \end{cases}$

3. The first general Zagreb index is given by,

$$M_\alpha(SDB(n,k,i)) = \begin{cases} n(n-1)^\alpha + \dfrac{n(n-1)}{2}\,2^\alpha \;\; if \;\; k=i=1, \\ (n+1)n^\alpha + \dfrac{n(n-1)}{2}\,2^\alpha \;\; if \;\; k=n-1,\; i=1, \\ \binom{n}{k}n^\alpha + \left[\binom{n}{k-1}+\binom{n}{k+1}\right](k+1)^\alpha \;\; if \;\; k=\frac{n}{2},\; i=1, \\ \binom{n}{k-1}(n-k+1)^\alpha + \binom{n}{k}n^\alpha + \binom{n}{k+1}(k+1)^\alpha \;\; if\; k\neq\frac{n}{2},\; i=1. \end{cases}$$

   Hence,

$$M_\alpha(SDB(n,k,i)) = \begin{cases} n(n-1)^\alpha + \dfrac{n(n-1)}{2}\,2^\alpha \;\; if \;\; k=1, \\ \binom{n}{k}\left[\binom{k}{k-i}+\binom{n-k}{i}\right]^\alpha + \binom{n}{k-i}\binom{n-k+i}{i}^\alpha + \binom{n}{k+i}\binom{k+i}{k}^\alpha \;\; if \;\; k\neq 1. \end{cases}$$

   When $k \neq 1$, all other indices are obtained directly by substituting degrees of end vertices of each edge in the corresponding formulae. When $k = 1$, the indices are obtained as follows:

4. The atom-bond connectivity index is

$$\begin{aligned} ABC(SDB(n,1,1)) &= n(n-1)\sqrt{\frac{n-1+2-2}{2(n-1)}} \\ &= n(n-1)\sqrt{\frac{1}{2}} = \sqrt{2}\binom{n}{2}. \end{aligned}$$

5. The augmented Zagreb index is

$$\begin{aligned} AZI(SDB(n,1,1)) &= n(n-1)\left[\frac{n-1+2-2}{2(n-1)}\right]^3 \\ &= n(n-1)\left(\frac{1}{2}\right)^3 = \frac{n(n-1)}{8}. \end{aligned}$$

6. The geometric-arithmetic index is

$$\begin{aligned} GA(SDB(n,1,1)) &= n(n-1)\frac{2\sqrt{2(n-1)}}{n-1+2} \\ &= 2n\sqrt{2(n-1)}\ \ \frac{n-1}{n+1}. \end{aligned}$$

7. The harmonic index is

$$\begin{aligned} H(SDB(n,1,1)) &= n(n-1)\ \frac{2}{(n-1)+2} \\ &= 2n\ \frac{n-1}{n+1}. \end{aligned}$$

8. As the Narumi-Katayama index is the product of degrees of vertices, $NK(SDB(n,1,1)) = (n-1)^n 2^{\binom{n}{2}}$.

9. Since the first multiplicative Zagreb index is the product of squares of the degrees of vertices, from Lemma 2.7, $M_\alpha(SDB(n,1,1)) = (n-1)^{2n}\ 2^{n(n-1)}$.

10. The Sombor index,

$$\begin{aligned} SO(SDB(n,1,1)) &= n(n-1)\sqrt{(n-1)^2+2^2} \\ &= n(n-1)\sqrt{n^2-2n+5}. \end{aligned}$$

□

Corollary 3.2. *1. When $\alpha = 1$, $R_1(SDB(n,k,i))$ is the second Zagreb index.*

2. The Randic connectivity index is $R_{\frac{-1}{2}}(SDB(n,k,i))$.

3. $R_{-1}(SDB(n,k,i))$ is the modified Zagreb Index, $M_2^*(G)$.

4. In the general sum connectivity index, when $\alpha = 1$, $\chi_1(SDB(n,k,i))$ is the first Zagreb index.

5. The sum connectivity index is $\chi_{\frac{-1}{2}}(SDB(n,k,i))$.

6. The forgotten index is $M_3(SDB(n,k,i))$. Also,

$$M_3(SDB(n,1,1)) = n(n-1)(n^2-2n+5).$$

In this part, we derive *distance-based topological indices*, which incorporate the shortest path distances between vertex pairs. These indices serve to reveal the efficiency of information transfer and the compactness of the network encoded by $SDB(n,k,i)$.

Distance-based indices for the graph $SDB(n,k,i)$

The notion of distance provides a basic measure of relationship between two vertices. Distance-based indices serve as powerful tools to quantify various properties of a graph by considering this relationship.

Example 3.3. *Consider the graph* $SDB(3,1,1)$. *The vertex set* $V = W_1 \cup W_2$ *with partition* $W_1 = \{\{1\},\{2\},\{3\}\}$ *and* $W_2 = \{\{1,2\},\{1,3\},\{2,3\}\}$. *There are* 6 *edges and so the end vertices of each edge are at a distance* 1. *The distance between vertices within* W_1 *and within* W_2 *are at a distance* 2. *Six such pairs exist.*
Also, $d(\{1\},\{2,3\}) = d(\{2\},\{1,3\}) = d(\{3\},\{1,2\}) = 3$.

In the graph $SDB(3,2,1)$, there are 9 vertex pairs at a distance 1, nine pairs are at a distance 2 and three pairs are at a distance 3.

The following proposition gives the number of unordered pairs of vertices at a distance h.

Lemma 3.4. *For the symmetric difference bipartite graphs* $SDB(n,1,1)$, $n > 3$, *the number of unordered pairs of vertices with distance* h *is :*

$$d_h(U,W) = \begin{cases} n(n-1) & \text{if } h = 1, \\ (n-1)\binom{n}{2} & \text{if } h = 2, \\ 3\binom{n}{3} & \text{if } h = 3, \\ 3\binom{n}{4} & \text{if } h = 4. \end{cases}$$

Proof. Using the Definition 2.3, the vertex partition W_1 contains all one element subsets of $[n]$, and W_2 contains only 2-element subsets of $[n]$. In $SDB(n,1,1)$, $n(n-1)$ vertex pairs are adjacent. To find the number of vertex pairs with distance other than 1, consider the following cases:

Case (1):
When $U, W \in W_1$, then $U \to U \cup W \to W$ is a path of length 2. Number of such vertex pairs is $\binom{n}{2}$.
If $U, W \in W_2$ with $|U \cap W| = 1$, then $U \to U \cap W \to W$ is a path of length 2 so that $d(U,W) = 2$ and there are $\frac{1}{2}\left[\binom{n}{2}\binom{2}{1}\binom{n-2}{1}\right] = (n-2)\binom{n}{2}$ such pairs.
Hence $d_2(U,W) = \binom{n}{2} + (n-2)\binom{n}{2} = (n-1)\binom{n}{2}$.

Case (2):
If $U \in W_1$, $W \in W_2$, and $|U \cap W| = 0$, there exists $n\binom{n-1}{2}$ vertex pairs at a distance 3. Hence $d_3(U,W) = n\binom{n-1}{2} = 3\binom{n}{3}$.

Case (3):
When $U, W \in W_2$ and $|U \cap W| = 0$, then there are $\frac{1}{2}\left[\binom{n}{2}\binom{n-2}{2}\right] = 3\binom{n}{4}$ vertex pairs at a distance 4. □

Using the above proposition, the Wiener index, Wiener polarity index, and hyper Wiener index for the graph $SDB(n,1,1)$ are determined as follows:

Proposition 3.5. *The Wiener index of the graph $SDB(n,1,1)$, denoted by $W(SDB(n,1,1))$, where $n>3$ is $n^2\binom{n}{2}$.*

Proof.

$$\begin{aligned} W(SDB(n,1,1)) &= n(n-1)+2\left[(n-1)\binom{n}{2}\right]+3\left[3\binom{n}{3}\right]+4\left[3\binom{n}{4}\right] \\ &= n^2(n-1)+\frac{3}{2}n(n-1)(n-2)+\frac{1}{2}n(n-1)(n-2)(n-3) \\ &= n^2(n-1)+\frac{1}{2}n^2(n-1)(n-2) \\ &= n^2\binom{n}{2}. \end{aligned}$$

□

Proposition 3.6. *The Wiener polarity index of the graph $SDB(n,1,1)$ is $3\binom{n}{3}$.*

Proof. From the Lemma 3.4, the Wiener polarity index of the graph $SDB(n,1,1)$ is $d_3(U,W)=3\binom{n}{3}$. □

Proposition 3.7. *The hyper Wiener index for the graph $SDB(n,1,1), n>3$ is $(3n-1)\binom{n}{2}+18\binom{n}{3}+30\binom{n}{4}$.*

Proof. Using Lemma 3.4, the hyper Wiener index,

$$\begin{aligned} WW(SDB(n,1,1)) &= \frac{1}{2}\left[\sum d^2(U,W)+\sum d(U,W)\right] \\ &= \frac{1}{2}\left[2n(n-1)+6(n-1)\binom{n}{2}+36\binom{n}{3}+60\binom{n}{4}\right] \\ &= (3n-1)\binom{n}{2}+18\binom{n}{3}+30\binom{n}{4}. \end{aligned}$$

□

Lemma 3.8. *The number of unordered pairs of vertices with distance h, $d_h(U,W)$ for the graph $SDB(n,2,1)$ is as follows:*

$$d_h(U,W)=\begin{cases} n\binom{n}{2} & \text{if } h=1, \\ \binom{n}{2}+6\binom{n}{3}+6\binom{n}{4} & \text{if } h=2, \\ 3\binom{n}{3}+12\binom{n}{4} & \text{if } h=3, \\ 7\binom{n}{4}+15\binom{n}{5} & \text{if } h=4, \\ 10\binom{n}{5} & \text{if } h=5, \\ 10\binom{n}{6} & \text{if } h=6. \end{cases}$$

Proof. From the Proposition 2.6, there are $n\binom{n}{2}$ unordered pair of vertices at a distance 1. If both the vertices belong to the same partition, then the distance between them must be even. Otherwise, it is odd. Consider the first case. Then there may arise subcases as follows:
Case (1): When both the vertices U and W lie in the part W_1, then $|U| = 2 = |W|$ and $0 \leq |U \cap W| \leq 1$.
(a): If $|U \cap W| = 0$,
then there is no *Sym-i-nbd* common to them. Also, $|U \cup W| = 4$. In this case, there is a common *Sym*-2-*nbd* for elements in the *Sym-i-nbd*, $i \in \{1, 3\}$ of U and W. Then $d(U, W) = 4$. Number of unordered pairs of vertices with this property is $\frac{1}{2}\left[\binom{n}{2}\binom{n-2}{2}\right] = 3\binom{n}{4}$.
(b): If $|U \cap W| = 1$,
then there exists a *Sym-i-nbd* where $i \in \{1, 3\}$, through which the path from U to W passes. So $d(U, W) = 2$.
There are $\frac{1}{2}\left[\binom{n}{2}\binom{2}{1}\binom{n-2}{1}\right] = (n-2)\binom{n}{2} = 3\binom{n}{3}$ such vertex pairs.
Case (2):
Let $U, W \in W_2$. Then there are three subcases:
(a): If $|U| = 1 = |W|$,
then $U \to U \cup W \to W$ is a path of length 2. These are $\binom{n}{2}$ in numbers.
(b): If $|U| = 3 = |W|$, then $0 \leq |U \cap W| \leq 2$.
- Let $|U \cap W| = 0$.

Then $|U \cup W| = 6$.
For $n \geq 6$, the length of the shortest path between U and W is 6.
For example, $U = \{1, 2, 3\} \to \{1, 2\} \to \{1, 2, 4\} \to \{1, 4\} \to \{4\} \to \{4, 5\} \to \{4, 5, 6\} = W$ is one of the such paths.
There are $\frac{1}{2}\left[\binom{n}{3}\binom{n-3}{3}\right] = 10\binom{n}{6}$ unordered pairs of vertices at a distance 6.
- If $|U \cap W| = 1$.

Then there exists $\frac{1}{2}\left[\binom{n}{3}\binom{3}{1}\binom{n-3}{2}\right] = 15\binom{n}{5}$ vertex pairs at a distance 4.
- If $|U| = 3 = |W|$ and $|U \cap W| = 2$, then $U \to U \cap W \to W$ constitutes a path of length 2. The total count of such pairs is $\frac{1}{2}\left[\binom{n}{3}\binom{3}{2}\binom{n-3}{1}\right] = 6\binom{n}{4}$.

(c): If $|U| = 1$ and $|W| = 3$.
- If $U \subset W$, then there exists $n\binom{n-1}{2} = 3\binom{n}{3}$ pairs such that $d(U, W) = 2$.
- If $U \nsubseteq W$ and $|U| = 1, |W| = 3$,

then the distance between these vertices is 4 and the number of vertex pairs is $\binom{n}{1}\binom{n-1}{3} = 4\binom{n}{4}$.
Case (3):
Consider the case when $U \in W_1$ and $W \in W_2$.
Then either $|W| = 1$ or $|W| = 3$.
(a): $|W| = 1$.
- When $|U \cap W| = \phi$, then there exists an edge between atleast one member of *Sym-i-nbd*

of W and that of U so that $d(U,W)=3$.
The number of such pairs is $(n-2)\binom{n}{2}=3\binom{n}{3}$.

- If $|U\cap W|\neq\phi$, then U and W are adjacent vertices.

(b): $|W|=3$.

- $|U\cap W|=\phi$ implies there are $\binom{n}{2}\binom{n-2}{3}=10\binom{n}{5}$ vertex pairs at a distance 5.
- If $|U\cap W|=1$, then there are $\binom{n}{2}\binom{2}{1}\binom{n-2}{2}=12\binom{n}{4}$ unordered pairs of vertices at a distance 3.
- If $|U\cap W|=2$, then $UW\in E(SDB(n,2,1))$.

Combining all these cases and subcases, we get the result. □

Now, Wiener index for the graph $SDB(n,2,1)$ is given in the the following theorem.

Proposition 3.9. *The Wiener index of the symmetric difference bipartite graph* $SDB(n,2,1)$ *is given by* $(n+2)\binom{n}{2}+21\binom{n}{3}+76\binom{n}{4}+110\binom{n}{5}+60\binom{n}{6}$.

Proof. The proof follows from the Lemma 3.8.

$$\begin{aligned}W(SDB(n,2,1)) &= \sum_{U,W\in V(SDB(n,2,1))} d(U,W)\\ &= \sum_{h=1}^{h=6} h\,d_h(U,W),\ \text{where } U,W\in V(SDB(n,2,1))\\ &= 1.n\binom{n}{2}+2\left[\binom{n}{2}+6\binom{n}{3}+6\binom{n}{4}\right]+3\left[3\binom{n}{3}+12\binom{n}{4}\right]\\ &+4\left[7\binom{n}{4}+15\binom{n}{5}\right]+10\binom{n}{5}5+10\binom{n}{6}6\\ &= (n+2)\binom{n}{2}+21\binom{n}{3}+76\binom{n}{4}+110\binom{n}{5}+60\binom{n}{6}.\end{aligned}$$

□

Proposition 3.10. *The Wiener Polarity index for the symmetric difference bipartite graph* $SDB(n,2,1)$ *is* $3\binom{n}{3}+12\binom{n}{4}$.

Proof. From the Lemma 3.8, the Wiener polarity index is

$$\begin{aligned}W_p(SDB(n,2,1)) &= d_3(U,W)\\ &= 3\binom{n}{3}+12\binom{n}{4}.\end{aligned}$$

□

Theorem 3.11. *The hyper Wiener index for the symmetric difference bipartite graph* $SDB(n,2,1)$ *is given by* $(n+3)\binom{n}{2}+36\binom{n}{3}+160\binom{n}{4}+300\binom{n}{5}+210\binom{n}{6}$.

Proof.

$$\begin{aligned}WW(SDB(n,2,1)) &= \frac{1}{2}\left[\sum_{h=1}^{6} h\ d_h(U,W) + \sum_{h=1}^{6} h^2\ d_h(U,W)\right], \text{ where } U,W \in V(SDB(n,2,1))\\ &= \frac{1}{2}\Bigg[(2n+1)\binom{n}{2} + 12\binom{n}{3} + 12\binom{n}{4} + 4\binom{n}{2} + 24\binom{n}{3} + 24\binom{n}{4}\\ &+ 9\binom{n}{3} + 36\binom{n}{4} + 27\binom{n}{3} + 108\binom{n}{4} + 28\binom{n}{4} + 60\binom{n}{5} + 112\binom{n}{4}\\ &+ 240\binom{n}{5} + 50\binom{n}{5} + 250\binom{n}{5} + 60\binom{n}{6} + 360\binom{n}{6}\Bigg]\\ &= (n+3)\binom{n}{2} + 36\binom{n}{3} + 160\binom{n}{4} + 300\binom{n}{5} + 210\binom{n}{6}.\end{aligned}$$

□

Lemma 3.12. *The number of unordered pairs of vertices with distance h, $d_h(U,W)$ for the graph $SDB(n,3,1)$ is as follows:*

$$d_h(U,W) = \begin{cases} n\binom{n}{3} & \text{if } h=1,\\ 3\binom{n}{3} + 12\binom{n}{4} + 10\binom{n}{5} & \text{if } h=2,\\ 12\binom{n}{4} + 30\binom{n}{5} & \text{if } h=3,\\ 3\binom{n}{4} + 35\binom{n}{5} + 45\binom{n}{6} & \text{if } h=4,\\ 10\binom{n}{5} + 60\binom{n}{6} & \text{if } h=5,\\ 25\binom{n}{6} + 70\binom{n}{7} & \text{if } h=6,\\ 35\binom{n}{7} & \text{if } h=7,\\ 35\binom{n}{8} & \text{if } h=8.\end{cases}$$

Proof. The number of unordered pairs of vertices at a distance of one is the number of edges in the graph $SDB(n,3,1)$ and it is obtained from the Proposition 2.6.
As demonstrated in the proof of the Lemma 3.8, we observe that the distance between two vertices is even if both vertices belong to the same part of the vertex partition; otherwise, it is odd. Since $k=3$, the partition W_1 contains 3-element subsets of $[n]$ and, W_2 contains all 2-element and 4-element subsets of $[n]$.
Case (1): both U and W are in W_1,
Then $0 \le |U \cap W| \le 2$.
(a): If $|U \cap W| = 2$, then $U \cap W \in W_2$ is a common *Sym-i-nbd* of U and W so that $d(U,W) = 2$. Number of such common *Sym-i-nbd* is $\frac{1}{2}\left[\binom{n}{3}\binom{3}{2}\binom{n-3}{1}\right] = 6\binom{n}{4}$.
(b): If $|U \cap W| = 1$, then there are $\frac{1}{2}\left[\binom{n}{3}\binom{3}{1}\binom{n-3}{2}\right] = 15\binom{n}{5}$ pairs of vertices with $d(U,W) = 4$.
(c): $|U \cap W| = 0$ implies U and W are disjoint vertices that are at a distance 6. There exists $\frac{1}{2}\left[\binom{n}{3}\binom{n-3}{3}\right] = 10\binom{n}{6}$ vertex pairs with this property.

Case (2): U and W are in W_2.
Then they are two element or four element subsets of $[n]$.
(a): When $|U| = |W| = 2$, then $0 \leq |U \cap W| \leq 1$.
• If $|U \cap W| = 0$, then $\frac{1}{2}\left[\binom{n}{2}\binom{n-2}{2}\right] = 3\binom{n}{4}$ pairs of vertices are connected by a path of length 4.
• If $|U \cap W| = 1$, then $U \cup W$ is a common *Sym-i-nbd* of U and W such that $U \to U \cup W \to W$ is a path of length 2. Total pairs is $\frac{1}{2}\left[\binom{n}{2}\binom{2}{1}\binom{n-2}{1}\right] = 3\binom{n}{3}$.
(b): If $|U| = |W| = 4$, then $0 \leq |U \cap W| \leq 3$.
• If $|U \cap W| = 0$, then these vertices are at a distance 8 for $n \geq 8$. The number of such pairs is $\frac{1}{2}\left[\binom{n}{4}\binom{n-4}{4}\right] = 35\binom{n}{8}$.
• If $|U \cap W| = 1$, then there exists $\frac{1}{2}\left[\binom{n}{4}\binom{4}{1}\binom{n-4}{3}\right] = 70\binom{n}{7}$ vertex pairs at a distance 6.
• If $|U \cap W| = 2$, then $d(U, W) = 4$ with $\frac{1}{2}\left[\binom{n}{4}\binom{4}{2}\binom{n-4}{2}\right] = 45\binom{n}{6}$ such pairs.
• If $|U \cap W| = 3$, then $U \to U \cap W \to W$ is a path of length 2. Number of pairs is $\frac{1}{2}\left[\binom{n}{4}\binom{4}{3}\binom{n-4}{1}\right] = 10\binom{n}{5}$.
(c): If $|U| = 2$, and $|W| = 4$, then $0 \leq |U \cap W| \leq 2$.
• If $|U \cap W| = 0$, then for $n \geq 6$, there are $\left[\binom{n}{2}\binom{n-2}{4}\right] = 15\binom{n}{6}$ unordered pairs of vertices with distance 6.
• If $|U \cap W| = 1$, then $\binom{n}{2}\binom{2}{1}\binom{n-2}{3} = 20\binom{n}{5}$ pairs of vertices are connected by the shortest path of length 4.
• If $|U \cap W| = 2$, then $d(U, W) = 2$ and there are $\binom{n}{2}\binom{n-2}{2}$ such pairs.
Case (3): Let $U \in W_1$ and $W \in W_2$.
(a): If $|U| = 3$, and $|W| = 2$, then either $W \subseteq U$ or $W \not\subseteq U$.

- $W \subseteq U$ implies U and W are adjacent vertices.

- If $W \not\subseteq U$, then $0 \leq |U \cap W| \leq 1$.

If $|U \cap W| = 0$, then $d(U, W) = 5$ for $n \geq 5$. In this case the number of vertex pairs is $\binom{n}{3}\binom{n-3}{2} = 10\binom{n}{5}$.

If $|U \cap W| = 1$, then the number of vertex pairs at a distance 3 is

$$\binom{n}{3}\binom{3}{1}\binom{n-3}{1} = 12\binom{n}{4}$$

.

(b): $|U| = 3$, and $|W| = 4$

• If $|U \cap W| = 0$, then $d(U, W) = 7$, and the number of vertex pairs in this case is $\binom{n}{3}\binom{n-3}{4} = 35\binom{n}{7}$.

• If $|U \cap W| = 1$, then $\binom{n}{3}\binom{3}{1}\binom{n-3}{3} = 60\binom{n}{6}$ vertex pairs are at a distance 5.

• If $|U \cap W| = 2$, then $d(U, W) = 3$ with $\binom{n}{3}\binom{3}{2}\binom{n-3}{2} = 30\binom{n}{5}$ pairs. Hence by combining all these cases, we have the required result. □

Proposition 3.13. *The Wiener index of the symmetric difference bipartite graph* $SDB(n, 3, 1)$ *is given by* $(n+6)\binom{n}{3} + 72\binom{n}{4} + 300\binom{n}{5} + 630\binom{n}{6} + 665\binom{n}{7} + 280\binom{n}{8}$.

Proof. By Lemma 3.12,

$$\begin{aligned} W(SDB(n,3,1)) &= n\binom{n}{3} + 2\left[3\binom{n}{3} + 12\binom{n}{4} + 10\binom{n}{5}\right] + 3\left[12\binom{n}{4} + 30\binom{n}{5}\right] \\ &\quad + 4\left[3\binom{n}{4} + 35\binom{n}{5} + 45\binom{n}{6}\right] + 5\left[10\binom{n}{5} + 60\binom{n}{6}\right] \\ &\quad + 6\left[25\binom{n}{6} + 70\binom{n}{7}\right] + 7\left[35\binom{n}{7}\right] + 8\left[35\binom{n}{8}\right] \\ &= (n+6)\binom{n}{3} + 72\binom{n}{4} + 300\binom{n}{5} + 630\binom{n}{6} + 665\binom{n}{7} + 280\binom{n}{8}. \end{aligned}$$

□

Proposition 3.14. *The Wiener polarity index for the symmetric difference bipartite graph* $SDB(n, 3, 1)$ *is* $12\binom{n}{4} + 30\binom{n}{5}$.

Proof. Using the Lemma 3.12, the number of unordered pairs of vertices at a distance 3 is given by $12\binom{n}{4} + 30\binom{n}{5}$ and it is the Wiener polarity index. □

Next, we proceed to determine the minimum degree Wiener index for the symmetric difference bipartite graphs.

Theorem 3.15. *[20] The minimum degree Wiener index of the symmetric difference bipartite graphs* $SDB(n, k, 1)$ *is* $\dfrac{n(n-1)^2(n-2)}{2}$, *when* $n \geq 4$ *and* $k = 1$ *or* $n \geq 3$ *and* $k = n - 1$.

All the 6 vertices of the symmetric difference bipartite graph $SDB(3, 1, 1)$ are vertices with minimum degree 2. Therefore, the minimum degree Wiener index and the Wiener index are the same and it is 27 for the graph $SDB(3, 1, 1)$.

Example 3.16. *Consider the symmetric difference bipartite graph* $SDB(4, 2, 1)$. *Among the vertices in* $V(SDB(4, 2, 1))$, *all the* 8 *vertices in the partition* W_2 *have minimum degree* 3. *By indexing these vertices in rows and columns, an* 8×8 *minimum* δ*-distance matrix can*

be constructed with entries as distance between them. Based on Lemma 3.8, there are 24 *unordered pairs of vertices are at a distance* 2 *and four vertex pairs are at a distance* 4. *Hence minimum degree Wiener index for* $SDB(4,2,1)$ *is* 64.

For $n > 4$, the minimum degree Wiener index is obtained as follows:

Proposition 3.17. *The minimum degree Wiener index for the graph* $SDB(n,2,1)$, *where* $n \neq 4$ *is* $MDW(SDB(n,2,1)) = 12\binom{n}{4} + 60\binom{n}{5} + 60\binom{n}{6}$.

Proof. In the graph $SDB(n,2,1)$,

$$d(U) = \begin{cases} n & if \ \ U \in W_1, \\ n-1 & if \ \ U \in W_2 \text{ and } |U| = 1, \\ 3 & if \ \ U \in W_2 \text{ and } |U| = 3. \end{cases}$$

Since $n > 4$, $V_{min} = \{U \in W_2 : |U| = 3\}$ and $|V_{min}| = \binom{n}{3}$. So to find minimum degree Wiener index, it is enough to calculate the distance between vertices among the set V_{min}. This is the Case (2), (b) of the Lemma 3.8.

That is, for $U, W \in V_{min}$, $d_h(U,W) = \begin{cases} 6\binom{n}{4} & if \ h = 2, \\ 15\binom{n}{5} & if \ h = 4, \\ 10\binom{n}{6} & if \ h = 6. \end{cases}$

Hence, $MDW(SDB(n,2,1)) = 12\binom{n}{4} + 60\binom{n}{5} + 60\binom{n}{6}$. □

Consider the graph $SDB(n,3,1)$. When $n = 4$, then minimum degree Wiener index for $SDB(4,3,1)$ is obtained from the Theorem 3.15. Let us consider the graphs $SDB(5,3,1)$ and $SDB(6,3,1)$.

Example 3.18. *For each vertex* U *in* $V(SDB(5,3,1))$,

degree of U, $d(U) = \begin{cases} 5 & if \ U \in W_1, \\ 4 & if \ U \in W_2 \text{ and } |U| = 4, \\ 3 & if \ U \in W_2 \text{ and } |U| = 2. \end{cases}$

Thus $V_{min} = \{U \in W_2 : |U| = 2\}$ *with* $|V_{min}| = 10$. *Using Case (2),* (a) *of Lemma 3.12, for each unordered pair of vertices* $U, W \in V_{min}$, 15 *vertex pairs are at a distance* 4, *and* 30 *vertex pairs are at a distance* 2. *So* $MDW(SDB(5,3,1)) = 120$.

Example 3.19. *Different from the above example, all the vertices in the partition* W_2 *of the graph* $SDB(6,3,1)$ *have degree* 4 *which is the minimum. Then Case(2), of Lemma 3.12*

shows,

$$d_h(U,W) = \begin{cases} 210 & if\ h = 2, \\ 210 & if\ h = 4, \\ 15 & if\ h = 6. \end{cases}$$

Hence, $MDW(SDB(6,3,1)) = 1350$.

The generalisation of minimum degree Wiener index for the graphs $SDB(n,3,1)$ is given in the following proposition.

Proposition 3.20. *For* $n \geq 7$*, the minimum degree Wiener index for* $SDB(n,3,1)$*,*

$$MDW(SDB(n,3,1)) = 280\binom{n}{8} + 420\binom{n}{7} + 180\binom{n}{6} + 20\binom{n}{5}.$$

Proof. Since $n \geq 7$, minimum degree for the graph $SDB(n,3,1)$ is 4 and the set of vertices with minimum degree, $V_{min} = \{U \in W_2 : |U| = 4\}$. So, $|V_{min}| = \binom{n}{4}$. By Case (2), (b) of Lemma 3.12, for each pair (U,W) of vertices in V_{min},

$$d_h(U,W) = \begin{cases} 35\binom{n}{8} & if\ h = 8, \\ 70\binom{n}{7} & if\ h = 6, \\ 45\binom{n}{6} & if\ h = 4, \\ 10\binom{n}{5} & if\ h = 2. \end{cases}$$

Thus $MDW(SDB(n,3,1)) = 280\binom{n}{8} + 420\binom{n}{7} + 180\binom{n}{6} + 20\binom{n}{5}$. □

4 Conclusion

In this paper, some degree-based topological indices of symmetric difference bipartite graph such as the general Randic connectivity index, the general sum connectivity index, the first Zagreb index and Sombor index were examined. Distance based indices were also calculated. Minimum degree Wiener index for $SDB(n,1,1)$, $SDB(n,2,1)$, $SDB(n,3,1)$ and $SDB(n,n-1,1)$ were computed. Finding more topological indices that relate to this graph is intriguing. This graph may have applications similar to hypercube graphs, which are used for designing multi-computer interconnection networks.

Conflict of Interest

The authors hereby declare that there is no potential conflict of interest.

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Computation of Temperature Indices of Dendrimer Structures

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Abstract

In this study, we investigate the temperature indices for dendrimer structures such as porphyrin dendrimer and poly ether imine dendrimer, using graph-theoretical approaches. Dendrimers, as highly branched, tree-like macromolecules, can be modeled as molecular graphs, where atoms and bonds correspond to vertices and edges, respectively. The temperature index, a topological descriptor derived from the degrees of adjacent vertices, provides valuable insights into the stability and reactivity of molecular structures. Our findings contribute to the theoretical understanding of structure–property relationships in complex molecular architectures. Temperature indices of dendrimer structures help to evaluate their thermal stability and responsiveness by analyzing how their branched architecture influences heat resistance and temperature-dependent behavior.

Keywords: Temperature indices, Porphyrin dendrimer, Poly ether imine dendrimer
AMS Classification: 05C09, 05C07, 05C92

1 Introduction

Graph theory is a branch of mathematics that studies graphs, which are mathematical structures made up of nodes (also known as vertices) linked by edges. Recent years have seen the widespread use of graph theory in a variety of disciplines, such as social networks, computer science, biology, and chemistry. Characterizing and measuring graph characteristics using topological indices is a crucial component of graph theory [11, 12, 13, 15, 14]. Topological indices are numerical parameters associated with graphs that provide valuable information about their structural and chemical properties. These indices capture specific structural features of graphs and are widely used in different branches of science and engineering and many indices have some applications in chemistry, especially in QSPR/QSAR studies [8, 9, 3, 5, 10, 16, 17, 18].

For a simple graph $\mathcal{G}$, we denote the vertex set $\mathcal{V}(\mathcal{G}) = \{x_1, x_2, x_3, ..., x_n\}$ and the edge set by $\mathcal{E}(\mathcal{G}) = \{\epsilon_1, \epsilon_2, \epsilon_3, ...\epsilon_n\}$. The degree of a vertex $x \in \mathcal{V}(\mathcal{G})$ is denoted by d_x.

In [1], Fajtlowicz defined the temperature of a vertex x in a graph G as

$$\psi(x) = \frac{d_x}{n - d_x},$$

where n is the number of vertices of $\mathcal{G}$.

In [6], Kulli defined the temperature indices in a natural way as follows:

The general first temperature index is

$$\psi_1(\mathcal{G}) = \sum_{xy \in \mathcal{E}(\mathcal{G})} [\psi(x) + \psi(y)]^{\alpha}.$$

The first hyper temperature index is

$$HT_1(\mathcal{G}) = \sum_{xy \in \mathcal{E}(\mathcal{G})} [\psi(x) + \psi(y)]^2.$$

The sum connectivity temperature index is

$$ST(\mathcal{G}) = \sum_{xy \in \mathcal{E}(\mathcal{G})} [\psi(x) + \psi(y)]^{-\frac{1}{2}}.$$

The general second temperature index is

$$\psi_2(\mathcal{G}) = \sum_{xy \in \mathcal{E}(\mathcal{G})} [\psi(x) \times \psi(y)]^{\alpha}.$$

The second hyper temperature index is

$$HT_2(\mathcal{G}) = \sum_{xy \in \mathcal{E}(\mathcal{G})} [\psi(x) \times \psi(y)]^2.$$

The product connectivity index is

$$PT(\mathcal{G}) = \sum_{xy \in \mathcal{E}(\mathcal{G})} [\psi(x) \times \psi(y)]^{-\frac{1}{2}}.$$

The reciprocal product connectivity index is

$$RPT(\mathcal{G}) = \sum_{xy \in \mathcal{E}(\mathcal{G})} [\psi(x) \times \psi(y)]^{\frac{1}{2}}.$$

The general temperature index is

$$\psi_{\alpha}(\mathcal{G}) = \sum_{xy \in \mathcal{E}(\mathcal{G})} [\psi(x)^{\alpha} + \psi(y)^{\alpha}].$$

The F-temperature index is

$$FT(\mathcal{G}) = \sum_{xy \in \mathcal{E}(\mathcal{G})} [\psi(x)^2 + \psi(y)^2].$$

V. Lokesha et al. introduced VL-temperature index, [15], as

$$VLTI(\mathcal{G}) = \sum_{xy \in \mathcal{E}(\mathcal{G})} [\psi(x) + \psi(y) + \psi(x)\psi(y)] .$$

Farahani, [2], studied the generalized version of the first Zagreb index, product connectivity index, and other topological indices of dendrimer nanostars. Motivated by this studies, we formulate the results of various temperature indices of Porphyrin Dendrimers and Poly Ether Imine Dendrimers.

1.1 Methodology

We obtained the results by using analytical method, edge partition method, graph theoretical methods and degree sums method. Also we used MATLAB and MAPLE 2015 for graphical representations.

2 Main results

2.1 Porphyrin Dendrimers $\mathcal{D}_n$

Porphyrin Dendrimers form the unique class of Dendritic Macromolecules that incorporate Porphyrin units—aromatic, macrocyclic compounds—either at the core, in the branches, or at the surface of the Dendrimer structure [7, 4]. These systems combine the structural precision of Dendrimers with the rich photophysical and electrochemical properties of Porphyrins.

Key features

- Core or Peripheral Porphyrins: The Porphyrin can serve as the Dendrimer's core or be present on the outer branches.
- Highly Branched Architecture: Like other Dendrimers, they exhibit a tree-like structure built generation by generation.
- Tunable Properties: Their electronic, optical, and catalytic properties can be tuned by modifying the Porphyrin or Dendritic arms.

Properties

- Strong light absorption and emission (especially in visible range)
- Ability to generate reactive oxygen species (important in photo dynamic therapy)
- Electron-transfer and charge-transfer capabilities.

Applications

- Photodynamic therapy (PDT): As photosensitizers for cancer treatment
- Artificial light-harvesting systems: Mimicking photosynthesis
- Sensors and diagnostics
- Catalysis and molecular electronics

Porphyrin Dendrimers stand out in nanomedicine and materials science due to their multi-functionality, high degree of control in design, and potent photochemical behavior.

Let $\mathcal{D}_n$ be the molecular graph of Porphyrin Dendrimer of n-th generation.

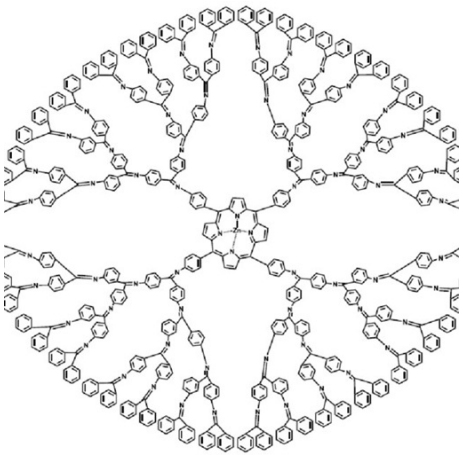

Figure 1: A Porphyrin Dendrimer

From general structure of this Porphyrin Dendrimer, we can observe $96n - 10$ atoms or vertices and $105n - 11$ number of bonds or edges of $\mathcal{D}_n$, i.e. for all n,

$$|V(\mathcal{D}_n)| = 96n - 10,$$
$$|\mathcal{E}(\mathcal{D}_n)| = 105n - 11.$$

There are six types of edges in $\mathcal{E}(\mathcal{D}_n)$ and the edge partition of Porphyrin Dendrimer is given below:

$$\mathcal{E}_{1,3} = 2n,\ \mathcal{E}_{1,4} = 24n,\ \mathcal{E}_{2,2} = 10n - 5,\ \mathcal{E}_{2,3} = 48n - 6,\ \mathcal{E}_{3,3} = 13n,\ \mathcal{E}_{3,4} = 8n.$$

If $d_x = 2$, the temperature of the vertex x is

$$\psi(x) = \frac{d_x}{n - d_x} = \frac{2}{96n - 12}.$$

If $d_x = 3$, the temperature of the vertex x is

$$\psi(x) = \frac{d_x}{n - d_x} = \frac{3}{96n - 13}.$$

If $d_x = 4$, the temperature of the vertex x is

$$\psi(x) = \frac{d_x}{n - d_x} = \frac{4}{96n - 14}.$$

Theorem 1. *The general first temperature index of Porphyrin Dendrimer $\mathcal{D}_n$ is given by*

$$\begin{aligned}\psi_1^{\alpha}(\mathcal{D}_n) = {} & 2n\left[\frac{384n-46}{(96n-11)(96n-13)}\right]^{\alpha} + 24n\left(\frac{480n-58}{(96n-11)(96n-14)}\right)^{\alpha} \\ & + (10n-5)\left(\frac{1}{24n-3}\right)^{\alpha} + 13n\left(\frac{6}{96n-13}\right)^{\alpha} + 8n\left[\frac{672n-94}{(96n-13)(96n-14)}\right]^{\alpha} \\ & + (48n-6)\left[\frac{480n-62}{(96n-12)(96n-13)}\right]^{\alpha}.\end{aligned}$$

Proof. From the edge partition of $\mathcal{D}_n$, the general first temperature index is obtained as

$$\begin{aligned}\psi_1^{\alpha}(\mathcal{D}_n) = {} & \sum_{x,y\in\mathcal{E}(\mathcal{G})} [\psi(x)+\psi(y)]^{\alpha} \\ & = \mathcal{E}_{1,3}\,[\psi(x)+\psi(y)]^{\alpha} + \mathcal{E}_{1,4}\,[\psi(x)+\psi(y)]^{\alpha} + \mathcal{E}_{2,2}\,[\psi(x)+\psi(y)]^{\alpha} \\ & + \mathcal{E}_{2,3}\,[\psi(x)+\psi(y)]^{\alpha} + \mathcal{E}_{3,3}\,[\psi(x)+\psi(y)]^{\alpha} + \mathcal{E}_{3,4}\,[\psi(x)+\psi(y)]^{\alpha} \\ & = 2n\left[\frac{1}{96n-11}+\frac{3}{96n-13}\right]^{\alpha} + 24n\left[\frac{1}{96n-11}+\frac{4}{96n-14}\right]^{\alpha} \\ & + (10n-5)\left[\frac{2}{96n-12}+\frac{2}{96n-12}\right]^{\alpha} + (48n-6)\left[\frac{2}{96n-12}+\frac{3}{96n-13}\right]^{\alpha} \\ & + 13n\left[\frac{3}{96n-13}+\frac{3}{96n-13}\right]^{\alpha} + 8n\left[\frac{3}{96n-13}+\frac{4}{96n-14}\right]^{\alpha} \\ & = 2n\left[\frac{384n-46}{(96n-11)(96n-13)}\right]^{\alpha} + 24n\left(\frac{480n-58}{(96n-11)(96n-14)}\right)^{\alpha} \\ & + (10n-5)\left(\frac{1}{24n-3}\right)^{\alpha} + 13n\left(\frac{6}{96n-13}\right)^{\alpha} \\ & + 8n\left[\frac{672n-94}{(96n-13)(96n-14)}\right]^{\alpha} + (48n-6)\left[\frac{480n-62}{(96n-12)(96n-13)}\right]^{\alpha}.\end{aligned}$$

□

Corollary 1. *The first hyper-temperature index of Porphyrin Dendrimer $\mathcal{D}_n$ is given by*

$$\begin{aligned} HT_1(\mathcal{D}_n) = 2n&\left[\frac{384n-46}{(96n-11)(96n-13)}\right]^2 + 24n\left(\frac{480n-58}{(96n-11)(96n-14)}\right)^2 \\ &+ (10n-5)\left(\frac{1}{24n-3}\right)^2 + 13n\left(\frac{6}{96n-13}\right)^2 \\ &+ 8n\left[\frac{672n-94}{(96n-13)(96n-14)}\right]^2 + (48n-6)\left[\frac{480n-62}{(96n-12)(96n-13)}\right]^2. \end{aligned}$$

Corollary 2. *The sum connectivity temperature index of Porphyrin Dendrimer $\mathcal{D}_n$ is*

$$\begin{aligned} ST_1(\mathcal{D}_n) = 2n&\left[\frac{384n-46}{(96n-11)(96n-13)}\right]^{-\frac{1}{2}} + 24n\left(\frac{480n-58}{(96n-11)(96n-14)}\right)^{-\frac{1}{2}} \\ &+ (10n-5)\left(\frac{1}{24n-3}\right)^{-\frac{1}{2}} + 13n\left(\frac{6}{96n-13}\right)^{-\frac{1}{2}} \\ &+ 8n\left[\frac{672n-94}{(96n-13)(96n-14)}\right]^{-\frac{1}{2}} + (48n-6)\left[\frac{480n-62}{(96n-12)(96n-13)}\right]^{-\frac{1}{2}}. \end{aligned}$$

Proof. In Theorem 1, put $\alpha = 2$ and $\alpha = -\frac{1}{2}$, we obtain Corollary 1 and Corollary 2, respectively. □

Theorem 2. *The general second temperature index of Porphyrin Dendrimer $\mathcal{D}_n$ is given by*

$$\begin{aligned} \psi_2^{\alpha}(\mathcal{D}_n) = 2n&\left[\frac{3}{(96n-11)(96n-13)}\right]^{\alpha} + 24n\left(\frac{4}{(96n-11)(96n-14)}\right)^{\alpha} \\ &+ (10n-5)\left(\frac{4}{(96n-12)^2}\right)^{\alpha} + 13n\left(\frac{9}{(96n-13)^2}\right)^{\alpha} \\ &+ 8n\left[\frac{12}{(96n-13)(96n-14)}\right]^{\alpha} + (48n-6)\left[\frac{6}{(96n-12)(96n-13)}\right]^{\alpha}. \end{aligned}$$

Proof. From the edge partition of Porphyrin Dendrimer $\mathcal{D}_n$, the general second temperature index is

$$\begin{aligned}\psi_2^{\alpha}(\mathcal{D}_n) &= \sum_{x,y\in\mathcal{E}(\mathcal{G})} [\psi(x)\psi(y)]^{\alpha} \\ &= \mathcal{E}_{1,3}\,[\psi(x)\psi(y)]^{\alpha} + \mathcal{E}_{1,4}\,[\psi(x)\psi(y)]^{\alpha} + \mathcal{E}_{2,2}\,[\psi(x)\psi(y)]^{\alpha} \\ &+ \mathcal{E}_{2,3}\,[\psi(x)\psi(y)]^{\alpha} + \mathcal{E}_{3,3}\,[\psi(x)\psi(y)]^{\alpha} + \mathcal{E}_{3,4}\,[\psi(x)\psi(y)]^{\alpha} \\ &= 2n\left[\frac{3}{(96n-11)(96n-13)}\right]^{\alpha} + 24n\left(\frac{4}{(96n-11)(96n-14)}\right)^{\alpha} \\ &+ (10n-5)\left(\frac{4}{(96n-12)^2}\right)^{\alpha} + 13n\left(\frac{9}{(96n-13)^2}\right)^{\alpha} \\ &+ 8n\left[\frac{12}{(96n-13)(96n-14)}\right]^{\alpha} + (48n-6)\left[\frac{6}{(96n-12)(96n-13)}\right]^{\alpha}.\end{aligned}$$

□

Corollary 3. *The second hyper-temperature index of Porphyrin Dendrimer $\mathcal{D}_n$ is given by*

$$\begin{aligned}HT_2(\mathcal{D}_n) =& 2n\left[\frac{3}{(96n-11)(96n-13)}\right]^{2} + 24n\left(\frac{4}{(96n-11)(96n-14)}\right)^{2} \\ &+ (10n-5)\left(\frac{4}{(96n-12)^2}\right)^{2} + 13n\left(\frac{9}{(96n-13)^2}\right)^{2} \\ &+ 8n\left[\frac{12}{(96n-13)(96n-14)}\right]^{2} + (48n-6)\left[\frac{6}{(96n-12)(96n-13)}\right]^{2}.\end{aligned}$$

Corollary 4. *The product connectivity temperature index of Porphyrin Dendrimer $\mathcal{D}_n$ is given by*

$$\begin{aligned}PT(\mathcal{D}_n) =& 2n\left[\frac{3}{(96n-11)(96n-13)}\right]^{-\frac{1}{2}} + 24n\left(\frac{4}{(96n-11)(96n-14)}\right)^{-\frac{1}{2}} \\ &+ (10n-5)\left(\frac{4}{(96n-12)^2}\right)^{-\frac{1}{2}} + 13n\left(\frac{9}{(96n-13)^2}\right)^{-\frac{1}{2}} \\ &+ 8n\left[\frac{12}{(96n-13)(96n-14)}\right]^{-\frac{1}{2}} + (48n-6)\left[\frac{6}{(96n-12)(96n-13)}\right]^{-\frac{1}{2}}.\end{aligned}$$

Corollary 5. *The reciprocal product connectivity temperature index of Porphyrin Dendrimer $\mathcal{D}_n$ is given by*

$$\begin{aligned}RPT(\mathcal{D}_n) =& 2n\left[\frac{3}{(96n-11)(96n-13)}\right]^{\frac{1}{2}} + 24n\left(\frac{4}{(96n-11)(96n-14)}\right)^{\frac{1}{2}} \\ &+ (10n-5)\left(\frac{4}{(96n-12)^2}\right)^{\frac{1}{2}} + 13n\left(\frac{9}{(96n-13)^2}\right)^{\frac{1}{2}} \\ &+ 8n\left[\frac{12}{(96n-13)(96n-14)}\right]^{\frac{1}{2}} + (48n-6)\left[\frac{6}{(96n-12)(96n-13)}\right]^{\frac{1}{2}}.\end{aligned}$$

Proof. In Equation (2), put $\alpha = 2, -\frac{1}{2}, \frac{1}{2}$ to obtain the Corollary 3, Corollary 4 and Corollary 5 respectively.

□

Theorem 3. *The general temperature index of Porphyrin Dendrimer $\mathcal{D}_n$ is given by*

$$\begin{aligned}\psi_\alpha(\mathcal{D}_n) = 2n\left[\frac{1}{(96n-11)^\alpha}+\frac{3^\alpha}{(96n-13)^\alpha}\right] + 24n\left[\frac{1}{(96n-11)^\alpha}+\frac{4^\alpha}{(96n-14)^\alpha}\right] \\ + (10n-5)\left[\frac{2^{\alpha+1}}{(96n-12)^\alpha}\right] + (48n-6)\left[\frac{2^\alpha}{(96n-12)^\alpha}+\frac{3^\alpha}{(96n-13)^\alpha}\right] \\ + 26n\left[\frac{3^\alpha}{(96n-13)^\alpha}\right] + 8n\left[\frac{3^\alpha}{(96n-13)^\alpha}+\frac{4^\alpha}{(96n-14)^\alpha}\right].\end{aligned}$$

Proof. From the edge partition of Porphyrin Dendrimer $\mathcal{D}_n$, we obtain the general temperature index as

$$\begin{aligned}\psi_\alpha(\mathcal{D}_n) &= \sum_{x,y\in\mathcal{E}(\mathcal{G})}[\psi(x)^\alpha+\psi(y)^\alpha] \\ &= \mathcal{E}_{1,3}[\psi(x)^\alpha+\psi(y)^\alpha] + \mathcal{E}_{1,4}[\psi(x)^\alpha+\psi(y)^\alpha] + \mathcal{E}_{2,2}[\psi(x)^\alpha+\psi(y)^\alpha] \\ &+ \mathcal{E}_{2,3}[\psi(x)^\alpha+\psi(y)^\alpha] + \mathcal{E}_{3,3}[\psi(x)^\alpha+\psi(y)^\alpha] + \mathcal{E}_{3,4}[\psi(x)^\alpha+\psi(y)^\alpha] \\ &= 2n\left[\frac{1}{(96n-11)^\alpha}+\frac{3^\alpha}{(96n-13)^\alpha}\right] + 24n\left[\frac{1}{(96n-11)^\alpha}+\frac{4^\alpha}{(96n-14)^\alpha}\right] \\ &+ (10n-5)\left[\frac{2^\alpha}{(96n-12)^\alpha}+\frac{2^\alpha}{(96n-12)^\alpha}\right] + (48n-6)\left[\frac{2^\alpha}{(96n-12)^\alpha}+\frac{3^\alpha}{(96n-13)^\alpha}\right] \\ &+ 13n\left[\frac{3^\alpha}{(96n-13)^\alpha}+\frac{3^\alpha}{(96n-13)^\alpha}\right] + 8n\left[\frac{3^\alpha}{(96n-13)^\alpha}+\frac{4^\alpha}{(96n-14)^\alpha}\right] \\ &= 2n\left[\frac{1}{(96n-11)^\alpha}+\frac{3^\alpha}{(96n-13)^\alpha}\right] + 24n\left[\frac{1}{(96n-11)^\alpha}+\frac{4^\alpha}{(96n-14)^\alpha}\right] \\ &+ (10n-5)\left[\frac{2^{\alpha+1}}{(96n-12)^\alpha}\right] + (48n-6)\left[\frac{2^\alpha}{(96n-12)^\alpha}+\frac{3^\alpha}{(96n-13)^\alpha}\right] \\ &+ 26n\left[\frac{3^\alpha}{(96n-13)^\alpha}\right] + 8n\left[\frac{3^\alpha}{(96n-13)^\alpha}+\frac{4^\alpha}{(96n-14)^\alpha}\right].\end{aligned}$$

□

Corollary 6. *The F-temperature index of Porphyrin Dendrimer $\mathcal{D}_n$ is given by*

$$\begin{aligned} FT(\mathcal{D}_n) &= 2n\left[\frac{1}{(96n-11)^2}+\frac{3^2}{(96n-13)^2}\right]+24n\left[\frac{1}{(96n-11)^2}+\frac{4^2}{(96n-14)^2}\right] \\ &+(10n-5)\left[\frac{2^3}{(96n-12)^2}\right]+(48n-6)\left[\frac{2^2}{(96n-12)^2}+\frac{3^2}{(96n-13)^2}\right] \\ &+26n\left[\frac{3^2}{(96n-13)^2}\right]+8n\left[\frac{3^2}{(96n-13)^2}+\frac{4^2}{(96n-14)^2}\right]. \end{aligned}$$

By replacing $\alpha = 2$ in Eqn. (3), we get the result.

Theorem 4. *VL-temperature index of Porphyrin Dendrimer $\mathcal{D}_n$ is given by*

$$\begin{aligned} VLTI(\mathcal{D}_n) &= 2n\left[\frac{384n-43}{(96n-11)(96n-13)}\right]+24n\left[\frac{480n-54}{(96n-11)(96n-14)}\right] \\ &+(10n-5)\left[\frac{4(96n-11)}{(96n-12)^2}\right]+13n\left[\frac{3(18n-23)}{(96n-13)^2}\right] \\ &+8n\left[\frac{672n-84}{(96n-13)(96n-14)}\right]+(48n-6)\left[\frac{480n-56}{(96n-12)(96n-13)}\right]. \end{aligned}$$

Proof. From the edge partition of Porphyrin Dendrimer $\mathcal{D}_n$, the VL-temperature index is

$$\begin{aligned} VLTI(\mathcal{D}_n) &= 2n\left[\frac{1}{96n-11}+\frac{3}{96n-13}+\frac{4}{(96n-11)(96n-13}\right] \\ &+24n\left[\frac{1}{96n-11}+\frac{4}{96n-14}+\frac{4}{(96n-11)(96n-14)}\right] \\ &+(10n-5)\left[\frac{2}{96n-12}+\frac{2}{96n-12}+\frac{4}{(96n-12)^2}\right] \\ &+(48n-6)\left[\frac{2}{96n-12}+\frac{3}{96n-13}+\frac{6}{(96n-12)(96n-13}\right] \\ &+13n\left[\frac{3}{96n-13}+\frac{3}{96n-13}+\frac{9}{(96n-13)^2}\right] \\ &+8n\left[\frac{3}{96n-13}+\frac{4}{96n-14}+\frac{12}{(96n-13)(96n-14)}\right] \\ &=2n\left[\frac{384n-43}{(96n-11)(96n-13)}\right]+24n\left[\frac{480n-54}{(96n-11)(96n-14)}\right] \\ &+(10n-5)\left[\frac{4(96n-11)}{(96n-12)^2}\right]+13n\left[\frac{3(18n-23)}{(96n-13)^2}\right] \\ &+8n\left[\frac{672n-84}{(96n-13)(96n-14)}\right]+(48n-6)\left[\frac{480n-56}{(96n-12)(96n-13)}\right]. \end{aligned}$$

□

2.2 Poly Ether Imine Dendrimers $\mathcal{DE}_n$

Poly Ether Imine (PETIM) Dendrimers form a class of synthetic, nanoscale, branched polymers known for their highly ordered and symmetric architecture [4]. These Dendrimers are built from a central core and expand outward through repetitive branching units composed of ether and imine linkages. Each layer of branching is called a "generation", and higher generations lead to an increased number of surface functional groups. PETIM Dendrimers exhibit several unique properties:

- Monodispersity: Uniform size and structure, making them predictable and reproducible.
- Multivalency: Numerous terminal functional groups on the surface allow for varied chemical modifications.
- Solubility & Biocompatibility: They can be engineered for solubility in different solvents and are often biocompatible, making them suitable for biomedical applications.

Their controlled architecture and functional versatility make PETIM Dendrimers useful in fields such as drug delivery, gene therapy, diagnostics, nonmaterial, and catalysis.

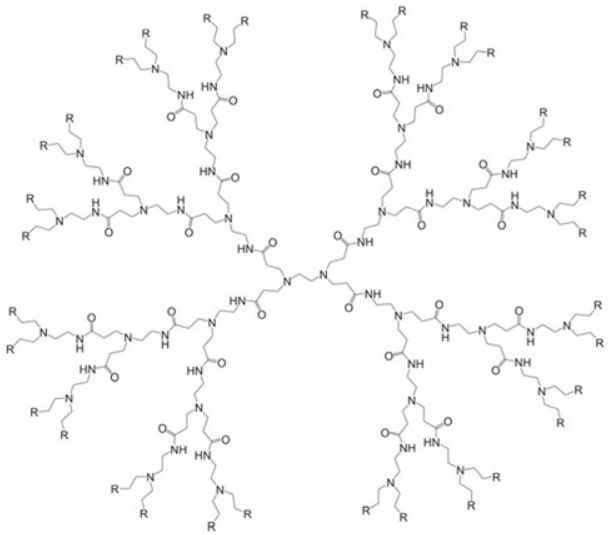

Figure 2: A Poly Ether Imine Dendrimer

From general structure of this Poly Ether Imine Dendrimer, we can observe that $24\times 2^n-23$ atoms (or vertices) and $24 \times 2^n - 24$ bonds (or edges) of $\mathcal{DE}_n$, i.e. for all n, we have

$$|V(\mathcal{DE}_n)| = 24 \times 2^n - 23,$$
$$|\mathcal{E}(\mathcal{DE}_n)| = 24 \times 2^n - 24.$$

There are three types of edges in $\mathcal{E}(\mathcal{DE}_n)$ and hence the edge partition of a Poly Ether Imine Dendrimer is given below:

$\mathcal{E}_{1,2} = 2^{n+1}$, $\mathcal{E}_{2,2} = 2^{n+4} - 18$, $\mathcal{E}_{2,3} = 6 \times 2^n - 6$.

If $d_x = 1$, temperature of the vertex x is

$$\psi(x) = \frac{d_x}{N - d_x} = \frac{1}{24 \times 2^n - 24}.$$

If $d_x = 2$, temperature of the vertex x is

$$\psi(x) = \frac{d_x}{N - d_x} = \frac{2}{24 \times 2^n - 25}.$$

If $d_x = 3$, temperature of the vertex x is

$$\psi(x) = \frac{d_x}{N - d_x} = \frac{3}{24 \times 2^n - 26}.$$

Theorem 5. *The general first temperature index of Poly Ether Imine Dendrimer $\mathcal{DE}_n$ is given by*

$$\psi_1^{\alpha}(\mathcal{DE}_n) = 2^{n+1}\left[\frac{72 \times 2^n - 73}{(24 \times 2^n - 24)(24 \times 2^n - 25)}\right]^{\alpha} + (2^{n+4} - 18)\left(\frac{4}{(24 \times 2^n - 25)}\right)^{\alpha}$$
$$+ 6(2^n - 1)\left(\frac{120 \times 2^n - 122}{(24 \times 2^n - 25)(24 \times 2^n - 26)}\right)^{\alpha}.$$

Proof. From the edge partition of $\mathcal{DE}_n$, the general first temperature index is obtained as

$$\psi_1^{\alpha}(\mathcal{DE}_n) = \sum_{x,y \in \mathcal{E}(\mathcal{G})} [\psi(x) + \psi(y)]^{\alpha}$$
$$= \mathcal{E}_{1,2}\,[\psi(x) + \psi(y)]^{\alpha} + \mathcal{E}_{2,2}\,[\psi(x) + \psi(y)]^{\alpha} + \mathcal{E}_{2,3}\,[\psi(x) + \psi(y)]^{\alpha}$$
$$= 2^{n+1}\left[\frac{1}{24 \times 2^n - 24} + \frac{2}{24 \times 2^n - 25}\right]^{\alpha} + (2^{n+4} - 18)\left[\frac{2 \times 2}{24 \times 2^n - 25}\right]^{\alpha}$$
$$+ 6(2^n - 1)\left[\frac{2}{24 \times 2^n - 25} + \frac{3}{24 \times 2^n - 26}\right]^{\alpha}$$
$$= 2^{n+1}\left[\frac{72 \times 2^n - 73}{(24 \times 2^n - 24)(24 \times 2^n - 25)}\right]^{\alpha} + (2^{n+4} - 18)\left(\frac{4}{(24 \times 2^n - 25)}\right)^{\alpha}$$
$$+ 6(2^n - 1)\left(\frac{120 \times 2^n - 122}{(24 \times 2^n - 25)(24 \times 2^n - 26)}\right)^{\alpha}.$$

□

Corollary 7. *The first hyper-temperature index of Poly Ether Imine Dendrimer $\mathcal{DE}_n$ is given by*

$$HT_1(\mathcal{DE}_n) = 2^{n+1}\left[\frac{72\times 2^n-73}{(24\times 2^n-24)(24\times 2^n-25)}\right]^2 + (2^{n+4}-18)\left(\frac{4}{(24\times 2^n-25)}\right)^2 + 6(2^n-1)\left(\frac{120\times 2^n-122}{(24\times 2^n-25)(24\times 2^n-26)}\right)^2.$$

Corollary 8. *The sum connectivity temperature index of Poly Ether Imine Dendrimer $\mathcal{DE}_n$ is given by*

$$ST_1(\mathcal{DE}_n) = 2^{n+1}\left[\frac{72\times 2^n-73}{(24\times 2^n-24)(24\times 2^n-25)}\right]^{-\frac{1}{2}} + (2^{n+4}-18)\left(\frac{4}{(24\times 2^n-25)}\right)^{-\frac{1}{2}} + 6(2^n-1)\left(\frac{120\times 2^n-122}{(24\times 2^n-25)(24\times 2^n-26)}\right)^{-\frac{1}{2}}.$$

Proof. In Theorem 5, put $\alpha = 2$ and $\alpha = -\frac{1}{2}$ to obtain Corollary 7 and Corollary 8, respectively. □

Theorem 6. *The general second temperature index of Poly Ether Imine Dendrimer $\mathcal{DE}_n$ is given by*

$$\psi_2^{\alpha}(\mathcal{DE}_n) = 2^{n+1}\left[\frac{2}{(24\times 2^n-24)(24\times 2^n-25)}\right]^{\alpha} + (2^{n+4}-18)\left(\frac{4}{(24\times 2^n-25)^2}\right)^{\alpha} + 6(2^n-1)\left(\frac{6}{(24\times 2^n-25)(24\times 2^n-26)}\right)^{\alpha}.$$

Proof. From the edge partition of a Poly Ether Imine Dendrimer $\mathcal{DE}_n$, the general second temperature index is found as

$$\psi_2^{\alpha}(\mathcal{DE}_n) = \sum_{x,y\in\mathcal{E}(\mathcal{G})} [\psi(x)\times\psi(y)]^{\alpha}$$

$$= \mathcal{E}_{1,2}\,[\psi(x)\times\psi(y)]^{\alpha} + \mathcal{E}_{2,2}\,[\psi(x)\times\psi(y)]^{\alpha} + \mathcal{E}_{2,3}\,[\psi(x)\times\psi(y)]^{\alpha}$$

$$= 2^{n+1}\left[\frac{1}{24\times 2^n-24}\times\frac{2}{24\times 2^n-25}\right]^{\alpha} + (2^{n+4}-18)\left[\frac{2\times 2}{(24\times 2^n-25)^2}\right]^{\alpha}$$
$$+ 6(2^n-1)\left[\frac{2}{24\times 2^n-25}\times\frac{3}{24\times 2^n-26}\right]^{\alpha}$$

$$= 2^{n+1}\left[\frac{2}{(24\times 2^n-24)(24\times 2^n-25)}\right]^{\alpha} + (2^{n+4}-18)\left(\frac{4}{(24\times 2^n-25)^2}\right)^{\alpha}$$

$$+ 6(2^n-1)\left(\frac{6}{(24\times 2^n-25)(24\times 2^n-26)}\right)^{\alpha}.$$

□

Corollary 9. *The second hyper-temperature index of Poly Ether Imine Dendrimer $\mathcal{DE}_n$ is given by*

$$HT_2(\mathcal{DE}_n) = 2^{n+1}\left[\frac{2}{(24\times 2^n-24)(24\times 2^n-25)}\right]^{2} + (2^{n+4}-18)\left(\frac{4}{(24\times 2^n-25)^2}\right)^{2}$$

$$+ 6(2^n-1)\left(\frac{6}{(24\times 2^n-25)(24\times 2^n-26)}\right)^{2}.$$

Corollary 10. *The product connectivity temperature index of Poly Ether Imine Dendrimer $\mathcal{DE}_n$ is given by*

$$PT(\mathcal{DE}_n) = 2^{n+1}\left[\frac{2}{(24\times 2^n-24)(24\times 2^n-25)}\right]^{-\frac{1}{2}} + (2^{n+4}-18)\left(\frac{4}{(24\times 2^n-25)^2}\right)^{-\frac{1}{2}}$$

$$+ 6(2^n-1)\left(\frac{6}{(24\times 2^n-25)(24\times 2^n-26)}\right)^{-\frac{1}{2}}.$$

Corollary 11. *The reciprocal product connectivity temperature index of Poly Ether Imine Den-*

drimer $\mathcal{DE}_n$ *is given by*

$$RPT(\mathcal{DE}_n) = = 2^{n+1}\left[\frac{2}{(24\times 2^n-24)(24\times 2^n-25)}\right]^{\frac{1}{2}} + (2^{n+4}-18)\left(\frac{4}{(24\times 2^n-25)^2}\right)^{\frac{1}{2}}$$
$$+ 6(2^n-1)\left(\frac{6}{(24\times 2^n-25)(24\times 2^n-26)}\right)^{\frac{1}{2}}.$$

Proof. In Theorem 6, put $\alpha = 2$, $\alpha = -\frac{1}{2}$ and $\alpha = \frac{1}{2}$ to obtain the Corollary 9, Corollary 10 and Corollary 11, respectively. □

Theorem 7. *The general temperature index of Poly Ether Imine Dendrimer* $\mathcal{DE}_n$ *is given by*

$$\psi_\alpha(\mathcal{DE}_n) = 2^{n+1}\left[\left(\frac{1}{24\times 2^n-24}\right)^\alpha + \left(\frac{2}{24\times 2^n-25}\right)^\alpha\right] + 2(2^{n+4}-18)\left[\frac{2}{24\times 2^n-25}\right]^\alpha$$
$$+ 6(2^n-1)\left[\left(\frac{2}{24\times 2^n-25}\right)^\alpha + \left(\frac{3}{24\times 2^n-26}\right)^\alpha\right].$$

Proof. From the edge partition of Poly Ether Imine Dendrimer $\mathcal{DE}_n$, the general temperature index

$$\psi_\alpha(\mathcal{DE}_n) = \sum_{x,y\in\mathcal{E}(\mathcal{G})}[\psi(x)^\alpha + \psi(y)^\alpha]$$
$$= \mathcal{E}_{1,2}[\psi(x)^\alpha + \psi(y)^\alpha] + \mathcal{E}_{2,2}[\psi(x)^\alpha + \psi(y)^\alpha] + \mathcal{E}_{2,3}[\psi(x)^\alpha + \psi(y)^\alpha]$$
$$+ \mathcal{E}_{1,2}[\psi(x)^\alpha + \psi(y)^\alpha] + \mathcal{E}_{2,2}[\psi(x)^\alpha + \psi(y)^\alpha] + \mathcal{E}_{2,3}[\psi(x)^\alpha + \psi(y)^\alpha]$$
$$= 2^{n+1}\left[\left(\frac{1}{24\times 2^n-24}\right)^\alpha + \left(\frac{2}{24\times 2^n-25}\right)^\alpha\right]$$
$$+ (2^{n+4}-18)\left[\left(\frac{2}{24\times 2^n-25}\right)^\alpha + \left(\frac{2}{24\times 2^n-25}\right)^\alpha\right]$$
$$+ 6(2^n-1)\left[\left(\frac{2}{24\times 2^n-25}\right)^\alpha + \left(\frac{3}{24\times 2^n-26}\right)^\alpha\right]$$
$$= 2^{n+1}\left[\left(\frac{1}{24\times 2^n-24}\right)^\alpha + \left(\frac{2}{24\times 2^n-25}\right)^\alpha\right] + 2(2^{n+4}-18)\left[\frac{2}{24\times 2^n-25}\right]^\alpha$$
$$+ 6(2^n-1)\left[\left(\frac{2}{24\times 2^n-25}\right)^\alpha + \left(\frac{3}{24\times 2^n-26}\right)^\alpha\right].$$

□

Corollary 12. *The F-temperature index of Poly Ether Imine Dendrimer $\mathcal{DE}_n$ is given by*

$$FT(\mathcal{DE}_n) = 2^{n+1}\left[\left(\frac{1}{24\times 2^n-24}\right)^2+\left(\frac{2}{24\times 2^n-25}\right)^2\right]+2(2^{n+4}-18)\left[\frac{2}{24\times 2^n-25}\right]^2 + 6(2^n-1)\left[\left(\frac{2}{24\times 2^n-25}\right)^2+\left(\frac{3}{24\times 2^n-26}\right)^2\right].$$

By replacing $\alpha = 2$ in Theorem 7, we get the result.

Theorem 8. *VL-temperature index of Poly Ether Imine Dendrimer $\mathcal{DE}_n$ is given by*

$$VLTI(\mathcal{DE}_n) = 2^{n+1}\left[\frac{72\times 2^n-71}{(24\times 2^n-24)(24\times 2^n-25)}\right] + (2^{n+4}-18)\left[\frac{96\times 2^n-96}{(24\times 2^n-25)^2}\right] + 6(2^n-1)\left[\frac{120\times 2^n-121}{(24\times 2^n-25)(24\times 2^n-26)}\right].$$

Proof. From the edge partition of Poly Ether Imine Dendrimer $\mathcal{DE}_n$, the VL-temperature index is found as

$$\begin{aligned}
VLTI(\mathcal{DE}_n) &= \sum_{x,y\in\mathcal{E}(\mathcal{G})}[\psi(x)+\psi(y)+\psi(x)\times\psi(y)]\\
&= 2^{n+1}\left[\frac{1}{24\times 2^n-24}+\frac{2}{24\times 2^n-25}+\frac{1}{24\times 2^n-24}\times\frac{2}{24\times 2^n-25}\right]\\
&+ (2^{n+4}-18)\left[\frac{2}{24\times 2^n-25}+\frac{2}{24\times 2^n-25}+\frac{2}{24\times 2^n-25}\times\frac{2}{24\times 2^n-25}\right]\\
&+ 6(2^n-1)\left[\frac{2}{24\times 2^n-25}+\frac{3}{24\times 2^n-26}+\frac{2}{24\times 2^n-25}\times\frac{3}{24\times 2^n-26}\right]\\
&= 2^{n+1}\left[\frac{72\times 2^n-71}{(24\times 2^n-24)(24\times 2^n-25)}\right]\\
&+ (2^{n+4}-18)\left[\frac{96\times 2^n-96}{(24\times 2^n-25)^2}\right]\\
&+ 6(2^n-1)\left[\frac{120\times 2^n-121}{(24\times 2^n-25)(24\times 2^n-26)}\right].
\end{aligned}$$

3 Conclusions

This study demonstrates that temperature indices effectively capture the topological characteristics of dendrimer structures. By analyzing their molecular graphs, we show how branching patterns and generations influence these indices. Here we computed temperature indices of the porphyrin dendrimer and poly ethyl imine dendrimer structures and given the graphical representation of temperature indices of dendrimer structures in Fig.s 3-16. Future work may extend these findings to modified dendrimer architectures and investigate experimental correlations to validate and enhance the applicability of temperature indices in molecular science.

Porphyrin Dendrimer ($\mathcal{D}_n$) generally shows higher values in most temperature indices because of its more complex edge connectivity.

Poly Ether Imine Dendrimer ($\mathcal{DE}_n$) performs better in product connectivity (PT) due to its more uniform and simpler edge partition.

Growth trends $\mathcal{D}_n$: Indices grow polynomially and are driven by dense multi-degree vertices.

$\mathcal{DE}_n$: Indices grow exponentially with 2^n but at a smoother, more predictable rate.

Acknowledgments The authors are thankful to the anonymous reviewers for their constructive comments and valuable suggestions, which have greatly helped to improve the quality and clarity of this review.

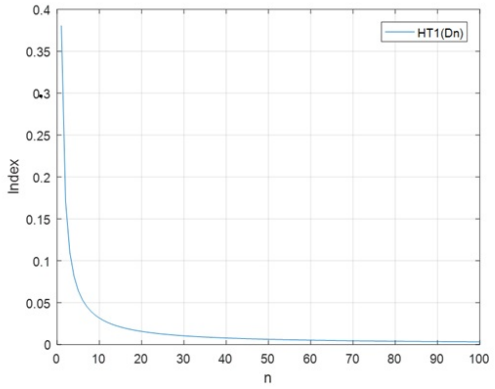

Figure 3: $HT_1(\mathcal{D}_n)$

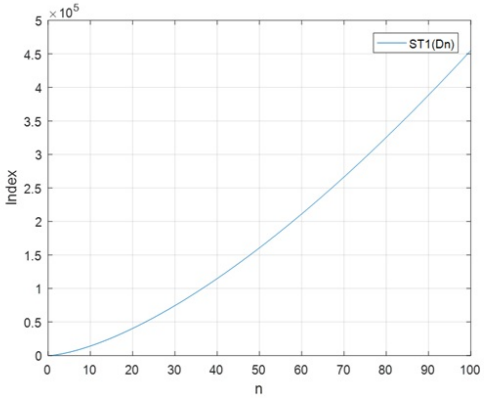

Figure 4: $ST_1(\mathcal{D}_n)$

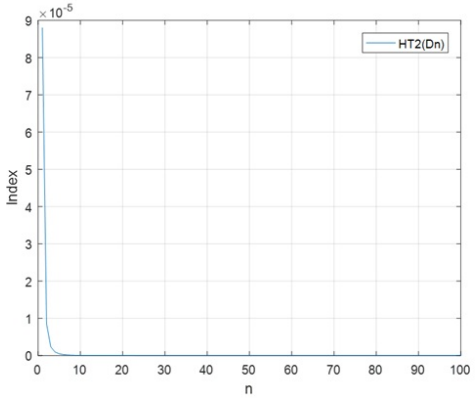

Figure 5: $HT_2(\mathcal{D}_n)$

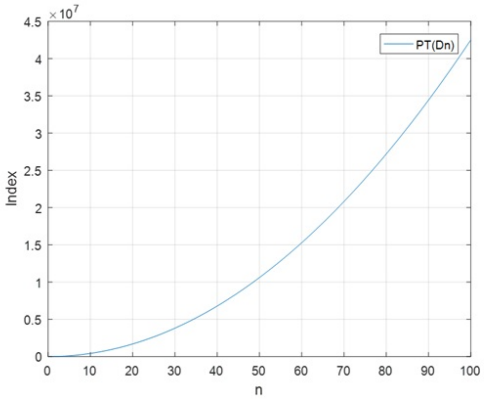

Figure 6: $PT(\mathcal{D}_n)$

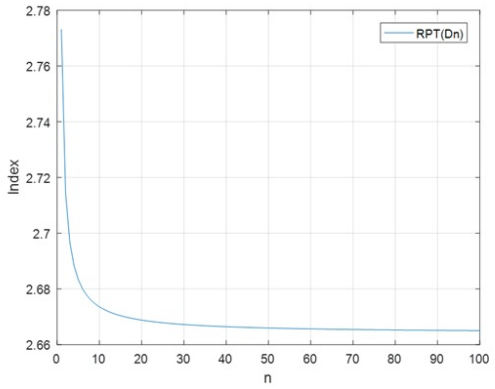

Figure 7: $RPT(\mathcal{D}_n)$

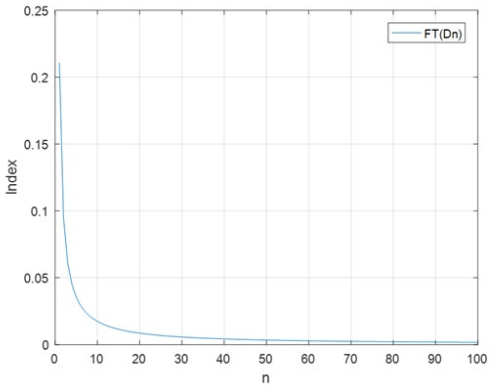

Figure 8: $FT(\mathcal{D}_n)$

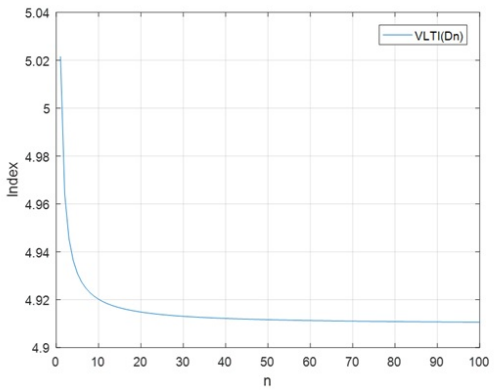

Figure 9: $VLTI(\mathcal{D}_n)$

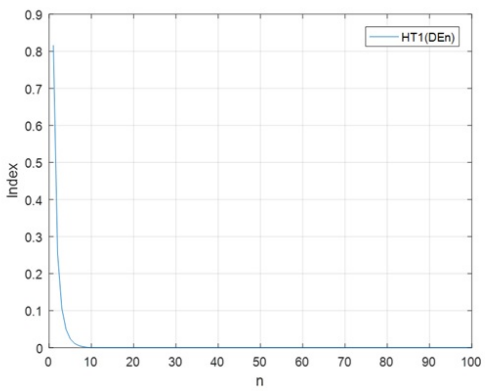

Figure 10: $HT_1(\mathcal{DE}_n)$

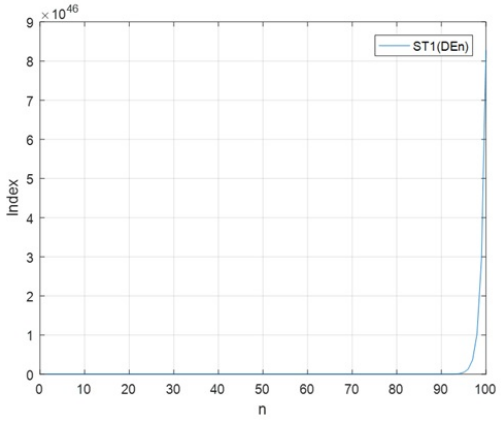

Figure 11: $ST_1(\mathcal{DE}_n)$

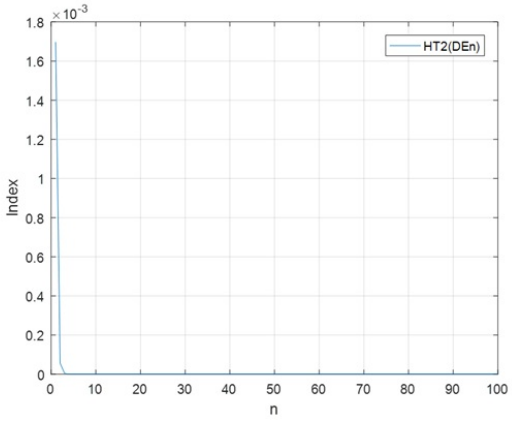

Figure 12: $HT_2(\mathcal{DE}_n)$

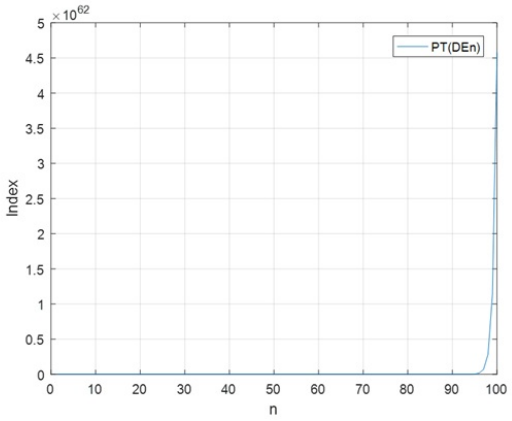

Figure 13: $PT(\mathcal{DE}_n)$

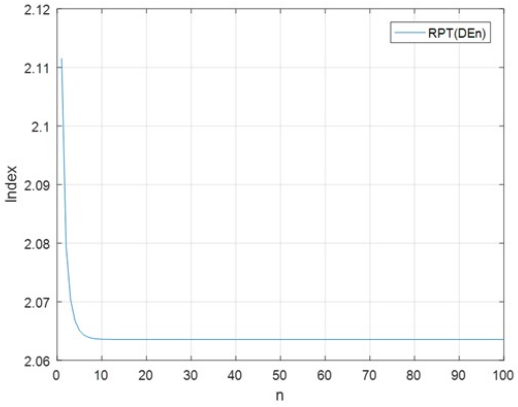

Figure 14: $RPT(\mathcal{DE}_n)$

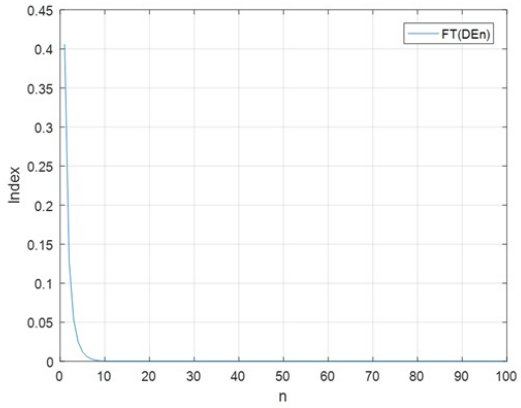

Figure 15: $FT(\mathcal{DE}_n)$

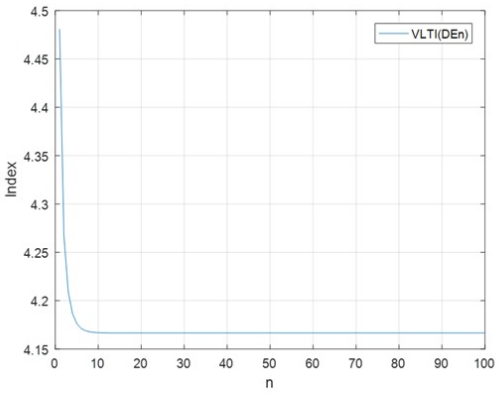

Figure 16: $VLTI(\mathcal{DE}_n)$

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Degree-Based Topological Indices on Nanotubes: Analytical Results for ABC and GA Measures

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Abstract

Topological indices encode structural information of molecular graphs into numerical descriptors with proven value in QSPR/QSAR modeling and nanomaterials design. This paper develops a unified, degree-based framework for deriving closed-form expressions of the Atom–Bond Connectivity (ABC) and Geometric–Arithmetic (GA) indices on two representative nanotubes: $SC_5C_7[p, q]$ and $TUC_4[m, n]$. Our methodology partitions bonds by local degree features (endpoint degree, degree-sum, and 2-distance counterparts), counts each class combinatorially, and substitutes into index definitions to yield compact formulae in the growth parameters p, q, m, n. Sanity checks at small sizes and comparative plots confirm monotone scaling with structural growth and delineate the distinct sensitivities of ABC (to degree heterogeneity) versus GA (to near-regular backbones). The resulting expressions furnish fast, interpretable predictors for properties linked to branching and framework regularity, with relevance to stability trends, adsorption capacity, and transport characteristics in graph-based nanotubes. The framework is modular and extends naturally to multiplicative and leap variants based on 2-distance degrees.

Keywords: Topological indices, Atom–bond connectivity (ABC), Geometric–arithmetic (GA), Degree-based descriptors, Nanotubes, Chemical graph theory
AMS Classification: 05C09, 05C12, 05C92

1 Introduction

Chemical graph theory provides a powerful framework for studying the structural properties of molecules and nanostructures by representing atoms as vertices and bonds as edges of a graph [7,

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20]. Within this framework, *topological indices*, numerical quantities derived from graph invariants, are used extensively in quantitative structure–property/activity relationships (QSPR/QSAR) to correlate molecular structure with physicochemical and biological properties. Among numerous classes of such indices, degree–based descriptors play a central role because of their direct relation to the degree of atoms.

Two particularly significant families of degree–based indices are the *Atom–Bond Connectivity (ABC)* index and the *Geometric–Arithmetic (GA)* index. The ABC index was originally introduced to predict enthalpies of formation of alkanes and has since been widely applied to study stability, branching, boiling points, and other molecular properties [4, 5]. The GA index, defined in terms of the arithmetic and geometric means of endpoint degrees, has been shown to possess strong predictive power in QSPR/QSAR models, especially for hydrophobicity, surface activity, and π–electron delocalization [10, 18]. Both indices have been extended in recent years to numerous variants, including multiplicative, fourth–version (ABC_4, GA_5), and leap versions based on 2–distance degree and degree–sums [13, 17, 19].

Applications. The ABC and GA indices have demonstrated relevance across a range of applied domains (see also the references in [1, 4, 5, 6, 10]).

- *Thermodynamic stability and enthalpy prediction*: ABC–based descriptors correlate with heat of formation and strain energy in hydrocarbons.
- *Nanomaterials design*: For nanotubes, dendrimers, and lattice–like frameworks, ABC and GA track growth in irregularity or regularity and thus inform predictions of stability, adsorption, and transport properties.
- *QSPR/QSAR modeling*: GA indices in particular have yielded robust correlations with solubility, hydrophobicity, and biological activity of organic compounds.

Scope of the present work. Motivated by these applications, this article develops closed–form expressions for the ABC and GA indices (together with selected variants) on two families of nanotubes of chemical and physical interest:

1. the SC5C7$[p, q]$ nanotube, and
2. the TUC4$[m, n]$ nanotube.

The approach relies on systematic bond partitions by local degree features, yielding compact parameterized formulae. Numerical tables and comparative plots illustrate scaling behavior, and the discussion highlights potential QSPR/QSAR and nanomaterial implications.

The remainder of the paper is organized as follows. In Section 2, we recall necessary definitions and variants of ABC and GA indices. Section 3 details the methodological framework for bond partitioning and index evaluation. Sections 4 and 5 present explicit results for each nanotube together with numerical results and comparison graphs. At the end concluding remarks is in Section 6.

2 Preliminaries and Formulae

Let $G = (V, E)$ be a simple connected graph, where $V = V(G)$ is the set of vertices and $E = E(G)$ is the set of edges. For a vertex $u \in V(G)$, the *degree* of u is denoted by $\deg(u)$ and equals the number of neighbors of u. The *neighborhood* of u is $N(u) = \{v \in V(G) : uv \in E(G)\}$. The *2–distance neighborhood* is $N_2(u) = \{v \in V(G) : d(u, v) = 2\}$, where $d(u, v)$ is the usual graph distance [3]. We further define the following sums:

$$S(u) = \sum_{v \in N(u)} \deg(v), \qquad S_2(u) = \sum_{v \in N_2(u)} \deg(v).$$

Similarly, the *2–distance degree* of u is $\deg_2(u) = |N_2(u)|$.

For an edge $uv \in E(G)$, we will often consider the degree–pair $(\deg(u), \deg(v))$, the degree–sum pair $(S(u), S(v))$, and their 2–distance counterparts $(\deg_2(u), \deg_2(v))$ and $(S_2(u), S_2(v))$.

Atom–Bond Connectivity (ABC) index. For a graph G, it is defined in [1, 4, 5, 6] as follows:

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{\deg(u) + \deg(v) - 2}{\deg(u)\deg(v)}}. \tag{1}$$

Geometric–Arithmetic (GA) index. The following formula to compute GA index of G is given by Gutman anf Furtula [10]

$$GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{\deg(u)\deg(v)}}{\deg(u) + \deg(v)}. \tag{2}$$

Fourth and Fifth versions. The following variants are obtained by replacing vertex degrees with neighbor–sum degrees as provided in [8, 9]

$$ABC_4(G) = \sum_{uv \in E(G)} \sqrt{\frac{S(u) + S(v) - 2}{S(u)S(v)}}, \qquad GA_5(G) = \sum_{uv \in E(G)} \frac{2\sqrt{S(u)S(v)}}{S(u) + S(v)}. \tag{3}$$

Multiplicative forms. The multiplicative versions of the indices are defined by Kulli [14, 15]

$$ABCII(G) = \prod_{uv \in E(G)} \sqrt{\frac{\deg(u) + \deg(v) - 2}{\deg(u)\deg(v)}}, \qquad GAII(G) = \prod_{uv \in E(G)} \frac{2\sqrt{\deg(u)\deg(v)}}{\deg(u) + \deg(v)}. \tag{4}$$

$$ABC_4II(G) = \prod_{uv \in E(G)} \sqrt{\frac{S(u) + S(v) - 2}{S(u)S(v)}}, \qquad GA_5II(G) = \prod_{uv \in E(G)} \frac{2\sqrt{S(u)S(v)}}{S(u) + S(v)}. \tag{5}$$

Leap variants. By employing 2–distance degrees and 2–distance degree sums, we define

$$ABC^2(G) = \sum_{uv\in E(G)} \sqrt{\frac{\deg_2(u)+\deg_2(v)-2}{\deg_2(u)\deg_2(v)}}, \qquad GA^2(G) = \sum_{uv\in E(G)} \frac{2\sqrt{\deg_2(u)\deg_2(v)}}{\deg_2(u)+\deg_2(v)}. \quad (6)$$

$$ABC_4^2(G) = \sum_{uv\in E(G)} \sqrt{\frac{S_2(u)+S_2(v)-2}{S_2(u)S_2(v)}}, \qquad GA_5^2(G) = \sum_{uv\in E(G)} \frac{2\sqrt{S_2(u)S_2(v)}}{S_2(u)+S_2(v)}. \quad (7)$$

$$ABC^2II(G) = \prod_{uv\in E(G)} \sqrt{\frac{\deg_2(u)+\deg_2(v)-2}{\deg_2(u)\deg_2(v)}}, \qquad GA^2II(G) = \prod_{uv\in E(G)} \frac{2\sqrt{\deg_2(u)\deg_2(v)}}{\deg_2(u)+\deg_2(v)}. \quad (8)$$

$$ABC_4^2II(G) = \prod_{uv\in E(G)} \sqrt{\frac{S_2(u)+S_2(v)-2}{S_2(u)S_2(v)}}, \qquad GA_5^2II(G) = \prod_{uv\in E(G)} \frac{2\sqrt{S_2(u)S_2(v)}}{S_2(u)+S_2(v)}. \quad (9)$$

These indices, together with their variants, will be evaluated in closed form for the nanotubes considered in the sequel.

3 Methodology

In this section, we outline the general framework adopted for computing the Atom–Bond Connectivity (ABC) and Geometric–Arithmetic (GA) indices, together with their multiplicative, fourth/fifth, and leap variants, on the considered nanotubes.

Graphical Modeling

Each nanotube under study is represented as a finite simple connected graph $G = (V, E)$, where the vertex set $V = A(G)$ corresponds to carbon atoms and the edge set $E = B(G)$ corresponds to covalent bonds. The construction parameters (p, q, m, n) describe the number of repeating units, layers, or growth stages, depending on the family (SC_5C_7 nanotube, or $TUC4$ nanotube).

Bond Partition Strategy

To evaluate indices systematically, the set of bonds $B(G)$ is partitioned into bond classes B_i according to degree features of end-atoms of a bond:

1. Degree pairs $(\deg(u), \deg(v))$.
2. Degree–sum pairs $(S(u), S(v))$, where $S(u)$ is the sum of neighbor degrees.

3. 2–distance degree pairs $(\deg_2(u), \deg_2(v))$.
4. 2–distance degree–sum pairs $(S_2(u), S_2(v))$.

For each bond class $B_i = B(\alpha, \beta) = \{uv \in B(G) \ ; \ x = \alpha, \ y = \beta\}$ with

$$(x, y) \in \{(\deg(u), \deg(v)), (S(u), S(v)), (\deg_2(u), \deg_2(v)), (S_2(u), S_2(v))\},$$

the number of bonds of that type is determined combinatorially from the geometry of the nanotube.

Index Evaluation

Given a partition $\{B_1, B_2, \ldots, B_k\}$ of the bond set $B(G)$, a topological index (TI) value is computed as

$$TI(G) \ = \sum_{i=1}^{k} \sum_{uv \in B_i} f(x, y)$$

for additive indices such as ABC and GA, where $f(x, y)$ denotes the local contribution of a bond depending on the chosen index. For multiplicative variants, the summation is replaced by the corresponding product over classes.

Validation and Scaling

The obtained closed–form expressions are validated through the following steps.

- Substituting small parameter values and checking against direct computation.
- Ensuring monotonicity and positivity of the indices with respect to structural growth parameters.
- Comparing asymptotic growth rates among families to highlight sensitivity to irregularity (for ABC) or backbone regularity (for GA).

Computational Support

To illustrate the formulas, numerical tables are generated for initial values of the parameters, and 2D comparison plots are drawn to visualize the scaling behavior. These computational checks confirm the correctness of derived formulas and provide insight into structural trends.

This methodology is uniform and modular, enabling application to diverse nanostructure families. In the next sections, we apply it case by case to SC_5C_7 and TUC_4 nanotubes.

4 $SC_5C_7[p, q]$ Nanotube

Construction

Our first molecular structure, denoted by $\mathbb{M}_1$, is the $SC_5C_7[p, q]$ nanotube with $p, q > 1$. Here p denotes the number of heptagons in the first period and q the number of periods in the entire lattice. A single period of $SC_5C_7[p, q]$ consists of three rows. This nanotube is a type of C_5C_7 net obtained by alternating pentagons (C_5) and heptagons (C_7) following a trivalent decoration, as illustrated in Figure 1. Such tiling can cover a torus [11, 12, 16] (see Figure 2).

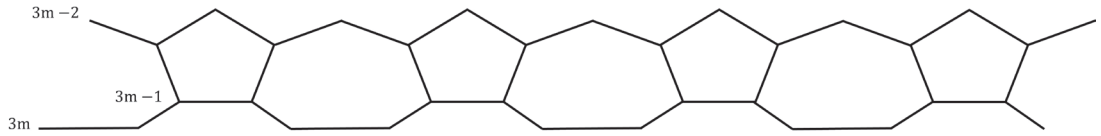

Figure 1: m^{th} period of $SC_5C_7[p, q]$ nanotube

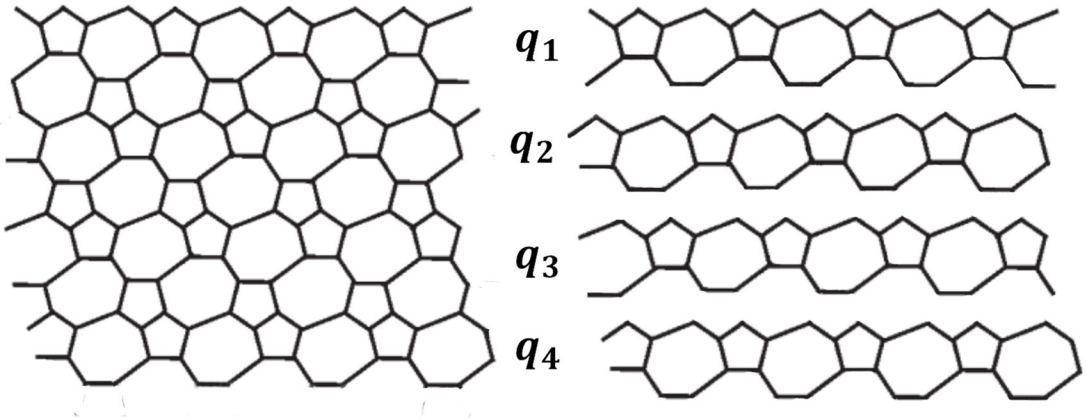

Figure 2: The structure of $SC_5C_7[p, q]$ nanotube with $p = 4$ and $q = 4$

There are $8p$ atoms in one period of the lattice. Hence, the whole nanotube contains $8pq$ atoms in total, of which $4p$ atoms are of degree 2 and $4p(2q - 1)$ atoms are of degree 3. Using hand shake lemma [3], the number of bonds in $\mathbb{M}_1$ is $12pq - 2p$.

Bond Partitions

- According to the degree of atoms incident with bonds, there are three types of bonds (2,2), (2,3) and (3,3) in $\mathbb{M}_1$. The corresponding partition of $B(\mathbb{M}_1)$ is given in Table 1.
- Based on degree sums, there are five distinct values $(5, 6, 7, 8, 9)$, which yield seven types of bonds. The corresponding partition is summarized in Table 2.

- With respect to the 2-distance degree, there are seven types of bonds in $\mathbb{M}_1$. The corresponding partition is presented in Table 3.
- According to the 2–distance degree sums, there are five distinct values $(8, 14, 16, 17, 18)$, which yield nine types of bonds. The partition is given in Table 4.

Table 1: Partition according to degrees

Bond class	Number of bonds
$B_1 = B(2,2)$	p
$B_2 = B(2,3)$	$6p$
$B_2 = B(3,3)$	$12pq - 9p$

Table 2: Partition according to degree sums

Bond class	Number of bonds
$B_1 = B(5,5)$	p
$B_2 = B(5,6)$	$2p$
$B_3 = B(6,7)$	$4p$
$B_4 = B(7,9)$	$2p$
$B_5 = B(8,8)$	p
$B_6 = B(8,9)$	$2p$
$B_7 = B(9,9)$	$12pq - 14p$

Table 3: Partition according to 2–distance degree

Bond class	Number of bonds
$B_1 = B(3,3)$	p
$B_2 = B(3,5)$	$2p$
$B_3 = B(4,4)$	$4p$
$B_4 = B(4,6)$	$2p$
$B_5 = B(5,5)$	p
$B_6 = B(5,6)$	$2p$
$B_7 = B(6,6)$	$12pq - 14p$

Table 4: Partition according to 2–distance degree sums

Bond class	Number of bonds
$B_1 = B(8,8)$	p
$B_2 = B(8,14)$	$6p$
$B_3 = B(14,14)$	p
$B_4 = B(14,16)$	$2p$
$B_5 = B(14,17)$	$2p$
$B_6 = B(16,16)$	p
$B_7 = B(16,18)$	$2p$
$B_8 = B(17,18)$	$4p$
$B_9 = B(18,18)$	$12pq - 21p$

Findings

In [11], the following results for ABC, ABC_4, GA, and GA_5 indices of $\mathbb{M}_1$ were reported:

$$ABC(\mathbb{M}_1) = \left(8q - \tfrac{12+7\sqrt{2}}{2}\right)p,$$

$$ABC_4(\mathbb{M}_1) = \left(\tfrac{16q}{3} + \tfrac{2\sqrt{2}}{5} + \tfrac{\sqrt{110}}{10} + \tfrac{\sqrt{14}}{8} + \tfrac{2\sqrt{462}}{21} + \tfrac{2\sqrt{2}}{3} + \tfrac{\sqrt{30}}{6} + \tfrac{56}{9}\right)p,$$

$$GA(\mathbb{M}_1) = \left(12q - \tfrac{40+12\sqrt{6}}{5}\right)p,$$

$$GA_5(\mathbb{M}_1) = \left(12q + \tfrac{8\sqrt{10}}{13} + \tfrac{8\sqrt{42}}{13} + \tfrac{3\sqrt{4}}{7} + \tfrac{24\sqrt{2}}{17} - 12\right)p.$$

Using the bond partitions in Tables 1–2 and formulas (4)–(5), we obtain the multiplicative versions:

$$ABCII(\mathbb{M}_1) = \left(\sqrt{\tfrac{1}{2}}\right)^{7p} \left(\tfrac{2}{3}\right)^{12pq-9p},$$

$$GAII(\mathbb{M}_1) = \left(\tfrac{24}{25}\right)^{3p},$$

$$ABC_4II(\mathbb{M}_1) = \left(\tfrac{11\sqrt{7}}{8640}\right)^{p} \left(\tfrac{11}{42}\right)^{2p} \left(\tfrac{4}{9}\right)^{12pq-14p},$$

$$GA_5II(\mathbb{M}_1) = \left(\tfrac{22680}{48841}\right)^{p} \left(\tfrac{168}{169}\right)^{2p}.$$

Using bond partitions in Tables 3–4 and formulas (6)–(7), the leap versions are obtained:

$$ABC^2(\mathbb{M}_1) = \left(\tfrac{3\sqrt{10}}{5} + \sqrt{6} + \tfrac{2\sqrt{3}}{3} + \tfrac{2\sqrt{2}}{5} + 3q - 4\right) p,$$

$$GA^2(\mathbb{M}_1) = \left(\tfrac{\sqrt{15}}{2} + \tfrac{4\sqrt{6}}{5} + \tfrac{4\sqrt{30}}{11} + 12q - 8\right) p,$$

$$ABC_4^2(\mathbb{M}_1) = \left(\tfrac{\sqrt{14}}{8} + \tfrac{3\sqrt{35}}{7} + \tfrac{\sqrt{26}}{14} + \tfrac{1}{\sqrt{2}} + 2\sqrt{\tfrac{29}{238}} + \tfrac{\sqrt{30}}{16} + \tfrac{2}{3} + \tfrac{4\sqrt{1122}}{102} + (4q-7)\tfrac{\sqrt{34}}{6}\right) p,$$

$$GA_5^2(\mathbb{M}_1) = \left(\tfrac{24\sqrt{7}}{11} + \tfrac{8\sqrt{14}}{15} + \tfrac{4\sqrt{238}}{31} + \tfrac{24\sqrt{2}}{17} + \tfrac{8\sqrt{306}}{35} + 12q - 18\right) p.$$

Similarly, using the bond partitions in Tables 3–4 and formulas (8)–(9), the multiplicative leap versions are:

$$ABC^2II(\mathbb{M}_1) = \left(\tfrac{3\sqrt{2}}{2000}\right)^{p} \left(\sqrt{\tfrac{5}{18}}\right)^{6pq-7p},$$

$$GA^2II(\mathbb{M}_1) = \left(\tfrac{108}{121}\right)^{p},$$

$$ABC_4^2II(\mathbb{M}_1) = \left(\tfrac{\sqrt{2730}}{896}\right)^{p} \left(\tfrac{\sqrt{35}}{14}\right)^{6p} \left(\tfrac{11\sqrt{3451}}{145656}\right)^{2p} \left(\tfrac{\sqrt{34}}{14}\right)^{12pq-21p},$$

$$GA_5^2II(\mathbb{M}_1) = \left(\tfrac{64\sqrt{1666}}{2635}\right)^{2p} \left(\tfrac{2\sqrt{306}}{35}\right)^{4p} \left(\tfrac{4\sqrt{7}}{11}\right)^{6p}.$$

These explicit closed–form expressions show that all indices grow linearly with q and scale proportionally with p, reflecting the geometric expansion of the nanotube. The ABC–type indices are more sensitive to degree heterogeneity from the C_5/C_7 alternation, while GA–type indices emphasize backbone regularity.

Numerical and Graphical Analysis

Numerical values and 2D plotting of results are presented in this section.

Table 5: $SC_5C_7[3,q]$ vs q

q	ABC	ABC_4	GA	GA_5
2	28.151	42.362	43.762	41.161
3	52.151	58.695	79.762	77.161
4	76.151	75.028	115.762	113.161
5	100.151	91.361	151.762	149.161
6	124.151	107.694	187.762	185.161
7	148.151	124.027	223.762	221.161
8	172.151	140.360	259.762	257.161
9	196.151	156.693	295.762	293.161
10	220.151	173.026	331.762	329.161
11	244.151	189.359	367.762	365.161
12	268.151	205.692	403.762	401.161
13	292.151	222.025	439.762	437.161

Table 6: $SC_5C_7[p,4]$ vs p

p	ABC	ABC_4	GA	GA_5
2	50.767	50.019	77.181	75.441
3	76.151	75.028	115.762	113.161
4	101.534	100.038	154.343	150.882
5	126.918	125.047	192.924	188.603
6	152.302	150.057	231.505	226.323
7	177.685	175.066	270.086	264.044
8	203.069	200.076	308.667	301.765
9	228.452	225.085	347.248	339.485
10	253.836	250.095	385.829	377.206
11	279.220	275.104	424.410	414.927
12	304.603	300.114	462.991	452.647
13	329.987	325.123	501.571	490.368

Table 7: $SC_5C_7[3,q]$ vs q

q	ABC^2	GA^2	ABC_4^2	GA_5^2
2	31.062	57.034	90.726	87.828
3	40.062	93.034	114.631	123.828
4	49.062	129.034	138.535	159.828
5	58.062	165.034	162.440	195.828
6	67.062	201.034	186.344	231.828
7	76.062	237.034	210.248	267.828
8	85.062	273.034	234.153	303.828
9	94.062	309.034	258.057	339.828
10	103.062	345.034	281.962	375.828
11	112.062	381.034	305.866	411.828
12	121.062	417.034	329.770	447.828
13	130.062	453.034	353.675	483.828

Table 8: $SC_5C_7[p,4]$ vs p

p	ABC^2	GA^2	ABC_4^2	GA_5^2
2	32.708	86.023	115.712	118.552
3	49.062	129.034	138.535	159.828
4	65.416	172.045	161.358	201.104
5	81.770	215.056	184.181	242.380
6	98.124	258.067	207.004	283.656
7	114.477	301.078	229.827	324.932
8	130.831	344.089	252.651	366.208
9	147.185	387.100	275.474	407.484
10	163.539	430.111	298.297	448.760
11	179.893	473.121	321.120	490.036
12	196.247	516.132	343.943	531.312
13	212.601	559.143	366.766	572.588

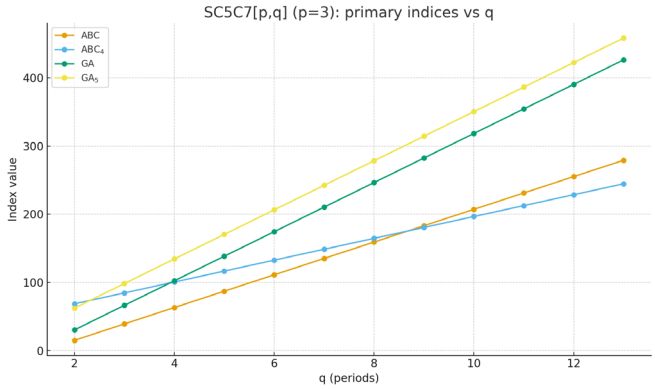

Figure 3: Classical indices vs q

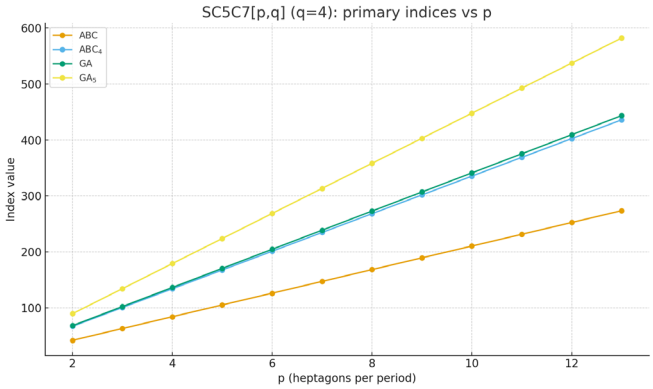

Figure 4: Classical indices vs p

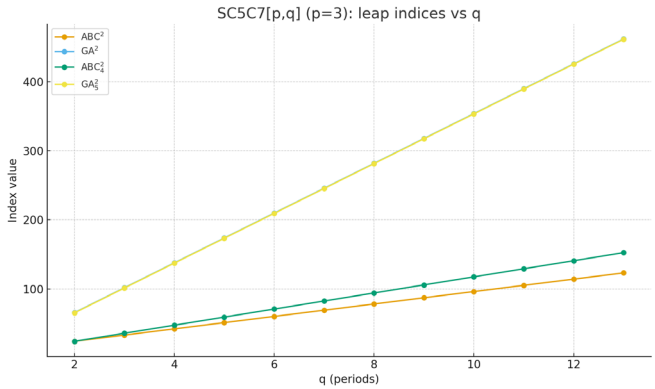

Figure 5: Leap indices vs q

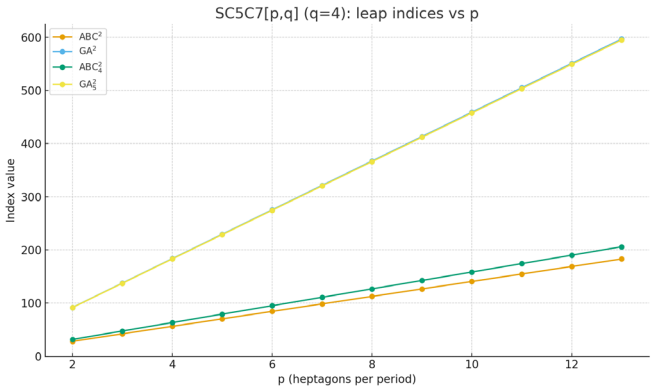

Figure 6: Leap indices vs p

Table 9: $SC_5C_7[3,q]$ vs q (scientific notation)

q	$ABCII$	$GAII$	ABC_4II	GA_5II
2	8.22e-12	6.93e-01	3.36e-22	9.66e-02
3	3.77e-18	6.93e-01	7.03e-35	9.66e-02
4	1.72e-24	6.93e-01	1.47e-47	9.66e-02
5	7.89e-31	6.93e-01	3.09e-60	9.66e-02
6	3.61e-37	6.93e-01	6.48e-73	9.66e-02
7	1.65e-43	6.93e-01	1.36e-85	9.66e-02
8	7.56e-50	6.93e-01	2.85e-98	9.66e-02
9	3.47e-56	6.93e-01	5.97e-111	9.66e-02
10	1.59e-62	6.93e-01	1.25e-123	9.66e-02
11	7.27e-69	6.93e-01	2.62e-136	9.66e-02
12	3.33e-75	6.93e-01	5.50e-149	9.66e-02
13	1.52e-81	6.93e-01	1.15e-161	9.66e-02

Table 10: $SC_5C_7[p,4]$ vs p (scientific notation)

p	$ABCII$	$GAII$	ABC_4II	GA_5II
2	1.44e-16	7.83e-01	6.01e-32	2.11e-01
3	1.72e-24	6.93e-01	1.47e-47	9.66e-02
4	2.07e-32	6.13e-01	3.61e-63	4.43e-02
5	2.48e-40	5.42e-01	8.86e-79	2.04e-02
6	2.97e-48	4.80e-01	2.17e-94	9.34e-03
7	3.56e-56	4.24e-01	5.33e-110	4.29e-03
8	4.27e-64	3.75e-01	1.31e-125	1.97e-03
9	5.12e-72	3.32e-01	3.20e-141	9.02e-04
10	6.14e-80	2.94e-01	7.85e-157	4.14e-04
11	7.37e-88	2.60e-01	1.93e-172	1.90e-04
12	8.83e-96	2.30e-01	4.72e-188	8.72e-05
13	1.06e-103	2.04e-01	1.16e-203	4.00e-05

Table 11: $SC_5C_7[3,q]$ vs q (scientific notation)

q	ABC^2II	GA^2II	ABC_4^2II	GA_5^2II
2	6.42e-13	7.11e-01	1.05e-28	4.71e-01
3	6.32e-18	7.11e-01	2.13e-42	4.71e-01
4	6.23e-23	7.11e-01	4.31e-56	4.71e-01
5	6.13e-28	7.11e-01	8.72e-70	4.71e-01
6	6.04e-33	7.11e-01	1.76e-83	4.71e-01
7	5.94e-38	7.11e-01	3.57e-97	4.71e-01
8	5.85e-43	7.11e-01	7.22e-111	4.71e-01
9	5.76e-48	7.11e-01	1.46e-124	4.71e-01
10	5.67e-53	7.11e-01	2.95e-138	4.71e-01
11	5.59e-58	7.11e-01	5.98e-152	4.71e-01
12	5.50e-63	7.11e-01	1.21e-165	4.71e-01
13	5.42e-68	7.11e-01	2.45e-179	4.71e-01

Table 12: $SC_5C_7[p,4]$ vs p (scientific notation)

p	ABC^2II	GA^2II	ABC_4^2II	GA_5^2II
2	1.57e-15	7.97e-01	1.23e-37	6.06e-01
3	6.23e-23	7.11e-01	4.31e-56	4.71e-01
4	2.47e-30	6.35e-01	1.51e-74	3.67e-01
5	9.78e-38	5.67e-01	5.30e-93	2.85e-01
6	3.87e-45	5.06e-01	1.86e-111	2.22e-01
7	1.54e-52	4.51e-01	6.60e-130	1.73e-01
8	6.09e-60	4.03e-01	2.28e-148	1.34e-01
9	2.41e-67	3.60e-01	8.00e-167	1.05e-01
10	9.56e-75	3.21e-01	2.81e-185	8.14e-02
11	3.79e-82	2.86e-01	9.83e-204	6.33e-02
12	1.50e-89	2.56e-01	3.45e-222	4.93e-02
13	5.95e-97	2.28e-01	1.21e-240	3.84e-02

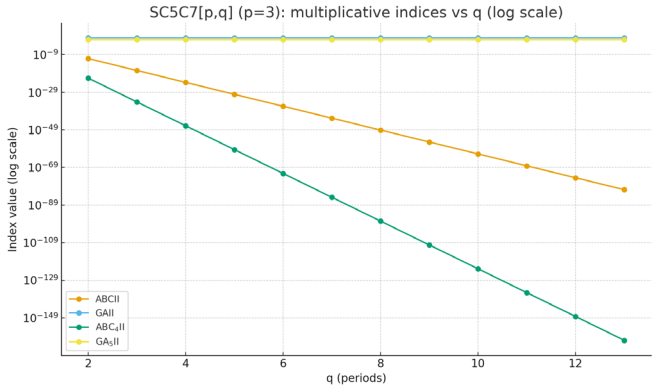

Figure 7: Multiplicative indices (log scale) vs q

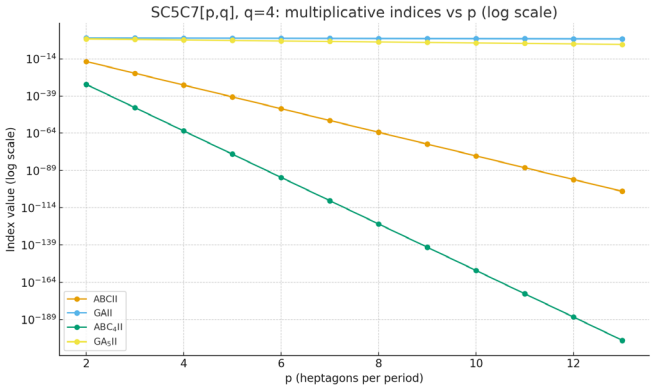

Figure 8: Multiplicative indices (log scale) vs p

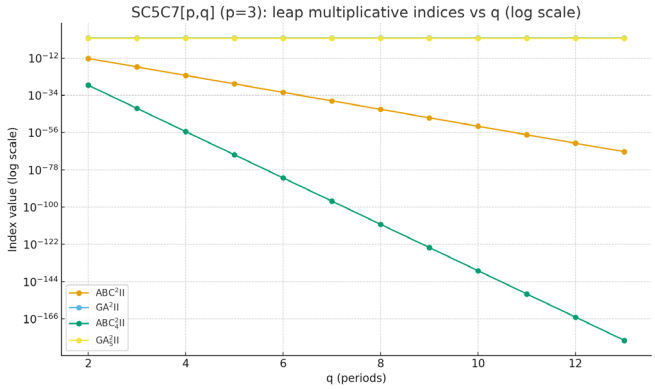

Figure 9: Multiplicative leap indices (log scale) vs q

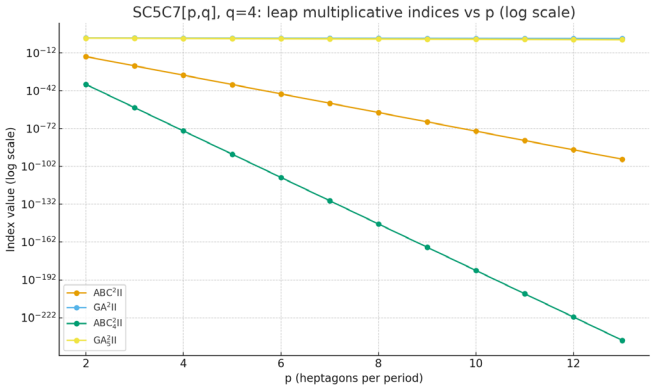

Figure 10: Multiplicative leap indices (log scale) vs p

Results and Discussion

The nanotube $SC_5C_7[p, q]$ was analyzed with respect to different families of atom–bond connectivity (ABC) and geometric–arithmetic (GA) indices. Based on the bond partitions derived in Tables 1–4, closed-form expressions were obtained for each family of indices, namely:

- classical additive indices (ABC, ABC_4, GA, GA_5),
- multiplicative indices ($ABCII$, $GAII$, ABC_4II, GA_5II),
- leap indices (ABC^2, GA^2, ABC_4^2, GA_5^2),
- multiplicative leap indices (ABC^2II, GA^2II, ABC_4^2II, GA_5^2II).

Numerical Evaluation

To illustrate the behavior of these indices, numerical values were computed for initial ranges of the parameters p (number of heptagons in the first period) and q (number of periods). For each

family of indices, Tables 5–12 of values are presented for fixed p and varying q, and vice versa. The corresponding plots in Figures 3–10 reveal consistent monotonic trends.

- For the classical additive indices, both ABC and GA grow linearly with q for fixed p, and likewise scale linearly with p for fixed q. This is in agreement with their dependence on the product pq.
- The leap indices exhibit a similar growth, but with larger coefficients, confirming that leap versions enhance the discriminative power of ABC- and GA-type measures in complex lattices.
- The multiplicative indices decay rapidly as p and q increase, with values approaching zero. This behavior, confirmed by log-scale plots, highlights their sensitivity to exponential terms. Such indices can therefore be useful in distinguishing nanotubes with small values of p and q, but become less effective for larger systems.
- The multiplicative leap indices also decay exponentially, but retain sharper separation between different parameter values than their non-leap counterparts, indicating a potential advantage for nano-material classification.

Graphical Comparisons

The comparison graphs further confirm these observations. For the additive and leap indices, the curves are nearly linear with respect to both p and q. In contrast, the multiplicative families show steep decays, captured clearly through log-scale plots. Together, the Figures 3–10 demonstrate how each index family emphasizes different structural aspects of the nanotube.

Implications

From an application viewpoint, additive and leap indices provide robust measures for modeling structure–property relationships in extended nanostructures, where size parameters are large. Conversely, multiplicative and leap multiplicative indices are more appropriate for analyzing smaller systems, where exponential sensitivity highlights fine structural variations. These complementary roles strengthen the utility of ABC- and GA-type indices in quantitative nanochemistry and materials informatics.

5 $TUC_4[m, n]$ Nanotube

Construction

Our second molecular structure, denoted by $\mathbb{M}_2$, is the $TUC_4[m, n]$ nanotube, which represents a plane tiling of C_4 [2]. Here m denotes the number of squares in a row, n is the number of squares in a column, and $m, n > 1$ (se the pictorial view in Figure 11). In the n^{th} growth of $\mathbb{M}_2$, the total number of atoms is $m(n + 1)$. Among these, $2m$ atoms have degree 3, while the remaining

$m(n-1)$ atoms have degree 4. By applying hand shake lemma [3], the total number of bonds in $\mathbb{M}_2$ is $|B(\mathbb{M}_2)| = m(2n+1)$.

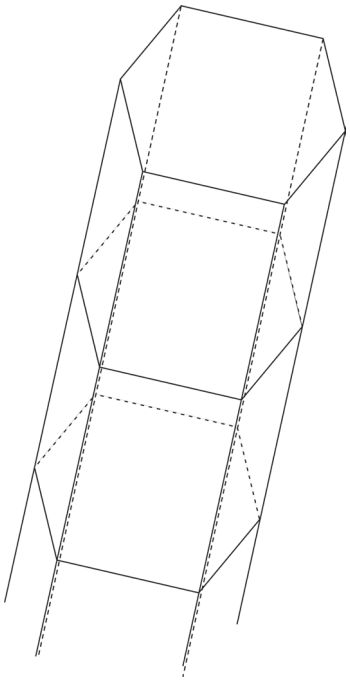

Figure 11: $TUC_4[6,n]$ nanotube covered by C_4

Bond Partitions

- Based on the degree of atoms incident to each bond, there are three distinct bond types in $\mathbb{M}_2$: (3,3), (3,4) and (4,4). The corresponding partition of $B(\mathbb{M}_2)$ is provided in Table 13.
- Considering the degree sums, three distinct values $(10, 15, 16)$ produce five bond classes. The corresponding bond partition is shown in Table 14.
- According to the 2-distance degree, there are five distinct bond types. The corresponding bond partition is presented in Table 15.
- The 2-distance degree sums $(17, 27, 31, 32)$ generate seven bond classes. This partition is displayed in Table 16.

Table 13: Partition according to degrees

Bond class	Number of bonds
$B_1 = B(3,3)$	$2m$
$B_2 = B(3,4)$	$2m$
$B_4 = B(4,4)$	$m(2n-3)$

Table 14: Partition according to degree sums

Bond class	Number of bonds
$B_1 = b(10,10)$	$2m$
$B_2 = B(10,15)$	$2m$
$B_3 = B(15,15)$	$2m$
$B_4 = B(15,16)$	$2m$
$B_5 = B(16,16)$	$2mn-7m$

Table 15: Partition according to 2-distance degrees

Bond class	Number of bonds
$B_1 = B(5,5)$	$2m$
$B_2 = B(5,7)$	$2m$
$B_3 = B(7,7)$	$2m$
$B_4 = B(7,8)$	$2m$
$B_5 = B(8,8)$	$2mn - 7m$

Table 16: Partition according to 2-distance degree sums

Bond class	Number of bonds
$B_1 = B(17,17)$	$2m$
$B_2 = B(17,27)$	$2m$
$B_3 = B(27,27)$	$2m$
$B_4 = B(27,31)$	$2m$
$B_5 = B(31,31)$	$2m$
$B_6 = B(31,32)$	$2m$
$B_7 = B(32,32)$	$2mn - 11m$

Findings

Using the bond partitions of Tables 13–14 in the definitions (1)–(5), the closed forms of the indices for $\mathbb{M}_2$ are obtained as:

$$ABC(\mathbb{M}_2) = \left(\frac{4}{3} + \sqrt{\frac{5}{3}} + \frac{(2n-3)\sqrt{6}}{4}\right) m,$$

$$GA(\mathbb{M}_2) = \left(\frac{8\sqrt{3}}{7} + (2n-1)\right) m,$$

$$ABC_4(\mathbb{M}_2) = \left(\frac{3\sqrt{2}}{5} + \frac{2\sqrt{138}}{15} + \frac{4\sqrt{7}}{15} + \frac{\sqrt{435}}{30} + \frac{(2n-7)\sqrt{30}}{16}\right) m,$$

$$GA_5(\mathbb{M}_2) = \left(\frac{4\sqrt{6}}{5} + \frac{16\sqrt{15}}{31} + (2n-3)\right) m.$$

Similarly, multiplicative versions are:

$$ABCII(\mathbb{M}_2) = \left(\frac{\sqrt{15}}{9}\right)^{2m} \left(\frac{\sqrt{6}}{4}\right)^{m(2n-3)}, \quad GAII(\mathbb{M}_2) = \left(\frac{2\sqrt{12}}{7}\right)^{2m}$$

$$ABC_4II(\mathbb{M}_2) = \left(\frac{1}{1500}\sqrt{\frac{14007}{15}}\right)^{2m} \left(\frac{\sqrt{30}}{16}\right)^{2mn-7m}, \quad GA_5II(\mathbb{M}_2) = \left(\frac{16\sqrt{90}}{155}\right)^{2m}.$$

Using Tables 15–16 and formulas (6)–(9), the leap versions are derived as follows:

$$ABC^2(\mathbb{M}_2) = \left(\frac{2\sqrt{2}}{5} + \frac{\sqrt{14}}{7} + \frac{\sqrt{588}}{49} + \frac{\sqrt{728}}{56} + \frac{(2n-7)\sqrt{14}}{8}\right) m,$$

$$GA^2(\mathbb{M}_2) = \left(\frac{2\sqrt{25}}{10} + \frac{2\sqrt{35}}{12} + \frac{2\sqrt{49}}{14} + \frac{2\sqrt{56}}{15} + (2n-7)\right) m,$$

$$ABC_4^2(\mathbb{M}_2) = \left(\frac{4\sqrt{2}}{17} + \frac{\sqrt{42}}{3} + \frac{6\sqrt{13}}{243} + \frac{6\sqrt{1302}}{837} + \frac{2\sqrt{15}}{31} + \frac{\sqrt{3782}}{248} + \frac{(2n-11)\sqrt{62}}{32}\right) m,$$

$$GA_5^2(\mathbb{M}_2) = \left(\frac{\sqrt{459}}{22} + \frac{\sqrt{837}}{29} + \frac{2\sqrt{992}}{63} + 2n - 5\right) m.$$

Similarly, multiplicative leap versions are:

$$ABC^2II(\mathbb{M}_2) = \left(\frac{2\sqrt{78}}{245}\right)^{2m}\left(\frac{\sqrt{14}}{8}\right)^{2mn-7m}, \quad GA^2II(\mathbb{M}_2) = \left(\frac{392}{405}\right)^{2m},$$

$$ABC_4^2II(\mathbb{M}_2) = \left(\frac{112}{3969891}\sqrt{\frac{122915}{527}}\right)^{2m}\left(\frac{\sqrt{62}}{32}\right)^{2mn-11m},$$

$$GA_5^2II(\mathbb{M}_2) = \left(\frac{12\sqrt{32647}}{2233}\right)^{2m}.$$

Numerical and Graphical Analysis

Numerical values and 2D plotting of results are presented in this section.

Table 17: $TUC_4[m,4]$ vs m

m	ABC	GA	ABC_4	GA_5
2	11.372	17.959	8.316	17.917
3	17.059	26.939	12.474	26.876
4	22.745	35.918	16.632	35.834
5	28.431	44.897	20.790	44.793
6	34.117	53.877	24.948	53.751
7	39.803	62.856	29.106	62.710
8	45.490	71.836	33.263	71.668
9	51.176	80.815	37.421	80.627
10	56.862	89.795	41.579	89.586
11	62.548	98.774	45.737	98.544
12	68.234	107.753	49.895	107.503
13	73.921	116.733	54.053	116.461

Table 18: $TUC_4[4,n]$ vs n

n	ABC	GA	ABC_4	GA_5
2	12.947	19.918	11.154	19.834
3	17.846	27.918	13.893	27.834
4	22.745	35.918	16.632	35.834
5	27.644	43.918	19.370	43.834
6	32.543	51.918	22.109	51.834
7	37.442	59.918	24.848	59.834
8	42.341	67.918	27.587	67.834
9	47.240	75.918	30.325	75.834
10	52.139	83.918	33.063	83.834
11	57.038	91.918	35.802	91.834
12	61.937	99.918	38.541	99.834
13	66.836	107.918	41.280	107.834

Table 19: $TUC_4[m,4]$ vs m

m	ABC^2	GA^2	ABC_4^2	GA_5^2
2	5.089	9.968	5.201	11.943
3	7.634	14.951	7.801	17.914
4	10.178	19.935	10.401	23.885
5	12.723	24.919	13.002	29.857
6	15.268	29.903	15.602	35.828
7	17.812	34.887	18.202	41.799
8	20.357	39.870	20.803	47.771
9	22.901	44.854	23.403	53.742
10	25.446	49.838	26.004	59.713
11	27.991	54.822	28.604	65.685
12	30.535	59.806	31.204	71.656
13	33.080	64.789	33.805	77.627

Table 20: $TUC_4[4,n]$ vs n

n	ABC^2	GA^2	ABC_4^2	GA_5^2
2	2.695	3.935	6.464	7.885
3	6.437	11.935	8.433	15.885
4	10.178	19.935	10.401	23.885
5	13.920	27.935	12.370	31.885
6	17.662	35.935	14.338	39.885
7	21.403	43.935	16.307	47.885
8	25.145	51.935	18.275	55.885
9	28.887	59.935	20.244	63.885
10	32.628	67.935	22.212	71.885
11	36.370	75.935	24.181	79.885
12	40.112	83.935	26.149	87.885
13	43.853	91.935	28.118	95.885

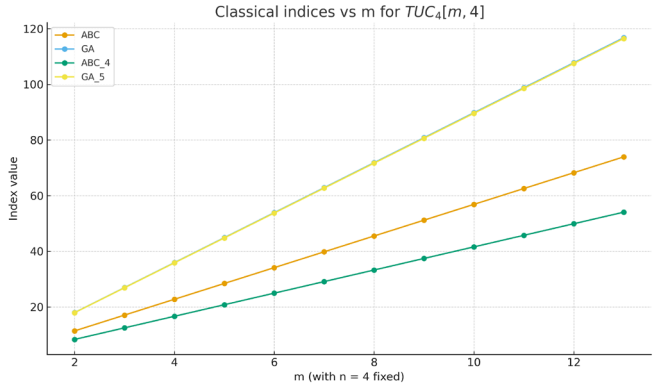

Figure 12: Classical indices vs m

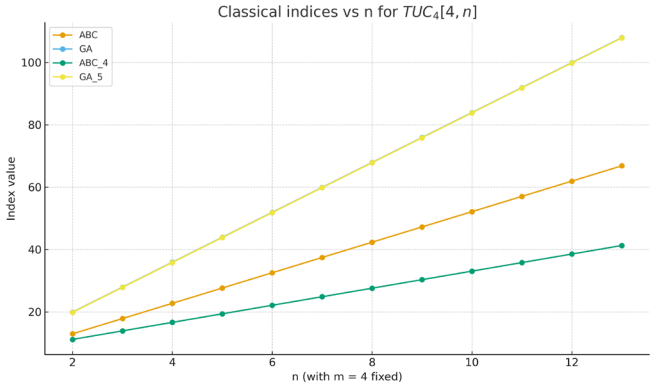

Figure 13: Classical indices vs n

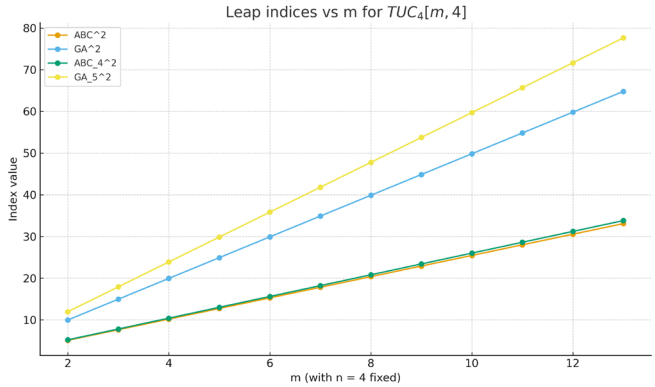

Figure 14: Leap indices vs m

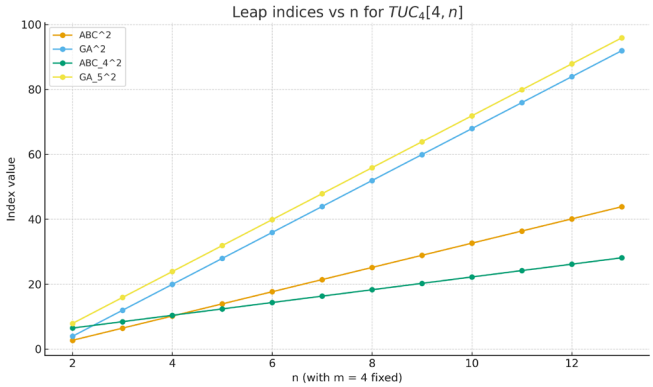

Figure 15: Leap indices vs n

Table 21: $TUC_4[m, 4]$ vs m (scientific notation)

m	$ABCII$	$GAII$	ABC_4II	GA_5II
2	2.54e-04	9.602e-01	2.02e-08	9.20e-01
3	4.06e-06	9.40e-01	2.87e-12	8.82e-01
4	6.47e-08	9.21e-01	4.07e-16	8.46e-01
5	1.03e-09	9.02e-01	5.79e-20	8.11e-01
6	1.65e-11	8.84e-01	8.22e-24	7.78e-01
7	2.62e-13	8.66e-01	1.17e-27	7.46e-01
8	4.18e-15	8.48e-01	1.66e-31	7.15e-01
9	6.67e-17	8.31e-01	2.36e-35	6.86e-01
10	1.06e-18	8.14e-01	3.35e-39	6.58e-01
11	1.69e-20	7.97e-01	4.76e-43	6.31e-01
12	2.71e-22	7.81e-01	6.76e-47	6.05e-01
13	4.31e-24	7.65e-01	9.61e-51	5.80e-01

Table 22: $TUC_4[4, n]$ vs n (scientific notation)

n	$ABCII$	$GAII$	ABC_4II	GA_5II
2	1.65e-04	9.21e-01	1.15e-08	8.46e-01
3	3.27e-06	9.21e-01	2.16e-12	8.46e-01
4	6.47e-08	9.21e-01	4.07e-16	8.46e-01
5	1.28e-09	9.21e-01	7.68e-20	8.46e-01
6	2.51e-11	9.21e-01	1.45e-23	8.46e-01
7	5.01e-13	9.21e-01	2.73e-27	8.46e-01
8	9.89e-15	9.21e-01	5.15e-31	8.46e-01
9	1.96e-16	9.21e-01	9.72e-35	8.46e-01
10	3.87e-18	9.21e-01	1.83e-38	8.46e-01
11	7.65e-20	9.21e-01	3.46e-42	8.46e-01
12	1.51e-21	9.21e-01	6.52e-46	8.46e-01
13	2.99e-23	9.21e-01	1.23e-49	8.46e-01

Table 23: $TUC_4[m,4]$ vs m (scientific notation)

m	ABC^2II	GA^2II	ABC_4^2II	GA_5^2II
2	5.91e-06	8.78e-01	1.55e-10	8.89e-01
3	1.44e-08	8.22e-01	1.94e-15	8.38e-01
4	3.49e-11	7.70e-01	2.41e-20	7.90e-01
5	8.49e-14	7.22e-01	3.01e-25	7.45e-01
6	2.06e-16	6.76e-01	3.74e-30	7.02e-01
7	5.02e-19	6.33e-01	4.66e-35	6.62e-01
8	1.22e-21	5.93e-01	5.81e-40	6.24e-01
9	2.97e-24	5.56e-01	7.24e-45	5.89e-01
10	7.21e-27	5.21e-01	9.02e-50	5.55e-01
11	1.75e-29	4.88e-01	1.12e-54	5.23e-01
12	4.26e-32	4.57e-01	1.40e-59	4.93e-01
13	1.04e-34	4.28e-01	1.75e-64	4.65e-01

Table 24: $TUC_4[4,n]$ vs n (scientific notation)

n	ABC^2II	GA^2II	ABC_4^2II	GA_5^2II
2	6.66e-06	7.70e-01	1.33e-10	7.90e-01
3	1.53e-08	7.70e-01	1.79e-15	7.90e-01
4	3.49e-11	7.70e-01	2.41e-20	7.90e-01
5	7.10e-14	7.70e-01	3.24e-25	7.90e-01
6	1.83e-16	7.70e-01	4.35e-30	7.90e-01
7	4.19e-19	7.70e-01	5.85e-35	7.90e-01
8	9.60e-22	7.70e-01	7.86e-40	7.90e-01
9	2.20e-24	7.70e-01	1.06e-44	7.90e-01
10	5.03e-27	7.70e-01	1.42e-49	7.90e-01
11	1.15e-29	7.70e-01	1.91e-54	7.90e-01
12	2.64e-32	7.70e-01	2.56e-59	7.90e-01
13	6.04e-35	7.70e-01	3.45e-64	7.90e-01

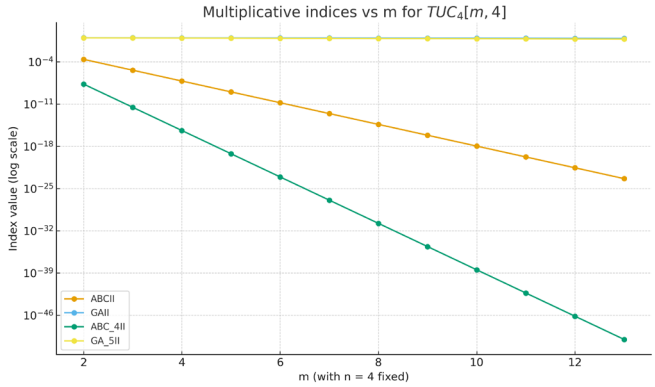

Figure 16: Multiplicative indices (log scale) vs m

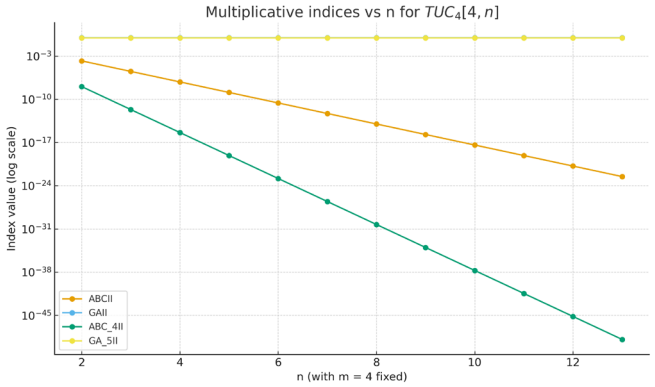

Figure 17: Multiplicative indices (log scale) vs n

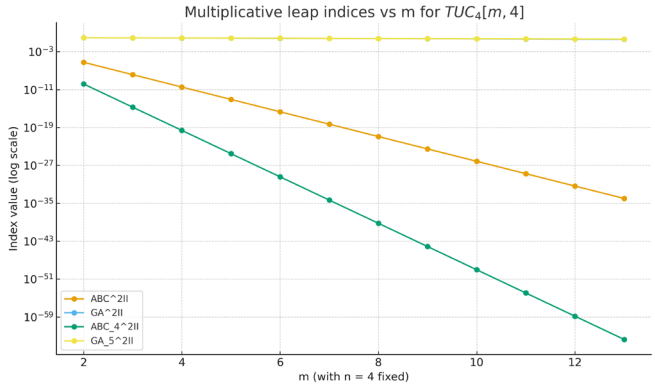

Figure 18: Multiplicative leap indices (log scale) vs m

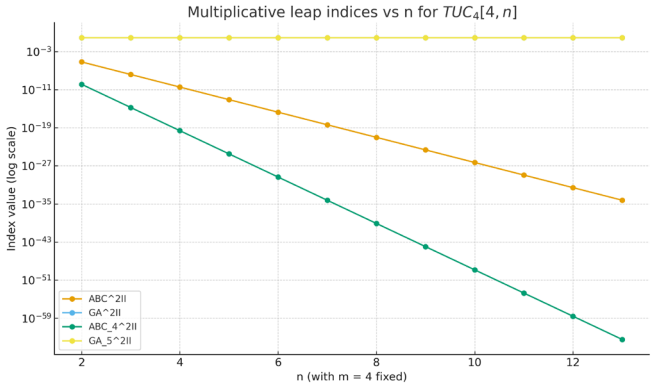

Figure 19: Multiplicative leap indices (log scale) vs n

Results and Discussion

The numerical tables and comparison plots for $TUC_4[m,n]$ (Slices: $n=4$ with $m=2,\ldots,13$ and $m=4$ with $n=2,\ldots,13$) reveal consistent scaling behaviors across all four descriptor families.

Additive indices. From the closed forms of classical indices ABC, GA, ABC_4, GA_5, it is clear that each additive index grows *linearly* in both m and n. The slopes with respect to n satisfy

$$\text{Slope}_n(GA) \approx \text{Slope}_n(GA_5) > \text{Slope}_n(ABC_4) > \text{Slope}_n(ABC),$$

consistent with the dominance of GA type descriptors at larger n. This ordering is confirmed in Figure 12 (varying m) and Figure 13 (varying n), where GA and GA_5 display the steepest linear rise.

Leap (additive) indices. The leap variants $ABC^2, GA^2, ABC_4^2, GA_5^2$ incorporate 2-distance degree sums, thereby amplifying long–range connectivity. Numerically, they increase faster than their classical counterparts, especially as m or n grows. Among them, GA^2 and GA_5^2 exhibit the steepest growth, reflecting the sensitivity of GA type families to larger degree sum pairs. These trends are illustrated in Figures 14 and 15.

Multiplicative indices. The multiplicative variants $ABCII, GAII, ABC_4II, GA_5II$ exhibit exponential behavior due to repeated edge–wise factors. For example, $GAII$ and GA_5II depend only on m and remain constant across n, while $ABCII$ and ABC_4II contain exponential factors in mn. Thus, for fixed $n=4$, they decay rapidly with m, and for fixed $m=4$, $GAII$ and GA_5II remain flat while $ABCII$ and ABC_4II fall steeply with n. Logarithmic scaling is required in Figures 16 and 17 to capture these trends.

Leap–multiplicative indices. The multiplicative leap family $ABC^2II, GA^2II, ABC_4^2II, GA_5^2II$ shows the strongest decay. Their closed forms include exponential factors in $(2mn-7m)$ or $(2mn-11m)$, which force the values toward zero quickly as either parameter increases. Among these, GA^2II drops most sharply, becoming negligible even at modest m or n. The suppression is evident in the log-scale plots of Figures 18 and 19.

Implications. Overall, the additive and leap families provide scalable, monotone growth indicators for $TUC_4[m,n]$, well suited for tracking structural expansion. In contrast, the multiplicative and leap–multiplicative indices decay exponentially, offering higher contrast only for small to moderate values of m,n but compressing differences at larger scales. Hence, a complementary perspective emerges: additive/leap indices are recommended for characterizing long range growth, while multiplicative/multiplicative leap families are best applied to detect subtle variations in early generations of the nanotube lattice.

6 Concluding Remarks

In this article, we developed closed–form expressions for the Atom–Bond Connectivity (ABC) and Geometric–Arithmetic (GA) indices, together with their notable variants, across two nanotube families: $SC_5C_7[p,q]$ and $TUC_4[m,n]$. The approach was grounded in systematic bond partitions according to degree, degree sums, and 2–distance degree, thereby enabling compact formulae that

reveal explicit scaling laws in parameters p, q, m, n. Numerical tables and comparative plots further clarified the growth behavior of additive, leap, multiplicative, and multiplicative leap indices.

The results demonstrate that additive and leap indices grow linearly (or super linearly) with system size, making them reliable indicators of structural expansion in extended nanotube. Conversely, multiplicative and multiplicative leap indices exhibit exponential decay, sharply distinguishing smaller systems but compressing differences for larger values of p, q, m, n. This complementary behavior underscores their utility: additive descriptors for global growth assessment, and multiplicative ones for capturing local or early generation variations. These trends align with established applications in QSPR/QSAR modeling, nanomaterials design, and the prediction of thermodynamic, diffusion, and adsorption properties.

From an applied perspective, these findings reinforce the utility of ABC and GA based indices for QSPR/QSAR modeling, thermodynamic prediction, and nanomaterials design. In particular, the systematic scaling observed here aligns with known correlations to solubility, hydrophobicity, and enthalpy of formation. The explicit formulae derived offer efficient tools for chemoinformatics pipelines, where repeated index evaluation on large parameter spaces is required.

Future Directions. Future work may extend this methodology to heteroatomic lattices, functionalized nanotubes, and stochastic graph models, as well as to explore direct statistical correlations with experimental physicochemical data. In this way, the present theoretical results provide a solid platform for further developments at the interface of chemical graph theory, molecular modeling, and nanostructured material design. Several avenues for further research emerge from this work:

- *Extension to functionalized and heteroatomic systems:* Incorporating heteroatoms or chemical substitutions into nanotubes and dendrimers to examine how ABC/GA descriptors capture heterogeneity and functional group effects.
- *Stochastic and dynamic graph models:* Studying ensembles of random lattices or time–evolving nanostructures to assess robustness of index scaling laws.
- *Integration with experimental datasets:* Systematic benchmarking of the closed–form indices against measured solubility, enthalpy, or conductivity data for nanotubes and dendrimers.
- *Machine learning applications:* Embedding the derived formulae into QSPR/QSAR pipelines as low–cost, high–interpretability descriptors to improve predictive performance.
- *Broader topological families:* Generalizing the present approach to other chemical graph classes such as graphene nanoribbons, fullerene derivatives, or cage polymers, where degree partitions can be exploited similarly.

Taken together, these directions point toward a broad agenda where the exact formulae developed here serve not only as theoretical contributions in chemical graph theory but also as practical tools in chemoinformatics, molecular design, and materials science.

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An Open-Source and Generalizable Linear Regression Framework for QSPR Using Topological Indices on Weighted Molecular Graphs

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Abstract

Topological indices derived from molecular graphs have proven to be efficient and widely adopted tools for Quantitative Structure–Property Relationship (QSPR) analysis. This study investigates both degree-based and distance-based topological indices and evaluates their relationships with fundamental molecular descriptors, such as molecular weight, exact mass, complexity, and polar surface area. The computational framework is constructed using vertex–edge weighted molecular graphs, which incorporate essential atomic and bond information directly into the graph representation. All calculations have been performed based on the Van der Waals atomic scheme. Furthermore, complete workflows and curated datasets have been made publicly available in an accompanying GitHub repository to ensure reproducibility and facilitate further research. The proposed methodology is designed to be general and has been structured to allow for seamless extension to alternative atomic schemes, including those parameterized by atomic radius or atomic mass. This flexibility significantly broadens the potential applications of topological indices in both QSPR and Quantitative Structure–Activity Relationship (QSAR) modeling.

Keywords: Quantitative structure–property relationship (QSPR), Molecular graph, Vertex–edge weighted graph, Topological index
AMS Classification: Primary: 05C09, Secondary: 05C92

1 Introduction

Graph theory has become an fundemantal mathematical framework for modeling complex structures across diverse scientific domains. In chemistry, graph-theoretical methods provide a natural representation of molecular structures, where atoms correspond to vertices and chemical bonds correspond to edges. This abstraction allows the application of combinatorial and algebraic tools to study molecular topology, predict chemical properties, and understand reactivity patterns without direct reliance on quantum mechanical computations [34]. In chemical terminology, this represantation is known as a *molecular graph* of the molecules [35]. The concept of a *vertex–edge weighted*

(VEW) molecular graph, introduced in [18], extends the traditional molecular graph model by assigning weights to both atoms and bonds. Formally, a VEW molecular graph is denoted as

$$\mathcal{G} = \mathcal{G}(V, E, Sym, Bo, Vw, Ew, w),$$

where $V = V(\mathcal{G})$ and $E = E(\mathcal{G})$ represent the sets of vertices (atoms) and edges (bonds), respectively. The set $Sym = Sym(\mathcal{G})$ contains the chemical symbols of all atoms in the molecule, while $Bo = Bo(\mathcal{G})$ stores the *topological bond order* of each edge, taking the values 1 for a single bond, 2 for a double bond, 3 for a triple bond, and 1.5 for an aromatic bond. The functions $Vw(w)$ and $Ew(w)$ represent the vertex and edge weight sets, respectively, both determined by a chosen weighting scheme w. In practice, the scheme w typically reflects an intrinsic atomic property such as atomic number, atomic radius, electronegativity, or valence electron count. These weights enable a more chemically informative representation, allowing the resulting graph to encode both structural connectivity and atom-specific or bond-specific characteristics.

The *weighted adjacency matrix* $A_w = A_w(\mathcal{G})$ of a vertex–edge weighted molecular graph $\mathcal{G}$ with n vertices is an $n \times n$ real symmetric matrix. Each entry encodes either a vertex weight, an edge weight, or zero, depending on the relationship between vertices. As formulated in [35], pp. 173–175, the entries are given by

$$(A_w)_{uv} = \begin{cases} V_w(w)_u, & \text{if } u = v, \\ E_w(w)_{uv}, & \text{if } uv \in E(\mathcal{G}), \\ 0, & \text{otherwise}, \end{cases} \tag{1}$$

where $V_w(w)_u$ denotes the weight assigned to vertex u under the scheme w, and $E_w(w)_{uv}$ represents the weight of the edge connecting u and v. This representation incorporates both atomic and bond information into a single matrix.

The *weighted distance matrix* $D_w = D_w(\mathcal{G})$ of a vertex–edge weighted molecular graph $\mathcal{G}$ encodes the weighted shortest-path distances between all pairs of vertices, while also incorporating vertex-specific weights along the diagonal. Formally, its entries are defined as

$$(D_w)_{uv} = \begin{cases} V_w(w)_u, & \text{if } u = v, \\ d_w(u, v), & \text{if } u \neq v, \end{cases} \tag{2}$$

where $V_w(w)_u$ is the weight assigned to vertex u and $d_w(u, v)$ denotes the weighted distance between vertices u and v under the weighting scheme w. This formulation integrates both local atomic characteristics and global connectivity into a single matrix representation. Here, $d_w(u, v)$ denotes the weighted distance between vertices u and v, where the weighting scheme w is applied to determine both the vertex weights V_w and the edge weights E_w. In a VEW graph $\mathcal{G}$, the length of a path p_{ij} connecting vertices v_i and v_j is expressed as

$$l(p_{ij}, w) = l\big(p_{ij}, w, \mathcal{G}\big),$$

and is computed as the sum of the edge weights $E_w(w)_{kl}$ over all consecutive edges (v_k, v_l) comprising the path. The weighted eccentricity of a vertex v_i in $\mathcal{G}$ is then given by

$$\epsilon_w(v_i) = \max_{v_j \in V(\mathcal{G})} d_w(v_i, v_j),$$

that is, the maximum weighted distance from v_i to any other vertex in the graph.

Topological indices (TIs) are numerical invariants extracted from graph representations of molecular structures, typically defined in terms of vertex degrees, edge relations, or other structural features of the underlying graph. These indices function as powerful descriptors in chemical graph theory. They provide a systematic means of quantifying molecular architecture and enable correlations between molecular structure and experimentally observed properties. Their importance arises from the fact that TIs capture both local and global structural characteristics, thereby linking abstract mathematical representations with practical chemical and biological behaviors.

The exploration of relationships between the structural features of molecules and their physicochemical or biological properties has long been a central focus in chemical graph theory. Within this context, TIs play a pivotal role in quantitative structure–property relationship (QSPR) and quantitative structure–activity relationship (QSAR) studies. The fundamental premise of these approaches is that the intrinsic structure of a molecule dictates its physicochemical properties and biological activity. QSPR/QSAR frameworks employ TIs as molecular descriptors. They transform molecular structures into mathematical forms encoding essential geometric, topological, and electronic information ([3, 22, 36]).

A key feature of QSPR/QSAR modeling lies in the establishment of predictive correlations between molecular descriptors and experimentally measured parameters. Such correlations are frequently expressed through regression-based statistical models, typically in the form

$$P = a + b \cdot \mathrm{TI}, \tag{3}$$

where P denotes the target property or activity under investigation and TI the selected topological index. This formulation yields interpretable and computationally efficient models that highlight the structural determinants of molecular behavior. Statistical approaches such as linear regression, among others, have therefore been widely applied to extract meaningful insights from TIs, supporting the systematic prediction of molecular efficacy.

Recent studies have demonstrated the broad applicability and predictive capability of TIs in various therapeutic domains, including drugs used in the treatment of blood, breast, and other cancer types [1, 6, 27, 30, 20, 24, 28]. By facilitating accurate predictions of properties such as solubility, reactivity, and toxicity, TIs not only accelerate drug discovery and materials design but also contribute to reducing laboratory costs and experimental efforts. Thus, topological indices have established themselves as indispensable tools in modern cheminformatics, bridging the gap between molecular structure and biological function.

In VEW molecular graph $\mathcal{G}$, $Vw(w)$ and $Ew(w)$ are vertex and edge weight sets, and w is a weighting scheme (e.g., atomic number, atomic radius). Vertex and edge weights relative to a reference atom (often carbon) are given by:

$$Vw(w)_i = 1 - \frac{w_C}{w_i}, \tag{4}$$

$$Ew(w)_{ij} = \frac{w_C^2}{Bo_{ij} w_i w_j}, \tag{5}$$

where $Vw(w)_i$ corresponds to atom i and $Ew(w)_{ij}$ to the bond between atoms i and j [35].

While classical TIs are computed on unweighted molecular graphs, more refined models incorporate atomic and bond-level information through *vertex–edge weighted* (VEW) graphs [10, 35, 32]. Hence unlike their classical definitions, VEW-based indices capture atomic-scale heterogeneity. So we recall several VEW-based degree and degree–distance topological indices defined on the graph

$\mathcal{G}$. Let A_w denote the weighted adjacency matrix of $\mathcal{G}$ and D_w denote the weighted distance matrix. For convenience, denote by $(A_w^2)_{uu}$ the VEW-based degree of the vertex u. Below, each index is expressed using these quantities.

The VEW-based first Zagreb and second Zagreb indices are defined by

$$M_1(\mathcal{G}) = \sum_{uv \in E} \left[(A_w^2)_{uu} + (A_w^2)_{vv} \right],$$

and

$$M_2(\mathcal{G}) = \sum_{uv \in E} (A_w^2)_{uu} (A_w^2)_{vv},$$

which parallel the classical definition given by Gutman and Das [13] and [4], respectively.
The hyper Zagreb index in VEW form is

$$HM(\mathcal{G}) = \sum_{uv \in E} \left[(A_w^2)_{uu} + (A_w^2)_{vv} \right]^2,$$

introduced in Shirdel et al. [31].

The VEW-based ABC index is

$$ABC(\mathcal{G}) = \sum_{uv \in E} \sqrt{\frac{(A_w^2)_{uu} + (A_w^2)_{vv} + 2}{(A_w^2)_{uu}(A_w^2)_{vv}}},$$

consistent with Estrada et al. [8].
The VEW-based GA index is given as

$$GA(\mathcal{G}) = \sum_{uv \in E} \frac{2\sqrt{(A_w^2)_{uu}(A_w^2)_{vv}}}{(A_w^2)_{uu} + (A_w^2)_{vv}},$$

following [5].

The AG index takes the form

$$AG(\mathcal{G}) = \sum_{uv \in E} \frac{(A_w^2)_{uu} + (A_w^2)_{vv}}{2\sqrt{(A_w^2)_{uu}(A_w^2)_{vv}}},$$

as proposed in [29].

The VEW-based harmonic index is

$$H(\mathcal{G}) = \sum_{uv \in E} \frac{2}{(A_w^2)_{uu} + (A_w^2)_{vv}},$$

introduced by Zhong [37].

$$R(\mathcal{G}) = \sum_{uv \in E} \sqrt{\frac{1}{(A_w^2)_{uu}(A_w^2)_{vv}}},$$

in accordance with Randić [23].

$$RR(\mathcal{G}) = \sum_{uv \in E} \sqrt{(A_w^2)_{uu}(A_w^2)_{vv}},$$

as considered in Gutman et al. [14].

$$F(\mathcal{G}) = \sum_{uv \in E} \left[(A_w^2)_{uu}^2 + (A_w^2)_{vv}^2\right],$$

introduced by Furtula and Gutman [9].

$$SC(\mathcal{G}) = \sum_{uv \in E} \sqrt{\frac{1}{(A_w^2)_{uu} + (A_w^2)_{vv}}},$$

proposed by Zhou and Trinajstić [38].

$$NI(\mathcal{G}) = \sum_{uv \in E} \sqrt{(A_w^2)_{uu} + (A_w^2)_{vv}},$$

introduced by Kulli [19].

$$ISI(\mathcal{G}) = \sum_{uv \in E} \frac{(A_w^2)_{uu}(A_w^2)_{vv}}{(A_w^2)_{uu} + (A_w^2)_{vv}},$$

due to An and Xiong [2].

$$ReZ1(\mathcal{G}) = \sum_{uv \in E} \frac{(A_w^2)_{uu} + (A_w^2)_{vv}}{(A_w^2)_{uu}(A_w^2)_{vv}},$$

introduced in Gutman et al. [15].

$$SO(\mathcal{G}) = \sum_{uv \in E} \sqrt{(A_w^2)_{uu}^2 + (A_w^2)_{vv}^2},$$

defined by Gutman [12].

$$mSO(\mathcal{G}) = \sum_{uv \in E} \sqrt{\frac{1}{(A_w^2)_{uu}^2 + (A_w^2)_{vv}^2}},$$

see Huang and Liu [17].

The VEW-based Wiener index is

$$W(\mathcal{G}) = \sum_{u<v} (D_w)_{uv},$$

consistent with Rouvray [25].

$$H(\mathcal{G}) = \frac{1}{2} \sum_{u<v} \frac{1}{(D_w)_{uv}},$$

introduced in Luvlić et al. [21].

$$TEI(\mathcal{G}) = \sum_{u \in V} \epsilon_w(u),$$

given by Sardana et al. [26].

$$ECI(\mathcal{G}) = \sum_{u \in V} \epsilon_w(u)(A_w^2)_{uu},$$

as introduced in [26].

$$DD(\mathcal{G}) = \sum_{uv \in E} \left[(A_w^2)_{uu} + (A_w^2)_{vv}\right](D_w)_{uv},$$

given by Dobrynin et al. [7].

$$G(\mathcal{G}) = \sum_{uv \in E} (A_w^2)_{uu}(A_w^2)_{vv}(D_w)_{uv},$$

introduced in Gutman [11].

$$RDD(\mathcal{G}) = \sum_{uv \in E} \left[(A_w^2)_{uu} + (A_w^2)_{vv}\right](D_w)_{uv},$$

considered by Hua and Zhang [16].

In contrast to the conventional QSPR studies that rely on unweighted molecular graphs, we introduce for the first time the following research question concerning the use of vertex- and edge-weighted molecular graphs in QSPR analysis [32]:

Question ([32]) Might enhanced correlations be achieved through QSPR analysis tailored to the atomic properties and inter-bond dynamics within these pharmaceutical compounds?

Sorgun and Birgin [32] examined 48 drugs employed in cancer treatment, where degree-based topological indices were computed by incorporating the physical properties of the constituent atoms (Table 1) through two distinct weighting schemes given in Eq. (5) and Eq. (4).

Table 1: Selected atomic properties of common elements relevant to QSPR analysis.

Property	**C**	**N**	**O**	**F**	**S**	**Cl**	**Pt**	**Br**	**P**	**I**
Atomic Number	6	7	8	9	16	17	78	35	15	53
Atomic Mass	12.011	14.007	15.999	18.998	32.066	35.453	195.079	79.904	30.974	126.90
Atomic Radius (pm)	70	65	60	50	100	100	135	115	100	140
Electronegativity	2.55	3.12	3.62	4.23	2.49	2.82	2.28	2.56	2.22	2.66
Van der Waals Radius (pm)	170	155	152	135	180	175	209	183	180	198

Furthermore, an extensive QSPR analysis was carried out by examining the correlations between the physical properties of these structures and their corresponding topological indices. In a similar vein, Sorgun and Ullah ([33]) performed QSPR analyses on selected drugs and compared their findings with those reported in the literature for unweighted molecular graphs.

In QSPR studies, the completeness and quality of the underlying data play a crucial role in the reliability of the analysis. When datasets are incomplete or contain excessive, noisy entries, the predictive power of topological indices can be significantly compromised. Missing data may lead to biased correlations, underestimation of molecular effects, or inability to compute certain indices, while overly large or redundant datasets can introduce noise that masks meaningful relationships. Therefore, careful preprocessing, including normalization, imputation, and selection of relevant features, is essential to ensure that the QSPR models remain robust and interpretable.

Unlike the studies in [[33]] and [[32]], in this work we calculated numerous degree- and degree–distance-based topological indices for 1895 drugs belonging to the antibiotic class by weighting according to the properties of the atoms they contain, and the correlations between these indices and the physicochemical properties of this drug class are presented.

2 Data Collection and Preprocessing

We curated 1895 SMILES representations of antibiotics from the open-access PubChem database. (The list of antibiotic classes employed in this study is publicly available at https://github.com/ssorgun/Antibiotic-datas-and-QSPR-analysis). To perform subsequent calculations, we utilized `Python`. A portion of the code used in our implementation is given below.

Imported Packages

```
import numpy as np
import networkx as nx
import pandas as pd
from rdkit import Chem
```

The code snippet below defines the fundamental atomic properties (mass, radius, van der Waals radius, electronegativity, atomic number, and ionization energy). These properties were obtained from data sources such as PubChem and SpyderChem, and are also tabulated in [32].

Atomic Properties

```
# Atomic properties table
atomicProperties = {
 "C": {"AtomicMass":12.011, "AtomicRadius": 70,
  "VanDerWaals": 170,"Electronegativity": 2.55,
  "AtomicNumber": 6, "Ionization":11.260},
 "N": {"AtomicMass": 14.007, "AtomicRadius": 65,
  "VanDerWaals": 155, "Electronegativity": 3.12,
  "AtomicNumber": 7, "Ionization":14.534},
 "O": {"AtomicMass": 15.999, "AtomicRadius": 60,
  "VanDerWaals": 152, "Electronegativity": 3.62,
  "AtomicNumber": 8, "Ionization":13.618},
 "F": {"AtomicMass": 18.998, "AtomicRadius": 50,
  "VanDerWaals": 135, "Electronegativity": 4.23,
  "AtomicNumber": 9, "Ionization":17.423},
 "S": {"AtomicMass": 32.066, "AtomicRadius": 100,
  "VanDerWaals": 180, "Electronegativity": 2.49,
  "AtomicNumber": 16, "Ionization":10.36},
 "Cl": {"AtomicMass": 35.453, "AtomicRadius": 100,
  "VanDerWaals": 175,"Electronegativity": 2.82,
  "AtomicNumber": 17, "Ionization":12.968},
 "Br": {"AtomicMass": 79.904, "AtomicRadius": 115,
  "VanDerWaals": 183,"Electronegativity": 2.56,
  "AtomicNumber": 35,"Ionization":11.814},
 "I": {"AtomicMass": 126.90, "AtomicRadius": 140,
   "VanDerWaals": 198,"Electronegativity": 2.66,
   "AtomicNumber": 53,"Ionization":10.451}
}
```

The vertex weights defined in Equation (3) are implemented as a function. Here, the vertex weight of an atom is calculated with respect to its atomic mass. Alternatively, other atomic properties can be substituted in place of the atomic mass.

Vertex Weight Function (based on Atomic Mass)

```
atomic_VanDerWaals = atomicProperties[atom]["VanDerWaals"]
return 1 - (atomicProperties["C"]["VanDerWaals"] / atomic_VanDerWaals)
```

Next, the SMILES strings of the antibiotics were integrated into the model. As an illustration, click here for the antibiotic IV-3, which is used in cardiovascular treatment.

List of SMILES Strings Representing Chemical Graphs

```
smiles_list = [
"CCC1=C(CN(C1=O)C(=O)NCCc2ccc(cc2)S(=O)(=O)NC(=O)N[C@H]3CC[C@@H](CC3)C)C"]
```

The edge weights are computed as a function of atomic properties and bond order. The following function defines the edge weighting scheme, followed by the initialization of a list to store weighted graphs.

Function for Edge Weights and Graph Initialization

```
def calculate_edge_weight(bond):
atom1, atom2, bond_type = bond.GetBeginAtom().GetSymbol(), \
bond.GetEndAtom().GetSymbol(), \
bond.GetBondTypeAsDouble()
atomic_VanDerWaals1 = atomicProperties[atom1]["VanDerWaals"]
atomic_VanDerWaals2 = atomicProperties[atom2]["VanDerWaals"]
bond_order = int(bond_type)
return (atomicProperties["C"]["VanDerWaals"]**2) / \
(bond_order * atomic_VanDerWaals1 * atomic_VanDerWaals2)

weighted_graphs = []
```

The following loop converts SMILES strings into weighted molecular graphs, where each atom corresponds to a vertex with its weight, and each bond corresponds to an edge with the calculated weight.

Loop for Graph Construction from SMILES

```
for smiles in smiles_list:
molecule = Chem.MolFromSmiles(smiles)
graph = nx.Graph()
for atom in molecule.GetAtoms():
graph.add_node(atom.GetIdx(),
weight=calculate_vertex_weight(atom.GetSymbol()))

for bond in molecule.GetBonds():
edge_weight = calculate_edge_weight(bond)
graph.add_edge(bond.GetBeginAtomIdx(),
bond.GetEndAtomIdx(), weight=edge_weight)

weighted_graphs.append(graph)
```

For the computation of degree-based topological indices, we define the adjacency matrix of the molecular graph, its square, and the trace of the matrix. These serve as the basis for determining the atomic degrees.

Adjacency Matrix and Degree Calculation

```
def graph_to_adjacency_matrix(graph):
num_nodes = len(graph.nodes)
adjacency_matrix = np.zeros((num_nodes, num_nodes))
for u, v, data in graph.edges(data=True):
adjacency_matrix[u][v] = data['weight']
adjacency_matrix[v][u] = data['weight']  # undirected

# Assign vertex weights to diagonal entries
for node in graph.nodes(data=True):
node_index = node[0]
vertex_weight = node[1]['weight']
adjacency_matrix[node_index][node_index] = vertex_weight

return adjacency_matrix

# Square of the adjacency matrix
def compute_adjacency_square(adjacency_matrix):
return np.dot(adjacency_matrix, adjacency_matrix)

# Extract diagonal entries
def extract_diagonal_entries(matrix):
return np.diag(matrix)

# Atom degrees from adjacency square
def calculate_atom_degrees(adjacency_square):
return np.diag(adjacency_square)
```

With these definitions, we are now ready to compute degree-based topological indices of the molecular graphs. For the complete implementation of the remaining code, please follow the supplementary material.

3 Results and Discussion

3.1 Outputs

In this paper, molecules were weighted according to the Van der Waals radius values of atoms for our outputs. The outputs were obtained based on this scheme. For results under other schemes, the code available on https://github.com/ssorgun/Antibiotic-datas-and-QSPR-analysis/tree/main can be executed to view the results.

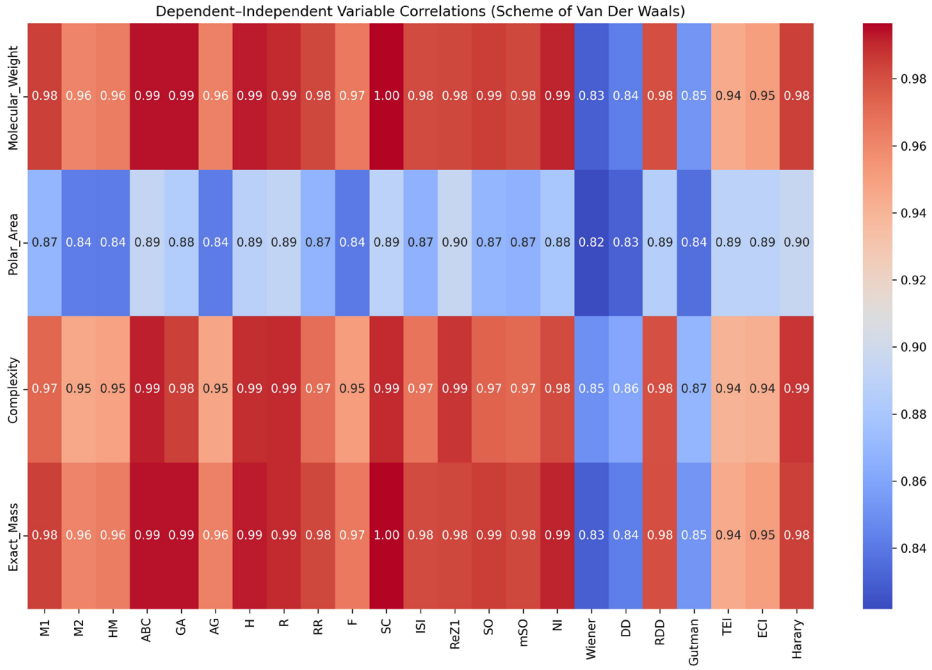

Figure 1: Correlation Heat Map of Topological Indices with Physicochemical Properties (Atomic Mass Scheme)

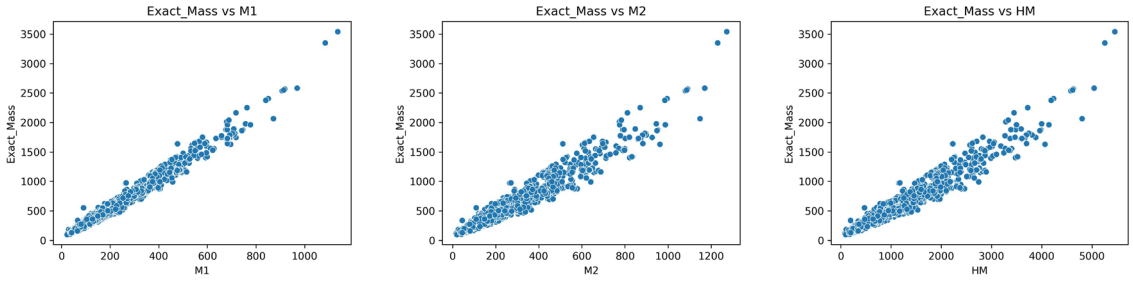

Figure 2: Linear Relationship Between ExactMass and M1,M2,HM indices, respectively.

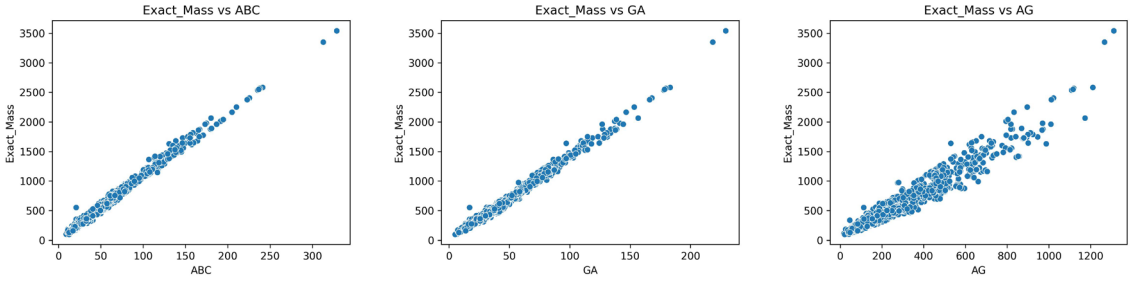

Figure 3: Linear Relationship Between ExactMass and ABC, GA, AG indices, respectively.

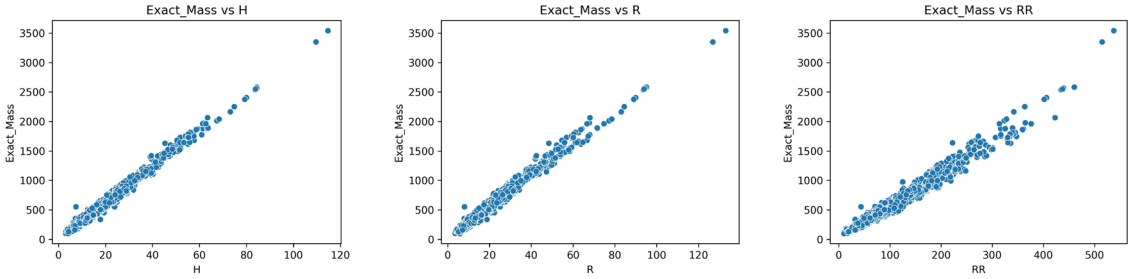

Figure 4: Linear Relationship Between ExactMass and H, R, RR indices, respectively.

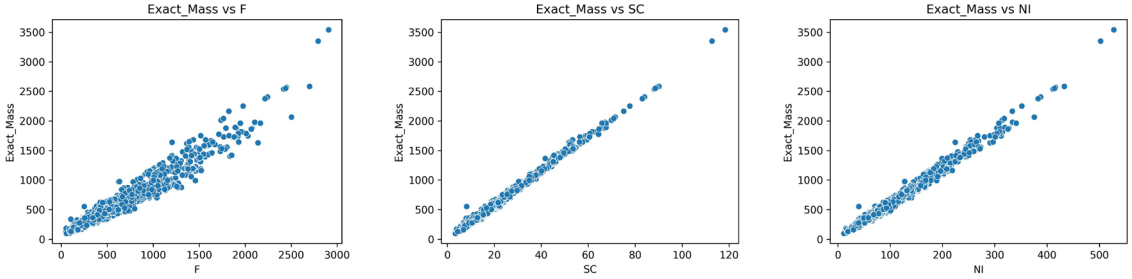

Figure 5: Linear Relationship Between ExactMass and F, SC, NI indices, respectively.

Figure 6: Linear Relationship Between ExactMass and ISI, ReZ1, SO indices, respectively.

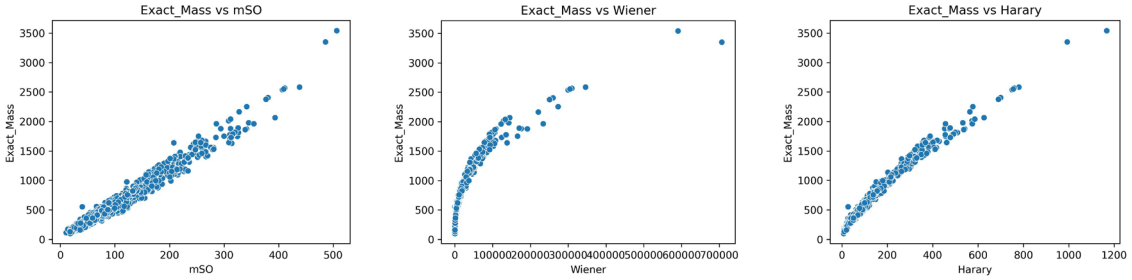

Figure 7: Linear Relationship Between ExactMass and mSO, Wiener, Harary indices, respectively.

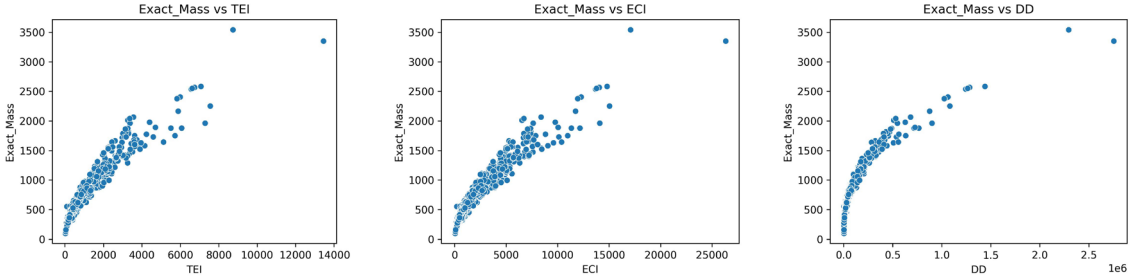

Figure 8: Linear Relationship Between ExactMass and TEI, ECI, DD indices, respectively.

Figure 9: Linear Relationship Between ExactMass and Gutman, RDD indices, respectively.

3.2 Interpretation of the Graphics

This section presents scatter plots with linear regression lines that analyze the relationship between various degree- and distance-based topological indices and the *Exact Mass* of molecular structures. Each figure (Fig 2)-9 is discussed in terms of correlation strength, data distribution, and predictive suitability.

- **M1 (First Zagreb):** Clear linear pattern, strongly correlated with mass.
- **M2 (Second Zagreb):** Positive correlation, though slightly more scatter at higher values.
- **HM (Harmonic Index):** Also exhibits an almost perfect fit, confirming its strong predictive ability.
- **ABC (Atom Bond Connectivity):** Shows a nearly perfect linear relationship. Data points cluster tightly along the regression line, making ABC a very strong predictor of mass.
- **AG (Arithmetic-Geometric):** Also demonstrates a strong positive correlation. Some scatter is visible for medium AG values, but the overall fit remains excellent.
- **GA (Geometric-Arithmetic):** Displays a strong positive linear trend, comparable to ABC, with points aligning closely with the regression line.
- **H (Hyper Zagreb):** Shows a positive correlation, though with more scatter compared to F and HM, indicating moderate reliability.
- **R (Randić):** Positive correlation, but with noticeable variance, making it weaker than RR.
- **RR (Reciprocal Randić):** Strong correlation, with points following an upward linear trend.
- **F (Forgotten Index):** Perfect linear alignment with mass, making it one of the top-performing indices.
- **SC (Sum-Connectivity):** Positive trend but with greater scatter, suggesting moderate predictive utility.
- **NI (Nirmala Index):** Nearly perfect linear relationship, with points forming a clean line. Excellent predictor.

- **ISI (Inverse Sum Indeg):** Strong linear correlation, with tightly clustered points.
- **ReZ1 (Redefined Zagreb First):** Tightly clustered points with a strong linear relationship, confirming its predictive strength.
- **SO (Sombor):** Exhibits an exceptionally strong correlation. Data align almost perfectly with the regression line, making SO one of the best predictors in the study.
- **mSO (Modified Sombor):** Strong correlation, with well-clustered data points confirming reliability.
- **Wiener Index:** Strong correlation, with data clustered along the regression line. Its classic use as a molecular descriptor is validated here as a robust predictor of mass.
- **Harary Index:** Shows a positive correlation with some scatter, making it a reasonably good, but weaker, predictor compared to DD or Gutman.
- **TEI (Total Eccentricity Index):** Exhibits a strong positive linear relationship, with data closely following the regression line. Reliable and effective predictor.
- **ECI (Eccentric Connectivity):** Strong positive correlation, tightly clustered points, and a well-fitting regression line confirm its predictive value.
- **DD (Degree Distance):** Shows a perfect linear correlation, with very large values scaling directly with mass. One of the strongest predictors overall.
- **Gutman Index:** Displays a mathematically near-perfect linear relationship, similar to DD. Large index values scale directly with mass, confirming excellent predictive capacity.
- **RDD (Reciprocal Degree Distance):** Very strong correlation, with tightly aligned data points and excellent predictive accuracy.

3.3 Comparative Insights and Conclusion

Both degree-based and distance-based topological indices demonstrate a strong ability to predict the *Exact Mass* of molecular structures. Among them, the Arithmetic–Geometric index (AG), the Forgotten index (F), the Harmonic index (HM), the Nirmala index (NI), and the Sombor index (SO) from the degree-based family, together with the Degree Distance (DD) and Gutman indices from the distance-based family, stand out as exceptional predictors. These indices exhibit almost perfect linear correlations, with data points aligning very closely to the regression lines.

Several other indices, including the Atom Bond Connectivity (ABC), Geometric–Arithmetic (GA), First Zagreb (M1), Second Zagreb (M2), Redefined Zagreb (ReZ1), Modified Sombor (mSO), Eccentric Connectivity (ECI), Reciprocal Degree Distance (RDD), Total Eccentricity (TEI), and the Wiener index, also show strong predictive capacity. While the correlations are slightly weaker than those of the top performers, these indices still maintain minimal scatter around the regression lines and provide highly reliable results.

In contrast, some indices, such as the Randić index (R), the Sum-Connectivity index (SC), the Hyper Zagreb index (H), and the Harary index, present more variance in their data distributions. Although they maintain positive correlations with molecular mass, their predictive power is noticeably lower compared to the stronger indices.

Overall, degree-based indices offer the advantage of computational efficiency while still achieving excellent predictive performance, with SO, F, and NI emerging as particularly effective. Distance-based indices, though more computationally demanding, include outstanding predictors such as DD and Gutman, which display nearly perfect linear scaling with molecular mass. These findings suggest that combining selected degree-based and distance-based indices in a hybrid framework could provide the most accurate and robust models for quantitative structure–property relationship (QSPR) studies.

4 Discussion

The correlation heatmap in Figure 1 (Scheme of Van der Waals) provides a comprehensive overview of the relationships between dependent molecular descriptors (Molecular Weight, Polar Area, Complexity, and Exact Mass) and a wide range of independent topological indices. Several important trends can be observed.

First, **Molecular Weight** and **Exact Mass** show nearly identical correlation patterns, with correlation coefficients consistently exceeding 0.95 across most indices. This strong similarity arises because both descriptors are linearly dependent on atomic composition, differing only in the use of isotopic weights. Therefore, their strong alignment with indices such as ABC, GA, R, and Harary suggests that these topological indices capture size-related molecular features effectively.

Similarly, **Complexity** demonstrates a very high correlation ($r > 0.95$) with most indices, especially ABC, GA, R, and Harary. This indicates that graph-based indices reflecting connectivity and branching patterns strongly align with molecular complexity. Interestingly, the highest correlations are observed with indices that account for neighborhood connectivity (e.g., ReZ1, mSO, Harary), suggesting that complexity is best described not only by molecular size but also by the intricacies of atom-to-atom relationships.

In contrast, **Polar Area** behaves differently. Its correlation values are comparatively lower, ranging between 0.82 and 0.90, with certain indices (e.g., Wiener, Gutman) showing weaker associations. This suggests that topological indices are less effective in capturing polarity-related features, which are influenced by functional groups and heteroatom distributions rather than purely by molecular topology. Nonetheless, indices such as ABC, GA, and Harary still maintain relatively strong correlations, reflecting that while topology cannot fully describe polar area, it provides partial predictive power through its indirect link to molecular size and branching.

Another important observation is the role of the **Wiener and Gutman indices**, which consistently display the weakest correlations (≈ 0.82–0.87). These indices emphasize distance-based structural features, which may not scale directly with mass or complexity. Their weaker performance suggests that while useful in certain contexts, they may be less suitable for predicting properties directly tied to Van Der Waals schemes.

Overall, the results show that most topological indices are very strong predictors of molecular weight, exact mass, and structural complexity, with correlations close to one. In contrast, the polar surface area is less well predicted, since purely graph-based descriptors cannot fully capture the effects of electronic structure or functional groups. This suggests that for polarity-sensitive properties, topological indices should be combined with physicochemical descriptors.

In short, the heatmap highlights two clear patterns:

- Some physicochemical properties (Molecular Weight, Exact Mass, Complexity) accurately predicted by a wide range of topological indices.

- Polar Surface Area) only moderately predicted, requiring extra non-topological information.

These findings confirm that topological indices are highly valuable in QSAR/QSPR research, especially for properties linked to molecular size and complexity, while also reminding us of their limits when it comes to polarity.

Declaration

In this study, all calculations were carried out using the Van der Waals scheme, where atomic properties were encoded according to Van der Waals radius. The complete computational workflow, including scripts for calculating both degree-based and distance-based topological indices and performing regression analysis, is provided in the accompanying GitHub repository. (https://github.com/ssorgun/Antibiotic-datas-and-QSPR-analysis). It is important to note that the same methodology can be extended beyond the Van der Waals framework. By substituting the underlying atomic parameters (e.g., atomic radius, atomic mass, covalent radius), the same set of topological indices and regression analyses can be recomputed. This flexibility enables researchers to investigate how different atomic schemes influence the predictive performance of topological indices, thereby broadening the scope of QSPR/QSAR applications.

The GitHub repository currently provides data and results specifically for the Van der Waals scheme, while also serving as a template for applying the same calculations under alternative atomic descriptors.

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Author Biography

Sezer Sorgun received his B.Sc. (2002) and Ph.D. (2011) degrees in Mathematics from Erciyes University and his M.Sc. degree from Gazi University (2007). He previously served as a research assistant at Gazi University and as a mathematician at the Turkish Statistical Institute. In 2012, he joined Nevşehir Hacı Bektaş Veli University, where he is currently a Full Professor. He conducted postdoctoral research at Sungkyunkwan University (South Korea, 2012–2013) and at the University of Delaware (USA, 2018–2019) as a visiting faculty member. His research interests include spectral graph theory, matrix theory, chemical graph theory, and applications of graph neural networks and machine learning.

Degree Based Indices of Möbius Function Graph of Finite Groups

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Abstract

The Möbius function graph of finite groups possess several algebraic and topological properties. The concept of topological indices play a crucial role for quantifying molecular structure properties. Here we focus on topological indices of Möbius function graph of finite groups. In this paper, we mainly explores the relationships between the degree-based topological indices specifically Randić Index, Atom Bond Connectivity Index, Geometric-Arithmetic Index, and Sum Connectivity index for Möbius function graphs of finite groups.

Keywords: Randić index, ABC index, Geometric-arithmetic index, Sum connectivity index, Möbius function graphs
AMS Classification: 92E10, 05C92

1 Introduction

Algebraic graph theory has gained significant attention in modern mathematical research due to its diverse applications in areas such as molecular structure chemistry, complex network optimization, social network analysis, data mining, coding theory, and quantum computing. The concept of Cayley graphs linked algebraic structures with graph theory, leading to the development of many new types of graphs [1, 2, 10, 12]. Based on this, we introduced Möbius function graphs of finite groups, denoted by $M(G)$ [4] and explored their properties in [5, 6, 7, 8, 9].
Topological indices are important tools in mathematical chemistry and graph theory. They help us to study the properties of chemical compounds by representing them

as graphs. Degree-based indices are especially useful, to focus on the connections between atoms in a molecule. Let Γ be a connected graph then, some of the degree based indices [3, 11, 13, 14] that are under considerations are:

a) Randić Index: Measures molecular branching, calculated as the sum of the reciprocal square roots of the product of degrees of adjacent vertices.

$$R(\Gamma) = \sum_{xy \in E(\Gamma)} \frac{1}{\sqrt{deg(x)deg(y)}}$$

b) Atom Bond Connectivity (ABC) Index: Quantifies molecular stability, calculated as

$$ABC(\Gamma) = \sum_{xy \in E(\Gamma)} \sqrt{\frac{deg(x) + deg(y) - 2}{deg(x)deg(y)}}$$

c) Geometric-Arithmetic (GA) Index: Compares geometric and arithmetic means of vertex degrees, calculated as

$$GA(\Gamma) = \sum_{xy \in E(\Gamma)} \frac{2\sqrt{deg(x) \cdot deg(y)}}{deg(x) + deg(y)}$$

d) Sum Connectivity Index: Measures the sum of the reciprocal square roots of the sum of degrees of adjacent vertices

$$\chi(\Gamma) = \sum_{xy \in E(\Gamma)} \frac{1}{\sqrt{deg(x) + deg(y)}}$$

In this paper we compute some degree-based topological indices of Möbius function graphs.
Note: In this paper, we use "e" to represent the identity element of a group.

2 Some Degree Based Indices of $M(G)$

In this section we first collect some definition and results of the Möbius function graphs. Then we calculate Randić index, Atom Bond Connectivity index, Geometric-Arithmetic index and Sum Connectivity index of $M(G)$.

Definition 2.1. [4] The Mobius function graph of a finite group G (denoted by $M(G)$) is a simple graph whose vertex set is same as the elements of G and any two distinct vertices x, y are adjacent in $M(G)$ if and only if $\mu(|a|\ |b|) = \mu(|a|)\mu\ (|b|)$.

Theorem 2.2. [4]For any group G of prime order p, $M(G) \cong K_{1,p-1}$

Theorem 2.3. [4] For a cyclic group G of order 2^k , $k \in Z^+$, $M(G)$ is isomorphic to a complete graph of order 2^k.

Also, let $\Gamma_1 = (V_1(\Gamma_1), E_1(\Gamma_1))$ and $\Gamma_2 = (V_2(\Gamma_2), E_2(\Gamma_2))$ be two simple graphs which are vertex- disjoint. The join $\Gamma_1 + \Gamma_2$ of Γ_1 and Γ_2 is defined as the graph where every vertex of Γ_1 is adjacent to every vertex of Γ_2.

Theorem 2.4. [4] For a finite group G of order $|G| = p^k$, where p is an odd prime and $k > 1$, the Möbius function graph $M(G)$ is a split graph.

Theorem 2.5. [4] Let $G = \mathbb{Z}_p \times \mathbb{Z}_q$, where p and q are distinct primes. Then $M(G) \cong (\overline{K_n} + \overline{K_m}) + K_1 + \overline{K_t}$, where $n,\ m,\ t$ denote the number of elements of order $p,\ q,\ pq$ respectively.

Theorem 2.6. [6] For a prime $p > 2$, $M(D_{2p}) \cong (\overline{K_{p-1}} + \overline{K_p}) + K_1$.

In the following theorems, we will determine the indices of certain p-groups.

Theorem 2.7. For a group G of prime order p then, $M(G)$ has the following indices:

a) Randić index : $R(M(G)) = \sqrt{(p-1)}$

b) Atom Bond Connectivity index : $ABC(M(G)) = \sqrt{(p-1)(p-2)}$

c) Geometric Arithmetic index : $GA(M(G)) = \dfrac{2(p-1)\sqrt{p-1}}{p}$

d) Sum Connectivity index : $\chi(M(G)) = \dfrac{p-1}{\sqrt{p}}$

Proof. Let G be any group with $|G| = p$, where p is prime. Using Theorem 2.2, $M(G)$ is isomorphic to the star graph $K_{1,p-1}$.

a) The Randić index can be calculated as

$$\begin{aligned} R(M(G)) &= \sum_{ex \in E(M(G))} \frac{1}{\sqrt{deg(e)deg(x)}} \\ &= \sum_{xy \in E(M(G))} \frac{1}{\sqrt{(p-1)\cdot 1}} \\ &= (p-1)\cdot \frac{1}{\sqrt{(p-1)\cdot 1}} \\ &= \sqrt{(p-1)} \end{aligned}$$

b) The Atom Bond Connectivity index can be calculated as

$$\begin{aligned} ABC(M(G)) &= \sum_{ex \in E(M(G))} \sqrt{\frac{deg(e) + deg(x) - 2}{deg(e)deg(x)}} \\ &= \sum_{ex \in E(M(G))} \sqrt{\frac{(p-1) + 1 - 2}{(p-1) \cdot 1}} \\ &= (p-1)\sqrt{\frac{(p-2)}{(p-1)}} \\ &= \sqrt{(p-1)(p-2)} \end{aligned}$$

c) The Geometric Arithmetic index can be calculated as

$$\begin{aligned} GA(M(G)) &= \sum_{ex \in E(M(G))} \frac{2\sqrt{deg(e) \cdot deg(x)}}{deg(e) + deg(x)} \\ &= \sum_{ex \in E(M(G))} \frac{2\sqrt{(p-1) \cdot 1}}{(p-1) + 1} \\ &= (p-1) \cdot \frac{2\sqrt{(p-1)}}{p} \end{aligned}$$

d) The Sum Connectivity index can be calculated as

$$\begin{aligned} \chi(M(G)) &= \sum_{ex \in E(M(G))} \frac{1}{\sqrt{deg(e) + deg(x)}} \\ &= \sum_{xy \in E(M(G))} \frac{1}{\sqrt{(p-1) + 1}} \\ &= (p-1) \cdot \frac{1}{\sqrt{p}} \end{aligned}$$

□

Theorem 2.8. For a finite cyclic group G of order 2^k, $k \in \mathbb{Z}^+$ then, $M(G)$ has the following indices:

a) Randić index : $R(M(G)) = 2^{k-1}$

b) Atom Bond Connectivity index : $ABC(M(G)) = 2^k\sqrt{(2^{k-1}-1)(2^k-1)}$

c) Geometric Arithmetic index : $GA(M(G)) = \binom{2^k}{2}$

d) Sum Connectivity index : $\chi(M(G)) = \dfrac{2^{k-1}(2^k-1)}{\sqrt{2}\cdot\sqrt{2^k-1}}$

Proof. Given that G be a finite cyclic group of order 2^k, $k \in \mathbb{Z}^+$. From Theorem 2.3, we get $M(G) \cong K_{2^k}$

a) The Randić index can be calculated as

$$\begin{aligned} R(M(G)) &= \sum_{xy\in E(M(G))} \frac{1}{\sqrt{deg(x)deg(y)}} \\ &= \sum_{xy\in E(M(G))} \frac{1}{\sqrt{(2^k-1)\cdot(2^k-1)}} \\ &= \binom{2^k}{2}\frac{1}{2^k-1} \\ &= 2^{k-1} \end{aligned} \tag{3.1}$$

b) The Atom Bond Connectivity index can be calculated as

$$\begin{aligned} ABC(M(G)) &= \sum_{xy\in E(M(G))} \sqrt{\frac{deg(x)+deg(y)-2}{deg(x)deg(y)}} \\ &= \sum_{xy\in E(M(G))} \sqrt{\frac{(2^k-1)+(2^k-1)-2}{(2^k-1)(2^k-1)}} \\ &= \binom{2^k}{2} 2\sqrt{\frac{2^{k-1}-1}{2^k-1}} \\ &= 2^k\sqrt{(2^{k-1}-1)(2^k-1)} \end{aligned}$$

c) The Geometric Arithmetic index can be calculated as

$$\begin{aligned} GA(M(G)) &= \sum_{xy\in E(M(G))} \frac{2\sqrt{deg(x)\cdot deg(y)}}{deg(x)+deg(y)} \\ &= \sum_{xy\in E(M(G))} \frac{2\sqrt{(2^k-1)(2^k-1)}}{(2^k-1)+(2^k-1)} \\ &= \binom{2^k}{2} \end{aligned}$$

d) The Sum Connectivity index can be calculated as

$$\begin{aligned}\chi(M(G)) &= \sum_{xy\in E(M(G))} \frac{1}{\sqrt{deg(x)+deg(y)}} \\ &= \sum_{xy\in E(M(G))} \frac{1}{\sqrt{(2^k-1)+(2^k-1)}} \\ &= \binom{2^k}{2} \frac{1}{\sqrt{2(2^k-1)}} \\ &= \frac{2^{k-1}(2^k-1)}{\sqrt{2}\cdot\sqrt{2^k-1}}\end{aligned}$$

□

Theorem 2.9. For a group G of order p^k, where p is an odd prime number with $k > 1$ then, $M(G)$ has the following indices:

a) Randić index : $R(M(G)) = \dfrac{rs}{\sqrt{s(r+s-1)}} + \dfrac{s(s-1)}{2(r+s-1)}$

b) Atom Bond Connectivity index :

$$ABC(M(G)) = rs\sqrt{\frac{2s+r-3}{m(r+s-1)}} + \frac{s(s-1)}{2(r+s-1)}\sqrt{2(r+s-2)}$$

c) Geometric Arithmetic index : $GA(M(G)) = \dfrac{2rs\sqrt{s(r+s-1)}}{2s+r-1} + \dfrac{s(s-1)}{2}$

d) Sum Connectivity index : $\chi(M(G)) = \dfrac{rs}{\sqrt{2s+r-1}} + \dfrac{s(s-1)}{2\sqrt{2(r+s-1)}}$

Where r being the number of elements in G of order p and $s = p^k - r$.

Proof. Given G be a group of order p^k with p an odd prime and $k > 1$. By Theorem 2.4, $M(G)$ is a split graph. We can partition the vertex set of $M(G)$ into two subsets:

$$\Theta_1 = \{u : |u| = p\} \quad and \quad \Theta_2 = \{v : |v| \neq p\}$$

with cardinalities $|\Theta_1| = r$ and $|\Theta_2| = s$.

a) The Randić index can be calculated as

$$R(M(G)) = \sum_{xy\in E(M(G))} \frac{1}{\sqrt{deg(x)deg(y)}}$$

$$= \sum_{\substack{x\in\Theta_1\\ y\in\Theta_2}} \frac{1}{\sqrt{deg(x)deg(y)}} + \sum_{x,y\in\Theta_2} \frac{1}{\sqrt{deg(x)deg(y)}}$$

$$= \sum_{\substack{x\in\Theta_1\\ y\in\Theta_2}} \frac{1}{\sqrt{s\cdot(r+s-1)}} + \sum_{x,y\in\Theta_2} \frac{1}{\sqrt{(r+s-1)\cdot(r+s-1)}}$$

$$= \frac{rs}{\sqrt{s\cdot(r+s-1)}} + \binom{s}{2}\frac{1}{(m+n-1)}$$

$$= \frac{rs}{\sqrt{s(r+s-1)}} + \frac{s(s-1)}{2(r+s-1)}$$

b) The Atom Bond Connectivity index can be calculated as

$$ABC(M(G)) = \sum_{xy\in E(M(G))} \sqrt{\frac{deg(x)+deg(y)-2}{deg(x)deg(y)}}$$

$$= \sum_{\substack{x\in\Theta_1\\ y\in\Theta_2}} \sqrt{\frac{deg(x)+deg(y)-2}{deg(x)deg(y)}} + \sum_{x,y\in\Theta_2} \sqrt{\frac{deg(x)+deg(y)-2}{deg(x)deg(y)}}$$

$$= \sum_{\substack{x\in\Theta_1\\ y\in\Theta_2}} \sqrt{\frac{s+(r+s-1)-2}{s\cdot(r+s-1)}} + \sum_{x,y\in\Theta_2} \sqrt{\frac{(r+s-1)+(r+s-1)-2}{(r+s-1)\cdot(r+s-1)}}$$

$$= rs\sqrt{\frac{2s+r-3}{s\cdot(r+s-1)}} + \binom{s}{2}\frac{\sqrt{2(r+s-2)}}{(r+s-1)}$$

$$= rs\sqrt{\frac{2s+r-3}{s(r+s-1)}} + \frac{s(s-1)}{2(r+s-1)}\sqrt{2(r+s-2)}$$

c) The Geometric Arithmetic index can be calculated as

$$GA(M(G)) = \sum_{xy\in E(M(G))} \frac{2\sqrt{deg(x)\cdot deg(y)}}{deg(x)+deg(y)}$$

$$= \sum_{\substack{x\in\Theta_1\\ y\in\Theta_2}} \frac{2\sqrt{s\cdot(r+s-1)}}{s+(r+s-1)} + \sum_{x,y\in\Theta_2} \frac{2\sqrt{(r+s-1)\cdot(r+s-1)}}{(r+s-1)+(r+s-1)}$$

$$= rs\frac{2\sqrt{s\cdot(r+s-1)}}{(2s+r-1)} + \binom{s}{2}\cdot 1$$

$$= \frac{2rs\sqrt{s(r+s-1)}}{2s+r-1} + \frac{s(s-1)}{2}$$

d) The Sum Connectivity index can be calculated as

$$\begin{aligned}
\chi(M(G)) &= \sum_{xy\in E(M(G))} \frac{1}{\sqrt{deg(x)+deg(y)}} \\
&= \sum_{\substack{x\in\Theta_1 \\ y\in\Theta_2}} \frac{1}{\sqrt{deg(x)+deg(y)}} + \sum_{x,y\in\Theta_2} \frac{1}{\sqrt{deg(x)+deg(y)}} \\
&= \sum_{\substack{x\in\Theta_1 \\ y\in\Theta_2}} \frac{1}{\sqrt{s+(r+s-1)}} + \sum_{x,y\in\Theta_2} \frac{1}{\sqrt{(r+s-1)+(r+s-1)}} \\
&= \frac{rs}{\sqrt{2s+r-1}} + \binom{s}{2}\frac{1}{\sqrt{2(r+s-1)}} \\
&= \frac{rs}{\sqrt{2s+r-1}} + \frac{s(s-1)}{2\sqrt{2(r+s-1)}}
\end{aligned}$$

□

In the next theorem, we will determine the indices of the product group $\mathbb{Z}_p \times \mathbb{Z}_q$, where p and q are distinct primes.

Theorem 2.10. For a group $G \cong \mathbb{Z}_p \times \mathbb{Z}_q$, where p and q are distint primes. Then, $M(G)$ has the following indices:

a) Randić index :

$$R(M(G)) = \frac{r}{\sqrt{(r+s+t)(s+1)}} + \frac{s}{\sqrt{(r+s+t)(r+1)}} + \frac{t}{\sqrt{(r+s+t)\cdot 1}} + \frac{rs}{\sqrt{(s+1)(r+1)}}$$

b) Atom Bond Connectivity index :

$$ABC(M(G)) = r\sqrt{\frac{r+2s+t-1}{(r+s+t)(s+1)}} + s\sqrt{\frac{2r+s+t-1}{(r+s+t)(r+1)}} + t\sqrt{1-\frac{1}{r+s+t}} + rs\sqrt{\frac{r+s}{(r+1)(s+1)}}$$

c) Geometric Arithmetic index :

$$GA(M(G)) = r \cdot \frac{2\sqrt{(r+s+t)(s+1)}}{r+2s+t+1} + s \cdot \frac{2\sqrt{(r+s+t)(r+1)}}{2r+s+t+1} + t \cdot \frac{2\sqrt{r+s+t}}{r+s+t+1} + rs \cdot \frac{2\sqrt{(r+1)(s+1)}}{r+s+2}$$

d) Sum Connectivity index :

$$\chi(M(G)) = \frac{r}{\sqrt{r+2s+t+1}} + \frac{s}{\sqrt{2r+s+t+1}} + \frac{t}{\sqrt{r+s+t+1}} + \frac{rs}{\sqrt{r+s+2}}$$

Where r, s and t denote the number of elements of G with order p, q and pq respectively.

Proof. Let us consider a group $G \cong \mathbb{Z}_p \times \mathbb{Z}_q$ with $|G| = pq$, then by Theorem 2.5, we can partition the vertex set of Möbius function graph as

$$\Theta_1 = \{e\}$$
$$\Theta_2 = \{u : |u| = p\}$$
$$\Theta_3 = \{v : |v| = q\}$$
$$\Theta_4 = \{w : |w| = pq\}$$

with cardinality $1, r, s, t$ respectively. Also $\Theta_2, \Theta_3, \Theta_4$ are isomorphic to $\overline{K_r}, \overline{K_s}, \overline{K_t}$ respectively. Here each element of $\Theta_1, \Theta_2, \Theta_3$ and Θ_4 has degree $(r+s+t)$, $(s+1)$, $(r+1)$ and 1 respectively.

a) The Randić index can be calculated as

$$\begin{aligned} R(M(G)) &= \sum_{xy \in E(M(G))} \frac{1}{\sqrt{deg(x)deg(y)}} \\ &= \sum_{i=2}^{4} \sum_{\substack{ex \in E \\ x \in \Theta_i}} \frac{1}{\sqrt{deg(e)deg(x)}} + \sum_{\substack{xy \in E \\ x \in \Theta_2 \\ y \in \Theta_3}} \frac{1}{\sqrt{deg(x)deg(y)}} \\ &= \sum_{\Theta_2} \frac{1}{\sqrt{(r+s+t)(s+1)}} + \sum_{\Theta_3} \frac{1}{\sqrt{(r+s+t)(r+1)}} \\ &+ \sum_{\Theta_4} \frac{1}{\sqrt{(r+s+t)\cdot 1}} + \sum_{\Theta_2\ \Theta_3} \frac{1}{\sqrt{(r+1)(s+1)}} \\ &= \frac{r}{\sqrt{(r+s+t)(s+1)}} + \frac{s}{\sqrt{(r+s+t)(r+1)}} + \\ &\frac{t}{\sqrt{(r+s+t)\cdot 1}} + \frac{rs}{\sqrt{(r+1)(s+1)}} \end{aligned}$$

b) The Atom Bond Connectivity index can be calculated as

$$\begin{aligned}
ABC(M(G)) &= \sum_{xy\in E(M(G))} \sqrt{\frac{deg(x)+deg(y)-2}{deg(x)deg(y)}} \\
&= \sum_{i=2}^{4} \sum_{\substack{ex\in E \\ x\in\Theta_i}} \sqrt{\frac{deg(e)+deg(x)-2}{deg(e)deg(x)}} + \sum_{\substack{xy\in E \\ x\in\Theta_2 \\ y\in\Theta_3}} \sqrt{\frac{deg(x)+deg(y)-2}{deg(x)deg(y)}} \\
&= \sum_{\Theta_2} \sqrt{\frac{(r+s+t)+(s+1)-2}{(r+s+t)(s+1)}} + \sum_{\Theta_3} \sqrt{\frac{(r+s+t)+(r+1)-2}{(r+s+t)(r+1)}} + \\
&\quad \sum_{\Theta_4} \sqrt{\frac{(r+s+t)+1-2}{(r+s+t)1}} + \sum_{\substack{xy\in E \\ x\in\Theta_2 \\ y\in\Theta_3}} \sqrt{\frac{(r+1)+(s+1)-2}{(r+1)(s+1)}} \\
&= r\sqrt{\frac{(r+s+t)+(s+1)-2}{(r+s+t)(s+1)}} + s\sqrt{\frac{(r+s+t)+(r+1)-2}{(r+s+t)(r+1)}} + \\
&\quad t\sqrt{\frac{(r+s+t)+1-2}{(r+s+t)1}} + rs\sqrt{\frac{(r+1)+(s+1)-2}{(r+1)(s+1)}} \\
&= r\sqrt{\frac{r+2s+t-1}{(r+s+t)(s+1)}} + s\sqrt{\frac{2r+s+t-1}{(r+s+t)(r+1)}} + \\
&\quad t\sqrt{1-\frac{1}{r+s+t}} + rs\sqrt{\frac{r+s}{(r+1)(s+1)}}
\end{aligned}$$

c) The Geometric Arithmetic index can be calculated as

$$\begin{aligned}
GA(M(G)) &= \sum_{xy\in E(M(G))} \frac{2\sqrt{deg(x)\cdot deg(y)}}{deg(x)+deg(y)} \\
&= \sum_{i=2}^{4} \sum_{\substack{ex\in E \\ x\in\Theta_i}} \frac{2\sqrt{deg(e)\cdot deg(x)}}{deg(e)+deg(x)} + \sum_{\substack{xy\in E \\ x\in\Theta_2 \\ y\in\Theta_3}} \frac{2\sqrt{deg(x)\cdot deg(y)}}{deg(x)+deg(y)} \\
&= \sum_{\Theta_2} \frac{2\sqrt{(r+s+t)\cdot(s+1)}}{(r+s+t)+(s+1)} + \sum_{\Theta_3} \frac{2\sqrt{(r+s+t)\cdot(r+1)}}{(r+s+t)+(r+1)} +
\end{aligned}$$

$$\sum_{\Theta_4} \frac{2\sqrt{(r+s+t)\cdot 1}}{(r+s+t)+1} + \sum_{\substack{xy\in E\\ x\in\Theta_2\\ y\in\Theta_3}} \frac{2\sqrt{(r+1)\cdot(s+1)}}{(r+1)+(s+1)}$$

$$= r\frac{2\sqrt{(r+s+t)\cdot(s+1)}}{(r+s+t)+(s+1)} + s\frac{2\sqrt{(r+s+t)\cdot(r+1)}}{(r+s+t)+(r+1)} +$$
$$t\frac{2\sqrt{(r+s+t)\cdot 1}}{(r+s+t)+1} + rs\frac{2\sqrt{(r+1)\cdot(s+1)}}{(r+1)+(s+1)}$$

$$= r\cdot\frac{2\sqrt{(r+s+t)(s+1)}}{r+2s+t+1} + s\cdot\frac{2\sqrt{(r+s+t)(r+1)}}{2r+s+t+1} +$$
$$t\cdot\frac{2\sqrt{r+s+t}}{r+s+t+1} + rs\cdot\frac{2\sqrt{(r+1)(s+1)}}{r+s+2}$$

d) The Sum Connectivity index can be calculated as

$$\chi(M(G)) = \sum_{xy\in E(M(G))} \frac{1}{\sqrt{deg(x)+deg(y)}}$$

$$= \sum_{i=2}^{4} \sum_{\substack{ex\in E\\ x\in\Theta_i}} \frac{1}{\sqrt{deg(x)+deg(y)}} + \sum_{\substack{xy\in E\\ x\in\Theta_2\\ y\in\Theta_3}} \frac{1}{\sqrt{deg(x)+deg(y)}}$$

$$= \sum_{\Theta_2} \frac{1}{\sqrt{(r+s+t)+(s+1)}} + \sum_{\Theta_3} \frac{1}{\sqrt{(r+s+t)+(r+1)}} +$$
$$\sum_{\Theta_4} \frac{1}{\sqrt{(r+s+t)+1}} + \sum_{\Theta_2\ \Theta_3} \frac{1}{\sqrt{(r+1)+(s+1)}}$$

$$= r\frac{1}{\sqrt{(r+s+t)+(s+1)}} + s\frac{1}{\sqrt{(r+s+t)+(r+1)}} +$$
$$t\frac{1}{\sqrt{(r+s+t)+1}} + rs\frac{1}{\sqrt{(r+1)+(s+1)}}$$

$$= \frac{r}{\sqrt{r+2s+t+1}} + \frac{s}{\sqrt{2r+s+t+1}} +$$
$$\frac{t}{\sqrt{r+s+t+1}} + \frac{rs}{\sqrt{r+s+2}}$$

□

In the following theorem, we calculate the indices of the dihedral group D_{2p}, where p is a prime number.

Theorem 2.11. For a dihedral group D_{2p} , p being prime. Then $M(D_{2p})$ has the following indices:

a) Randić index : $R(M(D_{2p})) = \dfrac{p-1}{\sqrt{(2p-1)(p+1)}} + \dfrac{\sqrt{p}}{\sqrt{2p-1}} + \dfrac{(p-1)\sqrt{p}}{\sqrt{p+1}}$

b) Atom Bond Connectivity index :

$$ABC(M(D_{2p})) = (p-1)\sqrt{\frac{3p-2}{(2p-1)(p+1)}} + \sqrt{\frac{3p-3}{2p-1}} + (p-1)\sqrt{\frac{p(2p-1)}{p+1}}$$

c) Geometric Arithmetic index :

$$GA(M(D_{2p})) = \frac{2(p-1)\sqrt{(2p-1)(p+1)}}{3p} + \frac{2p\sqrt{(2p-1)p}}{3p-1} + \frac{2p(p-1)\sqrt{(p+1)p}}{2p+1}$$

d) Sum Connectivity index : $\chi(M(D_{2p})) = \dfrac{p-1}{\sqrt{3p}} + \dfrac{p}{\sqrt{3p-1}} + \dfrac{p(p-1)}{\sqrt{2p+1}}$

Proof. In case of dihedral group D_{2p} , p being prime by Theorem 2.6, $M(D_{2p}) \cong (\overline{K_{p-1}} + \overline{K_p}) + K_1$. we can partition vertex set of $M(D_{2p})$ as $\Theta_1 = \{e\}$, $\Theta_2 = \{x : |x| = p\}$ and $\Theta_3 = \{y : |y| = 2\}$. Here each element of Θ_1, Θ_2 and Θ_3 has degree $(2p-1)$, $(p+1)$ and p respectively.

a) The Randić index can be calculated as

$$\begin{aligned}
R(M(D_{2p})) &= \sum_{xy \in E(M(D_{2p}))} \frac{1}{\sqrt{deg(x)deg(y)}} \\
&= \sum_{\substack{ex \in E \\ x \in \Theta_2}} \frac{1}{\sqrt{deg(e)deg(x)}} + \sum_{\substack{ey \in E \\ y \in \Theta_3}} \frac{1}{\sqrt{deg(e)deg(y)}} + \sum_{\substack{xy \in E \\ x \in \Theta_2 \\ y \in \Theta_3}} \frac{1}{\sqrt{deg(x)deg(y)}} \\
&= \sum_{\substack{ex \in E \\ x \in \Theta_2}} \frac{1}{\sqrt{(2p-1)(p+1)}} + \sum_{\substack{ey \in E \\ y \in \Theta_3}} \frac{1}{\sqrt{(2p-1)p}} + \sum_{\substack{xy \in E \\ x \in \Theta_2 \\ y \in \Theta_3}} \frac{1}{\sqrt{p(p+1)}} \\
&= \frac{p-1}{\sqrt{(2p-1)(p+1)}} + \frac{p}{\sqrt{(2p-1)p}} + \frac{p(p-1)}{\sqrt{p(p+1)}} \\
&= \frac{p-1}{\sqrt{(2p-1)(p+1)}} + \frac{\sqrt{p}}{\sqrt{2p-1}} + \frac{(p-1)\sqrt{p}}{\sqrt{p+1}}
\end{aligned}$$

b) The Atom Bond Connectivity index can be calculated as

$$\begin{aligned}
ABC(M(D_{2p})) &= \sum_{xy\in E(M(D_{2p}))} \sqrt{\frac{deg(x)+deg(y)-2}{deg(x)deg(y)}} \\
&= \sum_{\substack{ex\in E\\ x\in\Theta_2}} \sqrt{\frac{deg(e)+deg(x)-2}{deg(e)deg(x)}} + \sum_{\substack{ey\in E\\ y\in\Theta_3}} \sqrt{\frac{deg(e)+deg(y)-2}{deg(e)deg(y)}} + \\
&\quad \sum_{\substack{xy\in E\\ x\in\Theta_2\\ y\in\Theta_3}} \sqrt{\frac{deg(x)+deg(y)-2}{deg(x)deg(y)}} \\
&= \sum_{\substack{ex\in E\\ x\in\Theta_2}} \sqrt{\frac{(2p-1)+(p+1)-2}{(2p-1)(p+1)}} + \sum_{\substack{ey\in E\\ y\in\Theta_3}} \sqrt{\frac{(2p-1)+p-2}{(2p-1)p}} + \\
&\quad \sum_{\substack{xy\in E\\ x\in\Theta_2\\ y\in\Theta_3}} \sqrt{\frac{(p+1)+p-2}{(p+1)p}} \\
&= (p-1)\sqrt{\frac{(2p-1)+(p+1)-2}{(2p-1)(p+1)}} + p\sqrt{\frac{(2p-1)+p-2}{(2p-1)p}} + \\
&\quad p(p-1)\sqrt{\frac{(p+1)+p-2}{(p+1)p}} \\
&= (p-1)\sqrt{\frac{3p-2}{(2p-1)(p+1)}} + \sqrt{\frac{3p-3}{2p-1}} + (p-1)\sqrt{\frac{p(2p-1)}{p+1}}
\end{aligned}$$

c) The Geometric Arithmetic index can be calculated as

$$\begin{aligned}
GA(M(D_{2p})) &= \sum_{xy\in E(M(D_{2p}))} \frac{2\sqrt{deg(x)\cdot deg(y)}}{deg(x)+deg(y)} \\
&= \sum_{\substack{ex\in E\\ x\in\Theta_2}} \frac{2\sqrt{deg(e)\cdot deg(x)}}{deg(e)+deg(x)} + \sum_{\substack{ey\in E\\ y\in\Theta_3}} \frac{2\sqrt{deg(e)\cdot deg(y)}}{deg(e)+deg(y)} +
\end{aligned}$$

$$\sum_{\substack{xy\in E\\ x\in\Theta_2\\ y\in\Theta_3}} \frac{2\sqrt{deg(x)\cdot deg(y)}}{deg(x)+deg(y)}$$

$$= \sum_{\substack{ex\in E\\ x\in\Theta_2}} \frac{2\sqrt{(2p-1)\cdot(p+1)}}{(2p-1)+(p+1)} + \sum_{\substack{ey\in E\\ y\in\Theta_3}} \frac{2\sqrt{(2p-1)\cdot p}}{(2p-1)+p} +$$

$$\sum_{\substack{xy\in E\\ x\in\Theta_2\\ y\in\Theta_3}} \frac{2\sqrt{(p+1)\cdot p}}{(p+1)+p}$$

$$= (p-1)\frac{2\sqrt{(2p-1)\cdot(p+1)}}{(2p-1)+(p+1)} + p\frac{2\sqrt{(2p-1)\cdot p}}{(2p-1)+p} +$$

$$p(p-1)\frac{2\sqrt{(p+1)\cdot p}}{(p+1)+p}$$

$$= \frac{2(p-1)\sqrt{(2p-1)(p+1)}}{3p} + \frac{2p\sqrt{(2p-1)p}}{3p-1} + \frac{2p(p-1)\sqrt{(p+1)p}}{2p+1}$$

d) The Sum Connectivity index can be calculated as

$$\chi(M(D_{2p})) = \sum_{xy\in E(M(D_{2p}))} \frac{1}{\sqrt{deg(x)+deg(y)}}$$

$$= \sum_{\substack{ex\in E\\ x\in\Theta_2}} \frac{1}{\sqrt{deg(e)+deg(x)}} + \sum_{\substack{ey\in E\\ y\in\Theta_3}} \frac{1}{\sqrt{deg(e)+deg(y)}} +$$

$$\sum_{\substack{xy\in E\\ x\in\Theta_2\\ y\in\Theta_3}} \frac{1}{\sqrt{deg(x)+deg(y)}}$$

$$= \sum_{\substack{ex\in E\\ x\in\Theta_2}} \frac{1}{\sqrt{(2p-1)+(p+1)}} + \sum_{\substack{ey\in E\\ y\in\Theta_3}} \frac{1}{\sqrt{(2p-1)+p}} +$$

$$\sum_{\substack{xy\in E\\ x\in\Theta_2\\ y\in\Theta_3}} \frac{1}{\sqrt{(p+1)+p}}$$

$$= \frac{p-1}{\sqrt{(2p-1)+(p+1)}} + \frac{p}{\sqrt{(2p-1)+p}} + \frac{p(p-1)}{\sqrt{(p+1)+p}}$$

$$= \frac{p-1}{\sqrt{3p}} + \frac{p}{\sqrt{3p-1}} + \frac{p(p-1)}{\sqrt{2p+1}}$$

□

3 Conclusions

The present paper computes the topological indices, including the Randić Index, Atom-Bond Connectivity Index, Geometric-Arithmetic Index, and Sum Connectivity Index, for Möbius function graphs derived from finite groups. These indices enable structural comparisons between Möbius function graphs and other algebraically defined graphs. The results contribute to the classification of such graphs based on their topological characteristics, thereby emphasizing the connections between group theory and graph theory.

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Partial Mycielskian Graph

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Abstract

One of the intense application areas of graphs is modeling communication networks. The graph-theoretic parameters can be used in determining the stability of graphs. The connectivity plays a vital role in this regard. In this paper, we define a new construction which we call Partial Mycielskian graph (PM-graph) which will be more stable than the given graph with more number of nodes as well as links. The graph we define in this paper is more stable than Mycielskian of a graph, [40]. Further, we investigate its basic properties. In addition, we find the M-polynomial of this new graph and derive its degree-based topological indices.

Keywords: Partial Mycielskian graph, Mycielskian graph, Connectivity
AMS Classification: 05C07, 05C15, 05C40, 05C45

1 Introduction

The connectivity $\kappa(G)$ of a connected graph G is the least positive integer k such that there exists $S \subset \mathcal{V}$, $|S| = k$ and $G \setminus S$ is disconnected or reduces to the trivial graph K_1, [31]. The two graphs G and H are *isomorphic* (written $G \cong H$) if there exists a one-to-one correspondence between their point sets which preserves adjacency, [31].

For a graph $G = (\mathcal{V}, \mathcal{E})$, a *dominating set* is denoted by D where $D \subseteq \mathcal{V}$ and every $v \in \mathcal{V} \setminus D$ is adjacent to at least one vertex in D, [33]. The dominating set D is *minimal dominating set* of G if no proper subset of D is a dominating set. The *domination number* $\gamma(G)$ *of a graph* is the cardinality of the smallest minimal dominating set of G. Basic graph theoretic terminologies and notations can be found in [7, 31, 33].

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Nomenclature	
$\mathcal{V}$	Vertex set
$\mathcal{E}$	Edge set
$G = (\mathcal{V}, \mathcal{E})$	Graph G with vertex set $\mathcal{V}$ and edge set $\mathcal{E}$
$\mathcal{N}_G(v)$	open neighbourhood of $v \in \mathcal{V}$
$\mathcal{N}_G[v]$	closed neighbourhood of $v \in \mathcal{V}$
$d_G(v)$	degree of $v \in \mathcal{V}$
$d_G(u, v)$	distance from u to v in G

Mycielski gave a fascinating construction to obtain a triangle-free graph with large chromatic number known as the *Mycielskian of a graph*, [40]. For more details regarding Mycielskian graph and its related studies, refer to [2, 6, 40].

Definition 1. *[40] Let $G = (\mathcal{V}, \mathcal{E})$ be a graph. Then the Mycielskian $\mu(G)$ of G is the graph $\mu(G) = (\mathcal{V}_\mu, \mathcal{E}_\mu)$, where the vertex set $\mathcal{V}_\mu = \mathcal{V} \cup \mathcal{V}' \cup \{u\}$ ($\mathcal{V}, \mathcal{V}'$ and $\{u\}$ are mutually disjoint), with $\mathcal{V}' = \{x' : x \in \mathcal{V}\}$, and the edge set $\mathcal{E} \cup \{x'y : xy \in \mathcal{E}\} \cup \{x'u : x' \in \mathcal{V}'\}$. The triad $(\mathcal{V}, \mathcal{V}', u)$ denotes the vertex set of $\mu(G)$. Here, we call x' the twin of x in $\mu(G)$ and vice versa, u is called the root of $\mu(G)$ (See Fig. 1.)*

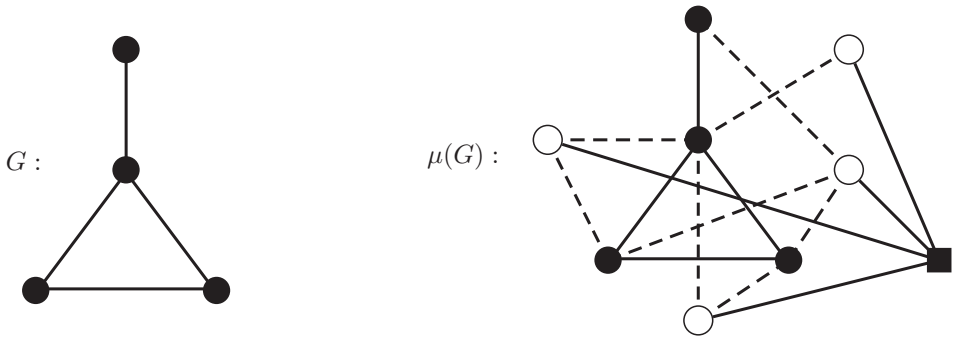

Figure 1: The graph G and its Mycielskian

Now, we propose a new construction which is more stable than Mycielskian graph. This newly constructed graph is called *Partial Mycielskian graph (PM-graph)* $\overline{\mu}(G)$. This $\overline{\mu}(G)$ builds a stronger and stable network than Mycielskian $\mu(G)$ of a graph G since $\overline{G}$ is an induced graph of $\overline{\mu}(G)$.

Definition 2. *For a graph $G = (\mathcal{V}, \mathcal{E})$, the PM-graph of G, denoted by $\overline{\mu}(G)$, is the graph with vertex set consisting of the disjoint union $\mathcal{V} \cup \mathcal{V}' \cup \{u\}$ where $\mathcal{V}' = \{x' : x \in \mathcal{V}\}, u$ is the newly added vertex as in $\mu(G)$ and the edge set $\overline{\mathcal{E}} \cup \mathcal{E}' \cup \mathcal{E}''$, where $\overline{\mathcal{E}} = \{xy : xy \notin \mathcal{E}\}, \mathcal{E}' = \{x'y : xy \in \mathcal{E}\}$ and $\mathcal{E}'' = \{x'u : x' \in \mathcal{V}'\}$. The triad $(\mathcal{V}, \mathcal{V}', u)$ denote the vertex set of $\overline{\mu}(G)$. Here, we call x' the twin of x in $\overline{\mu}(G)$ and vice versa, u is called the root vertex of $\overline{\mu}(G)$ (See Fig. 2).*

Remark 1.1. *[2] Let G be a graph such that $\delta(G) > 1$, then Mycielskian of G is connected.*

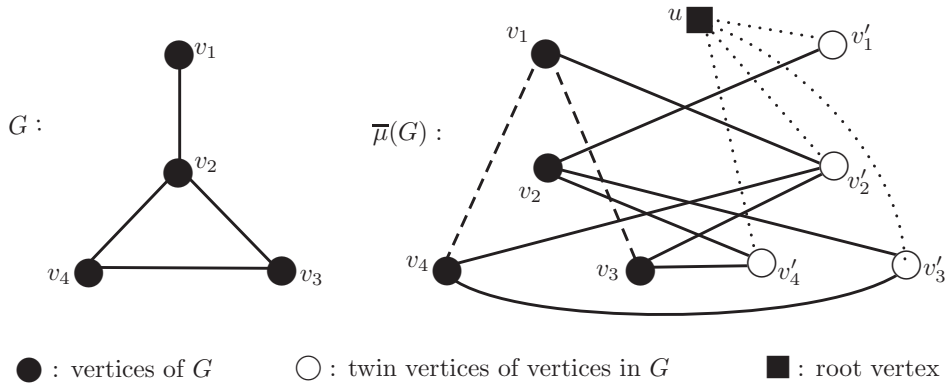

Figure 2: The graph G and its PM-graph.

Theorem 1.1. *[22] Let G be a graph such that $\kappa(G) \geq 1$ and $|\mathcal{V}| = n$. Then*

$$\alpha_0 + \beta_0 = \alpha_1 + \beta_1 = n.$$

2 Main results

In this section, we shall obtain some fundamental properties of the PM-graph.

Theorem 2.1. *Let G be a graph with $|\mathcal{V}| = n$ and $|\mathcal{E}| = m$. Then*

(a) $|\mathcal{V}_{\overline{\mu}}| = 2n + 1$,

(b) $|\mathcal{E}_{\overline{\mu}}| = m + \frac{n(n+1)}{2}$.

Proof. Using Definition 2, we have

(a) $\mathcal{V}_{\overline{\mu}} = \mathcal{V} \cup \mathcal{V}' \cup \{u\} \implies |\mathcal{V}_{\overline{\mu}}| = 2n + 1$,

(b) $\mathcal{E}_{\overline{\mu}} = \overline{\mathcal{E}} \cup \mathcal{E}' \cup \mathcal{E}''$. Therefore,

$$\begin{aligned} |\mathcal{E}_{\overline{\mu}}| &= |\overline{\mathcal{E}}| + |\mathcal{E}'| + |\mathcal{E}''| \\ &= \frac{n(n-1)}{2} - m + \sum_{v \in \mathcal{V}} d_G(v) + n \\ &= m + \frac{n(n+1)}{2}. \end{aligned}$$

□

The degree sequence of a graph is the sequence of all vertex degrees in the graph. There are many problems related to degree sequences. One of the most important problems related to degree sequences is the number and structure of the realizations of the given degree sequence. For example, there is no rule for determining the connectedness, the number of components, cyclicness or any other graph theoretical parameter or property of the realizations of any degree sequence. Recently, a new graph theoretical invariant called omega invariant was defined in [9].

The following theorem gives the degrees of vertices in the PM-graph.

Theorem 2.2. *Let G be a graph with $|\mathcal{V}| = n$ and $|\mathcal{E}| = m$. Then*

$$d_{\overline{\mu}(G)}(v) = \begin{cases} n-1 & if \ \ v \in \mathcal{V}, \\ d_G(v)+1 & if \ \ v \in \mathcal{V}', \\ n & if \ \ v = u. \end{cases}$$

Proof. Using Definition 2, we can get the desired result. □

Corollary 2.3. *Let G be a graph with $|\mathcal{V}| = n$. Then*

$$\Delta(\overline{\mu}(G)) = n,$$
$$\delta(\overline{\mu}(G)) = \begin{cases} n-1 & \text{if } \delta(G) = n-1, \\ \delta(G)+1 & \text{otherwise.} \end{cases}$$

Observation 1. *If G is any graph, then complement $\overline{G}$ of G is an induced subgraph of PM-graph of G.*

Observation 2. *If G is any graph with $|\mathcal{V}| = n$, then the star $K_{1,n}$ is an induced subgraph of PM-graph of G.*

Theorem 2.4. *If G is any graph such that $G \ncong \overline{K_n}$, then PM-graph $\overline{\mu}(G)$ is connected.*

Proof. Let $G \cong \overline{K_n}$. Then by Definition 2, $\overline{\mu}(G)$ is not connected as it has two components viz., K_n and $\overline{K_n} + K_1$, where $\mathcal{V}(K_n) = \mathcal{V}$, $\mathcal{V}(\overline{K_n}) = \mathcal{V}'$, K_1 is the graph having a single vertex $\{u\}$.

Suppose $G \ncong \overline{K_n}$. Then following cases will arise.

Case 1. If G is connected, then obviously $\overline{\mu}(G)$ is also connected.

Case 2. If G is not connected, then G has at least two components. Suppose $u, v \in \mathcal{V}(\overline{\mu}(G))$ such that u and v are not in the same component. Then clearly the are adjacent in $\overline{\mu}(G)$ by Definition 2. Now, if v and w' are not adjacent in $\overline{\mu}(G)$, then there exist a path $vxy'uw'$, where xy is an edge in one of the components of G such that v is not a vertex in that component.

Hence, $\overline{\mu}(G)$ is connected. □

Theorem 2.5. *If G is any graph such that $G \ncong \overline{K_n}$, then*

$$diam(\overline{\mu}(G)) \leq 4.$$

Proof. **Case 1.** Let $v, w \in \mathcal{V}$. If $vw \notin \mathcal{E}$, then $vw \in \mathcal{E}_{\overline{\mu}}$. Thus, $d_{\overline{\mu}(G)}(v, w)) = 1$. If $vw \in \mathcal{E}$, then we have the following situations.

(i) if there exists a point $x \in \mathcal{V}$ such that $xv \in \mathcal{E}$ and $xw \in \mathcal{E}$, then there exists a path $vx'w$. Therefore, $d_{\overline{\mu}(G)}(v, w)) = 2$.

(ii) if there exists no vertex $x \in \mathcal{V}$ such that $xv \in \mathcal{E}$ and $xw \in \mathcal{E}$, then there exists a path $vw'uv'w$. Therefore, $d_{\overline{\mu}(G)}(v, w)) = 4$.

(iii) if there exists a vertex $x \in \mathcal{V}$ such that either $xv \in \mathcal{E}$ or $xw \in \mathcal{E}$ but not both, then there exists a path $vx'uv'w$ or $wx'uw'v$. Therefore, $d_{\overline{\mu}(G)}(v, w)) = 4$.

Case 2. Let $v \in \mathcal{V}$ and $w \in \mathcal{V}'$. Suppose $w \in \mathcal{V}'$ is the twin vertex of v, then there will

be following situations.
(i) If there exists a vertex $x \in \mathcal{V}$ such that $vx \in \mathcal{E}$, then there will be a path $wux'v$. Thus, $d_{\overline{\mu}(G)}(v,w)) = 3$.
(ii) If there exists no vertex $x \in \mathcal{V}$ such that $vx \in \mathcal{E}$, then there will be a path $wuz'xv$, where $z' \in \mathcal{V}'$ is the twin vertex of any vertex $z \in \mathcal{V}$ such that $xz \in \mathcal{E}$ as $G \ncong \overline{(K_n)}$. Thus, $d_{\overline{\mu}(G)}(v,w)) = 4$.
Case 3. Let $v, w \in \mathcal{V}'$. Then there will be a path vuw and $d_{\overline{\mu}(G)}(v,w)) = 2$.
Case 4. Let $v \in \mathcal{V}$ and $w = u$. then there will be two situations as follows.
(i) If $v \in \mathcal{V}$ is isolated vertex, then there exists a path $vxy'w$ of length three in $\overline{\mu}(G)$, where $xy \in \mathcal{E}$. (ii) If $v \in \mathcal{V}$ is not isolated vertex, then there will be a path $vx'w$, where $vx \in \mathcal{E}$ and $d_{\overline{\mu}(G)}(v,w)) = 2$.
Case 5. Let $v \in \mathcal{V}'$ and $w = u$. Then $d_{\overline{\mu}(G)}(v,w)) = 1$ by Definition 2. Hence, for $G \ncong \overline{K_n}$, $diam(\overline{\mu}(G)) \leq 4$. □

Corollary 2.6. *If $G \ncong \overline{K_n}$ and $diam(G) \geq 4$, then*

$$diam(\overline{\mu}(G)) = 4.$$

The following lemma is useful to prove theorem for isomorphism of PM-graphs.

Lemma 2.7. *[2] Let $f : G \to H$ be a graph isomorphism of G onto H. Then $f(\mathcal{N}_G(x)) = \mathcal{N}_H(f(x))$. Furthermore, $G - x \cong H - f(x)$, and $G - \mathcal{N}_G[x] \cong H - \mathcal{N}_H[f(x)]$ under the restriction maps of f to the respective domains.*

Theorem 2.8. *For any two graphs $G \ncong \overline{K_n}$ and $H \ncong \overline{K_m}$, $\overline{\mu}(G) \cong \overline{\mu}(H)$ if and only if $G \cong H$.*

Proof. If $G \cong H$, then $\overline{\mu}(G) \cong \overline{\mu}(H)$ is trivial. So assume that $G \ncong \overline{K_n}$ and $H \ncong \overline{K_n}$ are two graphs such that $\overline{\mu}(G) \cong \overline{\mu}(H)$. For $n = 2$ or 3 the result is trivial. So, assume that $n \geq 4$. If G is of order n, then $\overline{\mu}(G)$ and $\overline{\mu}(H)$ are both of order $2n + 1$, hence H is also of order n.

Let $F : \overline{\mu}(G) \to \overline{\mu}(H)$ be the given isomorphism, where $\mathcal{V}(\overline{\mu}(G))$ and $\mathcal{V}(\overline{\mu}(H))$ are given by the triads $(\mathcal{V}_1, \mathcal{V}_1', \{u_1\})$ and $(\mathcal{V}_2, \mathcal{V}_2', \{u_2\})$, respectively.

Now, we look at the possible images of the vertex u_1 of $\overline{\mu}(G)$ under f. Here, both the vertices u_1 and u_2 are of degree n. If $f(u_1) = u_2$, then by Lemma 2.7,

$$G = \overline{\mu}(G) - N[u_1] \cong \overline{\mu}(H) - N[u_2] = H.$$

Next, we claim that $f(u_1) \notin \mathcal{V}_2$. Suppose $f(u_1) \in \mathcal{V}_2$. Since $d_{\overline{\mu}(H)}(f(u_1)) = d_{\overline{\mu}(G)}(u_1) = n$, it follows from the Definition 2 that, in $\overline{\mu}(H)$, $\frac{n}{2}$ neighbours of $f(u_1)$ belong to $\mathcal{V}_2$ while another $\frac{n}{2}$ neighbours (the twins) belong to $\mathcal{V}_2'$. (This forces n to be even.) These n neighbours of $f(u_1)$ form an independent subset of $\overline{\mu}(H)$. Then $H' = \overline{\mu}(H) - \mathcal{N}_{\overline{\mu}(H)}[f(u_1)] \cong \overline{\mu}(G) - \mathcal{N}_{\overline{\mu}(G)}[u_1] = G$. Now , if $x \in \mathcal{V}_2$ is adjacent to $f(u_1)$ in $\overline{\mu}(H)$, then x is adjacent to $f(u_i)'$, the twin of $f(u_i)$ belonging to $\mathcal{V}_2'$ in $\overline{\mu}(H)$. Further, $d_{H'}(f(u_1)') = 1 = d_G(v)$, where $v \in \mathcal{V}_1$ (the vertex set of G) corresponds to $f(u_1)'$ in $\overline{\mu}(H)$, then $d_{\overline{\mu}(G)}(v) = 2$, while $d_{\overline{\mu}(H)}(f(u_1)') = \frac{n}{2} + 1 > 2$, as $n \geq 4$. Hence, this case cannot arise.

Finally, suppose $f(u_1) \in \mathcal{V}_2'$. Set if $f(u_1) = y'$. Then y, the twin of y' in $\overline{\mu}(H)$, belongs to $\mathcal{V}_2$. As $d_{\overline{\mu}(G)}(u_1) = n, d_{\overline{\mu}(H)}(y') = n$. The vertex y' has $n-1$ neighbours in $\mathcal{V}_2$, say, $x_1, x_2, ..., x_{n-1}$. Then $\mathcal{N}_H(y) = \{x_1, x_2, ..., x_{n-1}\}$, and hence y is also adjacent to $x_1', x_2', ..., x_{n-1}'$ in $\mathcal{V}_2'$. Further, as $\mathcal{N}_{\overline{\mu}(G)}(u_1)$ is independent, $\mathcal{N}_{\overline{\mu}(H)}(y')$ is also independent. Therefore, $H = K_{1,n-1}$ consisting of the edges $\{yx_i : 1 \leq i \leq n-1\}$. Thus,

$$G \cong K_{1,n-1} \cong H.$$

□

Theorem 2.9. *For any graph G, $\gamma(\overline{\mu}(G)) = \gamma(\overline{G}) + 1$.*

Proof. From Definition 2, $\overline{G}$ is an induced subgraph of $\overline{\mu}(G)$. Thus, $\gamma(\overline{G})$ vertices dominate all vertices of $\mathcal{V}$ and the root vertex u will dominate the remaining vertices of $\overline{\mu}(G)$. Hence, $\gamma(\overline{\mu}(G)) = \gamma(\overline{G}) + 1$. □

Corollary 2.10. *For any graph G,*

$$\gamma(\overline{\mu}(G)) \leq \begin{cases} n+1 & \text{if } \delta(G) = n-1, \\ \delta(G)+3 & \text{otherwise.} \end{cases}$$

Theorem 2.11. *For any graph G,*

$$\chi(\overline{\mu}(G)) \leq \begin{cases} \chi(\overline{G_c}) + k & if \ \ \delta(G) = 0, \\ \chi(\overline{G}) + 1 & otherwise, \end{cases}$$

where $G_c = G - \cup_{a=1}^{k}\{i_a\}$, k is the number of isolated vertices in G and $\cup_{a=1}^{k}\{i_a\}$ is the union of all isolated vertices in G.

Proof. From Definition 2, the vertices in $\overline{\mu}(G)$ can be categorized in three categories. The points of $\mathcal{V}$ receive the same colour as in $\overline{G}$. The points of $\mathcal{V}'$ can be coloured using less than the colours that colour their twin vertices. The remaining root vertex may receive any of the coloures used for the members of $\mathcal{V}$ or one colour different from the colours already used. Thus, $\chi(\overline{\mu}(G)) = \chi(\overline{G}) + 1$. □

From Theorem 2.2, we have the following result.

Theorem 2.12. *The PM-graph of any graph is not Eulerian.*

Theorem 2.13. *If G is any graph of order n, then*

$$\alpha_0(\overline{\mu}(G)) = \begin{cases} n & if \ \ G \cong K_n, \\ n_c + 1 & if \ \ G \text{ has isolated vertices}, \\ n+1 & otherwise, \end{cases}$$

where $n_c = n - k, k$ is the number of isolated vertices in G.

Proof. The proof has the following cases.
Case 1: If $G \cong \overline{K_n}$, then it is easy to see that $n-1$ members of $\mathcal{V}$ together with the root vertex u forms the smallest point cover for $\overline{\mu}(G)$.
Case 2: Suppose G has isolated vertices. Then $n_c = n - k$ members of $\mathcal{V}$ (where k is the number of isolated vertices) together with the root vertex u forms the smallest point cover for $\overline{\mu}(G)$.
Case 3: If $G \ncong K_n$ and has no isolated vertices, then all the members of $\mathcal{V}$ together with the root vertex u forms the smallest point cover for $\overline{\mu}(G)$. Thus, the desired result follows from the above cases. □

Theorem 2.14. *If G is any graph of order n, then*

$$\beta_0(\overline{\mu}(G)) = \begin{cases} n+1 & if\ \ G \cong K_n, \\ 2n - n_c & if\ \ G \text{ has isolated vertices}, \\ n & otherwise. \end{cases}$$

Proof. The result follows from the Theorems 1.1 and 2.13. □

3 Topological indices of PM-graph

A mathematically derived numerical parameter related to the graph structure is termed as topological index. It is an invariant, which will not depend on labeling or pictorial representation of graph. These indices play a useful role in chemical graphs. For more details refer [25, 27, 36] and references cited there in. These topological indices can be obtained from an expression called graph polynomial. In fact, there are several graph polynomials like Tutte polynomial [19], matching polynomial [20, 26], Schultz polynomial [23, 32], Zang-Zang polynomial [46], etc., Among them, the Hosoya polynomial [34] is the best and well-known polynomial which plays a vital role in determining distance-based indices such as Wiener index [45], hyper Wiener index [8] of graphs. Similarly, M-polynomial which was introduced in 2015 by Deutsch et al., [18] is useful in determining many of the degree-based indices (listed in Table 1). Recently, the study of M-polynomial are reported in [4, 5, 37, 38, 39].

Definition 3. *[18] Let G be a graph. Then M-polynomial of G is defined as*

$$M(G; x, y) = \sum_{i \le j} m_{ij}(G) x^i y^j, \tag{3.1}$$

where $m_{ij}, i, j \ge 1$, is the number [29] of edges uv of G such that $\{d_G(u), d_G(v)\} = \{i, j\}$.
where $D_x = x\frac{\partial f(x,y)}{\partial x}$, $D_y = y\frac{\partial f(x,y)}{\partial y}$, $S_x = \int_0^x \frac{f(t,y)}{t}dt$, $S_y = \int_0^y \frac{f(x,t)}{t}dt$ and $J(f(x,y)) = f(x,x)$ are the operators.

The first and second Zagreb indices are amongst the oldest and best known topological indices defined in 1972 by Gutman [28] as follows:

$$M_1(G) = \sum_{v \in \mathcal{V}(G)} d_G^2(v), \tag{3.2}$$

$$\text{and } M_2(G) = \sum_{vw \in \mathcal{E}(G)} d_G(v) \cdot d_G(w), \text{ respectively.} \tag{3.3}$$

Table 1: Operations on M-polynomial to Derive degree-based topological indices [18].

Notation	Name of the Index	$f(x,y)$	Operation on $M(G;x,y)$
$M_1(G)$	First Zagreb	$x+y$	$(D_x+D_y)(M(G;x,y))\|_{x=y=1}$
$M_2(G)$	Second Zagreb	xy	$(D_xD_y)(M(G;x,y))\|_{x=y=1}$
${}^mM_2(G)$	Second modified Zagreb	$\frac{1}{xy}$	$(S_xS_y)(M(G;x,y))\|_{x=y=1}$
$S_D(G)$	Symmetric division index	$\frac{x^2+y^2}{xy}$	$(D_xS_y+D_yS_x)(M(G;x,y))\|_{x=y=1}$
$H(G)$	Harmonic	$\frac{2}{x+y}$	$2S_xJ(M(G;x,y))\|_{x=1}$
$I_n(G)$	Inverse sum index	$\frac{xy}{x+y}$	$S_xJD_xD_y(M(G;x,y))\|_{x=1}$

The vertex-degree-based graph invariant,

$$F(G)=\sum_{v\in\mathcal{V}(G)} d_G^3(v) \tag{3.4}$$

was encountered in [28]. This index is called "forgotten topological index"[21].

Recently, Shirdel et al. [3, 42] introduced a new version of Zagreb index called hyper-Zagreb index, which is defined for a graph G as

$$HM(G)=\sum_{vw\in\mathcal{E}(G)} (d_G(v)+d_G(w))^2. \tag{3.5}$$

Recently, Gutman et al. [30] put forward a new index called sigma index, which is defined as

$$\sigma(G)=\sum_{vw\in\mathcal{E}(G)} (d_G(v)-d_G(w))^2. \tag{3.6}$$

The following results are useful to prove our results.

Theorem 3.1. *[30] If G is any graph, then*

$$\sigma(G)=F(G)-2M_2(G).$$

Theorem 3.2. *If G is a graph with n vertices and m edges, then*

$$M_1(\overline{\mu}(G))=M_1(G)+n(n^2-n+2)+4m.$$

Proof. By using Eq. (3.2), we have

$$\begin{aligned} M_1(\overline{\mu}(G)) &= \sum_{v\in\mathcal{V}(\overline{\mu}(G))} d^2_{\overline{\mu}(G)}(v) \\ &= \sum_{v\in\mathcal{V}(G)} (n-1)^2 + \sum_{v\in\mathcal{V}(G)} (d_G(v)+1)^2 + n^2 \\ &= n(n-1)^2 + \sum_{v\in\mathcal{V}(G)} \left[d^2_G(v) + 1 + 2d_G(v)\right] + n^2 \\ &= M_1(G) + n(n^2-n+2) + 4m. \end{aligned}$$

□

Theorem 3.3. *If G is a graph with n vertices and m edges, then*

$$M_2(\overline{\mu}(G)) = \frac{n(n-1)^3}{2} + (n-1)M_1(G) + m(6n-n^2-3).$$

Proof. By using Eq. (3.3), we have

$$\begin{aligned} M_2(\overline{\mu}(G)) &= \sum_{vw\in\mathcal{E}(\overline{\mu}(G))} d_{\overline{\mu}(G)}(v)\cdot d_{\overline{\mu}(G)}(w) \\ &= \sum_{vw\notin\mathcal{E}} d_{\overline{\mu}(G)}(v)\cdot d_{\overline{\mu}(G)}(w) + \sum_{vx'\in\mathcal{E}'} d_{\overline{\mu}(G)}(v)\cdot d_{\overline{\mu}(G)}(x') + \sum_{ux'\in\mathcal{E}''} d_{\overline{\mu}(G)}(u)\cdot d_{\overline{\mu}(G)}(x') \\ &\quad \text{(where u is the root vertex)} \\ &= \sum_{vw\notin\mathcal{E}} (n-1)\cdot(n-1) + \sum_{vx'\in\mathcal{E}'} (n-1)\cdot(d_G(x)+1) + \sum_{ux'\in\mathcal{E}''} n\cdot(d_G(x)+1) \\ &= \left[\frac{n(n-1)}{2} - m\right](n-1)^2 + (n-1)\sum_{vx'\in\mathcal{E}'} (d_G(x)+1) + n\sum_{ux'\in\mathcal{E}''} (d_G(x)+1) \\ &= \left[\frac{n(n-1)}{2} - m\right](n-1)^2 + (n-1)\sum_{x\in\mathcal{V}} d_G(x)\,(d_G(x)+1) + n\sum_{x\in\mathcal{V}} (d_G(x)+1) \\ &= \frac{n(n-1)^3}{2} + (n-1)M_1(G) + m(6n-n^2-3). \end{aligned}$$

□

Theorem 3.4. *If G is a graph with n vertices and m edges, then*

$$F(\overline{\mu}(G)) = n(n^3-2n^2+3n) + 6m + F(G) + 3M_1(G).$$

Proof. By using Eq. (3.4), we have

$$\begin{aligned} F(\overline{\mu}(G)) &= \sum_{v\in\mathcal{V}(\overline{\mu}(G))} d^3_{\overline{\mu}(G)}(v) \\ &= \sum_{v\in\mathcal{V}} (n-1)^3 + \sum_{v\in\mathcal{V}'} (d_G(v)+1)^3 + n^3, \text{ where } d_{\overline{\mu}(G)}(u) = n,\ u \text{ is the root vertex.} \\ &= n(n^3-2n^2+3n) + 6m + F(G) + 3M_1(G). \end{aligned}$$

□

Now, we provide M-polynomial of PM-graph from which we can get degree-based topological indices (quoted in Table 1) of PM-graph.

Theorem 3.5. *If G is a graph of order n and size m with the M-polynomial $M(G;x,y) = \sum_{i\leq j} m_{ij}(G)x^iy^j$, then*

$$M(\overline{\mu}(G);x,y) = \left[\frac{n(n-1)}{2} - m\right] x^{n-1}y^{n-1} + \sum_{i\in Deg} im_i(G)x^{i+1}y^{n-1} + \sum_{i\in Deg} m_i(G)x^{i+1}y^n,$$

where Deg is the set of distinct degrees in G and m_i is the number of vertices v in G such that $d_G(v) = i$.

Proof. From Definition 2, the degree of $v \in \mathcal{V}$ in $\overline{\mu}(G)$ is $n-1-d_G(v)$ while $d_{\overline{\mu}(G)}(v') = d_G(v)+1$ of the twin v' of $v \in \mathcal{V}$ and the degree of the root vertex u is n. Therefore, we have edge distribution of PM-graph as in the following table.

$\mathbf{m_{ij}}$	**Number of edges**
$m_{n-1,n-1}$	$\frac{n(n-1)}{2} - m$
$m_{i+1,n-1}$	im_i
$m_{i+1,n}$	m_i.

Thus, the desired result can obtained by switching these values in Eq. (3.1). □

Corollary 3.6. *If M-polynomial of PM-graph is*

$$M(\overline{\mu}(G);x,y) = \left[\frac{n(n-1)}{2} - m\right] x^{n-1}y^{n-1} + \sum_{i\in Deg} im_i(G)x^{i+1}y^{n-1} + \sum_{i\in Deg} m_i(G)x^{i+1}y^n,$$

then

$$M_1(\overline{\mu}(G)) = 2(n-1)\left[\frac{n(n-1)}{2} - m\right] + \sum_{i\in Deg}\left((i+1)^2 + (n-1)i + n\right)m_i,$$

$$M_2(\overline{\mu}(G)) = (n-1)^2\left[\frac{n(n-1)}{2} - m\right] + \sum_{i\in Deg}\left((n-1)i+n\right)(i+1)m_i,$$

$${}^mM_2(\overline{\mu}(G)) = \frac{1}{n^2}\left[\frac{n(n-1)}{2} - m\right] + \sum_{i\in Deg}\frac{1}{(i+2)}\left(\frac{i}{n} + \frac{1}{(n+1)}\right)m_i,$$

$$S_D(\overline{\mu}(G)) = \frac{2(n-1)}{n}\left[\frac{n(n-1)}{2} - m\right] + \sum_{i\in Deg}\left(\frac{(i+1)}{n} + \frac{(i+1)}{(n+1)} + \frac{(n-1)i}{(i+2)} + \frac{n}{(i+2)}\right)m_i,$$

$$H(\overline{\mu}(G)) = \frac{2}{(2n-1)}\left[\frac{n(n-1)}{2} - m\right] + \sum_{i\in Deg}\left(\frac{i}{(n+i+1)} + \frac{1}{(n+i+2)}\right)m_i,$$

$$I_n(\overline{\mu}(G)) = \frac{(n-1)^2}{(2n-3)}\left[\frac{n(n-1)}{2} - m\right] + \sum_{i\in Deg}\left(\frac{(n-i)(i+1)i}{(n+i-1)} + \frac{n(i+1)}{(n+i)}\right)m_i.$$

Proof. These results can be obtained by using the proper operations quoted in Table 1 on M-polynomial of $\overline{\mu}(G)$. □

4 Conclusion

In this paper, we have proposed a new construction of a graph called PM-graph which can be more stable than original graph with more number of nodes (or vertices) as well as links (or edges). We have studied its basic properties. In addition, obtained M-polynomial of PM-graph and derived the formulae for degree-based topological indices.

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On Domination Zagreb Indices of Monogenic Semigroup Graphs

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Abstract

In this paper, we give domination Zagreb indices of graphs obtained by monogenic semi-groups with zero.

Keywords: Topological indices, Domination Zagreb indices, Monogenic semi-group graphs
AMS Classification: 05C07, 05C12, 05C76

1 Introduction

Graph theory has become a fundamental tool in chemistry, network analysis, computer science, electrical engineering and geography to sociology and architecture. Topological indices are numerical parameters that characterize the topology of a molecule and are generally invariant under graph isomorphism. Topological indices are generally divided into two main classes: degree-based and distance-based. The Zagreb indices [16, 17, 12, 18], Randić index [28], Wiener index [33, 22], and the more recently introduced Sombor index [19] have demonstrated utility in Quantitative Structure–Activity Relationships (QSAR) and Quantitative Structure–Property Relationships (QSPR), providing numerical descriptors that correlate with chemical and physical properties [31, 29, 10, 32].

Another fundamental topic in graph theory is theory of domination. A set $D \subseteq V$ is said to be a dominating set of G, if for any vertex $v \in V - D$ there exists a vertex $u \in D$ such that u and v are adjacent. The domination number $\gamma(G)$ of G is the minimum cardinality of a minimal dominating set in G. A dominating-set $D = \{v_1, v_2, ..., v_r\}$ is minimal if $D - v_i$ is not a dominating set. For a survey of domination in graphs, refer to [20, 21] .

Definition 1.1. For each vertex $v \in V(G)$, the domination degree denoted by $d_d(v)$ and defined as the number of minimal dominating sets of G which contains v.

Based on this new degree definition, a new family of topological indices called "domination topological indices" has been proposed as follows.

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Definition 1.2. [3] Let G be a simple connected graph, the first domination, second domination Zagreb and modified first Zagreb indices are defined as :

$$DM_1(G) = \sum_{u \in V(G)} d_d^2(u),$$
$$DM_2(G) = \sum_{uv \in E(G)} d_d(u) d_d(v),$$
$$DM_1^*(G) = \sum_{uv \in E(G)} [d_d(u) + d_d(v)].$$

The introduction of these indices has spurred research in this area, leading to the rapid development of other related indices such as the forgotten domination [4], hyper domination [4], second domination hyper [4], and domination Sombor indices [30], as well as new concepts like domination Zagreb polynomials [27, 1, 2]. Domination entropy derived from domination topological indices has been shown to exhibit better correlation than classical indices in predicting the physicochemical properties and pi-electron energy of molecules in QSPR analyses on 29 benzenoids [23].

The concept of a zero-divisor graph was first introduced in Beck's [11] 1988 work on commutative rings. The concept of a zero-divisor graph was later extended to both commutative and non-commutative rings by authors such as Anderson [7, 8, 9].

This concept was generalized to commutative semigroups by DeMeyer and his colleagues [14, 15]. They defined a semigroup zero-divisor graph as a graph whose vertices have zero-divisors different from the semizero group, and where the product of two distinct vertices is zero if they are adjacent.

Based on this definition, in 2013, Das and etc. [13] introduced a new and special type of graph derived from a finite monogenic semigroup as follows. For a survey of monogenic semigroup graphs, refer to [24, 25, 26, 5].

Definition 1.3. [13] Let $S = \{a, a^2, a^3, \ldots, a^n\}$ be a monogenic semigroup (with zero). The monogenic semigroup graph, denoted $\Gamma(S)$, is a graph obtained from monogenic semigroup S. The vertex set of this graph consists of the elements of S, except for zero. Any two vertices a^i and a^j are adjacent if and only if $i + j \geq n$.

1.1 An Algorithm [6]

To simplify our calculations and hence the key results in Section 2 below, we will provide the following algorithm about the neighborhood of the vertices on $\Gamma(S_M^n)$ while keeping the description of this specific graph in mind.

I_n : Except for itself, the vertex x^n is adjacent to the all vertices $x^{i_1}(1 \leq i_1 \leq n-1)$ except itself.

I_{n-1} : Except for itself and the vertex x^n, the vertex x^{n-1} is adjacent to the all vertices $x^{i_2}(2 \leq i_2 \leq n-2)$.

I_{n-2} : The vertex x^{n-2} is adjacent to the all vertices $x^{i_3}(3 \leq i_3 \leq n-3)$, the vertex x^n and the vertex x^{n-1}.

If we continue with these steps in this algorithm, we will have two options at the final two stages depending on whether n is even or odd.:

n is even:

$I_{\frac{n}{2}+2}$: The vertex $x^{\frac{n}{2}+2}$ is adjacent to the vertices $x^{\frac{n}{2}-1}$, $x^{\frac{n}{2}}$, $x^{\frac{n}{2}+1}$, x^n, x^{n-1}, x^{n-2}, ..., $x^{\frac{n}{2}+3}$.

$I_{\frac{n}{2}+1}$: The vertex $x^{\frac{n}{2}+1}$ is adjacent to the vertices $x^{\frac{n}{2}}$, x^n, x^{n-1}, x^{n-2}, ..., $x^{\frac{n}{2}+2}$.

n is odd:

$I_{\frac{n+1}{2}+2}$: The vertex $x^{\frac{n+1}{2}+2}$ is adjacent to the vertices $x^{\frac{n+1}{2}-2}$, $x^{\frac{n+1}{2}-1}$, $x^{\frac{n+1}{2}}$, $x^{\frac{n+1}{2}+1}$, x^n, x^{n-1}, x^{n-2}, ..., $x^{\frac{n+1}{2}+3}$.

$I_{\frac{n+1}{2}+1}$: The vertex $x^{\frac{n+1}{2}+1}$ is adjacent to the vertices $x^{\frac{n+1}{2}-1}$, $x^{\frac{n+1}{2}}$, x^n, x^{n-1}, x^{n-2}, ..., $x^{\frac{n+1}{2}+2}$.

As a usual way, let $d_d(x), d_d(x^2), \ldots, d_d(x^n)$ denote the domination degrees of the vertices $x, x^2, \ldots, x^n$ in $\Gamma(S_M^n)$, respectively. By considering the above effective algorithm, we give the following lemma.

2 Domination Zagreb Indices of Monogenic Semi-Group Graphs

Lemma 2.1. *Let $\Gamma(S_M^n)$ be graph obtained by monogenic semi-group $S_M = \{x, x^2, x^3, \ldots, x^n\} \cup \{0\}$. Then, the domination degree sequences of this graph are given as follows:*

$$\begin{aligned} D(G) &= \{d_d(x), d_d(x^2), d_d(x^3), \ldots, d_d(x^{\lfloor \frac{n}{2} \rfloor - 2}), d_d(x^{\lfloor \frac{n}{2} \rfloor - 1}), d_d(x^{\lfloor \frac{n}{2} \rfloor}), \\ &\quad d_d(x^{\lfloor \frac{n}{2} \rfloor + 1}), \ldots, d_d(x^n)\} \\ &= \begin{cases} \{\frac{n}{2}, \frac{n}{2}-1, \frac{n}{2}-2, \ldots, 3, 2, 1, 1, \ldots, 1\} & , \text{if } n \text{ is even} \\ \{\frac{n-1}{2}, \frac{n-1}{2}-1, \frac{n-1}{2}-2, \ldots, 3, 2, 1, 1, \ldots, 1\} & , \text{if } n \text{ is odd.} \end{cases} \end{aligned}$$

Proof. Let $\Gamma(S_M^n)$ be a monogenic semigroup graph. In this case, according to the values that n will receive, two situations arise.
Let n be even. Now let's give the domination degrees of all vertices of the x graph respectively. Since $d_d(x)$ is the number of minimal dominant sets containing x, we can give these dominant sets as follows.

$$\begin{aligned} A_1 &= \{x, x^{n-1}\} \\ A_2 &= \{x, x^{n-2}, x^2\} \\ A_3 &= \{x, x^{n-3}, x^3, x^2\} \\ &\vdots \\ A_{\frac{n}{2}} &= \{x, x^{\frac{n}{2}}, x^{\frac{n}{2}-1}, x^{\frac{n}{2}-2}, \ldots, x^3, x^2\}. \end{aligned}$$

Therefore, the domination degree of the vertex x is $\frac{n}{2}$.

Since $d_d(x^2)$ is the number of minimal dominant sets containing x^2, we can give these dominant

sets as follows.

$$\begin{aligned}
A_1 &= \{x^2, x^{n-2}, x\} \\
A_2 &= \{x^2, x^{n-3}, x^3, x\} \\
A_3 &= \{x^2, x^{n-4}, x^4, x^3, x\} \\
&\vdots \\
A_{\frac{n}{2}-1} &= \{x^2, x^{\frac{n}{2}}, x^{\frac{n}{2}-1}, x^{\frac{n}{2}-2}, \ldots, x^3, x\}.
\end{aligned}$$

Therefore, the domination degree of the vertex x^2 is $\frac{n}{2}-1$. If we continue in this way, we will get $d_d(x^{\frac{n}{2}-1}) = 2$. It is seen that the domination set containing $x^{\frac{n}{2}}$ is only $A = \{x^{\frac{n}{2}}, x^{\frac{n}{2}-1}, \ldots, x^2, x\}$, so $d_d(x^{\frac{n}{2}}) = 1$. Similarly, it is seen that $d_d(x^{\frac{n}{2}+1}) = d_d(x^{\frac{n}{2}+2}) = d_d(x^{n-1}) = d_d(x^n) = 1$.

When n is odd, the proof is completed by following similar steps. □

In the following theorem, we give the exact formula for the first domination Zagreb index.

Theorem 2.2. *Let $\Gamma(S_M^n)$ be monogenic semi-group graph. Then, we have*

$$DM_1(\Gamma(S_M^n)) = \begin{cases} \frac{1}{24}n(n^2+3n+14) & , \text{if } n \text{ is even} \\ \frac{1}{24}(n+1)(n^2-n+12) & , \text{if } n \text{ is odd.} \end{cases}$$

Proof. In the proof, we will mainly consider Lemma 2.1. By the definition of first domination Zagreb index, we have

$$\begin{aligned}
DM_1(\Gamma(S_M^n)) &= \sum_{x^i \in V(\Gamma(S_M^n))} d_d(x^i) \\
&= d_d^2(x) + d_d^2(x^2) + \ldots + d_d^2(x^{\lfloor \frac{n}{2} \rfloor}) + d_d^2(x^{\lfloor \frac{n}{2} \rfloor + 1}) + \ldots + d_d^2(x^n) \\
&= \left(\left\lfloor \frac{n}{2} \right\rfloor\right)^2 + \left(\left\lfloor \frac{n}{2} \right\rfloor - 1\right)^2 + \ldots + 1^2 + \underbrace{1^2 + \ldots + 1^2}_{\lfloor \frac{n}{2} \rfloor} \\
&= \frac{\lfloor \frac{n}{2} \rfloor (\lfloor \frac{n}{2} \rfloor + 1)(2\lfloor \frac{n}{2} \rfloor + 1)}{6} + \lfloor \frac{n}{2} \rfloor
\end{aligned}$$

We recall that, for a real number n, we denote by $\lfloor n \rfloor$ the greatest integer $\leq n$. For a natural number n, we clearly have

$$\left\lfloor \frac{n}{2} \right\rfloor = \begin{cases} \frac{n}{2} & , \text{if } n \text{ is even} \\ \frac{n-1}{2} & , \text{if } n \text{ is odd.} \end{cases} \tag{2.1}$$

Now depends on the status of n in $\lfloor \frac{n}{2} \rfloor$, we have to consider (2.1) which implies the result as desired. □

Theorem 2.3. *Let $\Gamma(S_M^n)$ be monogenic semi-group graph. Then, we have*

$$DM_2(\Gamma(S_M^n)) = \begin{cases} \frac{1}{48}(n^3+12n^2-4n) & , \text{if } n \text{ is even} \\ \frac{1}{48}(n^3+9n^2-n-9) & , \text{if } n \text{ is odd.} \end{cases}$$

Proof. Since the main goal in here to characterize $DM_2(\Gamma(S_M^n))$ depending on the total number of degrees, we need to think the summation as the sum of different blocks and then calculate each of them separately. During our calculations, we will mainly focus on the algorithm defined in Section 1.1 since it presents very systematically way to decide degrees of the vertices. Additionally, we will

use Equation (2.1) and Lemma 2.1.

Assume that n is even:

$$\begin{aligned}DM_2(\Gamma(S_M^n)) =& d_d(x^n)d_d(x) + d_d(x^n)d_d(x^2) + \ldots + d_d(x^n)d_d(x^{n-2}) + d_d(x^n)d_d(x^{n-1}) + \\ & \text{(which is written by } I_n\text{. Let us say } J_n \text{ to this sum)} \\ & + d_d(x^{n-1})d_d(x^2) + d_d(x^{n-1})d_d(x^3) + \ldots + d_d(x^{n-1})d_d(x^{n-2}) + \\ & \text{(which is written by } I_{n-1}\text{. Say } J_{n-1} \text{ to this sum)} \\ & + \ldots + \\ & + d_d(x^{\frac{n}{2}+2})d_d(x^{\frac{n}{2}-1}) + d_d(x^{\frac{n}{2}+2})d_d(x^{\frac{n}{2}}) + d_d(x^{\frac{n}{2}+2})d_d(x^{\frac{n}{2}+1}) + \\ & \text{(written by } I_{\frac{n}{2}+2}\text{. Say } J_{\frac{n}{2}+2} \text{ to this sum)} \\ & + d_d(x^{\frac{n}{2}+1})d_d(x^{\frac{n}{2}}) \\ & \text{(written by } I_{\frac{n}{2}+1}\text{. Say } J_{\frac{n}{2}+1} \text{ to this sum).}\end{aligned}$$

As a result, the second domination Zagreb index is written as the sum

$$\sum_{x^ix^j \in \Gamma(S_M^n)} = J_n + J_{n-1} + \ldots + J_{\frac{n}{2}+2} + J_{\frac{n}{2}+1}.$$

Now to reach the aim, we also need to investigate each $J_t(\frac{n}{2}+1 \leq t \leq n)$ separately, as indicated at the beginning of this proof.

$$\begin{aligned}J_n &= 1\left(\frac{n}{2}\right) + 1\left(\frac{n}{2}-1\right) + \ldots + 1(2) + 1(1) + \underbrace{1(1) + \ldots + 1(1)}_{\frac{n}{2}-1} \\ &= \frac{1}{2}\frac{n}{2}(\frac{n}{2}+1) + \frac{n}{2} - 1,\end{aligned}$$

By applying similar arguments as in J_n, we get

$$\begin{aligned}J_{n-1} &= 1\left(\frac{n}{2}-1\right) + 1\left(\frac{n}{2}-2\right) + \ldots + 1(2) + 1(1) + \underbrace{1(1) + \ldots + 1(1)}_{\frac{n}{2}-2} \\ &= \frac{1}{2}(\frac{n}{2}-1)(\frac{n}{2}) + \frac{n}{2} - 2,\end{aligned}$$

$$\begin{aligned}J_{n-2} &= 1\left(\frac{n}{2}-2\right) + 1\left(\frac{n}{2}-3\right) + \ldots + 1(2) + 1(1) + \underbrace{1(1) + \ldots + 1(1)}_{\frac{n}{2}-3} \\ &= \frac{1}{2}(\frac{n}{2}-2)(\frac{n}{2}-1) + \frac{n}{2} - 3,\end{aligned}$$

$$\vdots$$

$$J_{\frac{n}{2}+2} = 1.2 + 1.1 + 1.1,$$

and finally

$$J_{\frac{n}{2}+1} = 1.1.$$

Thus,

$$J_n + J_{n-1} + J_{n-2} + \ldots + J_{\frac{n}{2}+2} + J_{\frac{n}{2}+1} = \sum_{k=0}^{\frac{n}{2}-1} \frac{1}{2}(\frac{n}{2} - k)(\frac{n}{2} - k + 1) + (\frac{n}{2} - k - 1)$$
$$= \frac{1}{48}(n^3 + 12n^2 - 4n).$$

Assume that n is odd:
By taking into account (2) and following same steps as in n is even case, we obtain

$$J_n + J_{n-1} + J_{n-2} + \ldots + J_{\frac{n+1}{2}+2} + J_{\frac{n+1}{2}+1}$$
$$= \sum_{k=0}^{\frac{n-1}{2}-1} \frac{1}{2}(\frac{n-1}{2} - k)(\frac{n-1}{2} - k + 1) + (\frac{n-1}{2} - k)$$
$$= \frac{1}{48}(n^3 + 9n^2 - n - 9).$$

□

Theorem 2.4. *Let $\Gamma(S_M^n)$ be monogenic semi-group graph. Then, we have*

$$DM_1^*(\Gamma(S_M^n)) = \begin{cases} \frac{1}{48}(n^3 + 24n^2 - 4n) & , \text{if } n \text{ is even} \\ \frac{1}{48}(n^3 + 21n^2 - n - 21) & , \text{if } n \text{ is odd.} \end{cases}$$

Proof. Since the main goal in here to characterize $DM_1^*(\Gamma(S_M^n))$ depending on the total number of degrees, we need to think the summation as the sum of different blocks and then calculate each of them separately. During our calculations, we will mainly focus on the algorithm defined in Section 1.1 since it presents very systematically way to decide degrees of the vertices. Additionally, we will use Equation (2.1) and Lemma 2.1.

Assume that n is even:

$$\begin{aligned} DM_1^*(\Gamma(S_M^n)) =& (d_d(x^n) + d_d(x)) + (d_d(x^n) + d_d(x^2)) + \ldots + (d_d(x^n) + d_d(x^{n-2})) \\ &+ (d_d(x^n) + d_d(x^{n-1}))+ \\ &\text{(which is written by } I_n\text{. Let us say } J_n \text{ to this sum)} \\ &+ (d_d(x^{n-1}) + d_d(x^2)) + (d_d(x^{n-1}) + d_d(x^3)) + \ldots + \\ &+ (d_d(x^{n-1}) + d_d(x^{n-2}))+ \\ &\text{(which is written by } I_{n-1}\text{. Say } J_{n-1} \text{ to this sum)} \\ &+ \ldots + \\ &+ (d_d(x^{\frac{n}{2}+2}) + d_d(x^{\frac{n}{2}-1})) + (d_d(x^{\frac{n}{2}+2}) + d_d(x^{\frac{n}{2}})) \\ &+ (d_d(x^{\frac{n}{2}+2}) + d_d(x^{\frac{n}{2}+1}))+ \\ &\text{(written by } I_{\frac{n}{2}+2}\text{. Say } J_{\frac{n}{2}+2} \text{ to this sum)} \\ &+ (d_d(x^{\frac{n}{2}+1}) + d_d(x^{\frac{n}{2}})) \\ &\text{(written by } I_{\frac{n}{2}+1}\text{. Say } J_{\frac{n}{2}+1} \text{ to this sum).} \end{aligned}$$

As a result, the second domination Zagreb index is written as the sum

$$\sum_{x^ix^j\in\Gamma(S_M^n)} = J_n + J_{n-1} + \ldots + J_{\frac{n}{2}+2} + J_{\frac{n}{2}+1}.$$

Now to reach the aim, we also need to investigate each $J_t(\frac{n}{2}+1 \leq t \leq n)$ separately, as indicated at the beginning of this proof.

$$J_n = (1+\frac{n}{2}) + (1+\frac{n}{2}-1) + \ldots + (1+2) + (1+1) + \underbrace{(1+1)+\ldots+(1+1)}_{\frac{n}{2}-1}$$

$$= \frac{1}{2}(\frac{n}{2}+1)(\frac{n}{2}+2) + 2(\frac{n}{2}-1) - 1,$$

By applying similar arguments as in J_n, we get

$$J_{n-1} = (1+\frac{n}{2}-1) + (1+\frac{n}{2}-2) + \ldots + (1+2) + (1+1) + \underbrace{(1+1)+\ldots+(1+1)}_{\frac{n}{2}-2}$$

$$= \frac{1}{2}(\frac{n}{2})(\frac{n}{2}+1) + 2(\frac{n}{2}-2) - 1,$$

$$J_{n-2} = (1+\frac{n}{2}-2) + (1+\frac{n}{2}-3) + \ldots + (1+2) + (1+1) + \underbrace{(1+1)+\ldots+(1+1)}_{\frac{n}{2}-3}$$

$$= \frac{1}{2}(\frac{n}{2}-1)(\frac{n}{2}) + 2(\frac{n}{2}-3) - 1,$$

$$\vdots$$

$$J_{\frac{n}{2}+2} = (1+2) + (1+1) + (1+1),$$

and finally

$$J_{\frac{n}{2}+1} = (1+1).$$

Thus,

$$\begin{aligned} &J_n + J_{n-1} + J_{n-2} + \ldots + J_{\frac{n}{2}+2} + J_{\frac{n}{2}+1} \\ &= \sum_{k=1}^{\frac{n}{2}} \left[\frac{1}{2}(\frac{n}{2}-k+2)(\frac{n}{2}-k+3) + 2(\frac{n}{2}-k)\right] - \frac{n}{2} \\ &= \frac{1}{48}(n^3+24n^2-4n). \end{aligned}$$

Assume that n is odd:

By taking into account (2) and following same steps as in n is even case, we obtain

$$\begin{aligned} & J_n + J_{n-1} + J_{n-2} + \ldots + J_{\frac{n+1}{2}+2} + J_{\frac{n+1}{2}+1} \\ &= \sum_{k=1}^{\frac{n-1}{2}} \left[\frac{1}{2}(\frac{n-1}{2} - k + 2)(\frac{n-1}{2} - k + 3) + 2(\frac{n+1}{2} - k) \right] - \frac{n-1}{2} \\ &= \frac{1}{48}(n^3 + 21n^2 - n - 21). \end{aligned}$$

□

3 Examples

In the following examples, we show that the domination Zagreb indices of monogenic semigroup graphs are easily computed with the help of the main theorems.

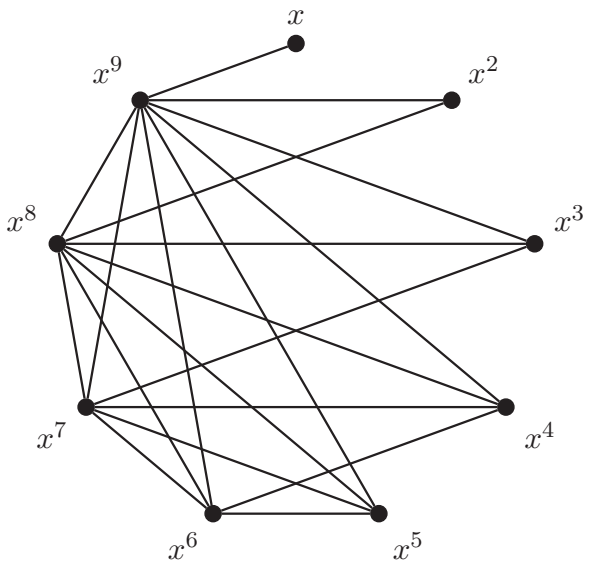

Figure 1: $\Gamma(S_M^9)$ monogenic semigroup graph.

Example 3.1. *Let us consider the monogenic semigroup graphs* $\Gamma(S_M^9)$ *with nine vertices as Figure 1. Then we get*

- $DM_1(\Gamma(S_M^9)) = \frac{1}{24}(9+1)(9^2 - 9 + 12) = 35$ *(by Theorem 2.2)*
- $DM_2(\Gamma(S_M^9)) = \frac{1}{48}(9^3 + 9.9^2 - 25.9 + 15) = 26$ *(by Theorem 2.3)*
- $DM_1^*(\Gamma(S_M^9)) = \frac{1}{48}(9^3 + 21.9^2 - 9 - 21) = 50$ *(by Theorem 2.4)*

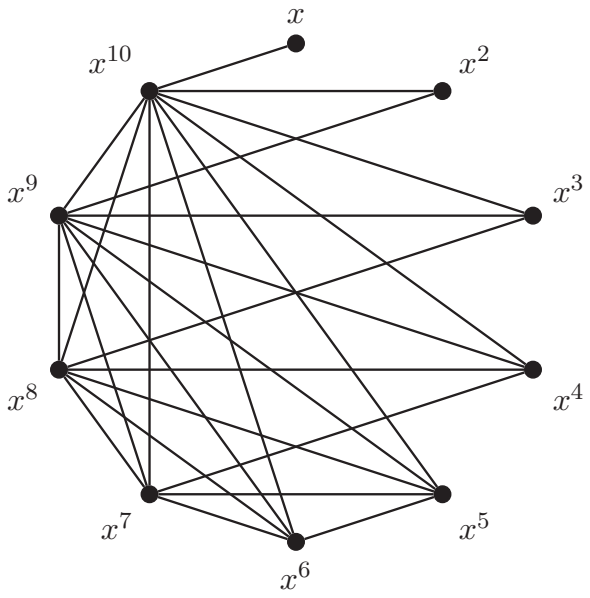

Figure 2: $\Gamma(S_M^{10})$ monogenic semigroup graph.

Example 3.2. *Let us consider the monogenic semigroup graphs* $\Gamma(S_M^{10})$ *with ten vertices as Figure 2. Then we get*

- $DM_1(\Gamma(S_M^{10})) = \frac{1}{24}.10.(10^2 + 3.10 + 14) = 60$ *(by Theorem 2.2)*
- $DM_2(\Gamma(S_M^{10})) = \frac{1}{48}(10^3 + 12.10^2 - 4.10) = 45$ *(by Theorem 2.3)*
- $DM_1^*(\Gamma(S_M^{10})) = \frac{1}{48}(10^3 + 24.10^2 - 4.10) = 70$ *(by Theorem 2.4)*

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Topological Indices of Order Sum Graphs

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Abstract

The study of graphs emerging from various algebraic structures like groups, rings, vector spaces, etc. is a well-known and prominent topic of research in algebraic graph theory. In this regard, several graphs have been constructed on finite groups. One such graph that has been recently defined on finite groups is the order sum graphs of finite groups. In this article, we discuss some of the topological indices of the order sum graphs of finite groups, defined based on distance, degree and vertex coloring.

Keywords: Order sum graphs, Topological index, Zagreb indices, Wiener index, Chromatic topological indices
AMS Classification: 05C25, 05C75, 05C12, O5C15

1 Introduction

For terminology in group theory, refer to [7]. For fundamentals in graph theory, see [23], and for definitions and concepts related to coloring in graphs, see [5].

The *order of a group* G, denoted by $|G|$, is the number of elements in the group, and if $|G|$ is finite, then we say G is a finite group of order $|G|$. For every $a \in G$, the *order* of a, denoted by $o(a)$ or $|a|$, is the least positive integer k such that $a^k = e$. A group G is said to be *cyclic* if there exists an element $a \in G$ such that $G = \langle a \rangle$ and a is called the *generator* of G. In view of Cayley's theorem, any cyclic group of order n is isomorphic to the additive group of integer modulo n, denoted by $\mathbb{Z}_n$ and there are $\phi(n)$ generators of the group $\mathbb{Z}_n$, where $\phi(n)$ represents the *Euler's totient function* that gives the number of relatively prime numbers that are less than n.

Graph indices, commonly known as the *topological indices* of graphs, are numerical graph invariants which do not vary with respect to isomorphism. The Wiener index of a graph was the first graph index introduced and it was based on the

shortest distance between the vertices. Following this, several variants of topological indices are being defined using different properties of vertices like their degrees, eccentricities, the geodesic between them, etc (see [4]).

Algebraic graph theory is an emerging research field in which the properties of graphs defined on algebraic structures are studied (see [10, 14, 20]). One of the recently introduced graphs on finite groups is the order sum graphs (see [3]), which is defined as follows.

Definition 1.1. [3] The *order sum graph* of a finite group G, denoted by $\Gamma_{os}(G)$, is a graph with $V(\Gamma_{os}(G)) = \{v_a : a \in G\}$ and any two distinct vertices $v_a, v_b \in V(\Gamma_{os}(G))$ are adjacent, if the sum of the orders of the group elements to which they correspond is greater than the order of the group; that is, for all $v_a, v_b \in V(\Gamma_{os}(G)), v_a v_b \in E(\Gamma_{os}(G))$, when $|a|+|b|> |G|$, where $a, b \in G$ and $v_a, v_b \in V(\Gamma_{os}(G))$ correspond to the elements $a, b \in G$, respectively.

An illustration of the order sum graph associated with a finite group is given in Figure 1.

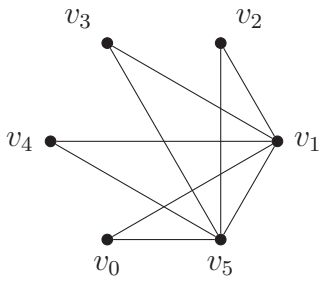

Figure 1 *The order sum graph of a cyclic group of order* 6.

After the initial study on the order sum graphs of finite groups in [3], further study on different types of domination, coloring and other structural properties were done in [2, 12, 13]. On defining an algebraic graph, various structural properties including coloring, domination, and spectra are investigated, in the literature (see [11,15–19]). In this line, determining various topological indices of algebraic graphs have also gained momentum, in recent days (ref. [1,9,10,21]). Hence, in this article, we determine certain distance, degree and coloring-based topological indices of order sum graphs of finite groups.

2 Degree and Distance-based Topological Indices of the Order Sum Graphs

In this section, we compute certain prominent degree-based and distance-based topological indices of the order sum graphs of finite groups. In [3], it has been proved that the order sum graph of any finite group is non-empty if and only if it is cyclic. Hence, we consider only the cyclic groups $\mathbb{Z}_n$ for the study, and denote the set of all generators of $\mathbb{Z}_n$ as G_n.

The oldest topological graph indices related to irregularity of graphs are the first the second Zagreb indices (ref. [6, 24]). These topological indices of a graph X are defined as follows.

(i) The *first Zagreb index* of a graph X, denoted by $M_1(X)$, is defined as $M_1(X) = \sum_{v \in V(G)} d(v)^2$ (see [24]).

(ii) The *second Zagreb index* of a graph X, denoted by $M_2(X)$, is defined as $M_2(X) = \sum_{uv \in E(G)} d(u)d(v)$ (*c.f.* [6]).

Theorem 2.1. *For $n \in \mathbb{N}$,*

$$(i)\ M_1(\Gamma_{os}(\mathbb{Z}_n)) = \begin{cases} n(n-1)^2, & \text{if } n \text{ is prime;} \\ \phi(n)(n-1)^2 + (n-\phi(n))\phi(n)^2, & \text{otherwise.} \end{cases}$$

$$(ii)\ M_2(\Gamma_{os}(\mathbb{Z}_n)) = \begin{cases} (n-1)^4, & \text{if } n \text{ is prime;} \\ (n-1)^2\binom{\phi(n)}{2} + (n-1)\left(n - \phi(n)\binom{\phi(n)+1}{2}\right), & \text{otherwise.} \end{cases}$$

Proof. By Definition 1, we see that any two vertices $v_a, v_b \in V(\Gamma_{os}(\mathbb{Z}_n))$ are adjacent if and only if both a and b are not generators of $\mathbb{Z}_n$. Hence, $d(v_a) = n-1$, when a is a generator of $\mathbb{Z}_n$ and $d(v_a) = \phi(n)$, otherwise.

(i) Based on this, the first Zagreb index of $\Gamma_{os}(\mathbb{Z}_n)$, is computed as follows. When n is prime, $\Gamma_{os}(\mathbb{Z}_n) \cong K_n$. Hence, $M_1(\Gamma_{os}(\mathbb{Z}_n)) = n(n-1)^2$, in this case. When n is composite,

$$M_1(\Gamma_{os}(\mathbb{Z}_n)) = \sum_{a \in G_n} d(v_a)^2 + \sum_{a \notin G_n} d(v_a)^2. \tag{1}$$

As there are $\phi(n)$ generators and $n - \phi(n)$ non-generators of $\mathbb{Z}_n$, Equation (1) becomes

$$M_1(\Gamma_{os}(\mathbb{Z}_n)) = \phi(n)(n-1)^2 + (n-\phi(n))\phi(n)^2. \tag{2}$$

(ii) We can see that the second Zagreb index of $\Gamma_{os}(\mathbb{Z}_n)$ becomes $(n-1)^4$, when n is prime, by (i). Hence, consider the case when n is composite. Each vertex v_a that corresponds to a generator a of $\mathbb{Z}_n$ has $n-1$ neighbours in $\Gamma_{os}(\mathbb{Z}_n)$. Among these $n-1$ neighbours, $\phi(n)-1$ correspond to the generators of $\mathbb{Z}_n$, other than a, and these vertices have degree $n-1$. The remaining $n-\phi(n)$ neighbours of v_a correspond to the non-generators of $\mathbb{Z}_n$, whose degrees are $\phi(n)$. As there are $\phi(n)$ generators of any cyclic group of order n,

$$\sum_{a \in G_n} d(v_a)d(v_b) = \phi(n)(n-1)\Big((n-1)(\phi(n)-1) + (n-\phi(n))\phi(n)\Big), \tag{3}$$

where $b \in \mathbb{Z}_n - \{a\}$. Any vertex v_a that corresponds to a non-generator a of $\mathbb{Z}_n$ has $\phi(n)$ neighbours, which correspond to the generators of $\mathbb{Z}_n$, having degree $n-1$. There are $n-\phi(n)$ non-generators of $\mathbb{Z}_n$, and hence,

$$\sum_{a \notin G_n} d(v_a)d(v_b) = (n-\phi(n))\phi(n)(n-1). \tag{4}$$

We know that $M_2(\Gamma_{os}(\mathbb{Z}_n)) = \sum_{a \in G_n} d(v_a)d(v_b) + \sum_{a \notin G_n} d(v_a)d(v_b)$. Therefore, by Equation (3) and Equation (4),

$$\begin{aligned} M_2(\Gamma_{os}(\mathbb{Z}_n)) &= \frac{1}{2}\Bigg((n-1)((n-1)(\phi(n)-1)+(n-\phi(n))\phi(n)) + \\ &\quad (n-\phi(n))\phi(n)(n-1)\Bigg) \\ &= \frac{1}{2}\Bigg((n-1)^2\phi(n)(\phi(n)-1)+(n-1)\phi(n)^2(n-\phi(n)) + \\ &\quad (n-1)\phi(n)(n-\phi(n))\Bigg) \\ &= \frac{1}{2}(n-1)^2\binom{\phi(n)}{2} + (n-1)\left(n-\phi(n)\binom{\phi(n)+1}{2}\right). \end{aligned}$$

□

Proposition 2.2. *For any composite integer n,*

$$M_2(\Gamma_{os}(\mathbb{Z}_n)) = \phi(n)(n-1)\Big(2|E(\Gamma_{os}(\mathbb{Z}_n))|-\phi(n)+1\Big).$$

Proof. Each vertex v_a that corresponds to a generator a of $\mathbb{Z}_n$ has $n-1$ neighbours in $\Gamma_{os}(\mathbb{Z}_n)$. Therefore, $\sum_{v_a \sim v_b} d(v_a)d(v_b) = (n-1)\sum_{b \in \mathbb{Z}_n - \{a\}} d(v)$. The value of $\sum_{b \in \mathbb{Z}_n - \{a\}} d(v) = \left(\sum_{a \in \mathbb{Z}_n} d(v)\right) - (n-1)$. Therefore, by handshaking lemma, $M_2(\Gamma_{os}(\mathbb{Z}_n)) = \phi(n)(n-1)\Big(2|E(\Gamma_{os}(\mathbb{Z}_n))|-\phi(n)+1\Big)$. □

Following the first and the second Zagreb indices of graphs, the third and the fourth Zagreb indices of graphs, were introduced in the literature, based on the difference between the degrees of the vertices in a graph. These indices which also measure the irregularity in a graph are defined as follows.

(i) The *third Zagreb index*, also known as the *irregularity index*, of a graph X, denoted by $M_3(X)$, is defined as $M_3(X) = \sum_{uv \in E(G)} |d(v) - d(u)|$ (ref. [6]).

(ii) The *fourth Zagreb index* or the *total irregularity index* of a graph X, denoted by $M_4(X)$, is defined as $M_4(X) = \frac{1}{2} \sum_{u,v \in V(G)} |d(v) - d(u)|$ (*c.f.* [8]).

In the following results, we determine the first, second, third and fourth Zagreb indices of the order sum graphs of finite cyclic groups.

Theorem 2.3. *For* $n \in \mathbb{N}$, $M_3(\Gamma_{os}(\mathbb{Z}_n)) = \begin{cases} 0, & \text{if } n \text{ is prime;} \\ 2\phi(n)\binom{n-\rho(n)}{2}, & \text{otherwise.} \end{cases}$

Proof. When n is prime, we can see that the order sum graph of $\mathbb{Z}_n$ is regular. Hence, the irregularity index $M_3(\Gamma_{os}(\mathbb{Z}_n)) = 0$, in this case. Hence, we consider the case when n is composite, for further discussion.

For any two elements $a, b \in \mathbb{Z}_n$,

$$|d(v_a) - d(v_b)| = \begin{cases} n - 1 - \phi(n), & \text{if either } a \text{ or } b \text{ is a generator;} \\ 0, & \text{otherwise.} \end{cases}$$

When a is a generator $\mathbb{Z}_n$,

$$\sum_{v_b \in N(v_a)} |d(v_a) - d(v_b)| = |(n-1)(n-1) - \sum_{v_b \in N(v_a)} d(v_b)| = (n - \phi(n))(n - 1 - \phi(n)).$$

This is because v_a has $n-1$ neighbours, of which only there is degree difference only with the $\phi(n)$ neighbours which correspond to the non-generators of $\mathbb{Z}_n$. On the other hand, when a is a non-generator of $\mathbb{Z}_n$, v_a has a degree difference with all its $\phi(n)$ neighbours. Hence, when a is a non-generator of $\mathbb{Z}_n$,

$$\sum_{v_b \in N(v_a)} |d(v_a) - d(v_b)| = |\phi(n)(n - \phi(n)) - \sum_{v_b \in N(v_a)} d(v_b)| = \phi(n)(n - 1 - \phi(n)).$$

The fact that a degree difference exists between two vertices v_a and v_b in $\Gamma_{os}(\mathbb{Z}_n)$ only when either when a is a generator of $\mathbb{Z}_n$ and b is a non-generator of $\mathbb{Z}_n$, or vice-versa, the expressions $\sum_{v_b \in N(v_a)} |d(v_a) - d(v_b)|$, when $a \in G_n$ and $\sum_{v_b \in N(v_a)} |d(v_a) - d(v_b)|$, when $a \notin G_n$ overlap. Owing to the presence of $\phi(n)$ generators and $n - \phi(n)$ non-generators of $\mathbb{Z}_n$, the result follows. □

Proposition 2.4. *For* $n \geq 2$, $M_4(\Gamma_{os}(\mathbb{Z}_n)) = M_3(\Gamma_{os}(\mathbb{Z}_n))$.

Proof. To compute the fourth Zagreb index of the order sum graph of $\mathbb{Z}_n$, the distance between the degrees of every pair of vertices in $\Gamma_{os}(\mathbb{Z}_n)$ must be computed. A degree difference exists between two vertices v_a and v_b in $\Gamma_{os}(\mathbb{Z}_n)$ only when either when a is a generator of $\mathbb{Z}_n$ and b is a non-generator of $\mathbb{Z}_n$, or vice-versa. Also, this degree difference is $n - \phi(n) - 1$. Hence, $M_4(\Gamma_{os}(\mathbb{Z}_n)) = 0$, when n is prime. When

n is composite, there are no edges between the vertices of $\Gamma_{os}(\mathbb{Z}_n)$ that correspond to two non-generators of $\mathbb{Z}_n$. Also, all the remaining pairs vertices in $\Gamma_{os}(\mathbb{Z}_n)$ are adjacent, and the sum of the degree differences between these vertices have been calculated in Theorem 2.3. Hence the result. □

Following these degree-based topological indices of the order sum graphs of finite groups, certain distance-based topological indices of these graphs, whose definitions are given below, are analysed. The first topological index that has been defined in the literature is the *Wiener indices* of graphs. The *Wiener index* of a graph X, denoted by $W(X)$, is defined as $W(X) = \sum_{u,v \in V(G)} d(u,v)$ (see [22]).

Theorem 2.5. *For $n \in \mathbb{N}$,*

$$W(\Gamma_{os}(\mathbb{Z}_n)) = \begin{cases} \binom{n}{2}, & \text{if } n \text{ is prime;} \\ \frac{1}{2}\left(\phi(n)^2 - (2n-1)\phi(n) + 4\binom{n+1}{2}\right), & \text{otherwise.} \end{cases}$$

Proof. The distance between any two vertices in the order sum graph of a finite cyclic group is at most 2. Except in the case when both the vertices of a considered pair are non-generators of the cyclic group, the distance between them is 2. Hence, when n is prime, $\sum_{a,b \in \mathbb{Z}_n} d(v_a, v_b) = \frac{n}{2}(n-1)$.

Let n be a composite number. If a is a generator of $\mathbb{Z}_n$, $d(v_a, v_b) = 1$, for all $b \in \mathbb{Z}_n - \{a\}$. Therefore, $\sum_{b \in \mathbb{Z}_n - \{a\}} d(v_a, v_b) = n - 1$, for any $a \in G_n$.

If a is not a generator of $\mathbb{Z}_n$, the $\phi(n)$ vertices of $\Gamma_{os}(\mathbb{Z}_n)$ that correspond to the generators of $\mathbb{Z}_n$ are at distance 1 from v_a. Also, the remaining $n - \phi(n) - 1$ vertices of $\Gamma_{os}(\mathbb{Z}_n)$ that correspond to the non-generators of $\mathbb{Z}_n$ are at distance 2 from v_a, in this case. Hence, $\sum_{b \in \mathbb{Z}_n - \{a\}} d(v_a, v_b) = \phi(n) + 2(n - \phi(n) - 1)$, for any $a \notin G_n$. As $|G_n| = \phi(n)$,

$$\begin{aligned} W(\Gamma_{os}(\mathbb{Z}_n)) &= \frac{1}{2}\Big(\phi(n)(n-1) + (n-\phi(n))(\phi(n) + 2(n-\phi(n)-1)\Big) \\ &= \frac{1}{2}\Big(\phi(n)(n-1) + (n-\phi(n))(2n + \phi(n) - 2)\Big) \\ &= \frac{1}{2}\Big(\phi(n)^2 - (2n-1)\phi(n) + 4\binom{n+1}{2}\Big). \end{aligned}$$

□

Following these indices of graphs, we analyse the eccentric connectivity index and modified eccentric connectivity index of the order sum graphs of groups, which are defined as follows.

(i) The *eccentric connectivity index*, of a graph X, denoted by $Ec_1(X)$, is defined as $Ec_1(X) = \sum_{v \in V(G)} ecc(v)d(v)$ (ref. [22]).

(ii) The *modified eccentric connectivity index* of a graph X, denoted by $Ec_2(X)$, is defined as $Ec_2(X) = \sum_{v \in V(G)} ecc(v) \left(\sum_{uv \in E(G)} d(u) \right)$ (*c.f.* [25]).

In the next result, these above defined eccentricity-based topological indices of the order sum graphs of finite cyclic groups are calculated.

Theorem 2.6. *For $n \geq 2$,*

$$(i)\ Ec_1(\Gamma_{os}(\mathbb{Z}_n)) = \begin{cases} 2\binom{n}{2}, & \text{if } n \text{ is prime;} \\ \phi(n)\Big(3n - 2\phi(n) - 1\Big), & \text{otherwise.} \end{cases}$$

$$(ii)\ Ec_2(\Gamma_{os}(\mathbb{Z}_n)) = \begin{cases} n(n-1)^2, & \text{if } n \text{ is prime;} \\ \phi(n)\,(n - \phi(n))\,(2n - 2 + \phi(n)) + & \\ 2(n-1)\binom{\phi(n))}{2}, & \text{otherwise.} \end{cases}$$

Proof. The eccentricity of a vertex $v_a \in V(\Gamma_{os}(\mathbb{Z}_n))$ is 2 if and only if a is a non-generator of $\mathbb{Z}_n$, and n is composite. Based on this, the eccentric connectivity index and modified eccentric connectivity index of the order sum graph of cyclic groups are computed as follows.

(i) When n is prime, $ecc(v_a) = 1$, for all $a \in \mathbb{Z}_a$. Hence, the eccentric connectivity index of $\Gamma_{os}(\mathbb{Z}_n)$ in this case is given as $\sum_{a \in \mathbb{Z}_n} ecc(v_a)d(v_a) = \sum_{a \in \mathbb{Z}_n} d(v_a) = n(n-1)$.

When n is composite, each of the $\phi(n)$ vertices that correspond to any generator a of $\mathbb{Z}_n$ have $ecc(v_a)d(v_a) = n - 1$. Also, for any vertex $v_a \in V(\Gamma_{os}(\mathbb{Z}_n))$ that corresponds to a non-generator of $\mathbb{Z}_n$, $ecc(v_a)d(v_a) = 2\phi(n)$. Therefore, the sum of $ecc(v_a)d(v_a)$, for all the n vertices in $V(\Gamma_{os}(\mathbb{Z}_n))$, is given as follows.

$$\begin{aligned} Ec_1(\Gamma_{os}(\mathbb{Z}_n)) &= \phi(n)(n-1) + 2\phi(n)(n - \phi(n)) \\ &= \phi(n)(n - 1 + 2(n - \phi(n))) \\ &= \phi(n)\Big(3n - 2\phi(n) - 1\Big). \end{aligned}$$

(ii) Now, to compute the modified eccentric connectivity index of $\Gamma_{os}(\mathbb{Z}_n)$, we need the sum of the degrees of the vertices in the neighbourhood of each of the vertex in the graph. If v_a is a vertex in $\Gamma_{os}(\mathbb{Z}_n)$ that corresponds to a non-generator a

of $\mathbb{Z}_n$, then all its neighbours are the vertices that correspond to the generators of $\mathbb{Z}_n$, that have degree $n-1$. Hence, for any such v_a,

$$\sum_{v_a \sim v_b} d(v_b) = \phi(n)(n-1).$$

Let v_a be a vertex in $\Gamma_{os}(\mathbb{Z}_n)$ that corresponds to a generator a of $\mathbb{Z}_n$ that has $n-1$ neighbours. Among these $n-1$, $\phi(n)-1$ neighbours are the vertices that correspond to the generators of $\mathbb{Z}_n$, that have degree $n-1$, and the remaining $n-\phi(n)$ neighbours are the vertices that correspond to the non-generators of $\mathbb{Z}_n$, that have degree $\phi(n)$. Hence, for any such v_a,

$$\sum_{v_a \sim v_b} d(v_b) = (\phi(n)-1)(n-1) + (n-\phi(n))\phi(n).$$

On account of the number of generators and non-generators of $\mathbb{Z}_n$ being $\phi(n)$ and $n-\phi(n)$, respectively,

$$\begin{aligned} Ec_2(\Gamma_{os}(\mathbb{Z}_n)) &= \phi(n)(\phi(n)-1)(n-1) + (n-\phi(n))\phi(n) + (n-\phi(n))(n-1)\phi(n) \\ &= \phi(n)\Big((\phi(n)-1)(n-1) + (n-\phi(n)) + (n-1)(n-\phi(n))\Big) \\ &= \phi(n)\left(n-\phi(n)\right)\left(2n-2+\phi(n)\right) + 2(n-1)\binom{\phi(n)}{2}. \end{aligned}$$

When n is taken as prime, $ecc(v_a) = 1$, for all $a \in \mathbb{Z}_a$. Thus, the modified eccentric connectivity index of $\Gamma_{os}(\mathbb{Z}_n)$ reduces to $\sum_{v_a \in V(\Gamma_{os}(\mathbb{Z}_n))} \sum_{v_b \in V(\Gamma_{os}(\mathbb{Z}_n))} d(v_b) = n(n-1)^2$, in this case.

□

3 Chromatic Topological Indices of the Order Sum Graphs

In [8], the idea of defining topological indices based on a proper vertex coloring c of a graph, rather than distance or degree of the vertices was put-forth. The variation of the well-known Zagreb indices by utilizing the parameter as the color index assigned to a vertex was introduced, in this article. In this section, we compute these chromatic variants of Zagreb indices of the order sum graphs of finite groups.

Let $c : V(X) \to \{c_1, c_2, \ldots, c_k\}$ be a minimum coloring of a graph X. The set of all vertices assigned a particular color in a coloring c is called a *color class*, and the number of vertices given a color c_i is called the *strength* of the color class of the color c_i. We denote the strength of the color class of the color c_i with the notation θ_i.

A vertex coloring of X consisting of the colors having minimum subscripts is called a *minimum parameter coloring*. Among all the minimum parameter colorings possible, a coloring in which θ_i is a non-decreasing (resp. non-increasing) function of i, is called a ψ^- (resp. ψ^+) coloring of X (see [8]).

Let c be a minimum parameter vertex coloring of the graph X. Then,

(i) the *first chromatic Zagreb index* of X, denoted by $M_1^c(X)$, is defined as $M_1^c(X) = \sum_{v \in V(G)} c(v)^2$ (see [8]).

(ii) the *second chromatic Zagreb index* of X, denoted by $M_2^c(X)$, is defined as $M_2^c(X) = \sum_{uv \in E(G)} c(u)c(v)$ (*c.f.* [8]).

(iii) the *third chromatic Zagreb index* of a graph X, denoted by $M_3(X)$, is defined as $M_3^c(X) = \sum_{uv \in E(G)} |c(v) - c(u)|$ (ref. [8]).

(iv) the *fourth chromatic Zagreb index* of a graph X, denoted by $M_4(X)$, is defined as $M_4^c(X) = \frac{1}{2} \sum_{u,v \in E(G)} |c(v) - c(u)|$ (*c.f.* [8]).

Note that as we consider only a minimum parameter coloring of X to compute the chromatic topological indices of graphs, we take the set of all k colors used in such a coloring of X to be the first k natural numbers, in this study.

For any graph X that admits a minimum parameter coloring using k colors, there are $k!$ such minimum parameter assignments possible. Among these $k!$ colorings, the minimum and maximum values of these variants of chromatic Zagreb indices occur when the coloring considered becomes a ψ^- and ψ^+ coloring of X. Therefore, these variants of the chromatic Zagreb indices are denoted as $M_i^{\psi^-}(X)$ and $M_i^{\psi^+}(X)$, respectively, for $1 \leq i \leq 4$.

Theorem 3.1. *For $n \geq 2$,*

$$(i)\ M_1^{\psi^-}(\Gamma_{os}(\mathbb{Z}_n)) = \begin{cases} \frac{n(n+1)(2n+1)}{6}, & \text{if } n \text{ is prime;} \\ n + \frac{1}{3}\binom{\phi(n)+1}{2}(2\phi(n)+7), & \text{otherwise.} \end{cases}$$

$$(ii)\ M_2^{\psi^-}(\Gamma_{os}(\mathbb{Z}_n)) = \begin{cases} \frac{1}{12}n(n^2-1)(3n+2), & \text{if } n \text{ is prime;} \\ (n-\phi(n)-2)a_\phi + \frac{1}{2}\sum_{i=1}^{1+\phi(n)} i(a_\phi - i), & \text{otherwise,} \end{cases}$$

where $a_\phi = \phi(n) + \sum_{i=1}^{\phi(n)} i = \frac{\phi(n)(\phi(n)+3)}{2}$.

Proof. In any chromatic coloring of the order sum graph of a cyclic group, all the vertices that correspond to the generators of $\mathbb{Z}_n$ are universal vertices and they must be assigned unique colors. Also, all the vertices of $\Gamma_{os}(\mathbb{Z}_n)$ that correspond to the non-generators of $\mathbb{Z}_n$ form an independent set and they are adjacent only

to the universal vertices. Hence, all these $n-\phi(n)$ vertices can be assigned the same color. Hence, the colors 1 to $\phi(n)+1$ are used in any minimum parameter chromatic coloring of $\Gamma_{os}(\mathbb{Z}_n)$.

In a ψ^- coloring c of $\Gamma_{os}(\mathbb{Z}_n)$, $c(v_a)=1$, when $a\in G_n$, and the colors $2,3,4\ldots$, $\phi(n)+1$ are assigned to the $\phi(n)$ vertices of $\Gamma_{os}(\mathbb{Z}_n)$ that correspond to the generators of $\mathbb{Z}_n$. With respect to this assignment, the first and the second chromatic Zagreb indices of $\Gamma_{os}(\mathbb{Z}_n)$ are determined as follows.

(i) When n is prime, it is easy to see that $\sum\limits_{a\in\mathbb{Z}_n} c(v_a)^2=\sum\limits_{i=1}^{n} i^2=\frac{n(n+1)(2n+1)}{6}$. When n is composite, as $(n-\phi(n))$ vertices of $\Gamma_{os}(\mathbb{Z}_n)$ are assigned the color 1,

$$\begin{aligned}\sum_{a\notin G_n} c(v_a)^2 &= (n-\phi(n))1^2+2^2+3^2+\ldots+\phi(n)^2+(\phi(n)+1)^2\\ &= n+\phi(n)+\phi(n)^2+\frac{\phi(n)(\phi(n)+1)(2\phi(n)+1)}{6}\\ &= \frac{\phi(n)+1}{6}\Big(6n+(6n-5)\phi(n)+\phi(n)^2\Big).\end{aligned}$$

(ii) The second chromatic Zagreb index of $\Gamma_{os}(\mathbb{Z}_n)$ is computed as follows. First, consider n to be prime. In this case, $\Gamma_{os}(\mathbb{Z}_n)\cong K_n$. Hence, as per the coloring protocol mentioned above,

$$\begin{aligned}M_2^{\psi^-}(\Gamma_{os}(\mathbb{Z}_n)) &= \sum_{1\le i<j\le n} ij\\ &= \frac{1}{2}\Big(\sum_{i=1}^{n}\sum_{j=1}^{n} ij-\sum_{i=1}^{n} i^2\Big)\\ &= \frac{1}{2}\left(\Big(\frac{n(n+1)}{2}\Big)^2-\frac{n(n+1)(2n+1)}{6}\right)\\ &= \frac{1}{12}n(n^2-1)(3n+2).\end{aligned}$$

When n is composite, the are $\phi(n)$ generators are assigned colors i; $2\le i\le \phi(n)+1$. Hence, for any generator a of $\mathbb{Z}_n$,

$$c(v_a)\sum_{v_b\sim v_a} c(v_b)=i((n-\phi(n))1+\left(\sum_{j=2}^{\phi(n)+1} j\right)-i).$$

In the case when a is a non-generator of $\mathbb{Z}_n$, all the $\phi(n)$ neighbours of v_a are assigned unique colors $2,3,\ldots,\phi(n)+1$. Thus,

$$c(v_a)\sum_{v_b\sim v_a} c(v_b)=\sum_{j=2}^{\phi(n)+1} j.$$

In view of this,

$$M_2^{\psi^-}(\Gamma_{os}(\mathbb{Z}_n)) = (n-\phi(n))a_\phi + \sum_{1\le i<j\le 1+\phi(n)} ij$$

$$= (n-\phi(n)-2)a_\phi + \frac{1}{2}\left(\sum_{i=1}^{1+\phi(n)}\sum_{j=1}^{1+\phi(n)} ij - \sum_{i=1}^{1+\phi(n)} i^2\right)$$

$$= \left((n-\phi(n)-2)a_\phi\right) + \frac{1}{2}\sum_{i=1}^{1+\phi(n)} i(a_\phi - i).$$

Hence the result. □

Theorem 3.2. *For $n \geq 2$,*

(i) $$M_1^{\psi^+}(\Gamma_{os}(\mathbb{Z}_n)) = \begin{cases} \frac{n(n+1)(2n+1)}{6}, & \text{if } n \text{ is prime;} \\ \frac{\phi(n)+1}{6}\left(6n + (6n-5)\phi(n) + \phi(n)^2\right), & \text{otherwise.} \end{cases}$$

(ii)

$$M_2^{\psi^+}(\Gamma_{os}(\mathbb{Z}_n)) = \begin{cases} \frac{1}{12}n(n^2-1)(3n+2), & \text{if } n \text{ is prime;} \\ \left((n-\phi(n)-2)(\phi(n)+1)(a_\phi-\phi(n))\right) - & \\ \frac{1}{2}\sum_{i=1}^{1+\phi(n)} i(a_\phi - i), & \text{otherwise} \end{cases}$$

where $a_\phi = \phi(n) + \sum_{i=1}^{\phi(n)} i = \frac{\phi(n)(\phi(n)+3)}{2}$.

Proof. By Theorem 3.1, we know that $\phi(n)+1$ colors are required in any chromatic coloring of $\Gamma_{os}(\mathbb{Z}_n)$. In a ψ^+ coloring of $\Gamma_{os}(\mathbb{Z}_n)$, each of the colors $1, 2, 3, \ldots, \phi(n)$ are assigned to one of the $\phi(n)$ vertices of $\Gamma_{os}(\mathbb{Z}_n)$ that correspond to the generators of $\mathbb{Z}_n$. Also, all the remaining $n-\phi(n)$ vertices of $\Gamma_{os}(\mathbb{Z}_n)$ that correspond to the non-generators of $\mathbb{Z}_n$ are assigned the color $\phi(n)+1$.

It can be seen that the number of vertices of $\Gamma_{os}(\mathbb{Z}_n)$ assigned a particular color in the ψ^+ and ψ^1 coloring of $\Gamma_{os}(\mathbb{Z}_n)$ are same, when n is prime. Hence, $M_1^{\psi^+}(\Gamma_{os}(\mathbb{Z}_n)) = M_1^{\psi^-}(\Gamma_{os}(\mathbb{Z}_n))$ and $M_2^{\psi^+}(\Gamma_{os}(\mathbb{Z}_n)) = M_2^{\psi^-}(\Gamma_{os}(\mathbb{Z}_n))$, when n is prime. Thus, we consider the case when n is composite, for further discussions. Based on the above mentioned ψ^+ coloring of $\Gamma_{os}(\mathbb{Z}_n)$, the first and the second chromatic Zagreb indices of $\Gamma_{os}(\mathbb{Z}_n)$ are determined as follows.

(i) Based on the above mentioned ψ^+ coloring of $\Gamma_{os}(\mathbb{Z}_n)$, the first chromatic Zagreb index of $\Gamma_{os}(\mathbb{Z}_n)$ is computed as

$$\sum_{a\in\mathbb{Z}} c(v_a)^2 = (1^2 + 2^2 + \ldots + \phi(n)^2) + (n-\phi(n)(\phi(n)+1)^2$$

$$= \frac{\phi(n)(\phi(n)+1)(2\phi(n)+1)}{6} + (n-\phi(n)(\phi(n)+1))^2$$
$$= \frac{\phi(n)+1}{6}\Big(6n+(6n-5)\phi(n)+\phi(n)^2\Big).$$

(ii) When n is prime, the coloring protocol is exactly the same as that of the corresponding part of Theorem 3.1, and hence

$$M_2^{\psi^+}(\Gamma_{os}(\mathbb{Z}_n)) = \sum_{1\le i<j\le n} ij = \frac{1}{2}\Big(\sum_{i=1}^{n}\sum_{j=1}^{n} ij - \sum_{i=1}^{n} i^2\Big) = \frac{1}{12}n(n^2-1)(3n+2).$$

When n is composite, we have

$$M_2^{\psi^+}(\Gamma_{os}(\mathbb{Z}_n)) = \Big((n-\phi(n))(\phi(n)+1)\sum_{i=1}^{\phi(n)} i\Big) + \Big(\sum_{1\le i<j\le 1+\phi(n)} ij\Big)$$
$$= \Big((n-\phi(n)-2)(\phi(n)+1)(a_\phi-\phi(n))\Big) - \frac{1}{2}\sum_{i=1}^{1+\phi(n)} i(a_\phi-i),$$

by Theorem 3.1 and the coloring mentioned in (i); completing the proof. □

Theorem 3.3. *For $n \ge 2$,*

$$(i)\ M_3^{\psi^-}(\Gamma_{os}(\mathbb{Z}_n)) = \begin{cases} \sum_{i,j=1}^{n} |i-j|, & \text{if } n \text{ is prime;} \\ (n-\phi(n))\binom{\phi(n)+1}{2} + \frac{1}{2}\sum_{i,j=2}^{\phi(n)+1} |i-j|, & \text{otherwise.} \end{cases}$$

$$(ii)\ M_3^{\psi^+}(\Gamma_{os}(\mathbb{Z}_n)) = \begin{cases} \sum_{i,j=1}^{n} |i-j|, & \text{if } n \text{ is prime;} \\ (n-\phi(n))\binom{\phi(n)+1}{2} + \frac{1}{2}\sum_{i,j=1}^{\phi(n)} |i-j|, & \text{otherwise.} \end{cases}$$

Proof. In the case when n is prime, there is a difference between the colors of any pair of vertices if $\Gamma_{os}(\mathbb{Z}_n)$. Also, of i is the color assigned to a vertex v_a, for some $a \in \mathbb{Z}_n$, by a ψ^- or ψ^+ coloring c of $\Gamma_{os}(\mathbb{Z}_n)$, $\sum_{b\in\mathbb{Z}_n} |c(v_a)-c(v_b)| = |i-1|+|i-2|+\ldots+|i-(i-1)|+|i-(i+1)|+\ldots+|i-n|$, where $b \in \mathbb{Z}_n - \{a\}$. Hence, $M_3^{\psi^1}(\Gamma_{os}(\mathbb{Z}_n)) = M_3^{\psi^+}(\Gamma_{os}(\mathbb{Z}_n)) = \sum_{a,b\in\mathbb{Z}_n} |c(v_a)-c(v_b)| = \sum_{i,j=1}^{n} |i-j|$, in this case.

Let n be composite. If a is a non-generator of $\mathbb{Z}_n$, then v_a is assigned the color 1 by any ψ^- coloring c of $\Gamma_{os}(\mathbb{Z}_n)$. Hence,

$$|c(v_a)-c(v_b)| = \sum_{j=1}^{\phi(n)+1} |1-j|$$

$$= \frac{\phi(n)(\phi(n)+1)}{2},$$

where $b \in G_n$. If a is a generator of $\mathbb{Z}_n$, then v_a is assigned a color i, where $2 \leq i \leq \phi(n)+1$, by any ψ^- coloring c of $\Gamma_{os}(\mathbb{Z}_n)$. If $c(v_a) = i$, then

$$\begin{aligned}|c(v_a) - c(v_b)| &= |i-1|(n-\phi(n)) + |i-2| + \ldots + |i-(i-1)| + \\ &\quad |i-(i+1)| + \ldots + |i-(\phi(n)+1)| \\ &= (n-\phi(n))(i-1) + \sum_{j=2}^{\phi(n)+1} |i-j|.\end{aligned}$$

Therefore, in view of the $\phi(n)$ number of generators assigned the colors $2 \leq i \leq \phi(n)+1$, we get

$$\begin{aligned}\sum_{a \in G_n} |c(v_a) - c(v_b)| &= \sum_{i=2}^{n} (n-\phi(n))(i-1) + \sum_{j=2}^{\phi(n)+1} |i-j| \\ &= (n-\phi(n))\frac{\phi(n)(\phi(n)+1)}{2} + \sum_{i=2}^{n}\sum_{j=2}^{n} |i-j| \\ &= (n-\phi(n))\binom{\phi(n)+1}{2} + \sum_{i,j=2}^{\phi(n)+1} |i-j|.\end{aligned}$$

Based on the above discussions, we deduce the third chromatic Zagreb index of the order sum graphs of cyclic group of composite order as follows.

$$\begin{aligned}M_3^{\psi^1}(\Gamma_{os}(\mathbb{Z}_n)) &= \frac{1}{2}\left((n-\phi(n))\binom{\phi(n)+1}{2} + (n-\phi(n))\binom{\phi(n)+1}{2} + \sum_{i,j=2}^{\phi(n)+1} |i-j|\right) \\ &= (n-\phi(n))\binom{\phi(n)+1}{2} + \frac{1}{2}\sum_{i,j=2}^{\phi(n)+1} |i-j|.\end{aligned}$$

Now, when we consider a ψ^- coloring of $\Gamma_{os}(\mathbb{Z}_n)$, the color assigned to the vertices corresponding to the $n-\phi(n)$ non-generators of $\mathbb{Z}_n$ is $\phi(n)+1$, Hence, for any $b \in \mathbb{Z} - n - \{a\}$,

(a) if a is a non-generator of $\mathbb{Z}_n$,

$$|c(v_a) - c(v_b)| = \sum_{j=1}^{\phi(n)} |\phi(n)+1-j| = \frac{\phi(n)(\phi(n)+1)}{2}.$$

(b) if a is a generator of $\mathbb{Z}_n$ such that i is the color assigned to v_a, for some $1 \leq i \leq \phi(n)$,

$$|c(v_a) - c(v_b)| = (n - \phi(n))(\phi(n) + 1 - i) + \sum_{j=1}^{\phi(n)} |i - j|.$$

Therefore, based on (a) and (b), we get

$$\begin{aligned} M_3^{\psi^1}(\Gamma_{os}(\mathbb{Z}_n)) &= \frac{1}{2}\left(2(n - \phi(n))\binom{\phi(n)+1}{2} + \frac{1}{2}\sum_{i,j=1}^{\phi(n)} |i - j|\right). \\ &= (n - \phi(n))\binom{\phi(n)+1}{2} + \frac{1}{2}\sum_{i,j=1}^{\phi(n)} |i - j|. \end{aligned}$$

□

When we compute the third chromatic Zagreb index of the order sum graph of $\mathbb{Z}_n$, we can see that there is no difference in the color assigned to the vertices that correspond to the non-generators of $\mathbb{Z}_n$). Also, all the pairs of vertices between which there is a color difference are adjacent. Hence, using the formula of the fourth chromatic Zagreb index of graphs, the following result is obtained.

Proposition 3.4. *For any $n \geq 2$,*

$$M_4^{\psi^-}(\Gamma_{os}(\mathbb{Z}_n)) = \frac{1}{2}M_3^{\psi^-}(\Gamma_{os}(\mathbb{Z}_n)) \text{ and } M_4^{\psi^+}(\Gamma_{os}(\mathbb{Z}_n)) = \frac{1}{2}M_3^{\psi^+}(\Gamma_{os}(\mathbb{Z}_n)).$$

4 Conclusion

In this article, we have determined certain distance, degree and coloring-based topological indices for the order sum graph of finite groups based on its structural properties. As the order sum graph of a finite group has a very clear structure of a split graph, it gives scope for further extension of studies. Also, computing chromatic topological indices for algebraic graphs is a novel research topic. This offers plethora of opportunities to explore further, in this direction.

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Some New Properties of the Second Omega Coindex

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Abstract

We present a comprehensive theoretical study of the second omega coindex and derive a fundamental identity that connects index and coindex values. Our main result shows that for any simple graph G, the sum $\Omega_2(G) + \overline{\Omega}_2(G)$ depends only on the degree sequence of G, thereby providing an invariant determined solely by degree distribution. We establish Nordhaus–Gaddum type inequalities for regular graphs, prove general upper bounds whose growth is of order n^6, and characterize extremal cases. This study enhances the understanding of omega-type indices and contributes to the classification of topological indices according to their structural properties.

Keywords: Second omega index, Coindex, Nordhaus–Gaddum inequalities, Topological indices, Degree sequence, Regular graphs
AMS Classification: 05C09, 05C92

1 Introduction and Preliminaries

Graph theory has emerged as a fundamental branch of discrete mathematics with profound applications across diverse scientific domains, from chemistry and biology to computer science and social network analysis, [3]. Central to many graph-theoretic investigations is the study of topological indices—numerical invariants that capture essential structural properties of graphs and enable quantitative analysis of complex networks.

Among the extensive family of topological indices, degree-based indices have attracted considerable attention due to their computational simplicity and meaningful interpretations in various contexts, [9, 20]. The classical Zagreb indices, introduced by Gutman and Trinajstić, [11], in the 1970s, pioneered this area by establishing connections between molecular structure and chemical properties. Subsequently, numerous variants and generalizations have been developed, each offering unique insights into graph structure, [2, 10].

The second omega index was recently formulized as a new degree–based topological descriptor, [19]. It emerges as an extension of the original omega invariant, which was first introduced by Delen and Cangül as a novel graph invariant in 2018, [4]. While the classical omega invariant describes structural aspects of

graphs, the second omega index uses degree sequence data in a multiplicative way, making it more effective for the study of graph properties.

Let $G = (V, E)$ denote a simple graph with vertex set $V = V(G)$ and edge set $E = E(G)$. We use $n = |V(G)|$ to denote the order of G and $m = |E(G)|$ to denote its size. For a vertex $v \in V$, we denote by $d(v) = d_G(v)$ the degree of v in G, and by $\Delta(G) = \Delta$ the maximum degree of G.

The *degree sequence* of G is denoted as

$$DS(G) = \{1^{(a_1)}, 2^{(a_2)}, \ldots, \Delta^{(a_\Delta)}\}, \tag{1}$$

where $a_i = |\{v \in V : d(v) = i\}|$ represents the number of vertices of degree i in G. Note that $\sum_{i=1}^{\Delta} a_i = n$ and $\sum_{i=1}^{\Delta} i \cdot a_i = 2m$ by the handshaking lemma.

The *omega index* of a graph G with degree sequence $DS(G) = \{1^{(a_1)}, 2^{(a_2)}, \ldots, \Delta^{(a_\Delta)}\}$ is defined as [19]

$$\Omega(G) = \sum_{i=3}^{\Delta} (i-2)\, a_i - a_1. \tag{2}$$

This invariant provides structural and combinatorial information about a graph solely in terms of its degree sequence, such as connectedness, cyclicness, and realizability.

The *second omega index* of G is defined as

$$\Omega_2(G) = \sum_{uv \in E(G)} [(d(u)-2)a_{d(u)}] \cdot [(d(v)-2)a_{d(v)}], \tag{3}$$

where the sum extends over all edges uv of G.

This index exhibits several remarkable properties that distinguish it from its predecessors. Unlike many traditional indices that depend solely on local vertex degrees, the second omega index not only incorporates global structural information through the degree sequence multiplicities a_i, but also takes into account the adjacency of vertices by summing over edges. In this way, it establishes a connection between local degree information, global degree distribution, and the edge structure of the graph.

A natural extension of any graph index is its corresponding coindex, which considers non-adjacent vertex pairs rather than edges. The *second omega coindex*, recently introduced in [17], is given by

$$\overline{\Omega_2}(G) = \sum_{\substack{u,v \in V(G) \\ uv \notin E(G)}} [(d(u)-2)a_{d(u)}] \cdot [(d(v)-2)a_{d(v)}], \tag{4}$$

where the sum extends over all non-adjacent pairs of vertices in G.

The systematic study of index-coindex relationships has proven invaluable in understanding the complete structural picture of graphs. Such relationships often reveal deep mathematical identities that connect seemingly disparate aspects of graph topology.

For a graph G, its *complement* $\overline{G}$ has the same vertex set $V(G)$ and edge set $\{\{u, v\} : u, v \in V(G), u \neq v, \{u, v\} \notin E(G)\}$. The development of Nordhaus–Gaddum type inequalities represents a classical theme in extremal graph theory, [1]. Named after the pioneering work of Nordhaus and Gaddum, [16], on chromatic

numbers, these results establish relationships between a graph parameter and its value on the complement graph, providing fundamental insights into how graph properties transform under complementation, [3, 12].

In this paper, we develop a theoretical basis for the second omega coindex and its connection with the corresponding index. First, we prove an *Index–Coindex Relation*, showing that for any simple graph G, the sum $\Omega_2(G) + \overline{\Omega_2}(G)$ depends only on the degree sequence of G, providing a fundamental invariant relationship that generalizes earlier results in topological index theory. We then present an *explicit computational formula*, which allows this sum to be expressed directly in terms of degree sequence multiplicities, making it possible to compute efficiently without constructing the graph itself. Furthermore, we derive *Nordhaus–Gaddum type inequalities* for the coindex values of a graph and its complement, with special emphasis on regular graphs where exact formulas can be obtained, [8]. We also investigate *extremal cases*, describing graphs that reach the minimum and maximum values of these measures, and show that for graphs with n vertices the maximum value grows on the order of n^6. Finally, we establish *general upper bounds* valid for all simple graphs and illustrate the sharpness of our results through explicit constructions.

The results of this work not only clarify the role of omega-type indices but also contribute to the broader effort of classifying topological indices according to their extremal and structural properties, [15]. The index–coindex relation we establish introduces a new type of invariant identity that may motivate similar studies for other graph parameters.

In addition, our findings have potential applications in chemical graph theory, where topological indices are widely used as molecular descriptors for predicting physical and chemical properties, [14]. By incorporating global degree sequence information, the second omega index can distinguish between molecules with the same local environments but different overall structures, [13, 6].

2 Main results

In this section, we present the central identity connecting the second omega index and its coindex. This result shows that their sum is determined entirely by the degree sequence of the graph, independent of its specific edge structure.

Theorem 2.1 (Index-Coindex Identity) *For every simple graph G, the following identity holds:*

$$\Omega_2(G) + \overline{\Omega}_2(G) = \sum_i \binom{a_i}{2}((i-2)a_i)^2 + \sum_{i<j} a_i a_j\,((i-2)a_i)((j-2)a_j). \tag{5}$$

In particular, the sum $\Omega_2(G) + \overline{\Omega}_2(G)$ depends only on the degree sequence of G.

Proof. For any unordered pair of distinct vertices $\{u, v\} \subseteq V$ define

$$W(u, v) := ((d(u) - 2)a_{d(u)})((d(v) - 2)a_{d(v)}).$$

Let $\mathcal{P}$ denote the set of all $\binom{|V|}{2}$ unordered vertex pairs, and consider the global sum

$$S := \sum_{\{u,v\}\in\mathcal{P}} W(u, v).$$

If both vertices lie in the same degree class $V_i = \{v : d(v) = i\}$ of size a_i, there are $\binom{a_i}{2}$ such pairs, each contributing $((i-2)a_i)^2$. If the vertices lie in distinct degree classes V_i and V_j with $i < j$, then there are $a_i a_j$ such pairs, each contributing $((i-2)a_i)((j-2)a_j)$. Hence

$$S = \sum_i \binom{a_i}{2}((i-2)a_i)^2 + \sum_{i<j} a_i a_j\,((i-2)a_i)((j-2)a_j). \tag{6}$$

On the other hand, every pair $\{u, v\} \in \mathcal{P}$ is either an edge or a non-edge, so

$$S = \sum_{uv\in E} W(u,v) + \sum_{uv\notin E} W(u,v) = \Omega_2(G) + \overline{\Omega}_2(G),$$

where the first term is exactly $\Omega_2(G)$ by 3, and the second term is $\overline{\Omega}_2(G)$ by definition. Combining this with (6) yields the desired identity (5). ■

Corollary 2.2 *For any realizable degree sequence DS, define*

$$S(DS) := \sum_i \binom{a_i}{2}((i-2)a_i)^2 + \sum_{i<j} a_i a_j\,((i-2)a_i)((j-2)a_j).$$

Then every realization G of this degree sequence satisfies

$$\overline{\Omega}_2(G) = S(DS) - \Omega_2(G).$$

In other words, for fixed degree sequence DS, the value of $\Omega_2(G) + \overline{\Omega}_2(G)$ is constant across all realizations G of DS.

To illustrate the identity, we now verify it on an example.

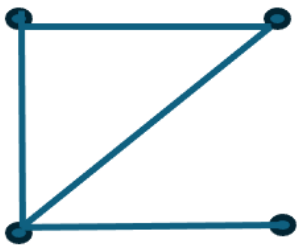

Figure 1: An example graph used to illustrate the Index–Coindex Relation.

Consider the graph in Figure 1, which has degree sequence

$$DS(G) = \{1^{(1)}, 2^{(2)}, 3^{(1)}\}.$$

A direct computation gives

$$\Omega_2(G) = -1, \qquad \overline{\Omega}_2(G) = 0,$$

while from the formula we obtain

$$S(DS) = a_1 a_3 ((1-2)a_1)((3-2)a_3) = 1 \cdot 1 \cdot (-1) \cdot 1 = -1.$$

Hence

$$\Omega_2(G) + \overline{\Omega}_2(G) = S(DS),$$

confirming the Index-Coindex relation for this graph.

2.1 Nordhaus–Gaddum-Type Results for the Second Omega Coindex

The study of Nordhaus–Gaddum type inequalities is a classical theme in extremal graph theory and has also been investigated for many topological indices [1]. Such results typically provide bounds on the sum or product of a graph parameter evaluated on a graph and its complement.

From Theorem 2.1, recall that for any graph G,

$$\overline{\Omega}_2(G) = S(DS(G)) - \Omega_2(G), \tag{7}$$

where $S(DS(G))$ is determined solely by the degree sequence of G.

Lemma 2.3 (Degree sequence of the complement) *Let $n = |V(G)|$. If $DS(G) = \{1^{(a_1)}, 2^{(a_2)}, \ldots, (n-1)^{(a_{n-1})}\}$, then*

$$DS(\overline{G}) = \{0^{(a_{n-1})}, 1^{(a_{n-2})}, \ldots, (n-1)^{(a_0)}\},$$

i.e., $\bar{a}_j = a_{n-1-j}$ for $0 \le j \le n-1$.

Proof. For every $v \in V(G)$, $d_{\overline{G}}(v) = n - 1 - d_G(v)$ [3]. Counting multiplicities gives $\bar{a}_j = |\{v : d_{\overline{G}}(v) = j\}| = |\{v : d_G(v) = n-1-j\}| = a_{n-1-j}$. ■

Proposition 2.4 *For every n-vertex graph G,*

$$\overline{\Omega}_2(G) + \overline{\Omega}_2(\overline{G}) = [S(DS(G)) + S(DS(\overline{G}))] - [\Omega_2(G) + \Omega_2(\overline{G})]. \tag{8}$$

Moreover, by Lemma 2.3,

$$S(DS(\overline{G})) = \sum_i \binom{a_i}{2} ((n-3-i)a_i)^2 + \sum_{i<j} a_i a_j ((n-3-i)a_i)((n-3-j)a_j), \tag{9}$$

so the right-hand side of (8) can be expressed purely in terms of the multiplicities a_i of G together with the index values $\Omega_2(G)$ and $\Omega_2(\overline{G})$.

Proof. Equation (8) follows by applying (7) to G and to $\overline{G}$ and then adding the results. For (9), substitute $\bar{a}_j = a_{n-1-j}$ for $\overline{G}$ and reindex using $j = n-1-i$, noting that $j-2 = n-3-i$. ■

Theorem 2.5 *Let G be k-regular on n vertices and $\overline{G}$ its complement (which is $(n-1-k)$-regular). Then*

$$\overline{\Omega}_2(G) + \overline{\Omega}_2(\overline{G}) = \frac{n^3}{2}\Big[(k-2)^2(n-1-k) + (n-3-k)^2 k\Big]. \tag{10}$$

In particular, for $n \geq 10$ the right-hand side is a concave quadratic in k whose maximum over $k \in \{0, 1, \ldots, n-1\}$ is attained at

$$k^\star = \arg\max_k \Big\{(-n+9)k^2 + (n^2 - 10n + 9)k + 4(n-1)\Big\} \approx \frac{n}{2} - \frac{1}{2},$$

and hence

$$\max_k \ (\overline{\Omega}_2(G) + \overline{\Omega}_2(\overline{G})) = \frac{n^6}{8} + O(n^5). \tag{11}$$

Proof. For a k-regular graph, by a direct count of non-edges ($\binom{n}{2} - \frac{kn}{2}$ many) and using the uniform degree k we get $\overline{\Omega}_2(G) = \frac{(k-2)^2 n^3 (n-1-k)}{2}$; the complement contributes $\frac{(n-3-k)^2 n^3 k}{2}$ analogously [8]. This proves (10). Expanding the bracket gives $(-n+9)k^2 + (n^2 - 10n + 9)k + 4(n-1)$, which is concave for $n \geq 10$, hence maximized at its vertex. Substituting $k^\star = \frac{n^2 - 10n + 9}{2(n-9)}$ and simplifying yields (11). ■

Proposition 2.6 *For any n-vertex simple graph G,*

$$\left|\overline{\Omega}_2(G)\right| \leq \frac{n(n-1)}{2}\,(n(n-3))^2 \quad \textit{and} \quad \left|\overline{\Omega}_2(G) + \overline{\Omega}_2(\overline{G})\right| \leq n(n-1)\,(n(n-3))^2. \tag{12}$$

Consequently, $\overline{\Omega}_2(G) + \overline{\Omega}_2(\overline{G}) = O(n^6)$, and Theorem 2.5 shows this order is sharp.

Proof. Each unordered pair contributes a weight $W(u,v) = ((d(u)-2)a_{d(u)})((d(v)-2)a_{d(v)})$. We have $|d(u)-2| \leq n-3$ and $a_{d(u)} \leq n$, hence $|W(u,v)| \leq (n(n-3))^2$. There are at most $\binom{n}{2}$ non-edges in G and at most $2\binom{n}{2}$ non-edges counting G and $\overline{G}$ together, which yields (12). ■

Remark 2.7

- K_n: $\overline{\Omega}_2(K_n) = \overline{\Omega}_2(\overline{K_n}) = 0$ *(tight lower endpoint for the sum).*
- S_n *(star graph):* $\overline{\Omega}_2(S_n) = \frac{(n-1)^3(n-2)}{2}$, *while* $DS(\overline{S_n}) = \{0^{(1)}, (n-2)^{(n-1)}\}$ *gives* $\overline{\Omega}_2(\overline{S_n}) = -(n-1)^2(2n-8)$*; hence*

$$\overline{\Omega}_2(S_n) + \overline{\Omega}_2(\overline{S_n}) = \frac{(n-1)^2}{2}\,(n^2 - 7n + 18) > 0 \quad (\textit{all } n \geq 3).$$

- C_n *(cycle): both coindices vanish, so the sum is* 0.

These examples illustrate that the sum can be zero *(complete/cycle),* positive and of order n^4 *(stars), and* as large as order n^6 *(near-$n/2$ regular graphs), coherently with Proposition 2.6 and Theorem 2.5. This diversity of behaviors demonstrates the richness of the second omega coindex family [7,* **?***].*

Product-type NG bounds Following the classical approach to Nordhaus–Gaddum inequalities, [1], we can derive multiplicative bounds. For any real numbers x, y, we have $xy \leq \frac{(x+y)^2}{4}$. Therefore,

$$\overline{\Omega}_2(G) \cdot \overline{\Omega}_2(\overline{G}) \leq \frac{(\overline{\Omega}_2(G) + \overline{\Omega}_2(\overline{G}))^2}{4}. \tag{13}$$

Combining (13) with Theorem 2.5 (regular case) or with the universal bound (12) yields immediate product-type NG inequalities, extending the classical framework to omega-type indices.

3 Conclusion and Future Work

We have established an index–coindex relation for the second omega index, showing that the sum $\Omega_2(G) + \overline{\Omega}_2(G)$ depends only on the degree sequence of G. Our Nordhaus–Gaddum analysis highlights the role of regular graphs in attaining extremal values, with the maximum sum growing on the order of n^6. These results demonstrate that omega-type indices possess a rich structural behavior.

Several directions remain open for future research, including the extension of our methods to other omega-type indices, the search for analogous relations in different index families, and computational studies of extremal graphs. In addition, applications to chemical graph theory appear promising, since the second omega index incorporates degree sequence information and thus can help distinguish molecules with similar local environments but different global structures.

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Interpretation of Fractional Dominating Parameters in Chemical Graphs

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Abstract

Benzenoid molecules are represented here as simple, connected graphs, with vertices corresponding to atoms and edges indicating chemical bonds. Our findings provide significant insights into the behavior of γ_f for polycyclic aromatic hydrocarbons, revealing its structural dependencies. Beyond benzenoid systems, we extend our study to other classes of chemical graphs, including dendrimers and fullerenes. In particular, we derive the exact values of γ_f for fullerene families under various modifications, offering a comprehensive analysis of how structural alterations influence their fractional domination properties. We also conduct a structural analysis of linear benzenoid chains by establishing bounds for other domination parameters, including the independence domination number(i), independence number(α), and cover number(β). Additionally, we examine the impact of structural modifications, such as vertex and edge additions or deletions on the γ_f of these chains. Our results contribute to the mathematical understanding of molecular graph theory and provide valuable implications for network science.

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1 Introduction

Extensive research on domination [16] has led to a wealth of documented findings and applications. Among these, fractional domination has emerged as a noteworthy variant, garnering considerable attention due to its theoretical advancements, [15].

Let G^* be a graph where the vertices correspond to atoms and the edges represent bonds. In a graph G^*, a vertex (or edge) independent set consists of vertices (or edges) where no two elements are adjacent. The vertex (or edge) independence number of G^*, denoted by $\beta(G^*)$ (or $\beta_1(G^*)$), represents the largest possible size of such an independent set. Similarly, a vertex (or edge) cover set is a collection of vertices (or edges) such that every edge (or vertex) of the graph is incident to at least one element of the set. The vertex (or edge) cover number of G^*, denoted by $\alpha(G^*)$ (or $\alpha_1(G^*)$), is the smallest possible size of such a cover set. For edge covers, it is assumed that the graph contains no isolated vertices.

A dominating set is a set of vertices such that every vertex in the graph either belongs to the set or is adjacent to a vertex in it. The domination number, denoted by $\gamma(G^*)$, is the smallest possible size of a dominating set. The independent domination number, $i(G^*)$, is defined as the minimum size of a maximal independent set [4, 11]. For any vertex $x_1 \in V(G^*)$, the open neighborhood $Z(x_1)$ is the set of vertices adjacent to x_1, while the closed neighborhood is $Z[x_1] = Z(x_1) \cup \{x_1\}$. Similarly, for any edge $m_1 \in E(G^*)$, the open neighborhood $Z(m_1)$ includes all edges adjacent to m_1, and the closed neighborhood is $Z[m_1] = Z(m_1) \cup \{m_1\}$, [8]. A function $f : V(G^*) \to [0,1]$ is called a Fractional Dominating Function (FDF) if, for every vertex $x_1 \in V(G^*)$, it satisfies $f(Z[x_1]) = \sum_{x_2 \in Z[x_1]} f(x_2) \geq 1$. The fractional domination number, $\gamma_f(G^*)$, is the minimum total weight among all FDFs, [17]. Similarly, a function $g : E(G^*) \to [0,1]$ is a Fractional Edge Dominating Function (FEDF) if, for every edge $m_1 \in E(G^*)$, $g(Z[m_1]) = \sum_{m_2 \in Z[m_1]} g(m_2) \geq 1$. The fractional edge domination number, denoted $\gamma'_g(G^*)$, is the minimum total weight of all FEDFs in G^*, [1].

Klobučar and Vukićević, [9], examined K-dominating sets on linear benzenoids and hexagonal grids, while Klobučar and Barišić, [10], studied total and double total domination in octagonal grids. Quadras et al., [13], analyzed domination in various chemical graphs, and Bukhary, [5], provided an in-depth exploration of domination in benzenoid systems. Hayat et al., [7], investigated predictive topological indices related to benzenoid hydrocarbons, and Raji and Jayalalitha [14] studied domination sequences in fractal-based linear benzenoid graphs. Although domination parameters and their structural roles have been extensively explored

in chemical graphs, the fractional domination properties of key molecular structures remain largely unaddressed. This presents a compelling opportunity to gain new structural insights and refine our understanding of molecular stability and reactivity.

In this study, to push the boundaries of this exploration, we extend our analysis to other classes of chemical graphs, such as polycyclic aromatic hydrocarbon, Balaban 10-cage, dendrimers and fullerenes. By determining the exact values of γ_f under specific structural modifications, we establish a broader framework for understanding fractional domination across diverse molecular structures and we also undertake a systematic structural analysis of linear benzenoid chains, establishing precise bounds for fractional domination-related parameters, including the independence domination number(i), independence number (α), and cover number (β). More importantly, we explore the impact of structural modifications on the γ_f, a crucial yet understudied property in PAHs. Our findings reveal intricate dependencies between molecular structure and fractional domination, challenging existing paradigms in molecular graph theory. Beyond theoretical advancements, our study demonstrates the practical relevance of fractional domination in computational chemistry. Minimizing γ_f allows for the identification of the most reactive atomic sites in complex molecules, providing a novel approach to optimizing reaction pathways, predicting catalytic behavior, and enhancing synthetic efficiency. This work not only addresses an uncharted aspect of chemical graph theory but also introduces a foundation for future explorations into fractional domination as a predictive tool in molecular design.

2 Fractional domination number in the family of chemical graphs

This section examines the γ_f for selected families of chemical graphs, including polycyclic aromatic hydrocarbons(PAHs), fullerenes, and dendrimers. Benzenoid hydrocarbons(BHs) are a specific subset of PAHs that consist solely of fused benzene rings, while PAHs encompass a broader range of compounds with multiple aromatic rings, not all exclusively composed of fused benzene rings, [6, 3]. Fullerene graphs represent the structure of fullerenes and these graphs are highly symmetric and planar. The dendrimer family of graphs consists of highly branched, tree-like macromolecules where each branching level represents a generation of the dendrimer. These graphs feature hierarchical, regular branch-

ing patterns and are used to model complex, structured polymers. Our investigation reveals a compelling insight for these PAHs, the γ_f is equal to the γ. This finding has significant theoretical and practical implications. After careful observation and thorough analysis of the fractional domination number in various BHs including pyrene networks, hexabenzocoronene, parallelogram benzenoids, triangulenes, benzene, naphthalene, and anthracene as well as in other PAHs like pyrene, chrysene, and coronene, we arrive at the following conclusion.

Theorem 1. *For any PAH,* $\gamma_f(PAH) = \gamma(PAH)$.

Proof. Let D_{PAH} be a minimum γ-set of a given PAH, meaning $|D_{PAH}| = \gamma(\text{PAH})$. Consider a FDF $f : V(\text{PAH}) \to [0,1]$ that satisfies $f(Z[x_1]) = \sum_{x_2 \in Z[x_1]} f(x_2) \geq 1$ for every $x_1 \in V(PAH)$. Assigning $f(x_i) = 1$ for all $x_i \in D_{PAH}$ and $f(x_i) = 0$ for all $x_i \notin D_{PAH}$ where $1 \leq i \leq n$ clearly forms a valid FDF, yielding $\gamma_f(\text{PAH}) \leq \gamma(\text{PAH})$. Suppose, in contrast, that $\gamma_f(\text{PAH}) < \gamma(\text{PAH})$, which implies the existence of FDF g satisfying $\sum_{x_i \in V(\text{PAH})} g(x_i) < |D_{PAH}|$. This implies that at least one vertex $\sum_{x_i \in Z[x_{i+1}]} g(x_i) < 1$, which violates the domination condition. Hence, no such FDF can exist, ensuring that no valid FDF achieves a strictly smaller value than $\gamma(\text{PAH})$. Therefore, we conclude that $\gamma_f(\text{PAH}) = \gamma(\text{PAH})$. □

Corollary 1. *For any BH,* $\gamma_f(BH) = \gamma(BH)$.

Proof. Since BHs form a subclass of PAHs, it follows directly from Theorem 1. $\gamma_f(\text{BH}) = \gamma(\text{BH})$. □

Balaban (3-10)-cage graph The Balaban (3,10)-cage, or simply the Balaban 10-cage, is a bipartite graph consisting of 70 vertices & 105 edges. Named after A. T. Balaban and first published in 1972 [2], this graph is significant in graph theory. Even though this was the first (3,10)-cage to be discovered, it does not stand as a unique graph. In chemistry, such cage structures and their associated graphs are used to simulate chemical processes and degenerate rearrangements[12].

Theorem 2. *Let BCG be the Balaban 10-cage graph. Then,* $\gamma_f(BCG) = \frac{70}{4}$.

Proof. We define $f : V(BCG) \to [0,1]$ as $f(x_i) = \frac{1}{4} \ \forall \ x_i \in V(BCG)$, satisfying $f(Z[x_i]) \geq 1$ for every $x_i \in V(BCG)$. The total weight of this function is $\sum_{x_i \in V(BCG)} f(x_i) = \frac{70}{4}$. Assume that there exists $g : V(BCG) \to [0,1]$ for which g is a FDF and $g < f$. Then, for some $x_i \in V(BCG)$, it follows that $g(Z[x_i]) < 1$, contradicting the definition of a FDF. Hence, f is a minimal FDF, which implies $\gamma_f(BCG) = \frac{70}{4} < \gamma(BCG)$. □

Similarly, an examination of other chemical graph families, including fullerenes and dendrimers, yields the following findings.

Theorem 3. *For each dendrimer D belonging to the family of chemical graphs,* $\gamma_f(D) = \gamma(D)$.

Proof. We need to show that for any D, $\gamma_f(D) = \gamma(D)$ is satisfied. First, denote by S a γ-set of D, so $|S| = \gamma(D)$. Define $f : V(D) \to [0,1]$ by $f(x_i) = \begin{cases} 1, & \text{if } x_i \in S \\ 0, & \text{otherwise} \end{cases}$ where $1 \leq i \leq n$. Because S forms a γ-set, each vertex $x_i \in V(D)$ satisfies $\sum_{x_{i+1} \in Z[x_i]} f(x_{i+1}) \geq 1$. Thus, f is a valid FDF of D, and $\sum_{x_i \in V(D)} f(x_i) = |S| = \gamma(D)$ for $(1 \leq i \leq n)$. Since $\gamma_f(D)$ indicates the minimum assigned weight of a FDF, we obtain $\gamma_f(D) \leq \gamma(D)$. Now, let f be an optimal FDF for D so that $\sum_{x_i \in V(D)} f(x_i) = \gamma_f(D)$. The fact that D is a hierarchical and highly branched structure ensures that fractional weight assignments do not provide an advantage over integer assignments. In any D, the domination constraints push fractional assignments to whole numbers because each leaf vertex must be dominated, forcing a nearby vertex to receive a weight of at least 1, and each internal vertex has limited neighbors, restricting possible fractional allocations. Because of the branching structure, the optimum is always realized by an integral function, ensuring the presence of a γ-set of cardinality bounded above by $\gamma_f(D)$. Hence, a γ-set S^* can be found with $|S^*| \leq \gamma_f(D)$, which implies $\gamma(D) \leq \gamma_f(D)$. Since we have established both inequalities, $\gamma_f(D) = \gamma(D)$ holds. □

Theorem 4. *For each Fullerene Graph(FG) consisting of n vertices,*

$$\gamma_f(FG) = \frac{n}{4}. \tag{1}$$

Proof. A fullerene graph is a cubic simple graph, meaning each vertex has exactly three neighbors. This structure arises from the presence of only pentagonal and hexagonal faces, forming a polyhedral carbon allotrope. Define $f : V(FG) \to [0,1]$ by assigning $f(x_i) = \frac{1}{4}$ for every vertex $x_i (1 \leq i \leq n) \in V(FG)$. This assignment assigns values such that, for each vertex $x_i \in V(FG)$, we have $f(Z[x_i]) \geq 1$. The total sum is $\sum_{x_i \in V(FG)} f(x_i) = \frac{n}{4}$. Now, suppose there exists another $g : V(FG) \to [0,1]$ that also a FDF but satisfies $g < f$. Thus, one can identify a vertex $x_i \in V(FG)$ where $1 \leq i \leq n$ for which $g(Z[x_i]) < 1$, contradicting the definition of a FDF. This contradiction confirms that f is a minimum FDF. Hence, $\gamma_f(FG) = \frac{n}{4}$. □

Theorem 5. *For every FG, we have*

$$\gamma_f(FG-e') = \lceil \frac{n}{4} \rceil \tag{2}$$

where $FG-e'$ denote the graph obtained after deleting the edge e' from $E(FG)$.

Proof. Let $FG-e'$ stand for the graph resulting from the deletion of an edge $e' \in E(FG)$. We aim to prove that the $\gamma_f(FG-e) = \lceil \frac{n}{4} \rceil$. Suppose we remove $e' \in E(FG)$. Let $f : V(G''-e') \longrightarrow [0,1]$ as the functional total value of $\lceil \frac{n}{4} \rceil$. This function satisfies the condition $f(Z[v']) \geq 1$ where $v' \in V(FG-e')$. Suppose not. Then there is another FDF g' so that $g' < f$. Hence, for a certain vertex $v' \in V(FG-e')$, we get $g'(v') < f(v')$. Let $u' \in Z[v']$ so that $f(Z[u']) = 1$. Then $g'(Z[u']) = g'(v') + \sum_{w' \in Z[u'], w' \neq v'} g'(w') < f(v') + \sum_{w' \in Z[u'], w' \neq v'} f(w') = f(Z[u']) = 1$ and hence $g'(Z[u']) < 1$. This contradicts with the claim that g' is a FDF which implies that f is a minimum FDF. Likewise, the theorem remains valid for the removal of any other edge in FG. Hence, $\gamma_f(FG-e') = \lceil \frac{1}{4} \rceil$.

□

Theorem 6. *For any FG with n vertices, we have*

$$\gamma_f(FG+e') = \lfloor \frac{n+3}{4} \rfloor \tag{3}$$

where $FG+e'$ refers to the graph of introducing a new edge $e' = v'_i v'$, with $v'_i \in V(FG)$ and v' being a new vertex added to the graph.

Proof. To construct $FG+e'$, a new edge $e' = v'_i v'$ is added, where $v'_i \in V(FG+e')$ and v' is a newly introduced vertex created by adding the edge. Let $f : V(FG+e') \longrightarrow [0,1]$ be such that $f(v'_i) = \frac{1}{4}$ for all $i \in V(FG+e')$ except the function value at the new vertex formed by adding an edge is assigned as $\frac{3}{4}$. When the minimality condition is not satisfied on the FG, then the γ_f is nothing but equal to the γ of $FG+e'$. The sum yields $\gamma_f(FG+e') = \lfloor \frac{n+3}{4} \rfloor$. Since this function holds $f(Z[v']) \geq 1$ where $v' \in V(FG+e')$, we get $\gamma_f(FG+e') = \lfloor \frac{n+3}{4} \rfloor$.

□

Theorem 7. *For any FG, $\gamma_f(FG) \leq \gamma_f(FG-e') \leq \gamma_f(FG+e')$. This inequality holds for all graphs G^* that do not contain isolated vertices.*

Proof. By equations (1), (2) and (3), it is obvious that for any FG, $\gamma_f(FG) \leq \gamma_f(FG-e') \leq \gamma_f(FG+e')$. We need to prove that $\gamma_f(G^*) \leq \gamma_f(G^*-e')$. To

derive a contradiction, assume that, $\gamma_f(G^*) > \gamma_f(G^* - e')$. From this, it follows that minimum FDF of $G^* - e'$ is strictly less than the minimum FDF of G^*. Let f be minimum FDF of $G^* - e'$. Because, f is a FDF of $G^* - e'$, it must also fractional dominating G^* because G^* contains all vertices and edges of $G^* - e'$ along with the additional edge e'. Therefore, f should also be an FDF for G^*, contradicting the assumption that $\gamma_f(G^*) > \gamma_f(G^* - e')$. Thus, $\gamma_f(G^*) \leq \gamma_f(G^* - e')$. Similarly, to prove $\gamma_f(G^* - e') \leq \gamma_f(G^* + e')$, observe that adding an edge e' to G^* cannot decrease the γ_f, as the additional edge can potentially require more value to the FDF to cover all vertices. Hence, $\gamma_f(G^* - e') \leq \gamma_f(G^* + e')$. Combining these results, we obtain, $\gamma_f(G^*) \leq \gamma_f(G^* - e') \leq \gamma_f(G^* + e')$ □

Theorem 8. *For any $v' \in V(FG - e')$. If $\gamma_f((FG - e') - v') < \gamma_f(FG - e')$, then: $\gamma_f(FG - e') - 1 \leq \gamma_f((FG - e') - v') < \gamma_f(FG - e')$.*

Proof. Assume $\gamma_f((FG - e') - v') < \gamma_f(FG - e')$, and let g' be a minimum FDF for the graph $(FG - e') - v'$. Suppose there exists a function g'' defined on $V(FG - e')$ with the same weights as g' but fails to serve as an FDF for $FG - e'$. Define g'' as follows $g''(v') = 0 \quad \& \quad g''(x') = g(x') \; \forall \; x' \neq v'$. The contribution of g'' to the closed neighborhood $Z[v']$ becomes $g''(Z[v']) = g''(v') + \sum_{w' \in Z(v')} g''(w') = 0 + \sum_{w' \in Z(v')} g''(w')$. Since g'' is a candidate for an FDF on $FG - e'$, it follows that $g''(Z[v']) \geq 1$. This would make g'' a valid FDF for $FG - e'$, contradicting the assumption that $\gamma_f((FG - e') - v') < \gamma_f(FG - e')$. Consequently, it must hold that: $\sum_{w' \in Z(v')} g'(w') < 1$.. Next, construct a new function h' on $V(FG - e')$ as, $h'(v') = 1 - \sum_{w' \in Z(v')} g'(w') \quad$ and $\quad h'(x') = g'(x') \; \forall \; x' \neq v'$. The function h' satisfies the condition, $h'(Z[v']) = h'(v') + \sum_{w' \in Z(v')} h'(w') = 1$. Thus, h' is an FDF for $FG - e'$. Its weights satisfy $\gamma_f((FG - e') - v') < \gamma_f(FG - e') \leq \text{weight}(h') \leq \text{weight}(g') + 1$. Therefore, the inequality $\gamma_f(FG - e') - 1 \leq \gamma_f((FG - e') - v') < \gamma_f(FG - e')$ is established. □

Theorem 9. *For any FG*

$$\gamma_f(FG - v') = \lceil \frac{n}{5} \rceil \tag{4}$$

where $FG - v'$ represents the graph formed by deleting the vertex $v' \in V(FG)$.

Proof. To obtain $FG - v'$, a vertex $v' \in V(FG)$ is removed from FG. Suppose we remove $v' \in V(FG)$, let $f : V(FG - v') \longrightarrow [0, 1]$ so that the functional total value of $\lceil \frac{n}{5} \rceil$. Since this function holds $f(Z[v']) \geq 1$ for all $v' \in V(FG - v')$. It's total weight is $\gamma_f(FG - v')$. Suppose not, there must exist an FDF g' for which $g' < f$. Consequently, for a certain vertex $v' \in V(FG - v')$, we get $g'(v') <$

$f(v')$. Let u' be a vertex $u' \in Z[v']$ where $f(Z[u']) = 1$. Then $g'(Z[u']) = g'(v') + \sum_{w' \in Z[u'], w' \neq v'} g'(w') < f(v') + \sum_{w' \in Z[u'], w' \neq v'} f(w') = f(Z[u']) = 1$ and hence, we get $g'(Z[u']) < 1$. This contradicts with the property that g' is an FDF. Therefore f is a minimum FDF. Similarly, the theorem holds for the removal of another vertex in G. Hence, $\gamma_f(FG - v') = \lceil \frac{n}{5} \rceil$.

□

3 Bounds of fractional and domination-related parameters in linear Benzenoid molecular graphs

In this section, we consider a member of a polycyclic aromatic hydrocarbons which is the linear benzenoid chains, which consists of a series of fused benzene rings. Let $Lb(n)$ represent the linear benzenoid chain, which has $4n+2$ vertices for $n \in \mathbb{N}$ hexagons, [14] (see Fig. 1).

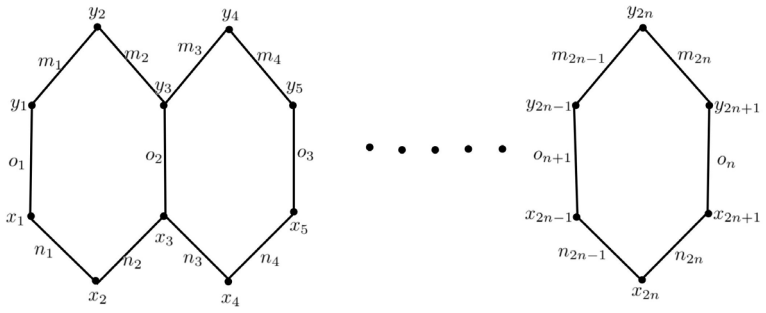

Figure 1: Linear benzenoid chain

We discuss the bounds and effects of fractional and related domination parameters for Lb(n). These parameters are crucial in understanding the structural properties and behavior of these molecular graphs.

Lemma 1. *[14] For a linear benzenoid chain with n hexagons, the γ_f of its molecular graph is $n+1$.*

Theorem 10. *For every even $n \in \mathbb{N}$, we have*

$$\gamma_f(Lb(n)+v) = \gamma_f(Lb(n)+e)$$

$$= \begin{cases} n+1 & \text{if } v \text{ is added to a vertex in } R_1 \cup R_2 \\ n+2 & \text{otherwise} \end{cases}$$

where $R_1 = \{y_1, x_3, y_5, \ldots, x_{2n-1}, y_{2n+1}\}$, $R_2 = \{x_1, y_3, x_5, \ldots, y_{2n-1}, x_{2n+1}\}$ *and* $Lb(n)+v$ *denotes the graph formed by attaching a new vertex* v *to an existing vertex in* $V(Lb(n))$, $Lb(n)+e$ *represents the graph formed by adding a new edge* $e = v_i v$, *where* $v_i \in V(Lb(n))$ *and* v *is a newly added vertex.*

Proof. Let n be an even number and $V(Lb(n)+v) = X \cup Y \cup \{v\}$, with v being the newly added vertex. The edge set $E(Lb(n)+e) = M \cup O \cup N \cup e$ of the linear benzenoid graph $Lb(n)$ is defined as follows:

$$X = \{x_1, x_2, x_3, \ldots, x_{2n}, x_{2n+1}\},$$
$$Y = \{y_1, y_2, y_3, \ldots, y_{2n}, y_{2n+1}\},$$
$$M = \{m_1, m_2, m_3, \ldots, m_{2n-1}, m_{2n}\},$$
$$O = \{o_1, o_2, o_3, \ldots, o_n, o_{n+1}\},$$
$$N = \{n_1, n_2, n_3, \ldots, n_{2n-1}, n_{2n}\}$$

where e represents an edge formed by connecting the new vertex v to another vertex in $V(Lb(n))$.

Case (i):

Subcase (i):

Assume we add vertex v to any vertex in the set $\{y_1, x_3, y_5, \ldots, x_{2n-1}, y_{2n+1}\}$ of $Lb(n)$. To find $\gamma_f(Lb(n)+v)$, consider $f : V(Lb(n)+v) \to [0,1]$ where $f(y_1) = f(x_3) = f(y_5) = \ldots = f(x_{2n-1}) = f(y_{2n+1}) = 1$, and all other remaining vertices, including v, are assigned a value of 0. The weight of this function f is $n+1$ when all function values are summed. Since the function satisfies $f(N[x_i]), f(N[y_i]) \geq 1$ for all $x_i, y_i \in V(Lb(n))$, it forms a minimum FDF. Suppose $\gamma_f(Lb(n)+v) \neq n+1$. Then, for every $x_i, y_i \in V(Lb(n))$, it follows that a vertex exists $f(N[x_i]) < 1$ or $f(N[y_i]) < 1$. This implies f is not a minimum FDF, contradicting the earlier assertion. Thus, $\gamma_f(Lb(n)+v) = n+1$. Consequently, if v is added to any vertex in the set $\{y_1, x_3, y_5, \ldots, x_{2n-1}, y_{2n+1}\}$, then $\gamma_f(Lb(n)+v) = n+1$.

Subcase (ii):

Now, suppose we add vertex v to any vertex in the set $\{x_1, y_3, x_5, \ldots, y_{2n-1}, x_{2n+1}\}$

of $Lb(n)$. Define $f : V(Lb(n)+v) \to [0,1]$ where $f(x_1) = f(y_3) = f(x_5) = \ldots = f(y_{2n-1}) = f(x_{2n+1}) = 1$, and all other vertices, including v, are assigned a value of 0. The total weight is $n+1$. Since f satisfies $f(N[x_i]), f(N[y_i]) \geq 1$ for all $x_i, y_i \in V(Lb(n))$, it forms a minimum FDF, with the function weight being $\gamma_f(Lb(n)+v)$. If $\gamma_f(Lb(n)+v) \neq n+1$, it follows that a vertex exists $f(N[x_i]) < 1$ or $f(N[y_i]) < 1$, implying f is not a minimum FDF. Thus, $\gamma_f(Lb(n)+v) = n+1$. Therefore, if v is added to any vertex in the set $\{x_1, y_3, x_5, \ldots, y_{2n-1}, x_{2n+1}\}$, then $\gamma_f(Lb(n)+v) = n+1$.

Case (ii):

Now, assume we add vertex v to the graph $Lb(n)$ such that it is not in the vertex set $R_1 \cup R_2$. Consider $f : V(Lb(n)+v) \to [0,1]$ defined by $f(y_1) = f(x_3) = f(y_5) = \ldots = f(x_{2n-1}) = f(y_{2n+1}) = f(v) = 1$, and all vertices not mentioned above are allocated a value of 0. Alternatively, $f(x_1) = f(y_3) = f(x_5) = \ldots = f(y_{2n-1}) = f(x_{2n+1}) = f(v) = 1$, with other vertices assigned 0. In both cases, the total weight is $n+2$. Since f satisfies $f(N[x_i]), f(N[y_i]) \geq 1$ for all $x_i, y_i \in V(Lb(n))$, it forms a minimum FDF. Thus, if v is added to a vertex not in $R_1 \cup R_2$ of $Lb(n)$, then $\gamma_f(Lb(n)+v) = n+2$. Similarly, if we add any edge e to any vertex in $V(Lb(n))$, the same cases and subcases as discussed above follow, and the theorem remains valid. Therefore, for every even $n \in \mathbb{N}$,

$$\gamma_f(Lb(n)+v) = \gamma_f(Lb(n)+e) = \begin{cases} n+1 & \text{if } v \text{ is added to a vertex in } R_1 \cup R_2 \\ n+2 & \text{otherwise} \end{cases}$$ □

Theorem 11. *For every $n \in \mathbb{N}$ and n is odd*

$$\gamma_f(Lb(n)+v) = \gamma_f(Lb(n)+e)$$

$$= \begin{cases} n+1 & \textit{if } v \textit{ is added to one of the vertices in } R_1 \cup R_2, \\ n+2 & \textit{otherwise} \end{cases}$$

where $R_1 = \{y_1, x_3, y_5, \ldots, x_{2n-1}, y_{2n+1}\}$, $R_2 = \{x_1, y_3, x_5, \ldots, y_{2n-1}, x_{2n+1}\}$ and $Lb(n)+v$ represents the graph formed by attaching a new vertex v to vertex in $V(Lb(n))$, $Lb(n)+e$ denotes adding an edge e to $E(Lb(n))$.

Proof. Analogous to Theorem 10's proof. □

Theorem 12. *For every $n \in \mathbb{N}$, we have*

$$\gamma_f(Lb(n)-e) = \begin{cases} n+1 & \textit{if } e \textit{ is one of the edges in } \{\{m_i, n_i\} \mid i = 1,2,3,\ldots,2n+1\} \\ n+2 & \textit{if } e \textit{ is one of the edges in } \{o_i \mid i = 1,2,3,\ldots,n+1\} \end{cases}$$

where $Lb(n)-e$ represents the graph $Lb(n)$ after removing the edge e.

Proof. **Case (i):**
Let n be an even number.
Subcase (i):
Suppose we remove one of the edges from the edge set $\{o_i \mid i = 1,2,3,...,2n+1\}$ of the graph $Lb(n)$. To calculate the fractional domination number, let $f : V(Lb(n)-e) \to [0,1]$ be such that $f(y_1) = f(x_3) = f(y_5) = \ldots = f(x_{2n-1}) = f(y_{2n+1}) = 1$ & the incident vertex of the removed edge is assigned a value of 1, with all other remaining vertices assigned a value of 0. Alternatively, let $f(x_1) = f(y_3) = f(x_5) = \ldots = f(y_{2n-1}) = f(x_{2n+1}) = 1$ with the incident vertex of the removed edge assigned a value of 1, & remaining vertices assigned 0. In either case, the total weight is $n+2$. For all $x_i, y_i \in V(Lb(n))$, $f(Z[x_i])$ and $f(Z[y_i]) \geq 1$ because this function satisfies the condition. Therefore, it is a minimum FDF, and the weight of the function is $\gamma_f(Lb(n)-e)$. If $\gamma_f(Lb(n)-e) \neq n+2$, then there would be a vertex such that $f(Z[x_i])$ and $f(Z[y_i]) < 1$ for some i, which would imply that f is not a minimum FDF and the weight of the function f is not $\gamma_f(Lb(n)-e)$. Thus, if removing one of the edges from $\{\{m_i,n_i\} \mid i = 1,2,3,...,2n+1\}$, then $\gamma_f(Lb(n)-e) = n+2$.
Subcase (ii):
Suppose we remove one of the edges from the edge set $\{\{m_i,n_i\} \mid i = 1,2,3,...,2n+1\}$ of the graph $Lb(n)$. Let $f : V(Lb(n)-e) \to [0,1]$ be such that $f(y_1) = f(x_3) = f(y_5) = \ldots = f(x_{2n-1}) = f(y_{2n+1}) = 1$ (or) $f(x_1) = f(y_3) = f(x_5) = \ldots = f(y_{2n-1}) = f(x_{2n+1}) = 1$ and all vertices not mentioned above are allocated a value of 0. Regardless of the case, the total weight is $n+1$. Since this function satisfies $f(Z[x_i]) \geq 1$ and $f(Z[y_i]) \geq 1$ for all $x_i, y_i \in V(Lb(n))$, it is a minimum FDF and the weight of the function is $\gamma_f(Lb(n)-e)$. Therefore, if removing one of the edges from $\{\{m_i,n_i\} \mid i = 1,2,3,...,2n+1\}$, then $\gamma_f(Lb(n)-e) = n+1$.
Case (ii):
Let n be an odd number. If we remove any one of the edges from the edge set $E(Lb(n))$ of the graph $Lb(n)$, by reasoning in the same way as Case (i), we get

$$\gamma_f(Lb(n)-e) = \begin{cases} n+1 & \text{if } e \text{ is one of the edges in } \{\{m_i,n_i\} \mid i = 1,2,3,...,2n+1\} \\ n+2 & \text{if } e \text{ is one of the edges in } \{o_i \mid i = 1,2,3,...,n+1\}. \end{cases}$$

□

Theorem 13. *For every $n \in \mathbb{N}$, $\gamma_f(Lb(n)-v) = n+1$, where $Lb(n)-v$ denotes the graph $Lb(n)$ with any vertex $v \in V(Lb(n))$ removed.*

Proof. Analogous to the proof provided for Theorem 12. □

Theorem 14. *For every $n \in \mathbb{N}$, $i(Lb(n)) = n+1$.*

Proof. The linear benzenoid chain $Lb(n)$ consists of $2n+1$ vertices. To determine the independence domination number, we need to identify the i-set
Case(i) If n is even, i(Lb(n))-set is either $\{y_1, x_3, y_5, x_7, \ldots, x_{2n-1}, y_{2n+1}\}$ or $\{x_1, y_3, x_5, \ldots, y_{2n-1}, x_{2n+1}\}$. Suppose $i(Lb(n)) < n+1$. This would imply the existence of some vertex that is neither independent nor dominating, which contradicts the minimal cardinality requirement. Thus, if n is even, $i(Lb(n)) = n+1$.
Case (ii) If n is odd, i(Lb(n))-set is either $\{y_1, x_3, y_5, x_7,$
$\ldots, y_{2n-1}, x_{2n+1}\}$ or $\{x_1, y_3, x_5, \ldots, x_{2n-1}, y_{2n+1}\}$. Suppose $i(Lb(n)) < n+1$. This would imply the presence of a vertex that is neither independent nor dominating, which contradicts the minimal cardinality requirement. Therefore, if n is odd, $i(Lb(n)) = n+1$. □

Theorem 15. *For every* $n \in \mathbb{N}$, $\gamma'_g(Lb(n)) = n+1$.

Proof. Consider the linear benzenoid graph $Lb(n)$ with edge set $E(Lb(n))$, partitioned into three sets $M = \{m_1, m_2, \ldots, m_{2n}\}$, $O = \{o_1, o_2, \ldots, o_{n+1}\}$, and $N = \{n_1, n_2, \ldots, n_{2n}\}$. Define a function $g : E(Lb(n)) \to [0,1]$ by setting $g(m_i) = 0$ and $g(n_i) = 0 \; \forall \; 1 \leq i \leq 2n$, and $g(o_i) = 1 \; \forall \; 1 \leq i \leq n+1$. The sum of the weights of this function g is $n+1$. Since this function g ensures that $g(Z[m]) \geq 1$ for every $m \in E(Lb(n))$, it constitutes a minimum FEDF. Thus, the weight of the function g is $\gamma'_g(Lb(n))$. Now, suppose $\gamma'_g(Lb(n)) \neq n+1$. There is some $m \in E(Lb(n))$ with $g(Z[m]) < 1$. This would imply that g is not a minimum FEDF, and hence, the weight of g does not represent the $\gamma'_g(Lb(n))$. Therefore, $\gamma'_g(Lb(n)) = n+1$ for n hexagons. □

Theorem 16. *For every* $n \in \mathbb{N}$, $\beta(Lb(n)) = 2n+1$

Proof. The linear benzenoid chain consists of $2n+1$ vertices. To calculate the $\beta(Lb(n))$, let $T = Z_1 \cup Z_2$, where $Z_1 = \{x_{2t} \mid t = 1, 2, \ldots, n\}$ and $|Z_1| = n$, and $Z_2 = \{y_{2t+1} \mid t = 0, 1, 2, 3, \ldots, n\}$ and $|Z_2| = n+1$. This forms the maximum vertex independence set consisting of $2n+1$ vertices for $Lb(n)$. Hence, $\beta(Lb(n)) = |T| = |Z_1| + |Z_2| = n+n+1 = 2n+1$. □

Theorem 17. *For every* $n \in \mathbb{N}$, $\gamma'_g(Lb(n)) < \beta(Lb(n)) = \alpha_1(Lb(n))$.

Proof. We know that if $Lb(n)$ has no isolated vertices, then $\beta(Lb(n)) = \alpha_1(Lb(n))$ [4]. Therefore, $\alpha_1(Lb(n)) = 2n+1$ for every $n \in \mathbb{N}$ hexagons. Thus, by Theorems 15 and 16, $\gamma'_g(Lb(n)) < \beta(Lb(n)) = \alpha_1(Lb(n))$. □

Theorem 18. *For every* $n \in \mathbb{N}$, $\alpha(Lb(n)) = 2n+1$.

Proof. The linear benzenoid chain consists of $2n+1$ vertices. To calculate $\alpha(Lb(n))$, let $T = Z_1 \cup Z_2$, where $Z_1 = \{x_{2t+1} \mid t = 0,1,2,\ldots,n\}$ and $|Z_1| = n+1$, and $Z_2 = \{y_{2t} \mid t = 1,2,3,\ldots,n\}$ and $|Z_2| = n$. This forms the minimum vertex covering set consisting of $2n+1$ vertices for $Lb(n)$. Hence, $\alpha(Lb(n)) = |T| = |Z_1| + |Z_2| = n+1+n = 2n+1$. □

Theorem 19. *For every $n \in \mathbb{N}$, $\gamma'_g(Lb(n)) < \alpha(Lb(n)) = \beta_1(Lb(n))$.*

Proof. We know that in any bipartite graph, the number of edges in a maximum matching equals the number of vertices in a minimum vertex cover[4]. Since the linear benzenoid chain is a bipartite graph, $\alpha(Lb(n)) = \beta_1(Lb(n)) = 2n+1$ for n hexagons. Therefore, by Theorems 15 and 18, $\gamma'_g(Lb(n)) < \alpha(Lb(n)) = \beta_1(Lb(n))$. □

Remark 1. *The following theorems lead us to the conclusion that for every $n \in \mathbb{N}$, $i(Lb(n)) = \gamma_f(Lb(n)) = \gamma_f(Lb(n)-v) = \gamma'_g(Lb(n)) \leq \gamma_f(Lb(n)+v) < \alpha(Lb(n)) = \beta_1(Lb(n)) = \alpha_1(Lb(n)) = \beta(Lb(n))$.*

4 Conclusion and future work

We extended our analysis of γ_f to other molecular graph families such as polycyclic aromatic hydrocarbon, Balaban 10-cage, dendrimers and fullerenes. Specifically, we determined the exact values of γ_f for fullerene graphs under structural modifications involving vertex and edge additions or deletions, demonstrating how such changes impact the domination properties of molecular networks. Furthermore, we analyzed the γ_f in dendrimers, revealing significant variations due to hierarchical branching and connectivity patterns with domination parameter. Also, we analyzed the structural properties of linear benzenoid chains and established bounds for key domination parameters, including the independence domination number(i), independence number(α), and cover number(β). We further examined the effect of structural modifications such as the addition or removal of vertices and edges on the γ_f, providing deeper insights into its behavior of linear benzenoid chain. Our findings provide novel insights into the fractional domination number in chemical graph families, establishing structural dependencies that have not been previously explored. Future research may focus to establish the bounds for fractional domination chain in chemical graphs, with specific focus on examining inequalities and identifying the conditions under which these parameters are equal.

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Predicting Properties of PAHs with Graph Indices and Graph-Based Machine Learning

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Abstract

Molecular graphs are obtained from 2D images of chemical structures. Molecular descriptors are mathematical values derived from the structure of molecular graphs. These descriptors are used to predict the physicochemical properties of chemical structures in QSPR and QSAR studies. In this paper, degree and distance-dependent molecular descriptors of 40 polycyclic aromatic hydrocarbons are calculated. Curvilinear regression models are developed with molecular descriptor values for mass weight, flash point, boiling point, enthalpy of vaporization, and polarized of these chemical structures. This study is limited to linear, quadratic, cubic, and multi-linear regression models. Regression models and graph indices are found that best predict the properties of the chemical structures.

Keywords: Graph index, Curvilinear regression models, Multilinear regression models, Polycyclic aromatic hydrocarbons, Machine learning
AMS Classification: 05C09, 05C92

1 Introduction

Chemical graph theory deals with the mathematical modeling of chemical structures. It focuses on molecular descriptors (graph indices, topological indices). The graph indices are numerical values of the molecular graphs. A molecular graph is a 2D image of a chemical structure that does not contain hydrogen. Atoms in a chemical structure are represented by the vertices of the graph, and chemical bonds are represented by the edges of the graph [21].

Graph indices are used to estimate the physical/chemical properties and biological activities of the chemical in QSPR/QSAR studies [15]. The first application of graph index was studied by H. Wiener in 1947 [29]. There are many graph indices in the

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literature and new ones are added every day. There are no definite criteria yet to stop or slow down these new indices. However, by comparing these indices, it is possible to obtain indices that are more valuable and have better predictive ability.

Polycyclic aromatic hydrocarbons (PAHs) are a group of organic compounds consisting of carbon and hydrogen atoms containing at least two condensed or fused aromatic rings. The simplest PAH is naphthalene. PAHs are low-volatility solids at room temperature and are relatively insoluble in water, and many of them are photo oxidized and decompose to simpler substances [1]. PAHs are spread to the environment by incomplete combustion and pyrolysis of wood and biomass through oil spills, volcanic eruptions, erosion from oil things, forest and grass fires. Since most PAHs are mutagenic and carcinogenic, they have been recognized as priority pollutants by many countries.The state of chemicals in the environment is controlled by their physical and chemical properties [16]. Therefore, it is important to predict the properties of PAHs. Kirana et al. calculated the Sombor index and its versions for some polycyclic aromatic hydrocarbons and obtained regression models [14]. Nikolic et al. obtained models with connectivity indices for the boiling points of 23 benzenoid hydrocarbons [17]. Tamilarasi et al. obtained linear models with some molecular descriptors for the properties of 16 priority PAHs [23]. In this study, 40 PAHs will be studied. These are; Coronene, Dibenzo [a,l] pyrene, 9,10- Diphenylanthracene, Perylene, Methylcholanthene, 9- Benzylidenefluorene, 7,10- Dihydrophenanthrene, Indeno (1,2,3:c,d) pyrene, Dibenz(a,h)anthracene, 6-Ethylchrysene, 6-Methylbenz (u) anthracene, Benzo (k) fluoranthene, 1- Ethylpyrene, Retene, 2-tert-Butylanthracene, 9,1O- Dihydroanthracene, 9- Phenylfluorene, 1,2,3,6,7-Hexahydropyrene, n-Butylpyrene, Triphenylene, Dibenz [a,c] anthracene, Benzo(c)-phenanthrene, 1-Methylpyrene, 3,9- Dimethyl benz (a) anthracene, 2,3- Benzofluorene, 9- Benzylfluorene, Pyrene, 2-Ethylanthracene, 10-Methylbenzo (a) pyrene, 1- Methylanthracene, 3,6- Dimethylphenanthrene, Fluorene, 2-Methylphenanthrene, 9- Ethylfluorene, 1- Methyl-phenanthrene, 9,10- Dihydrophenanthrene, 9-Vinylanthracene, Anthracene, 1- Methylfluorene, 4H- Cyclopenta (d,e,f lphenanthrene) polycyclic aromatic hydrocarbons are given in Figure 1, respectively.

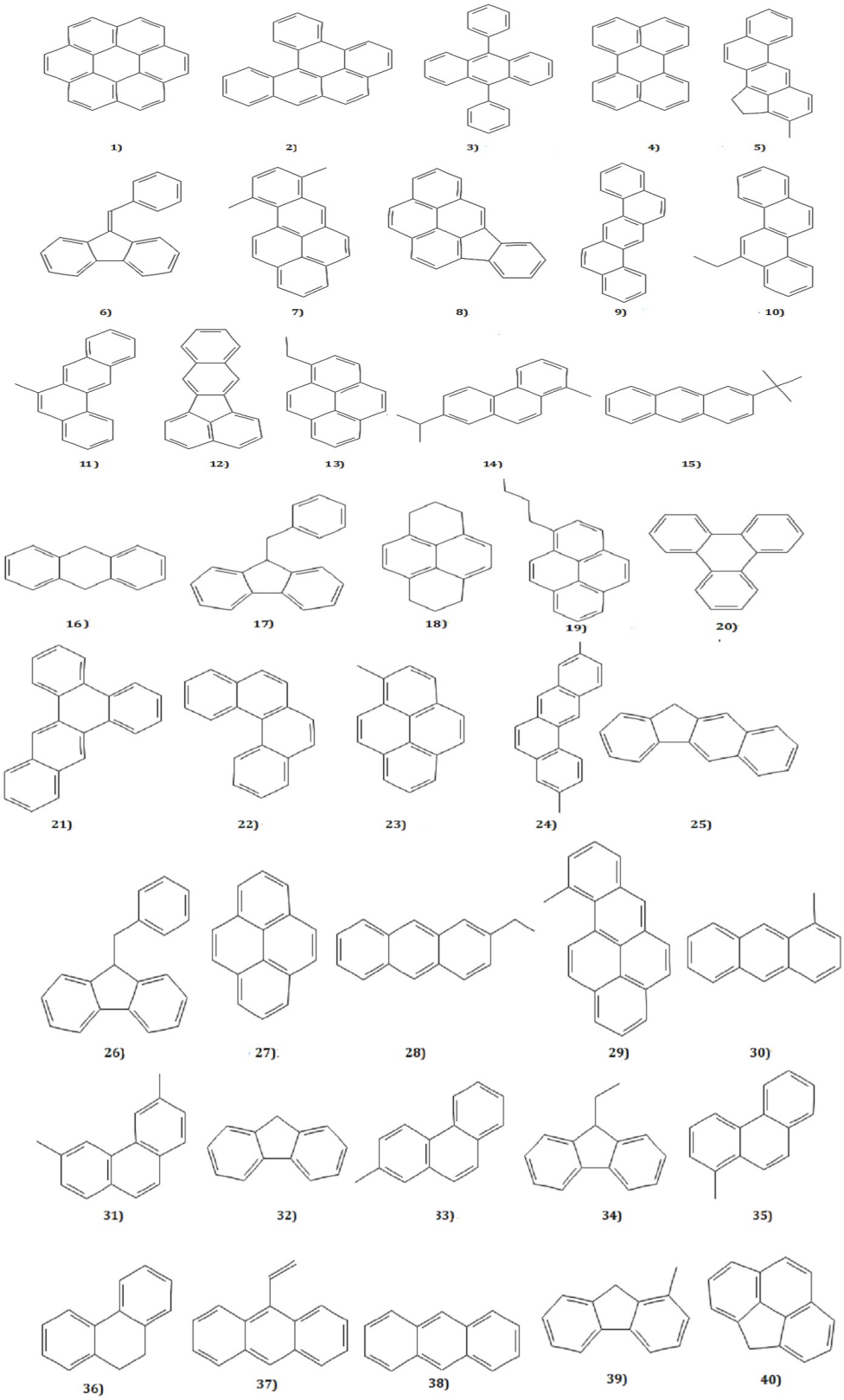

Figure 1: The chemical structures of PAHs [19].

Tablo 1 shows the boiling point (BP), enthalpy of vaporization (E), flash point (FP), polarize (P), and mass weight (MW) of these PAHs. The benchmark sets of the properties of 40 PAHs are taken from PubChem [19] and [12].

Table 1: The boiling point (BP), enthalpy of vaporization (E), flash point (FP), polarize (P), and mass weight (MW) of these PAHs.

PAHs No	BP	E	FP	P	MW
1	6.852	77	265.2	44.1	300.352
2	7,098	80,2	282	42,9	302,368
3	8,19	70,3	234,7	44,1	330,421
4	6,40	70,2	228,6	35,8	252,309
5	7,11	74.7	253,2	36,5	268,252
6	7,27	61,8	184,9	33,5	254,325
7	7,32	72,8	244,1	39,6	280,362
8	6,89	73,6	247,2	40,0	276,331
9	7,14	76,9	264,5	38,7	278,347
10	6,90	69,0	223,6	35,4	256,341
11	6,37	68,1	217,8	33,5	242,314
12	6,40	71,6	228,6	35,8	252,309
13	6,16	62,2	185,8	32,5	230,304
14	6,48	61,7	177,8	32,1	234,335
15	6,37	60	174,7	31,8	234,335
16	4,16	52,4	131,8	23,2	180,245
17	5,25	60,2	175,6	31	242,314
18	5,75	62,2	213,3	27,1	208,298
19	7,22	64,8	202	36,2	258,357
20	5,91	65,3	209,1	31,6	228,288
21	7,14	76,1	264,5	38,7	278,347
22	5,91	66,7	209,1	31,6	228,288
23	5,63	61,2	178,9	30,6	216,277
24	6,83	69,6	226,6	35,5	256,341
25	5,39	62,4	185,4	28,4	216,277
26	6,14	63,8	196,3	32,9	256,341
27	5,17	63	168,8	28,7	202,251
28	5,67	58,6	165,1	28,3	206,282
29	6,86	71,5	236,7	37,7	266,336
30	5,14	58,5	157,5	26,5	192,256
31	5,6	58,5	168,4	28,4	206,282
32	4,16	51,2	133,1	21,3	166,219
33	5,14	55,9	157,5	26,5	192,256
34	5,19	54,1	149,4	25	194,272
35	5,14	57,5	157,5	26,5	192,256
36	5,04	52,7	144,1	23,2	180,245
37	5,16	60	172,4	28,9	204,266
38	4,68	55,8	146,6	26,4	178,229
39	4,62	53,3	148,5	23,2	180,245
40	4,54	57,4	168,8	25,7	190,240

2 Graph Indices

Let G be a graph and its vertex (edge) set be denoted by $V(G)(E(G))$. The vertex degree of t is defined by $d(t)$. The distance between vertices of s and t is denoted by $d(s,t)$. $n(u)$ is defined by the number of vertices of G closer to u than to v [6].

The symmetric division deg index, and min-max rodeg index are the best predictors for many properties of the polychlorobiphenyls [26]. It is seen that the Wiener index and Mostar index predict the boiling point of the benzenoid hydrocarbons very well [5]. With the motivation of these studies, in this study, first Zagreb ($M_1(G)$) [11], second Zagreb ($M_2(G)$) [11], forgotten ($F(G)$) [8], sombor ($SO(G)$) [10], symmetric division deg index (SD(G)) [26], max-min rodeg ($Mm(G)$) [26], min-max rodeg index ($mM(G)$) [26], geometric-arithmetic ($GA(G)$) [27], hyper Zagreb ($HM(G)$) [22], Albertson index ($Al(G)$) [2], harmonic index ($H(G)$) [7],Wiener index ($W(G)$) [29], Mostar index ($Mo(G)$) [6], Gutman index ($Gut(G)$)[9] are discussed. Table 2 shows mathematical expressions of graph indices.

Table 2: Graph indices and theirs mathematical expressions.

Graph indices of G	**Mathematical Expressions**
$M_1(G)$	$\sum_{u\in V(G)} d(u)^2$
$M_2(G)$	$\sum_{uv\in E(G)} d(u)d(v)$
$F(G)$	$\sum_{uv\in E(G)} (d(u)^2+d(v)^2)$
$SO(G)$	$\sum_{uv\in E(G)} (\sqrt{d(u)^2+d(v)^2})$
$SD(G)$	$\sum_{uv\in E(G)} (\frac{d(u)}{d(v)}+\frac{d(v)}{d(u)})$
$Mm(G)$	$\sum_{uv\in E(G)} \sqrt{\frac{max(d(u),d(v))}{min(d(u),d(v))}}$
$mM(G)$	$\sum_{uv\in E(G)} \sqrt{\frac{min(d(u),d(v))}{max(d(u),d(v))}}$
$GA(G)$	$\sum_{uv\in E(G)} \frac{2\sqrt{d(u)d(v)}}{d(u)+d(v)}$
$HM(G)$	$\sum_{uv\in E(G)} (d(u)+d(v))^2$
$Al(G)$	$\sum_{uv\in E(G)} \lvert d(u)-d(v)\rvert$
$H(G)$	$\sum_{uv\in E(G)} \frac{2}{d(u)+d(v)}$
$W(G)$	$\sum_{u,v\in V(G)} d(u,v)$
$Gut(G)$	$\sum_{u,v\in V(G)} d(u)d(v)d(u,v)$
$Mo(G)$	$\sum_{uv\in E(G)} \lvert n(u)-n(v)\rvert$

3 Regression Models

This section discusses the method to be used in the analysis of graph indices obtained for PAHs. Here, curvilinear regression models will be generated using SPSS (IBM Statistics 20 license). The following curvilinear regression models (equations) are examined in this study:

$$y = a + b\tilde{\xi}$$
$$y = a + b\tilde{\xi} + c\tilde{\xi}^2$$
$$y = a + b\tilde{\xi} + c\tilde{\xi}^2 + d\tilde{\xi}^3$$
$$y = a + b\tilde{\xi} + c_i\tilde{\xi}_i$$

where y is the property of chemical structure, a is constant, b, c, d, c_i are the coefficients for the graph index, and $\tilde{\xi}$, $\tilde{\xi}_i$ are graph indices. R is the correlation coefficient [4].

If the theoretical result and the experimental result are close to each other, the correlation coefficient is close to 1 (see detail [28]). The closeness of the theoretical and experimental results to each other increases the prediction quality of the model. In this study, for the predictive ability and quality of the model will be discussed measures the maximum correlation and minimum root mean square error (RMSE). The root mean square error is defined as

$$RMSE = \sqrt{\frac{\sum_{k=1}^{n}(\rho_k - \vartheta_k)^2}{n}}$$

where ρ_k is the observed value of chemical properties, ϑ_k is predicted value, n is the samples number in the test.

4 Results and Discussion

The results in Table 3 and Table 4 are obtained from Table 2 and molecular graphs of chemical structures in Figure 1. Table 3 shows the values of the degree-dependent graph indices of 40 PAHs.

Table 3: Degree based on Graph indices of PAHs.

no	M_1	M_2	F	GA	H	HM	SO	Al	SDD	mM	Mm
1	156	204	420	29.74	11.80	828	111.13	12	62.00	27.79	32.68
2	146	186	382	28.79	11.83	826	103.92	10	59.66	27.16	31.24
3	144	176	360	29.83	12.86	712	102.36	8	61.33	28.52	31.79
4	120	152	312	23.83	9.86	616	85.40	8	49.33	22.52	25.79
5	126	159	332	24.65	10.16	650	90.12	12	53.00	22.73	27.97
6	110	133	274	22.83	14.66	540	78.33	8	56.33	21.52	24.79
7	132	167	352	25.52	10.50	686	94.69	14	47.33	23.31	29.70
8	138	178	366	26.79	10.83	722	98.26	10	55.66	25.16	29.24
9	128	158	328	25.74	10.80	644	91.33	12	54.00	23.79	28.68
10	113	139	291	22.67	9.60	569	80.85	11	48.83	20.92	25.74

Table 3: Degree based on Graph indices of PAHs (Cont.)

no	M_1	M_2	F	GA	H	HM	SO	Al	SDD	mM	Mm
11	108	132	278	21.65	10.00	542	77.39	12	47.00	19.73	24.97
12	120	151	312	23.79	9.83	614	85.54	10	49.66	22.16	26.24
13	103	130	270	20.75	8.76	530	74.27	10	44.00	19.05	23.43
14	98	118	256	19.65	8.36	492	70.84	14	45.33	17.25	23.98
15	96	112	246	19.61	8.50	470	69.57	16	45.66	16.89	24.43
16	76	90	188	15.83	6.86	368	54.29	8	33.33	14.52	17.79
17	110	133	274	22.83	9.86	540	78.33	8	47.33	21.52	24.79
18	94	117	242	18.83	7.86	476	67.01	8	39.33	17.52	20.79
19	109	136	281	21.81	9.10	562	77.69	9	45.50	20.34	24.01
20	102	126	258	20.87	8.90	510	72.53	6	43.00	19.89	22.34
21	128	159	328	25.79	9.50	646	91.19	10	32.12	24.16	28.24
22	95	113	235	19.81	8.60	461	67.79	9	41.50	18.34	22.01
23	100	125	262	19.69	8.20	512	78.66	10	42.66	18.10	22.52
24	114	138	298	22.43	9.43	574	82.24	18	51.00	19.57	27.60
25	98	120	250	19.79	8.33	490	69.98	10	41.66	18.16	22.24
26	110	133	274	22.83	9.86	540	78.33	8	47.33	21.52	24.79
27	94	117	242	18.83	7.86	476	67.01	8	39.33	17.52	20.79
28	86	102	221	17.71	7.73	420	61.68	6	38.33	15.68	20.87
29	125	156	327	24.63	10.23	639	89.47	10	53.16	22.55	28.19
30	81	95	203	16.67	7.26	393	58.23	6	36.83	14.92	19.74
31	88	105	228	17.52	7.50	438	63.58	11	37.00	15.31	21.70
32	72	87	180	14.87	6.40	354	51.32	14	31.00	13.89	16.34
33	82	98	208	16.69	7.20	404	58.86	6	36.66	15.10	19.52
34	82	101	208	16.83	7.33	410	58.43	8	35.33	15.78	18.53
35	82	99	208	16.74	7.23	406	58.72	6	36.33	15.47	19.07
36	76	91	188	15.87	6.90	370	54.15	8	33.00	14.89	17.34
37	86	104	216	17.79	7.80	424	61.40	8	37.66	16.41	19.98
38	82	99	206	16.83	7.20	404	58.53	8	35.33	15.52	18.79
39	78	95	200	15.74	6.73	390	55.90	8	34.33	14.47	18.07
40	90	113	234	17.83	7.36	460	64.19	8	37.33	16.52	16.12

Table 4 shows the values of the distance-dependent graph indices of 40 PAHs.

Table 4: Distance based on Graph indices of PAHs.

no	W	Mo	Gut
1	1006	252	5970
2	1067	296	5851
3	1444	408	7153
4	654	152	3540
5	808	205	4300
6	725	235	3703
7	876	230	4504
8	845	227	4805
9	971	224	5154
10	714	223	3509

Table 4: Distance based on Graph indices of PAHs (Cont.)

no	W	Mo	Gut
11	628	177	2783
12	703	176	3825
13	511	159	2559
14	573	152	2548
15	582	154	2636
16	279	64	1392
17	757	246	3766
18	362	102	1933
19	732	216	3521
20	513	144	2581
21	900	248	4786
22	513	180	2538
23	433	136	2210
24	764	196	3763
25	466	122	2459
26	761	240	3406
27	362	112	1929
28	425	106	1970
29	770	227	4122
30	334	89	1442
31	396	128	1840
32	220	68	1107
33	334	103	1599
34	319	87	1475
35	326	107	1559
36	271	88	1336
37	388	122	1728
38	265	107	1296
39	276	92	1353
40	301	92	1640

4.1 Curvilinear Regression Models

It is obtained the correlation coefficient in curvilinear regression models, between molecular descriptors and physicochemical properties of PAHs From Table 1, Table 3 and Table 4. The bolded values in the tables show the maximum correlation for each physicochemical property. Since the correlation for feature E was below 0.5, it was not included in the tables. Table 5 shows the correlation coefficient of linear equations.

Table 5: Corelation of TI with properties.

TI	BP	FP	P	MW
M_1	**0.933**	**0.930**	0.974	0.966
M_2	0.928	0.927	0.960	0.944
F	**0.933**	**0.930**	0.967	0.948
GA	0.921	0.919	0.975	**0.980**
H	0.747	0.741	0.848	0.883
HM	0.931	**0.930**	0.961	0.942
SO	0.930	0.925	0.973	0.962
Al	0.350	0.327	0.360	0.334
SDD	0.775	0.760	0.869	0.878
mM	0.901	0.903	0.955	0.964
Mm	0.920	0.907	**0.977**	0.974
W	0.848	0.845	0.947	0.983
Mo	0.776	0.776	0.901	0.952
Gut	0.878	0.880	0.958	0.979

There are multiple molecular descriptors with the same correlation for the BP, and FP properties. Therefore, not only the maximum correlation but also the minimum RMSE values for these properties should be examined. Linear equations and their RMSE values are given below.

$BP = 100.834 + 2.981M_1$, $SE = 25.172$, $RMSE = 0.783$

$BP = 120.410 + 1.087F$, $SE = 25.115$, $RMSE = 0.782$

$FP = 12.513 + 1.766M_1$, $SE = 15.216$, $RMSE = 14.831$

$FP = 24.185 + 0.644F$, $SE = 15.225$, $RMSE = 14.839$

$FP = 32.081 + 0.313HM$, $SE = 15.299$, $RMSE = 14.911$

The linear regression models with the best predictive ability from (maximum correlation) and minimum RMSE are as follows:

$BP = 120.410 + 1.087F$

$FP = 12.513 + 1.766M_1$

$P = 0.859 + 1.321Mm$ $MW = 31.155 + 9.594GA$,

The correlation coefficient obtained from the second-degree equations is given in Table 7. R^2, RMSE, SE of the model giving the best estimate for linear equation is given in Table 6 .

Table 6: Statistical values of the regression model.

Properties	Index	R^2	RMSE	SE
BP	F	0.871	0.782	25.115
FP	M_1	0.866	14.831	15.216
P	Mm	0.954	1.269	1.303
MW	GA	0.960	7.894	8.099

Table 7: Corelation of TI with properties for quadratic regression.

TI	BP	FP	P	MW
M_1	0.944	0.937	0.976	0.971
M_2	0.941	0.937	0.965	0.953
F	**0.945**	0.938	0.971	0.957
GA	0.934	0.926	0.976	0.981
H	0.915	0.895	0.942	0.955
HM	**0.945**	**0.940**	0.969	0.956
SO	0.938	0.930	0.974	0.965
Al	0.425	0.400	0.424	0.387
SDD	0.776	0.760	0.870	0.880
mM	0.920	0.915	0.957	0.966
Mm	0.920	0.908	**0.977**	0.975
W	0.901	0.886	0.963	**0.992**
Mo	0.847	0.835	0.922	0.962
Gut	0.919	0.912	0.969	0.988

There are two graph indices with the same correlation for the BP property from Table 7. Therefore, the model with the minimum RMSE values for the BP property has the best predictive power. The RMSE values of molecular descriptors in quadratic models for BP are as follows.

$$\text{BP} = -79.746 + 2.557F - 0.003F^2, \quad SE = 23.240, \quad RMSE = 22.351$$

$$\text{BP} = -69.415 + 1.279HM - 0.001HM^2, \quad SE = 23.154, \quad RMSE = 22.268$$

Best predictive models for quadratic equations:

$$\text{BP} = -69.415 + 1.279HM - 0.001HM^2,$$
$$FP = -69.359 + 0.687HM - 0.000HM^2,$$
$$P = 5.809 + 0.895Mm + 0.009Mm^2,$$
$$MW = 127.334 + 0.217W - (5.286 \times 10^5)W^2,$$

R^2, RMSE, SE of the model giving the best estimate for quadratic equation is given in Table 8 .

Table 8: Statistical values of the regression model.

Properties	Index	R^2	RMSE	SE
BP	HM	0.893	22.268	23.154
FP	HM	0.883	13.818	14.368
P	Mm	0.955	1.257	1.307
MW	W	0.984	4.940	5.137

Table 9 shows the correlation between the properties of PAHs and the graph index in third-order equations.

Table 9: Corelation of TI with properties for cubic regression.

TI	BP	FP	P	MW
M_1	0.944	0.937	0.976	0.971
M_2	0.941	0.937	0.965	0.953
F	**0.945**	**0.938**	0.971	0.958
GA	0.935	0.926	0.976	0.981
H	0.920	0.902	0.946	0.959
HM	**0.945**	0.940	0.969	0.957
SO	0.938	0.930	0.974	0.965
Al	0.425	0.400	0.424	0.388
SDD	0.776	0.760	0.871	0.881
mM	0.920	0.916	0.957	0.966
Mm	0.920	0.908	**0.977**	0.975
W	0.907	0.896	0.963	0.992
Mo	0.847	0.836	0.922	0.962
Gut	0.922	0.917	0.970	**0.993**

There are two graph indices with the same correlation for the BP and E properties from Table 9. The RMSE values of graph indices in cubic models for BP and E are as follows:

$$\text{BP} = -14.897 + 1.837F - (2.973 \times 10^{6})F^3, \quad SE = 23.146, \quad RMSE = 22.261$$

$$\text{BP} = -1.446 + 0.905HM - (3.741 \times 10^{7})HM^3, \quad SE = 23.134, \quad RMSE = 22.249$$

From min RMSE and max R, the cubic regression models that give the best prediction for each physicochemical property:

$$\text{BP} = -1.446 + 0.905HM - (3.741 \times 10^{7})HM^3,$$
$$FP = -36.351 + 0.503HM - (1.886 \times 10^{7})HM^3,$$
$$P = 4.205 + 1.104Mm + 0.000Mm^3,$$

$$MW = 96.383 + 0.079Gut - (1.314 \times 10^{5})Gut^2 + (9.326 \times 10^{-10})Gut^3,$$

R^2, RMSE, SE of the model giving the best estimate for cubic equations are given in Table 10.

Table 10: Statistical values of the regression models.

PB	Index	R^2	RMSE	SE
BP	HM	0.893	22.249	23.134
FP	HM	0.884	13.782	14.330
P	Mm	0.955	1.256	5.022
MW	Gut	0.985	4.764	5.022

4.2 Machine Learning

In recent years, machine learning (ML) techniques have become an essential complement to both experimental and theoretical studies in chemistry. Owing to advances in data generation capacity and computational power, ML-based approaches are increasingly employed to model structure-property relationships, predict reaction mechanisms, and design novel compounds. The literature shows that regression and classification algorithms can predict key molecular properties such as solubility, logP, melting and boiling points, toxicity, and biological activity with high accuracy ([3], [20]). Moreover, deep learning methods have been widely applied to the analysis of complex datasets from molecular dynamics simulations and to the estimation of potential energy surfaces ([24], [18]). Application domains such as drug discovery, catalyst development, and sustainable material design particularly benefit from ML, as it not only reduces experimental costs but also accelerates research processes, thereby enhancing scientific productivity ([25], [13]). Thus, the integration of ML into chemistry represents not merely a data-analysis tool, but a paradigm shift in the generation of scientific knowledge.

Multilinear equation obtained by the machine learning for the MW feature and its statistical values showing its predictive ability:

$$\begin{aligned} MW = {} & 64.35 - 1.94627\,M1 + 1.20171\,M2 + 0.00401851\,F + 13.8274\,GA \\ & + 1.30012\,H + 0.0173452\,HM - 0.243969\,SO - 0.0861282\,irr \\ & - 0.163142\,SDD - 6.92649\,mMs + 1.383\,Mms \\ & + 0.127428\,w + 0.0538977\,Mo - 0.0171918\,Gut \end{aligned}$$

In Figure 2, the graphical comparison of the actual and estimated values for the MW property of PAHs is given.

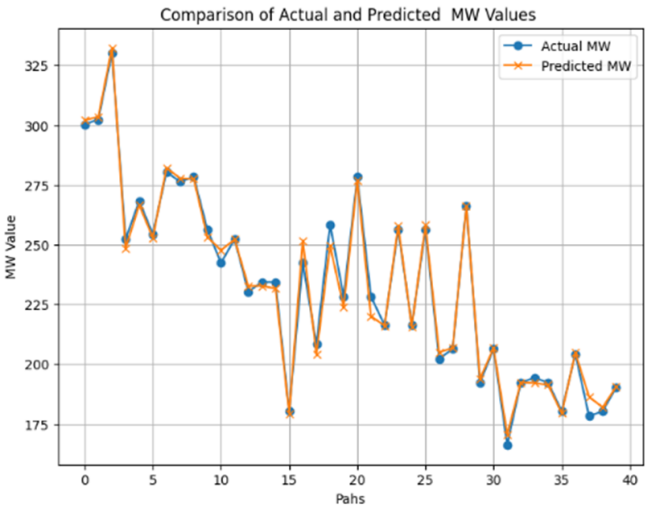

Figure 2: **The actual and estimated values for the MW property**

The best equation and its statistical values showing the prediction ability of the statistical values obtained by the machine learning for the E feature of PAHs:

$$\begin{aligned} E = {} & 3.5128 + 2.93563\,M1 + 0.078334\,M2 - 0.763063\,F + 1.30045\,GA \\ & - 0.387741\,H + 0.0627505\,HM - 0.206438\,SO - 0.0934716\,irr \\ & - 0.159235\,SDD - 4.21591\,mMs + 0.526035\,Mms \\ & + 0.00536468\,w - 0.0365286\,Mo - 0.00420849\,Gut \end{aligned}$$

In Figure 3, the graph comparing the predicted values obtained from the multilinear equation with the actual values for the E property of PAHs is given.

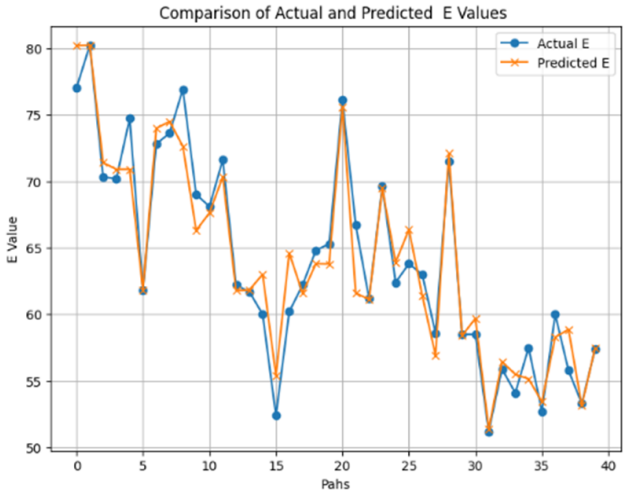

Figure 3: **Comparison of actual and estimated values for the E property**

The equation that gives the best estimate for the P property of PAHs is:

$$\begin{aligned} P = {} & 3.10322 + (-0.460307)M_1 + (0.45969)M_2 + (-0.106955)F + (4.00037)GA \\ & + (0.0855009)H + (0.0110938)HM + (0.0373753)SO + (-0.0828537)irr \\ & + (-0.0331577)SDD + (-2.84511)mM_{sde} + (0.380769)Mm_{sde} + (0.0148446)W \\ & + (0.0028935)Mo + (-0.0025852)Gut \end{aligned}$$

A graph comparing the predicted value from the equation obtained by machine learning for the P property of PAHs with the actual value is shown in Figure 4.

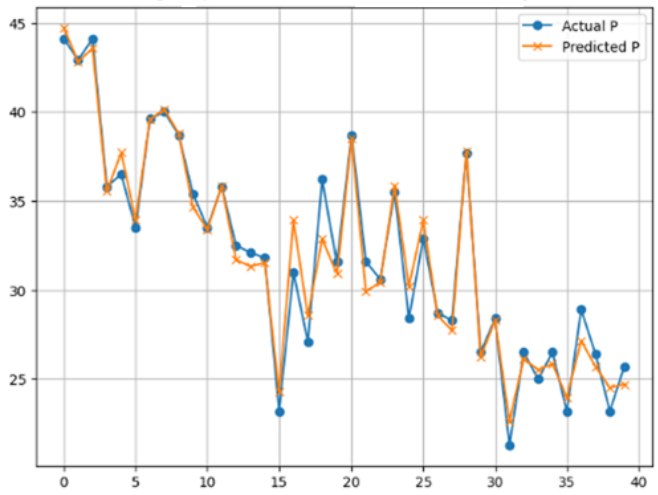

Figure 4: **Comparison of actual and estimated values for the P property**

The equation that gives the best prediction for the BP property obtained through machine learning is:

$$\begin{aligned} BP &= -146.382 + (26.022)M_1 + (0.83452)M_2 + (-6.76353)F + (15.2312)GA \\ &+ (-3.72316)H + (0.507789)HM + (-1.82103)SO + (-0.892031)irr \\ &+ (-1.32476)SDD + (-39.1636)mM_{sde} + (4.39131)Mm_{sde} + (0.0578344)W \\ &+ (-0.30341)Mo + (-0.0433978)Gut \end{aligned}$$

Figure 5 shows the graph comparing the actual value of the BP feature with its estimated value.

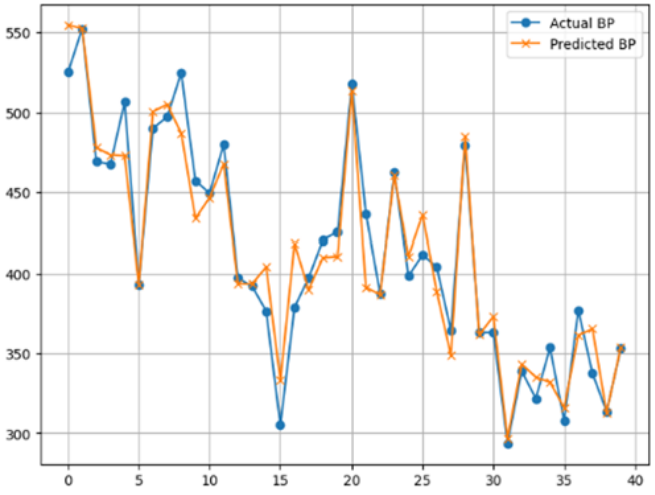

Figure 5: **Comparison of actual and estimated values for the BP property**

The multilinear equation that gives the best prediction for the FP feature obtained through machine learning is:

$$\begin{aligned} FP &= -92.9709 + (15.5609)M_1 + (-1.08424)M_2 + (-2.99096)F \\ &+ (-7.27113)GA + (-1.83136)H + (0.296999)HM + (-1.656)SO \\ &+ (0.29406)irr + (-1.00999)SDD + (-9.21067)mM_{sde} + (1.30174)Mm_{sde} \\ &+ (0.0251005)W + (-0.152534)Mo + (-0.0187646)Gut \end{aligned}$$

The graph comparing the estimated and actual values of the FP feature is given in Figure 6.

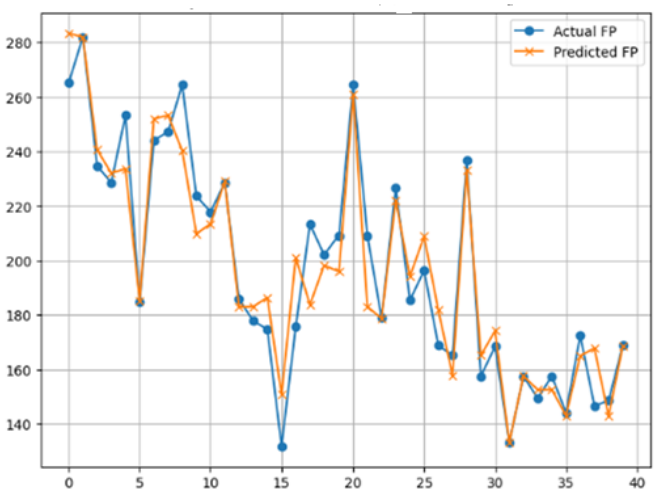

Figure 6: **Comparison of actual and estimated values for the BP property**

The statistical values of the multilinear equations obtained for the BP, FP, P, MW, E properties of PAHs obtained by machine learning are given in Table 11.

Table 11: Model performance metrics for different properties

Features	R^2	**RMSE**	**MAE**
BP	0.929155	18.135977	13.464609
P	0.974679	0.940340	0.702334
FP	0.912519	11.972476	8.781838
E	0.931010	2.002286	1.473012
MW	0.992347	3.433594	2.422730

5 Conclusions

The state of chemicals in the environment can be controlled by their physicochemical properties. Therefore, it is important to know the physicochemical properties of PAHs,

which are priority pollutants. Curvilinear regression models that give the best estimation are obtained for boiling point, enthalpy of vaporization, flash point, polarize, and mass weight of PAHs. These models are obtained with 40 PAHs and 11 degree and 3 distance based graph indices.

In linear regression models, the best estimator indices are

- the forgotten index (F) for boiling point (BP),
- the first Zagreb index for flashpoint
- the max-min rodeg index for polarize,
- the geometric arithmetic index for the mass weight of PAHs.

In quadratic regression models, the best estimator indices are

- the hyper Zagreb index for boiling point, flashpoint,
- the max-min rodeg index for polarize,
- the Wiener index for the mass weight of PAHs.

In cubic regression models, the best estimator molecular descriptors are

- the hyper Zagreb index for boiling point and flashpoint,
- the max-min rodeg index for polarize,
- the Gutman index for the mass weight of PAHs.

It seems that the correlation ability of the Albertson index is rather weak for some properties of PAHs, in this study. The molecular descriptors that make the best prediction in all models, except for the MW property, are degree-dependent descriptors. For MW property, the best predictor molecular descriptor in linear regression models is degree dependent, whereas in quadratic and cubic regression models it depends on distance.

For all properties of PAHs, multilinear regression models obtained by machine learning yielded better predictive equations than linear, quadratic, and cubic regression models. The value of the squared correlation coefficient is closer to 1 than the values of the other models.

The results show that as the degree of regression models increases, the observed value and the estimated value get closer to each other, and the predictive power of the models increases. This work contributes to slowing the duplication of molecular descriptors

Data Availability

In this article, no data were utilized.

Funding statement

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Conflicts of Interest

Authors declare no conflict of interest.

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The Wiener Index of Graphs Obtained from the Associate Graph of $\mathbb{Z}_n$

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Abstract

Let R be a commutative ring, the associate graph, $Ass(R)$ of ring R has the elements of ring R as vertices and two distinct vertices u and v are adjacent if u and v are associate elements of R, and the Wiener index is defined as the sum of the lengths of the shortest paths between all pairs of vertices in the graph. In this chapter, we investigate the Wiener index of the splitting graph, shadow graph, middle graph, and total graph of $Ass(\mathbb{Z}_n)$ for all $n \in \mathbb{N}$.

Keywords: Wiener Index, Associate Graph, Commutative Ring, Splitting Graph, Shadow Graph, Middle Graph, Total Graph
AMS Classification: 05C09, 05C25, 05C76, 05C12

1 Introduction

All the graph considered here are simple, connected and undirected. Clark and Holton [4], Herstein [14] and Burton [3] are the main source for the terminologies related to graph theory, algebra and number theory respectively.

Topological indices (also known as molecular descriptors) are numerical parameters of the graph that characterize its topology and are graph invariants.

The concept of the topological index was first introduced by Wiener [20] while doing research on the boiling points of paraffins. Later, many other indices were developed by researchers, such as Hyper-Wiener index [17], first and second Zagreb index [12], Gutman index [10], etc. These indices are generally classified into two major categories: degree-based and distance-based. Interesting results on topological indices are reported in [7, 8, 13, 6, 9, 5, 11, 1].

In this chapter, we focus on study of the Wiener index of a graph, Hosoya [15], in 1971, gave a mathematical representation of the Wiener index as follows:

Definition 1.1. *For a graph G, the* Wiener index *of G is denoted by $W(G)$ and defined as*

$$W(G) = \sum_{u,v \in V(G)} d_G(u,v)$$

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Yeh and Gutman [21] studied the Wiener index of graphs obtained using some binary operations. While Stevanović [18] generalized result using Wiener polynomial.

The idea of associating the elements of a ring with a graph and investigating the interplay between the ring structure and the graph-theoretical properties of the associated graph was first introduced by Beck [2] in 1988. The study of the associate graph of a commutative ring with unity was initiated by Subhakar [19] in 2010. Khalel and Ibrahiem [16] later modified the definition as follows:

Definition 1.2. *For ring R,* Associate graph *of R is denoted by $Ass(R)$ and is a graph with $V(Ass(R)) = R$ and $E(Ass(R)) = \{uv/u = rv$ and $v = su$ for some r and $s \in R\}$.*

Note that the zero element of R is adjacent to every other vertex in $Ass(R)$.

In this chapter, our main focus is to find the Wiener index for splitting, shadow, middle, and total graphs of an associate graph of a commutative ring $\mathbb{Z}_n$.

2 Preliminaries

In this section, we present a few definitions and results necessary for the advancement of our work.

Definition 2.1. *For a graph G the* splitting graph *$S'(G)$ is obtained by adding new vertex v' corresponding to each vertex of v of G such that $N(v) = N(v')$, where $N(v)$ and $N(v')$ are the neighbourhood sets of v and v' respectively.*

Remark 2.2.

$$deg_{S'(G)}(v) = \begin{cases} 2\,(deg_G(v)) & \text{if } v \in V(G) \\ deg_G(u) & \text{if } v \notin V(G) \end{cases}$$

Definition 2.3. *The* shadow graph *$D_2(G)$ of a connected graph G is constructed by taking two copies of G, say G' and G''. Join each vertex v' in G' to the neighbours of the corresponding vertex v'' in G''.*

Remark 2.4. *Let $D_2(G)$ be a shadow graph of G, then any $v \in V(D_2(G))$, there exist $u \in V(G)$ corresponding to v. Then, $deg_{D_2(G)}(v) = 2\,(deg_G(u))$.*

Definition 2.5. *The* middle graph *of a graph G, denoted by $M(G)$, is the graph whose vertex set is $V(G) \cup E(G)$ and in which two vertices are adjacent if and only if either they are adjacent edges of G or one is a vertex of G and the other is an incident on it.*

Definition 2.6. *The* total graph *of a graph G is the graph whose vertex set is $V(G) \cup E(G)$ and two vertices are adjacent whenever they are either adjacent or incident in G. The total graph of G is denoted by $T(G)$.*

Notations:

- $O = \{0\}$, $O' = \{0'\}$, and $O'' = \{0''\}$.

- For $n \in \mathbb{N}$. The Euler′s totient function of n is denoted by $\phi(n)$ and is given by the number of positive integers not exceeding n that are relatively prime to n.
- For $n \in \mathbb{N}, n \neq 1$, let $n = p_1^{\alpha_1} p_2^{\alpha_2} \dots p_k^{\alpha_k}$, where p_i's are distinct primes and $\alpha_i \in \mathbb{N}$ for all $i = 1, 2, \dots, k$.
  - $\phi(n) = n\left(1 - \frac{1}{p_1}\right)\left(1 - \frac{1}{p_2}\right)\dots\left(1 - \frac{1}{p_k}\right)$.
  - Let $\langle d_j \rangle$ be the sequence of proper divisors of n in increasing order.
  - Define $\tau(n) = \{d_j : \text{ for each } j\}$, $B_{d_j} = \{v \in \mathbb{Z}_n : gcd(v, n) = d_j\}$, $B'_{d_j} = \{v' \in \mathbb{Z}_n : gcd(v', n) = d_j\}$ and $B''_{d_j} = \{v'' \in \mathbb{Z}_n : gcd(v'', n) = d_j\}$
  - $|\tau(n)| = \prod_{i=1}^{k}(\alpha_i + 1) - 1$, $\left|B_{d_j}\right| = \phi\left(\frac{n}{d_j}\right)$, $\left|B'_{d_j}\right| = \phi\left(\frac{n}{d_j}\right)$ and $\left|B''_{d_j}\right| = \phi\left(\frac{n}{d_j}\right)$.

Proposition 2.7. *Let $v \in V(Ass(\mathbb{Z}_n))$ and $d = gcd(v, n)$. Then,*

$$deg\,(v) = \begin{cases} n-1 & \text{if } v \in O \\ \phi\left(\frac{n}{d}\right) & \text{if } v \notin O \end{cases}$$

Proposition 2.8. *The Wiener index of $Ass(\mathbb{Z}_n)$ is given by*

$$W\left(Ass(\mathbb{Z}_n)\right) = 2\binom{n}{2} - \sum_{j=1}^{|\tau(n)|}\binom{\phi\left(\frac{n}{d_j}\right)+1}{2}, \text{ where } d_j \in \tau(n).$$

Proposition 2.9. *Let $[u, v] \in V(L(Ass(\mathbb{Z}_n)))$. Then,*

$$deg\,([u,v]) = \begin{cases} n + \phi\left(\frac{n}{d_j}\right) - 3 & \text{if } u = 0 \text{ and } v \in B_{d_j} \\ 2\left(\phi\left(\frac{n}{d_j}\right) - 1\right) & \text{if } u, v \in B_{d_j} \end{cases}$$

Proposition 2.10.

$$\begin{aligned} W\left(L\left(Ass(\mathbb{Z}_n)\right)\right) = {} & \frac{n(n-1)}{2} + \frac{1}{4}\sum_{j=1}^{|\tau(n)|}\left[\left(\phi\left(\frac{n}{d_j}\right)\right)^4 - 3\cdot\left(\phi\left(\frac{n}{d_j}\right)\right)^2 + 2\cdot\phi\left(\frac{n}{d_j}\right)\right] \\ & + \sum_{j=1}^{|\tau(n)|}\left[\phi\left(\frac{n}{d_j}\right)\left(\sum_{k=1}^{|\tau(n)|}\left(\left(\phi\left(\frac{n}{d_k}\right)\right)^2 - \phi\left(\frac{n}{d_k}\right)\right)\right.\right. \\ & \left.\left. - \left(\left(\phi\left(\frac{n}{d_j}\right)\right)^2 - \phi\left(\frac{n}{d_j}\right)\right)\right)\right] \\ & + \frac{3}{4}\sum_{j=1}^{|\tau(n)|-1}\left[\sum_{k=j+1}^{|\tau(n)|}\left(\left(\phi\left(\frac{n}{d_j}\right)\right)^2 - \phi\left(\frac{n}{d_j}\right)\right)\right. \\ & \left. \times \left(\left(\phi\left(\frac{n}{d_k}\right)\right)^2 - \phi\left(\frac{n}{d_k}\right)\right)\right] \end{aligned}$$

3 Main Results

Theorem 3.1.

$$W\left(S'\left(Ass\left(\mathbb{Z}_n\right)\right)\right) = \begin{cases} 2\left(W\left(Ass\left(\mathbb{Z}_n\right)\right)\right) + 4n - 2 \\ + \sum_{j=1}^{|\tau(n)|} \left(\phi\left(\frac{n}{d_j}\right)\right)^2 + \sum_{j=1}^{|\tau(n)|} \binom{\phi\left(\frac{n}{d_j}\right)}{2} \quad ; \quad \text{if } n \text{ is odd} \\ +2\sum_{j=1}^{|\tau(n)|} \left(\phi\left(\frac{n}{d_j}\right)\left(n-1-\phi\left(\frac{n}{d_j}\right)\right)\right) \\ \\ 2\left(W\left(Ass\left(\mathbb{Z}_n\right)\right)\right) + 4n - 1 \\ + \sum_{j=1}^{|\tau(n)|} \left(\phi\left(\frac{n}{d_j}\right)\right)^2 + \sum_{j=1}^{|\tau(n)|} \binom{\phi\left(\frac{n}{d_j}\right)}{2} \quad ; \quad \text{if } n \text{ is even} \\ +2\sum_{j=1}^{|\tau(n)|} \left(\phi\left(\frac{n}{d_j}\right)\left(n-1-\phi\left(\frac{n}{d_j}\right)\right)\right) \end{cases}$$

Proof. Let $Ass\left(\mathbb{Z}_n\right)$ be the associate graph of $\mathbb{Z}_n$. To construct splitting graph $S'\left(Ass(\mathbb{Z}_n)\right)$, let v' be the added vertex corresponding to each $v \in V\left(Ass\left(\mathbb{Z}_n\right)\right)$.

The distance between any two vertices u and v of $S'\left(Ass(\mathbb{Z}_n)\right)$ is given by following ten cases:

Case 1: If $u \in O$ and $\left(v \in B_{d_j} \text{ or } v \in B'_{d_j}\right)$, then distance between u and v is 1. (There are $2(n-1)$ pairs of such vertices.)

Case 2: If $u \in O'$ and $v \in B_{d_j}$, then distance between u and v is 1. (There are $(n-1)$ pairs of such vertices.)

Case 3: For odd n, if $u \in O'$ and $\left(v \in O \text{ or } v \in B'_{d_j}\right)$, then distance between u and v is 2. (There are n pairs of such vertices.)

Case 4: For even n, if $u \in O'$ and $\left(v \in O \text{ or } v \in B'_{d_j} - \left\{\frac{n}{2}\right\}\right)$, then distance between u and v is 2. (There are $n-1$ pairs of such vertices.) If $u \in O'$ and $v = \frac{n}{2}$, then distance between u and v is 3. (There is one pair of such vertices.)

Case 5: If $u, v \in B_{d_j}$, then distance between u and v is 1. (There are $\sum_{j=1}^{|\tau(n)|} \binom{\phi\left(\frac{n}{d_j}\right)}{2}$ pairs of such vertices.)

Case 6: If $u, v \in B'_{d_j}$, then distance between u and v is 2. (There are $\sum_{j=1}^{|\tau(n)|} \binom{\phi\left(\frac{n}{d_j}\right)}{2}$ pairs of such vertices.)

Case 7: If $\left(u \in B_{d_j} \text{ and } v \in B_{d_k}\right)$ or $\left(u \in B'_{d_j} \text{ and } v \in B'_{d_k}\right)$, $j \neq k$, then distance between u and v is 2. (There are $2 \sum_{j=1}^{|\tau(n)|-1} \left(\sum_{k=j+1}^{|\tau(n)|} \phi\left(\frac{n}{d_j}\right) \phi\left(\frac{n}{d_k}\right) \right)$ pairs of such vertices.)

Case 8: If $u \in B_{d_j}$ and $\left(v \in B'_{d_j} \text{ and } v \neq u'\right)$, then distance between u and v is 1. (There are $\sum_{j=1}^{|\tau(n)|} \phi\left(\frac{n}{d_j}\right) \left(\phi\left(\frac{n}{d_j}\right) - 1\right)$ pairs of such vertices.)

Case 9: If $u \in B_{d_j}$ and $v = u' \in B'_{d_j}$, then distance between u and v is 2. (There are $\sum_{j=1}^{|\tau(n)|} \phi\left(\frac{n}{d_j}\right)$ pairs of such vertices.)

Case 10: If $u \in B_{d_j}$ and $v \in B'_{d_k}$, $j \neq k$, then distance between u and v is 2. (There are $\sum_{j=1}^{|\tau(n)|} \left(\phi\left(\frac{n}{d_j}\right)\left(n - 1 - \phi\left(\frac{n}{d_j}\right)\right)\right)$ pairs of such vertices.)

For odd n,

$$\begin{aligned}
W\left(S'\left(Ass(\mathbb{Z}_n)\right)\right) &= \sum_{u,v\in V(S'(Ass(\mathbb{Z}_n)))} d(u,v) \\
&= \sum_{u\in O \text{ and } \left(v\in B_{d_j} \text{ or } v\in B'_{d_j}\right)} d(u,v) + \sum_{u\in O' \text{ and } v\in B_{d_j}} d(u,v) \\
&\quad + \sum_{u\in O' \text{ and } \left(v\in O \text{ or } v\in B'_{d_j}\right)} d(u,v) + \sum_{u,v\in B_{d_j}} d(u,v) + \sum_{u,v\in B'_{d_j}} d(u,v) \\
&\quad + \sum_{\substack{\left(u\in B_{d_j} \text{ and } v\in B_{d_k}\right) \\ \text{or } \left(u\in B'_{d_j} \text{ and } v\in B'_{d_k}\right)}} d(u,v) + \sum_{u\in B_{d_j},\left(v\in B'_{d_j} \text{ and } v\neq u'\right)} d(u,v) \\
&\quad + \sum_{u\in B_{d_j},v=u'\in B'_{d_j}} d(u,v) + \sum_{u\in B_{d_j},v\in B'_{d_k},j\neq k} d(u,v) \\
&= 2(n-1)+(n-1)+2n+\sum_{j=1}^{|\tau(n)|}\binom{\phi\left(\frac{n}{d_j}\right)}{2}+2\sum_{j=1}^{|\tau(n)|}\binom{\phi\left(\frac{n}{d_j}\right)}{2} \\
&\quad +4\sum_{j=1}^{|\tau(n)|-1}\left(\sum_{k=j+1}^{|\tau(n)|}\phi\left(\frac{n}{d_j}\right)\phi\left(\frac{n}{d_k}\right)\right) \\
&\quad +\sum_{j=1}^{|\tau(n)|}\phi\left(\frac{n}{d_j}\right)\left(\phi\left(\frac{n}{d_j}\right)-1\right)+2\sum_{j=1}^{|\tau(n)|}\phi\left(\frac{n}{d_j}\right) \\
&\quad +2\sum_{j=1}^{|\tau(n)|}\left(\phi\left(\frac{n}{d_j}\right)\left(n-1-\phi\left(\frac{n}{d_j}\right)\right)\right) \\
&= 2\left(W\left(Ass\left(\mathbb{Z}_n\right)\right)\right)+4n-2+\sum_{j=1}^{|\tau(n)|}\left(\phi\left(\frac{n}{d_j}\right)\right)^2+\sum_{j=1}^{|\tau(n)|}\binom{\phi\left(\frac{n}{d_j}\right)}{2} \\
&\quad +2\sum_{j=1}^{|\tau(n)|}\left(\phi\left(\frac{n}{d_j}\right)\left(n-1-\phi\left(\frac{n}{d_j}\right)\right)\right)
\end{aligned}$$

Similarly, for even n,

$$\begin{aligned}
W\left(S'\left(Ass(\mathbb{Z}_n)\right)\right) &= 2\left(W\left(Ass\left(\mathbb{Z}_n\right)\right)\right)+4n-1+\sum_{j=1}^{|\tau(n)|}\left(\phi\left(\frac{n}{d_j}\right)\right)^2+\sum_{j=1}^{|\tau(n)|}\binom{\phi\left(\frac{n}{d_j}\right)}{2} \\
&\quad +2\sum_{j=1}^{|\tau(n)|}\left(\phi\left(\frac{n}{d_j}\right)\left(n-1-\phi\left(\frac{n}{d_j}\right)\right)\right)
\end{aligned}$$

□

Illustration 3.2. *For $n = 12 = 2^2 \cdot 3$. The Wiener index of $S'(Ass(\mathbb{Z}_{12}))$ is 493, when it is computed from graph structure.*
The number of proper divisor of 12 is 5. Then

d_j	$\lvert B_{d_j}\rvert = \phi\left(\frac{n}{d_j}\right)$	B_{d_j}	B'_{d_j}
1	4	$1, 5, 7, 11$	$1', 5', 7', 11'$
2	2	$2, 10$	$2', 10'$
3	2	$3, 9$	$3', 9'$
4	2	$4, 8$	$4', 8'$
6	1	6	$6'$

By Theorem 3.1,

$$\begin{aligned} W\left(S'\left(Ass\left(\mathbb{Z}_n\right)\right)\right) &= 2\left(W\left(Ass\left(\mathbb{Z}_n\right)\right)\right) + 4n - 1 + \sum_{j=1}^{|\tau(n)|}\left(\phi\left(\frac{n}{d_j}\right)\right)^2 + \sum_{j=1}^{|\tau(n)|}\binom{\phi\left(\frac{n}{d_j}\right)}{2} \\ &\quad +2\sum_{j=1}^{|\tau(n)|}\left(\phi\left(\frac{n}{d_j}\right)\left(n-1-\phi\left(\frac{n}{d_j}\right)\right)\right) \\ W\left(S'\left(Ass\left(\mathbb{Z}_{12}\right)\right)\right) &= 2(112) + (48-1) + 29 + 9 + 184 \\ &= 493 \end{aligned}$$

Thus, the Wiener index of $S'(Ass(\mathbb{Z}_{12}))$ computed from graph structure and using Theorem 3.1 are same.

Theorem 3.3.

$$\begin{aligned} W\left(D_2\left(Ass(\mathbb{Z}_n)\right)\right) &= 2\left(W\left(Ass\left(\mathbb{Z}_n\right)\right)\right) + 3n - 1 + \sum_{j=1}^{|\tau(n)|}\left(\phi\left(\frac{n}{d_j}\right)\right)^2 \\ &\quad +2\cdot\sum_{j=1}^{|\tau(n)|}\left(\phi\left(\frac{n}{d_j}\right)\left(n-1-\phi\left(\frac{n}{d_j}\right)\right)\right) \end{aligned}$$

Proof. Let $Ass\left(\mathbb{Z}_n\right)$ be the associate graph of $\mathbb{Z}_n$. To construct $D_2\left(Ass(\mathbb{Z}_n)\right)$, let v' and v'' be the vertices of first and second copies of $Ass\left(\mathbb{Z}_n\right)$ respectively, corresponding to $v \in V\left(Ass\left(\mathbb{Z}_n\right)\right)$.

The distance between any two vertices u and v of $D_2\left(Ass(\mathbb{Z}_n)\right)$ is given by following seven cases:

Case 1: If $u \in O'$ and $v \in O''$, then distance between u and v is 2. (There is 1 pair of such vertices.)

Case 2: If ($u \in O'$ or $u \in O''$) and $\left(v \in B'_{d_j}\right.$ or $\left.v \in B''_{d_j}\right)$, then distance between u and v is 1. (There are $4(n-1)$ pairs of such vertices.)

Case 3: If $\left(u, v \in B'_{d_j}\right)$ or $\left(u, v \in B''_{d_j}\right)$, then distance between u and v is 1. (There are $2\sum_{j=1}^{|\tau(n)|}\binom{\phi\left(\frac{n}{d_j}\right)}{2}$ pairs of such vertices.)

Case 4: If $\left(u \in B'_{d_j} \text{ and } v \in B'_{d_k}\right)$ or $\left(u \in B''_{d_j} \text{ and } v \in B''_{d_k}\right)$, $j \neq k$, then distance between u and v is 2. (There are $2\sum_{j=1}^{|\tau(n)|-1}\left(\sum_{k=j+1}^{|\tau(n)|}\phi\left(\frac{n}{d_j}\right)\phi\left(\frac{n}{d_k}\right)\right)$ pairs of such vertices.)

Case 5: If $u = u' \in B'_{d_j}$ and $\left(v \in B''_{d_j} \text{ and } v \neq u''\right)$, then distance between u and v is 1. (There are $\sum_{j=1}^{|\tau(n)|}\phi\left(\frac{n}{d_j}\right)\left(\phi\left(\frac{n}{d_j}\right)-1\right)$ pairs of such vertices.)

Case 6: If $u = u' \in B'_{d_j}$ and $v = u'' \in B''_{d_j}$, then distance between u and v is 2. (There are $\sum_{j=1}^{|\tau(n)|}\phi\left(\frac{n}{d_j}\right)$ pairs of such vertices for distance 2.)

Case 7: If $u \in B'_{d_j}$ and $v \in B''_{d_k}$, $j \neq k$, then distance between u and v is 2. (There are $\sum_{j=1}^{|\tau(n)|}\phi\left(\frac{n}{d_j}\right)\left(n-1-\phi\left(\frac{n}{d_j}\right)\right)$ pairs of such vertices.)

Hence,

$$\begin{aligned}
W\left(D_2\left(Ass(\mathbb{Z}_n)\right)\right) &= \sum_{u,v\in V(D_2(Ass(\mathbb{Z}_n)))} d(u,v) \\
&= \sum_{u\in O' \text{ and } v\in O''} d(u,v) + \sum_{(u\in O' \text{ or } u\in O'') \text{ and } \left(v\in B'_{d_j} \text{ or } v\in B''_{d_j}\right)} d(u,v) \\
&\quad + \sum_{\left(u,v\in B'_{d_j}\right) \text{ or } \left(u,v\in B''_{d_j}\right)} d(u,v) + \sum_{\substack{\left(u\in B'_{d_j} \text{ and } v\in B'_{d_k}\right) \\ \text{or } \left(u\in B''_{d_j} \text{ and } v\in B''_{d_k}\right), j\neq k}} d(u,v) \\
&\quad + \sum_{u\in B'_{d_j}, \left(v\in B''_{d_j} \text{ and } v\neq u''\right)} d(u,v) + \sum_{u\in B'_{d_j}, v=u''\in B''_{d_j}} d(u,v) \\
&\quad + \sum_{u\in B'_{d_j}, v\in B''_{d_k}, j\neq k} d(u,v) \\
&= 2\cdot 1 + 4(n-1) + 2\sum_{j=1}^{|\tau(n)|} \binom{\phi\left(\frac{n}{d_j}\right)}{2} \\
&\quad + 2\sum_{j=1}^{|\tau(n)|-1} 2\cdot\left(\sum_{k=j+1}^{|\tau(n)|} \phi\left(\frac{n}{d_j}\right)\phi\left(\frac{n}{d_k}\right)\right) \\
&\quad + \sum_{j=1}^{|\tau(n)|} \left(\phi\left(\frac{n}{d_j}\right)-1\right)\left(\phi\left(\frac{n}{d_j}\right)\right) + 2\cdot\sum_{j=1}^{|\tau(n)|}\left(\phi\left(\frac{n}{d_j}\right)\right) \\
&\quad + 2\cdot\sum_{j=1}^{|\tau(n)|}\left(\phi\left(\frac{n}{d_j}\right)\left(n-1-\phi\left(\frac{n}{d_j}\right)\right)\right) \\
&= 2\left(W\left(Ass\left(\mathbb{Z}_n\right)\right)\right) + 3n - 1 + \sum_{j=1}^{|\tau(n)|}\left(\phi\left(\frac{n}{d_j}\right)\right)^2 \\
&\quad + 2\cdot\sum_{j=1}^{|\tau(n)|}\left(\phi\left(\frac{n}{d_j}\right)\left(n-1-\phi\left(\frac{n}{d_j}\right)\right)\right)
\end{aligned}$$

□

Illustration 3.4. *For $n = 15 = 3\cdot 5$. The Wiener index of $D_2\left(Ass(\mathbb{Z}_{15})\right)$ is 674, when it is computed from graph structure.*
The number of proper divisor of 15 is 3. Then

d_j	$\lvert B_{d_j}\rvert = \phi\left(\frac{n}{d_j}\right)$	B'_{d_j}	B''_{d_j}
1	8	$1',2',4',7',8',11',13',14'$	$1'',2'',4'',7'',8'',11'',13'',14''$
3	4	$3',6',9',12'$	$3'',6'',9'',12''$
5	2	$5',10'$	$5'',10''$

By Theorem 3.3,

$$\begin{aligned} W\left(D_2\left(Ass(\mathbb{Z}_n)\right)\right) &= 2\left(W\left(Ass\left(\mathbb{Z}_n\right)\right)\right)+3n-1+\sum_{j=1}^{|\tau(n)|}\left(\phi\left(\frac{n}{d_j}\right)\right)^2 \\ &\quad +2\cdot\sum_{j=1}^{|\tau(n)|}\left(\phi\left(\frac{n}{d_j}\right)\left(n-1-\phi\left(\frac{n}{d_j}\right)\right)\right) \\ W\left(D_2\left(Ass(\mathbb{Z}_{15})\right)\right) &= 2(161)+44+84+224 \\ &= 674 \end{aligned}$$

Thus, the Wiener index of $D_2\left(Ass(\mathbb{Z}_{15})\right)$ computed from graph structure and using Theorem 3.3 are same.

Theorem 3.5. *Let $v \in V\left(M\left(Ass(\mathbb{Z}_n)\right)\right)$. Then,*

$$deg\left(v\right)=\begin{cases} n-1 & \text{if } v\in O \\ \phi\left(\frac{n}{d_j}\right) & \text{if } v\in B_{d_j} \\ n+\phi\left(\frac{n}{d_j}\right)-3 & \text{if } v=[u_1,v_1],\ \text{where } u_1=0 \text{ and } v_1\in B_{d_j} \\ 2\left(\phi\left(\frac{n}{d_j}\right)-1\right) & \text{if } v=[u_1,v_1],\ \text{where } u_1,v_1\in B_{d_j} \end{cases}$$

Proof. By definition of middle graph and Proposition 2.9 we get the result. □

Theorem 3.6.

$$\begin{aligned} W\left(M\left(Ass(\mathbb{Z}_n)\right)\right) &= \frac{3}{2}W\left(Ass\left(\mathbb{Z}_n\right)\right)+W\left(L\left(Ass\left(\mathbb{Z}_n\right)\right)\right)+\frac{1}{2}(n-1) \\ &\quad +\sum_{j=1}^{|\tau(n)|}\left[\left(\phi\left(\frac{n}{d_j}\right)\right)^3+\left(\phi\left(\frac{n}{d_j}\right)\right)^2\right]+\frac{1}{2}\sum_{j=1}^{|\tau(n)|}\binom{\phi\left(\frac{n}{d_j}\right)}{2} \\ &\quad +2\sum_{j=1}^{|\tau(n)|}\left(\phi\left(\frac{n}{d_j}\right)\left(n-1-\phi\left(\frac{n}{d_j}\right)\right)\right) \\ &\quad +\frac{3}{2}\sum_{j=1}^{|\tau(n)|}\left[\phi\left(\frac{n}{d_j}\right)\left(\sum_{k=1}^{|\tau(n)|}\left(\left(\phi\left(\frac{n}{d_k}\right)\right)^2-\phi\left(\frac{n}{d_k}\right)\right)\right.\right. \\ &\qquad \left.\left.-\left(\left(\phi\left(\frac{n}{d_j}\right)\right)^2-\phi\left(\frac{n}{d_j}\right)\right)\right)\right] \end{aligned}$$

Proof. Let $Ass(\mathbb{Z}_n)$ be the associate graph of $\mathbb{Z}_n$. To construct $M(Ass(\mathbb{Z}_n))$, $[u_1, v_1]$ denote the vertex added corresponding to each edge $u_1v_1 \in E(Ass(\mathbb{Z}_n))$.

The distance between any two vertices u and v of $M(Ass(\mathbb{Z}_n))$ is given by following fifteen cases:

Case 1: If $u \in O$, $v = [0, v_i]$, where $i = 1, 2, \ldots, n-1$, then distance between u and v is 1. (There are $(n-1)$ pairs of such vertices.)

Case 2: If $u, v \in \{[0, v_i] : i = 1, 2, \ldots, n-1\}$, then distance between u and v is 1. (There are $\binom{n-1}{2}$ pairs of such vertices.)

Case 3: If $u = [u_1, v_1]$ and $v = [u_2, v_2]$, where $(u_1 = 0), (v_1, u_2, v_2 \in B_{d_j})$ and ($v_1 = u_2$ or $v_1 = v_2$) for some d_j, then distance between u and v is 1.
(There are $\sum_{j=1}^{|\tau(n)|} \phi\left(\frac{n}{d_j}\right)\left(\phi\left(\frac{n}{d_j}\right) - 1\right)$ pairs of such vertices.)

Case 4: If $u = [u_1, v_1]$ and $v = [u_2, v_2]$, where $(u_1 = 0), (v_1, u_2, v_2 \in B_{d_j})$ and ($v_1 \neq u_2$ and $v_1 \neq v_2$) for some d_j, then distance between u and v is 2.
(There are $\sum_{j=1}^{|\tau(n)|} \frac{1}{2}\phi\left(\frac{n}{d_j}\right)\left(\phi\left(\frac{n}{d_j}\right) - 1\right)\left(\phi\left(\frac{n}{d_j}\right) - 2\right)$ pairs of such vertices.)

Case 5: If $u = [u_1, v_1]$ and $v = [u_2, v_2]$, where $u_1, v_1, u_2, v_2 \in B_{d_j}$, for some d_j then

$$d(u, v) = \begin{cases} 2 & \text{if } u_1, v_1, u_2, v_2 \text{ are distinct;} \\ 1 & \text{otherwise} \end{cases}$$

(There are $\sum_{j=1}^{|\tau(n)|} \frac{1}{2}\phi\left(\frac{n}{d_j}\right)\left(\phi\left(\frac{n}{d_j}\right) - 1\right)\left(\phi\left(\frac{n}{d_j}\right) - 2\right)$ pairs of such vertices for distance 1 and there are $\sum_{j=1}^{|\tau(n)|} \frac{1}{8}\phi\left(\frac{n}{d_j}\right)\left(\phi\left(\frac{n}{d_j}\right) - 1\right)\left(\phi\left(\frac{n}{d_j}\right) - 2\right)\left(\phi\left(\frac{n}{d_j}\right) - 3\right)$ pairs of such vertices for distance 2.)

Case 6: If $u = [u_1, v_1]$, where $u_1 = 0$ and $v_1 \in B_{d_j}$ and $v = [u_2, v_2]$, where $u_2, v_2 \in B_{d_k}$, $j \neq k$, then distance between u and v is 2.
(There are $\sum_{j=1}^{|\tau(n)|} \left[\frac{1}{2}\phi\left(\frac{n}{d_j}\right)\left(\sum_{k=1}^{|\tau(n)|}\left(\left(\phi\left(\frac{n}{d_k}\right)\right)^2 - \phi\left(\frac{n}{d_k}\right)\right) - \left(\left(\phi\left(\frac{n}{d_j}\right)\right)^2 - \phi\left(\frac{n}{d_j}\right)\right)\right)\right]$ pairs of such vertices.)

Case 7: If $u = [u_1, v_1]$ and $v = [u_2, v_2]$, where $u_1, v_1 \in B_{d_j}$ and $u_2, v_2 \in B_{d_k}$, $j \neq k$, then distance between u and v is 3. (There are

$$\sum_{j=1}^{|\tau(n)|-1}\left[\sum_{k=j+1}^{|\tau(n)|}\left(\frac{1}{2}\phi\left(\frac{n}{d_j}\right)\left(\phi\left(\frac{n}{d_j}\right)-1\right)\right)\left(\frac{1}{2}\phi\left(\frac{n}{d_k}\right)\left(\phi\left(\frac{n}{d_k}\right)-1\right)\right)\right]$$

pairs of such vertices.)

Case 8: If $u \in B_{d_j}$ and $v = [u_1, v_1]$, where $u_1 = u$ or $v_1 = u$, and $u_1, v_1 \in B_{d_j} \cup \{0\}$, then distance between u and v is 1. (There are $\sum_{j=1}^{|\tau(n)|}\left(\phi\left(\frac{n}{d_j}\right)\right)^2$ pairs of such vertices for distance 1.)

Case 9: If $u \in B_{d_j}$ and $v = [u_1, v_1]$, where $u_1 \neq u \neq v_1$, and $u_1, v_1 \in B_{d_j} \cup \{0\}$, then distance between u and v is 2. (There are $\sum_{j=1}^{|\tau(n)|}\frac{1}{2}\left(\phi\left(\frac{n}{d_j}\right)\right)^2\left(\phi\left(\frac{n}{d_j}\right)-1\right)$ pairs of such vertices for distance 2.)

Case 10: If $u, v \in B_{d_j}$. Then, distance between u and v is 2.
(There are $\sum_{j=1}^{|\tau(n)|}\binom{\phi\left(\frac{n}{d_j}\right)}{2}$ pairs of such vertices.)

Case 11: If $u \in B_{d_j}$ and $v \in B_{d_k}$ for $j \neq k$. Then, distance between u and v is 3.
(There are $\sum_{j=1}^{|\tau(n)|-1}\left(\sum_{k=j+1}^{|\tau(n)|}\phi\left(\frac{n}{d_j}\right)\phi\left(\frac{n}{d_k}\right)\right)$ pairs of such vertices.)

Case 12: If $u \in B_{d_j}$ and $v = [0, v_1]$, where $v_1 \in B_{d_k}$, $j \neq k$, then distance between u and v is 2. (There are $\sum_{j=1}^{|\tau(n)|}\phi\left(\frac{n}{d_j}\right)\left(n-1-\phi\left(\frac{n}{d_j}\right)\right)$ pairs of such vertices.)

Case 13: If $u \in O$ and $v \in B_{d_j}$. Then, distance between u and v is 2.
(There are $n-1$ pairs of such vertices.)

Case 14: If $u \in O$ and $v = [u_1, v_1]$, where $u_1, v_1 \in B_{d_j}$, for some d_j, then distance between u and v is 2. (There are $\sum_{j=1}^{|\tau(n)|}\frac{1}{2}\phi\left(\frac{n}{d_j}\right)\left(\phi\left(\frac{n}{d_j}\right)-1\right)$pairs of such vertices.)

Case 15: If $u \in B_{d_j}$ and $v = [u_1, v_1]$, where $u_1, v_1 \in B_{d_k}$, $j \neq k$, then distance between u and v is 3. (There are
$\sum_{j=1}^{|\tau(n)|}\left[\frac{1}{2}\phi\left(\frac{n}{d_j}\right)\left(\sum_{k=1}^{|\tau(n)|}\left(\left(\phi\left(\frac{n}{d_k}\right)\right)^2-\phi\left(\frac{n}{d_k}\right)\right)-\left(\left(\phi\left(\frac{n}{d_j}\right)\right)^2-\phi\left(\frac{n}{d_j}\right)\right)\right)\right]$ pairs of such vertices.)

Hence,

$$
\begin{aligned}
W\left(M\left(Ass(\mathbb{Z}_n)\right)\right) &= \sum_{u,v\in V(M(Ass(\mathbb{Z}_n)))} d(u,v) \\
&= \sum_{u\in O, v=[0,v_i],\ \text{where } i=1,2,\ldots,n-1} d(u,v) + \sum_{u,v\in\{[0,v_i]:i=1,2,\ldots,n-1\}} d(u,v) \\
&+ \sum_{\substack{u=[u_1,v_1], v=[u_2,v_2], \\ \text{where } (u_1=0), \left(v_1,u_2,v_2\in B_{d_j}\right) \\ \text{and } (v_1=u_2 \text{ or } v_1=v_2)}} d(u,v) + \sum_{\substack{u=[u_1,v_1], v=[u_2,v_2], \\ \text{where } (u_1=0), \left(v_1,u_2,v_2\in B_{d_j}\right) \\ \text{and } (v_1\neq u_2 \text{ and } v_1\neq v_2)}} d(u,v) \\
&+ \sum_{\substack{u=[u_1,v_1], v=[u_2,v_2], \\ \text{where } \left(u_1,v_1,u_2,v_2\in B_{d_j}\right)}} d(u,v) + \sum_{\substack{u=[u_1,v_1], \text{ where } u_1=0 \text{ and } v_1\in B_{d_j} \\ \text{and } v=[u_2,v_2], \\ \text{where } u_2,v_2\in B_{d_k}, j\neq k}} d(u,v) \\
&+ \sum_{\substack{u=[u_1,v_1] \text{ and } v=[u_2,v_2], \\ \text{where } u_1,v_1\in B_{d_j} \\ \text{and } u_2,v_2\in B_{d_k}, j\neq k}} d(u,v) + \sum_{\substack{u\in B_{d_j} \text{ and } v=[u_1,v_1], \\ \text{where } u_1=u \text{ or } v_1=u, \\ \text{and } u_1,v_1\in B_{d_j}\cup\{0\}}} d(u,v) \\
&+ \sum_{\substack{u\in B_{d_j} \text{ and } v=[u_1,v_1], \\ \text{where } u_1\neq u\neq v_1, \\ \text{and } u_1,v_1\in B_{d_j}\cup\{0\}}} d(u,v) + \sum_{u,v\in B_{d_j}} d(u,v) + \sum_{\substack{u\in B_{d_j} \text{ and } v\in B_{d_k} \\ \text{for } j\neq k}} d(u,v) \\
&+ \sum_{\substack{u\in B_{d_j} \text{ and } v=[0,v_1], \\ \text{where } v_1\in B_{d_k}, j\neq k}} d(u,v) + \sum_{u\in O \text{ and } v\in B_{d_j}} d(u,v) \\
&+ \sum_{\substack{u\in O \text{ and } v=[u_1,v_1], \\ \text{where } u_1,v_1\in B_{d_j}}} d(u,v) + \sum_{\substack{u\in B_{d_j} \text{ and } v=[u_1,v_2], \\ \text{where } u_1,v_1\in B_{d_k}, j\neq k}} d(u,v)
\end{aligned}
$$

$$
\begin{aligned}
&= (n-1)+\binom{n-1}{2}+\sum_{j=1}^{|\tau(n)|}\phi\left(\frac{n}{d_j}\right)\left(\phi\left(\frac{n}{d_j}\right)-1\right)\\
&+2\sum_{j=1}^{|\tau(n)|}\frac{1}{2}\phi\left(\frac{n}{d_j}\right)\left(\phi\left(\frac{n}{d_j}\right)-1\right)\left(\phi\left(\frac{n}{d_j}\right)-2\right)\\
&+\sum_{j=1}^{|\tau(n)|}\frac{1}{2}\phi\left(\frac{n}{d_j}\right)\left(\phi\left(\frac{n}{d_j}\right)-1\right)\left(\phi\left(\frac{n}{d_j}\right)-2\right)\\
&+2\sum_{j=1}^{|\tau(n)|}\frac{1}{8}\phi\left(\frac{n}{d_j}\right)\left(\phi\left(\frac{n}{d_j}\right)-1\right)\left(\phi\left(\frac{n}{d_j}\right)-2\right)\left(\phi\left(\frac{n}{d_j}\right)-3\right)\\
&+2\sum_{j=1}^{|\tau(n)|}\left[\frac{1}{2}\phi\left(\frac{n}{d_j}\right)\left(\sum_{k=1}^{|\tau(n)|}\left(\left(\phi\left(\frac{n}{d_k}\right)\right)^2-\phi\left(\frac{n}{d_k}\right)\right)-\left(\left(\phi\left(\frac{n}{d_j}\right)\right)^2-\phi\left(\frac{n}{d_j}\right)\right)\right)\right]\\
&+3\sum_{j=1}^{|\tau(n)|-1}\left[\sum_{k=j+1}^{|\tau(n)|}\left(\frac{1}{2}\phi\left(\frac{n}{d_j}\right)\left(\phi\left(\frac{n}{d_j}\right)-1\right)\right)\left(\frac{1}{2}\phi\left(\frac{n}{d_k}\right)\left(\phi\left(\frac{n}{d_k}\right)-1\right)\right)\right]\\
&+\sum_{j=1}^{|\tau(n)|}\left(\phi\left(\frac{n}{d_j}\right)\right)^2+2\sum_{j=1}^{|\tau(n)|}\frac{1}{2}\left(\phi\left(\frac{n}{d_j}\right)\right)^2\left(\phi\left(\frac{n}{d_j}\right)-1\right)+\sum_{j=1}^{|\tau(n)|}\binom{\phi\left(\frac{n}{d_j}\right)}{2}\\
&+3\sum_{j=1}^{|\tau(n)|-1}\left(\sum_{k=j+1}^{|\tau(n)|}\phi\left(\frac{n}{d_j}\right)\phi\left(\frac{n}{d_k}\right)\right)+2\sum_{j=1}^{|\tau(n)|}\left(\phi\left(\frac{n}{d_j}\right)\left(n-1-\phi\left(\frac{n}{d_j}\right)\right)\right)\\
&+2(n-1)+2\sum_{j=1}^{|\tau(n)|}\frac{1}{2}\phi\left(\frac{n}{d_j}\right)\left(\phi\left(\frac{n}{d_j}\right)-1\right)\\
&+3\sum_{j=1}^{|\tau(n)|}\left[\frac{1}{2}\phi\left(\frac{n}{d_j}\right)\left(\sum_{k=1}^{|\tau(n)|}\left(\left(\phi\left(\frac{n}{d_k}\right)\right)^2-\phi\left(\frac{n}{d_k}\right)\right)-\left(\left(\phi\left(\frac{n}{d_j}\right)\right)^2-\phi\left(\frac{n}{d_j}\right)\right)\right)\right]\\
&= \frac{3}{2}W\left(Ass\left(\mathbb{Z}_n\right)\right)+W\left(L\left(Ass\left(\mathbb{Z}_n\right)\right)\right)+\frac{1}{2}(n-1)+\sum_{j=1}^{|\tau(n)|}\left[\left(\phi\left(\frac{n}{d_j}\right)\right)^3+\left(\phi\left(\frac{n}{d_j}\right)\right)^2\right]\\
&+\frac{1}{2}\sum_{j=1}^{|\tau(n)|}\binom{\phi\left(\frac{n}{d_j}\right)}{2}+2\sum_{j=1}^{|\tau(n)|}\left(\phi\left(\frac{n}{d_j}\right)\left(n-1-\phi\left(\frac{n}{d_j}\right)\right)\right)\\
&+\frac{3}{2}\sum_{j=1}^{|\tau(n)|}\left[\phi\left(\frac{n}{d_j}\right)\left(\sum_{k=1}^{|\tau(n)|}\left(\left(\phi\left(\frac{n}{d_k}\right)\right)^2-\phi\left(\frac{n}{d_k}\right)\right)-\left(\left(\phi\left(\frac{n}{d_j}\right)\right)^2-\phi\left(\frac{n}{d_j}\right)\right)\right)\right]
\end{aligned}
$$

□

Illustration 3.7. *For $n = 12 = 2^2 \cdot 3$. The Wiener index of $M\left(Ass(\mathbb{Z}_{12})\right)$ is 1003, when it is computed from graph structure.*

The number of proper divisor of 12 *is* 5. *Then*

d_j	B_{d_j}	$[0,u], u \in B_{d_j}$	$[u,v], u,v \in B_{d_j}$
1	$1,5,7,11$	$[0,1],[0,5],[0,7],[0,11]$	$[1,5],[1,7],[1,11],[5,7],[5,11],[7,11]$
2	$2,10$	$[0,2],[0,10]$	$[2,10]$
3	$3,9$	$[0,3],[0,9]$	$[3,9]$
4	$4,8$	$[0,4],[0,8]$	$[4,8]$
6	6	$[0,6]$	–

By Theorem 3.6,

$$\begin{aligned} W\left(M\left(Ass(\mathbb{Z}_n)\right)\right) &= \frac{3}{2}W\left(Ass\left(\mathbb{Z}_n\right)\right) + W\left(L\left(Ass\left(\mathbb{Z}_n\right)\right)\right) + \frac{1}{2}(n-1) \\ &\quad + \sum_{j=1}^{|\tau(n)|}\left[\left(\phi\left(\frac{n}{d_j}\right)\right)^3 + \left(\phi\left(\frac{n}{d_j}\right)\right)^2\right] + \frac{1}{2}\sum_{j=1}^{|\tau(n)|}\binom{\phi\left(\frac{n}{d_j}\right)}{2} \\ &\quad + 2\sum_{j=1}^{|\tau(n)|}\left(\phi\left(\frac{n}{d_j}\right)\left(n-1-\phi\left(\frac{n}{d_j}\right)\right)\right) \\ &\quad + \frac{3}{2}\sum_{j=1}^{|\tau(n)|}\left[\phi\left(\frac{n}{d_j}\right)\left(\sum_{k=1}^{|\tau(n)|}\left(\left(\phi\left(\frac{n}{d_k}\right)\right)^2 - \phi\left(\frac{n}{d_k}\right)\right)\right.\right. \\ &\quad \left.\left. - \left(\left(\phi\left(\frac{n}{d_j}\right)\right)^2 - \phi\left(\frac{n}{d_j}\right)\right)\right)\right] \\ W\left(M\left(Ass(\mathbb{Z}_{12})\right)\right) &= \frac{3(112)}{2} + 316 + \frac{12-1}{2} + \frac{9}{2} + 118 + 2(92) + \frac{3(138)}{2} \\ &= 1003 \end{aligned}$$

Thus, the Wiener index of $M\left(Ass(\mathbb{Z}_{12})\right)$ *computed from graph structure and using Theorem 3.6 are same.*

Theorem 3.8. *Let* $v \in V\left(T\left(Ass(\mathbb{Z}_n)\right)\right)$. *Then,*

$$deg\left(v\right) = \begin{cases} 2(n-1) & \text{if } v \in O \\ 2\phi\left(\frac{n}{d_j}\right) & \text{if } v \in B_{d_j} \\ n + \phi\left(\frac{n}{d_j}\right) - 3 & \text{if } v = [u_1, v_1], \text{ where } u_1 = 0 \text{ and } v_1 \in B_{d_j} \\ 2\left(\phi\left(\frac{n}{d_j}\right) - 1\right) & \text{if } v = [u_1, v_1], \text{ where } u_1, v_1 \in B_{d_j} \end{cases}$$

Proof. By definition of total graph and Proposition 2.9 we get the result. □

Theorem 3.9.

$$\begin{aligned} W\left(T\left(Ass(\mathbb{Z}_n)\right)\right) &= W\left(Ass\left(\mathbb{Z}_n\right)\right) + W\left(L\left(Ass\left(\mathbb{Z}_n\right)\right)\right) \\ &\quad + \sum_{j=1}^{|\tau(n)|}\left[\left(\phi\left(\frac{n}{d_j}\right)\right)^3 + \left(\phi\left(\frac{n}{d_j}\right)\right)^2\right] \\ &\quad + 2\sum_{j=1}^{|\tau(n)|}\left(\phi\left(\frac{n}{d_j}\right)\left(n-1-\phi\left(\frac{n}{d_j}\right)\right)\right) \\ &\quad + \frac{3}{2}\sum_{j=1}^{|\tau(n)|}\left[\phi\left(\frac{n}{d_j}\right)\left(\sum_{k=1}^{|\tau(n)|}\left(\left(\phi\left(\frac{n}{d_k}\right)\right)^2 - \phi\left(\frac{n}{d_k}\right)\right)\right.\right. \\ &\quad \left.\left. - \left(\left(\phi\left(\frac{n}{d_j}\right)\right)^2 - \phi\left(\frac{n}{d_j}\right)\right)\right)\right] \end{aligned}$$

Proof. Let $Ass\left(\mathbb{Z}_n\right)$ be the associate graph of $\mathbb{Z}_n$. To construct $T\left(Ass(\mathbb{Z}_n)\right)$, $[u_1, v_1]$ denote the vertex added corresponding to each edge $u_1v_1 \in E\left(Ass\left(\mathbb{Z}_n\right)\right)$.

Distance between any two vertices u and v of $V\left(T\left(Ass\left(\mathbb{Z}_n\right)\right)\right)$ is given as follows: For cases 1 to 9, 12, 14 and 15 distance between u and v is as per Theorem 3.6, and for case 10, 11 and 13, the distance between u and v is 1, 2 and 1, respectively, and for all cases, pairs of such vertices are taking as per Theorem 3.6, then we get the result. □

4 Conclusion

It is a tedious job to compute the Wiener index of any graph. In this chapter, we have computed exact values of the Wiener index of large graphs obtained from the associate graph of $\mathbb{Z}_n$ using various graph operations and comparing them with $W\left(Ass\left(\mathbb{Z}_n\right)\right)$. Our results show that these larger graphs possess higher Wiener index values than the original associate graph

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Distance Based Topological Indices of Deleted Lexicographic Product of Graphs

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Abstract

The Szeged index of a connected graph G is defined as $Sz(G) = \sum_{e=uv\in E(G)} n_u(e)n_v(e)$, where $n_u(e)$ is number of vertices closer to u than to v, the quantity $n_v(e)$ is defined analogously. The Co-PI index of a connected graph G is defined as $Co-PI_v(G) = \sum_{e=uv\in E(G)} |n_u(e) - n_v(e)|$. In this study, we compute the exact values of the Szeged and Co-PI indices of deleted lexicographic product of two connected graphs.

Keywords: Co-PI index, Deleted lexicographic product, Szeged index
AMS Classification: 05C07, 05C09, 05C12, 05C99

1 Introduction and Preliminaries

Let G be a finite, connected, simple graph with vertex and edge sets $V(G)$ and $E(G)$, respectively. The number of vertices of G is denoted by n and number of edges of G is denoted by m. For $v \in V(G)$; the degree of the vertex v , denoted by $\deg(v)$. For vertices $u, v \in V$, the distance $d(u, v)$ is defined as the length of the shortest path between u and v in G. Other terminology and notations needed will be introduced as it naturally occurs in the following and we use [3, 4] for those not defined here.

A topological index is a number related to graph which is invariant under graph isomorphism. In theoretical chemistry, molecular structure descriptors (also called topological indices) are used for modeling physicochemical, pharmacologic, toxicologic, biological and other properties of chemical compounds [8]. There exist several types of such indices, especially those based on vertex degree and distance.

The first Zagreb index [6] of a connected graph G is denoted by $M_1(G)$ and defined by

$$M_1(G) = \sum_{e=uv\in E(G)} \deg(u) + \deg(v).$$

The second Zagreb index [7] of a connected graph G is denoted by $M_2(G)$ and defined by

$$M_2(G) = \sum_{e=uv\in E(G)} \deg(u)\deg(v).$$

The Albertson index [2] of a connected graph G is denoted by $Alb(G)$ and defined by

$$Alb(G) = \sum_{e=uv\in E(G)} |\deg(u) - \deg(v)|.$$

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The total irregularity measure [1] of a graph G is denoted by $irr_t(G)$ and defined by

$$irr_t(G) = \frac{1}{2}\sum_{u,v\in V(G)} |\deg(u) - \deg(v)|.$$

The vertex PI index [11] of a connected graph G is denoted by $PI_v(G)$ and defined by

$$PI_v(G) = \sum_{e=uv\in E(G)} n_u(e) + n_v(e),$$

the Szeged index [9] of a connected graph G is denoted by $Sz(G)$ and defined by

$$Sz(G) = \sum_{e=uv\in E(G)} n_u(e)n_v(e)$$

and the Co-PI index is introduced by Hasani et al. [10] of a connected graph G is denoted by $Co-PI_v(G)$ and defined by

$$Co-PI_v(G) = \sum_{e=uv\in E(G)} |n_u(e) - n_v(e)|$$

here the sum is taken over all edges of G, and for a given edge $e = uv$, the quantity $n_u(e)$ denotes the number of vertices closer to u than to v, the quantity $n_v(e)$ is defined analogously.

The deleted lexicographic product was studied first by Frelih and Miklavič [5] as follow:

For two graphs G and H with $|V(H)| = n$, the deleted lexicographic product $G[H]-nG$ of graphs G and H is a graph with vertex set $V(G)\times V(H)$ and $u = (u_1, v_1)$ is adjacent with $v = (u_2, v_2)$ whenever ($u_1 = u_2$ and v_1 is adjacent with v_2) or ($v_1 \neq v_2$ and u_1 is adjacent with u_2).

2 Main Results

In this section, some exact formulae for the Szeged and Co-PI indices of deleted lexicographic product are presented. We first give the following lemma which will used in main result.

Lemma 2.1 *[12] Let G and H be two graphs with at least two vertices and $\Gamma = G[H]-nG$. Then,*

1. $\deg_W((g,h)) = \deg_H(h) + (|V(H)|-1)\deg_G(g)$
2. *If H has at least three vertices, then*

$$d_W((g,h),(g',h')) = \begin{cases} 1, \text{ if } (g=g', hh'\in E(H)) \text{ or } (gg'\in E(G), h\neq h') \\ 2, \text{ if } (g=g', hh'\notin E(H)) \text{ or } (gg'\in E(G), h=h') \\ d_G(g,g'), \text{ if } (gg'\notin E(G) \text{ and } g\neq g') \end{cases}$$

3. *If H has exactly two vertices, then*

$$d_W((g,h),(g',h')) = \begin{cases} 1, \text{if } (g=g') \text{ or } (gg'\in E(G), h\neq h') \\ d_G(g,g'), \text{ if } (g\neq g', h=h', 2\mid d_G(g,g')) \text{ or } (g\neq g', h\neq h', 2\nmid d_G(g,g')) \\ d_G(g,g')+1, \text{ if } (g\neq g', h\neq h', 2\mid d_G(g,g')) \text{ or } (g\neq g', h=h', 2\nmid d_G(g,g')) \end{cases}$$

The next theorem gives a formula for the Szeged index of the deleted lexicographic product of G and H in terms of their parameters.

Theorem 2.2 *Let G and H be two connected graphs with n_G, n_H vertices and m_G, m_H edges, respectively and $n_H \geq 3$. Then*

$$\begin{aligned} Sz(G[H]-n_HG) &= n_GM_2(H)+M_1(H)(2m_G-3n_Gt_H)+3t_H(3n_Gt_H-4m_G)+m_HM_1(G)+n_H(n_H-1)Sz(G) \\ &\quad +12t_G(n_H-1)[2n_H+3n_Ht_G-m_Gm_H]-6t_Gn_H(n_H-1)[M_1(G)-PI_v(G)] \\ &\quad +4m_Gm_H(n_H+2)-n_H(n_H-1)[2M_1(G)-2PI_v(G)-M_2(G)] \\ &\quad +2m_H(n_H-1)M_1(G)-n_H(n_H-1)[PI_v(G)+m_H+m_G] \end{aligned}$$

where t_G and t_H denote the number of triangles of G and H, respectively.

Proof. Let $t_G(g,g')$ and $t_H(h,h')$ denote the number of triangles containing edge gg' of G and hh' of H, respectively. Using Lemma 2.1 and definition of deleted lexicographic product, we have

$$n_{(g_i,h_l)}((g_i,h_l)(g_j,h_k)) = \begin{cases} \deg_H(h_l)+\deg_G(g_i)-t_H(h_lh_k) & \text{if } i=j, h_lh_k \in E(H), \\ n_Hn_{g_i}(g_ig_j)-\deg_G(g_i)-\deg_H(h_k)+2t_G(g_ig_j)+2 & \text{if } i\neq j, h_lh_k \in E(H), \\ n_Hn_{g_i}(g_ig_j)-\deg_G(g_i)-\deg_H(h_k)+2t_G(g_ig_j) & \text{if } i\neq j, h_lh_k \notin E(H). \end{cases} \quad (1)$$

By definition of deleted lexicographic product, we partition the edge set of $\Gamma = G[H]-n_HG$ into two subsets as follows:

$$\begin{aligned} E_1 &= \{(g,h)(g',h') \mid g=g' \text{ and } hh' \in E(H)\}, \\ E_2 &= \{(g,h)(g',h') \mid h\neq h' \text{ and } gg' \in E(G)\}. \end{aligned} \quad (2)$$

Therefore $Sz(\Gamma) = Sz(\Gamma_1)+Sz(\Gamma_2)$,
where

$$Sz(\Gamma_1) = \sum_{i=1}^{n_G} \sum_{h_lh_k\in E(H)} n_{(g_i,h_l)}[(g_i,h_l)(g_j,h_k)]\, n_{(g_i,h_k)}[(g_i,h_l)(g_j,h_k)]$$

and

$$Sz(\Gamma_2) = \sum_{g_ig_j\in E(G)} \sum_{\substack{h_l,h_k\in V(H) \\ l\neq k}} n_{(g_i,h_l)}[(g_i,h_l)(g_j,h_k)]\, n_{(g_j,h_k)}[(g_i,h_l)(g_j,h_k)].$$

Thus,

$$\begin{aligned} Sz(\Gamma_1) &= \sum_{i=1}^{n_G} \sum_{h_lh_k\in E(H)} [\deg_H(h_l)+\deg_G(g_i)-t_H(h_lh_k)][\deg_H(h_k)+\deg_G(g_i)-t_H(h_lh_k)] \\ &= \sum_{i=1}^{n_G} \sum_{h_lh_k\in E(H)} \deg_H(h_l)\deg_H(h_k)+\sum_{i=1}^{n_G} \sum_{h_lh_k\in E(H)} \deg_H(h_l)\deg_G(g_i) \\ &\quad -\sum_{i=1}^{n_G} \sum_{h_lh_k\in E(H)} \deg_H(h_l)t_H(h_lh_k)+\sum_{i=1}^{n_G} \sum_{h_lh_k\in E(H)} \deg_G(g_i)\deg_H(h_k) \\ &\quad +\sum_{i=1}^{n_G} \sum_{h_lh_k\in E(H)} \deg_G^2(g_i)-\sum_{i=1}^{n_G} \sum_{h_lh_k\in E(H)} \deg_G(g_i)t_H(h_lh_k) \\ &\quad -\sum_{i=1}^{n_G} \sum_{h_lh_k\in E(H)} t_H(h_lh_k)\deg_H(h_k)-\sum_{i=1}^{n_G} \sum_{h_lh_k\in E(H)} t_H(h_lh_k)\deg_G(g_i) \\ &\quad +\sum_{i=1}^{n_G} \sum_{h_lh_k\in E(H)} t_H^2(h_lh_k) \\ &= n_GM_2(H)+2m_GM_1(H)-3n_GM_1(H)t_H-12m_Gt_H+m_HM_1(G)+9n_Gt_H^2. \end{aligned}$$

Let

$$\begin{aligned} A &= n_H n_{g_i}(g_i g_j) - \deg_G(g_i) - \deg_H(h_k) + 2t_G(g_i g_j) + 2, \\ B &= n_H n_{g_j}(g_i g_j) - \deg_G(g_j) - \deg_H(h_l) + 2t_G(g_i g_j) + 2. \end{aligned}$$

Then,

$$\begin{aligned} Sz(\Gamma_2) &= \sum_{g_i g_j \in E(G)} \sum_{\substack{h_l, h_k \in V(H) \\ l \neq k}} AB \\ &= n_H(n_H-1)Sz(G) + 12t_G(n_H-1)[2n_H + 3n_H t_G - m_G m_H] - 6t_G n_H(n_H-1)[M_1(G) - PI_v(G)] \\ &\quad -n_H(n_H-1)[2M_1(G) - 2PI_v(G) - M_2(G)] + 4m_G m_H(n_H+2) \\ &\quad +2m_H(n_H-1)M_1(G) - n_H(n_H-1)[PI_v(G) + m_H + m_G] \end{aligned}$$

By summation of $Sz(\Gamma_1)$ and $Sz(\Gamma_2)$,the proof is completed. ■

The next theorem gives a formula for the Co-PI index of the deleted lexicographic product of G and H in terms of their parameters.

Theorem 2.3 *Let G and H be two connected graphs with n_G and n_H vertices, respectively and $n_H \geq 3$. Then*

$$Co - PI_v(G[H] - n_H G) = n_G Alb(H) + n_H(n_H-1)(Co - PI_v(G) + Alb(G)) + 2m_G irr_t(H). \quad (3)$$

Proof. Using Lemma 2.1, (1) and (2), we have

$$Co - PI_v(\Gamma) = Co - PI_v(\Gamma_1) + Co - PI_v(\Gamma_2),$$

where

$$Co - PI_v(\Gamma_1) = \sum_{i=1}^{n_G} \sum_{h_l h_k \in E(H)} \left| \left(n_{(g_i,h_l)}[(g_i,h_l)(g_j,h_k)]\right) - \left(n_{(g_i,h_k)}[(g_i,h_l)(g_j,h_k)]\right) \right|$$

and

$$Co - PI_v(\Gamma_2) = \sum_{g_i g_j \in E(G)} \sum_{\substack{h_l, h_k \in V(H) \\ l \neq k}} \left| \left(n_{(g_i,h_l)}[(g_i,h_l)(g_j,h_k)]\right) - \left(n_{(g_j,h_k)}[(g_i,h_l)(g_j,h_k)]\right) \right|.$$

Thus we have,

$$\begin{aligned} Co - PI_v(\Gamma_1) &= \sum_{i=1}^{n_G} \sum_{h_l h_k \in E(H)} |[\deg_H(h_l) + \deg_G(g_i) - t_H(h_l h_k)] - [\deg_H(h_k) + \deg_G(g_i) - t_H(h_l h_k)]| \\ &= \sum_{i=1}^{n_G} \sum_{h_l h_k \in E(H)} |\deg_H(h_l) - \deg_H(h_k)| + \sum_{i=1}^{n_G} \sum_{h_l h_k \in E(H)} |\deg_G(g_i) - \deg_G(g_i)| \\ &\quad + \sum_{i=1}^{n_G} \sum_{h_l h_k \in E(H)} |t_H(h_l h_k) - t_H(h_l h_k)| \\ &= n_G Alb(H). \end{aligned}$$

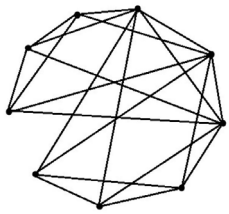

Figure 1. The deleted lexicographic product of P_3 and C_3.

Let

$$\begin{aligned} A &= n_H n_{g_i}(g_i g_j) - \deg_G(g_i) - \deg_H(h_k) + 2t_G(g_i g_j) + 2, \\ B &= n_H n_{g_j}(g_i g_j) - \deg_G(g_j) - \deg_H(h_l) + 2t_G(g_i g_j) + 2. \end{aligned}$$

Then we have,

$$\begin{aligned} Co - PI_v(\Gamma_2) &= \sum_{g_i g_j \in E(G)} \sum_{\substack{h_l, h_k \in V(H) \\ l \neq k}} |A - B| \\ &= n_H(n_H - 1)(Co - PI_v(G) + Alb(G)) + m_G irr_t(H). \end{aligned}$$

By summation of $Co - PI_v(\Gamma_1)$ and $Co - PI_v(\Gamma_2)$,the proof is completed. ■

Example 2.4 *Consider the deleted lexicographic product of P_3 and C_3 shown in Figure 1. So, by Theorem 2.2, by replacing $Sz(P_3) = 4, PI_v(P_3) = 6, M_1(P_3) = 6, M_2(P_3) = 4, M_1(C_3) = 12, M_2(C_3) = 12, t_{P_3} = 0, t_{C_3} = 1$ in relation, we get $Sz(P_3[C_3] - 3P_3) = 147$.*

Also, by Theorem 2.3 we have

$$Co - PI_v(P_3[C_3] - 3P_3) = n_{P_3} Alb(C_3) + n_{C_3}(n_{C_3} - 1)(Co - PI_v(P_3) + Alb(P_3)) + 2m_{P_3} irr_t(C_3). \quad (4)$$

Then, by replacing $Alb(C_3) =, Co - PI_v(P_3) = 6, Alb(P_3) = 6, irr_t(C_3) = 4$ in relation (4), $Co - PI_v(P_3[C_3] - 3P_3) = 24$.

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Reduced first Zagreb index of graphs with added edges

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Abstract

Adding or deleting an edge or a vertex gives a smaller or larger graph compared to the original graph and hence the calculations on smaller graph helps us to get the information of larger graph. In this paper, we compute the change in the reduced first Zagreb index of a simple graph G when an arbitrary edge is added is considered. In particular, some statements for the change of reduced first Zagreb indices of path, cycle, star, complete, complete bipartite and tadpole graphs are obtained to illustrate the affect of this operation.

Keywords: Graphs, Pendant edge, Vertex degrees, Graph index, Reduced first Zagreb index, Edge addition.
2010 AMS Classification: 05C07, 05C09, 05C30, 05C38

1 Introduction

Throughout this paper, we consider $G = (V, E)$ as connected and simple graphs which are finite and undirected graphs without any loops and multiple edges. The notation $d_G(v)$ denotes the degree of a vertex $v \in V(G)$. A vertex having degree one will be called as a pendant vertex. Here the notations P_n, C_n, S_n, K_n, $K_{r,s}$ and $T_{r,s}$ denote the path, cycle, star, complete, complete bipartite and tadpole graphs, respectively.

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2 Zagreb indices

Since 1947, several degree based graph topological indices have been defined in many areas to study required properties of different objects such as atoms and molecules. The most studied degree based topological indices are the family of Zagreb indices. Two of the most important indices are called the first and second Zagreb indices denoted by $M_1(G)$ and $M_2(G)$, respectively in [3]:

$$M_1(G) = \sum_{u \in V(G)} d_G^2(u) \quad \text{and} \quad M_2(G) = \sum_{uv \in E(G)} d_G(u) d_G(v). \tag{1}$$

In a similar way, reduced first and second Zagreb indices are introduced and they are denoted by $M_1^R(G)$ and $M_2^R(G)$.

The reduced first Zagreb index is defined by

$$M_1^R(G) = \sum_{i=1}^{n} (d_i - 1)^2$$

And the reduced second Zagreb index is defined by

$$M_2^R(G) = \sum_{e=uv} (du - 1)(dv - 1)$$

Reduced first and second Zagreb indices interms of first and second Zagreb indices are as follows:

Reduced first Zagreb index satisfies the following relation in terms of the first Zagreb index and the order and size of the given graph:

$$\begin{aligned} M_1^R(G) &= \sum_{i=1}^{n} (d_i - 1)^2 \\ &= \sum_{i=1}^{n} d_i^2 - 2 \sum_{i=1}^{n} d_i + \sum_{i=1}^{n} 1 \end{aligned}$$

and hence

$$M_1^R(G) = M_1(G) - 4m + n. \tag{2}$$

Reduced second Zagreb index also has a similar expression in terms of the first and second Zagreb indices together with the size of the graph as

$$\begin{aligned} M_2^R(G) &= \sum_{uv \in E} dudv - \sum_{uv \in E} (du + dv) + \sum_{uv \in E} 1 \\ &= M_2(G) - M_1(G) + m. \end{aligned}$$

In this work, we find the effect of the reduced first Zagreb index when an edge e is added to a given graph. Finally we give examples to the change of reduced first Zagreb index for some well-known graphs when a new edge is added.

3 Change in the reduced first Zagreb index when a new edge is added

In this section, we will determine the amount of change in the reduced first Zagreb index when a new edge is added to a simple graph. We have

Theorem 3.1. *Let G be a connected simple graph and let $G+e$ be the connected graph obtained by adding an edge e to the graph G.*

i) *If e is a pendant edge joining the vertex $v_i \in V(G)$ of degree d_i with a new pendant vertex v_{n+1}, then*

$$M_1^R(G+e) = M_1(G) + 2(1 + d_G v_i) - 4m(G) + n(G). \tag{3}$$

ii) *If the added edge e connects two vertices v_i, v_j of the graph G with degrees d_i, d_j respectively, then*

$$M_1^R(G+e) = M_1(G) + 2(1 + d_G v_i + d_G v_j) - 4m(G) + n(G). \tag{4}$$

Proof. ***i)*** Let G be the graph having the vertices $v_1, v_2, \cdots, v_n$ of degrees $d_1, d_2, \cdots, d_n$, respectively. Let us add a new pendant edge e between the vertex $v_i \in V(G)$ of degree d_i in G and a new vertex v_{n+1} of degree $d_{n+1} = 1$ which is clearly not a vertex of G. By Eqn. (2), we can write

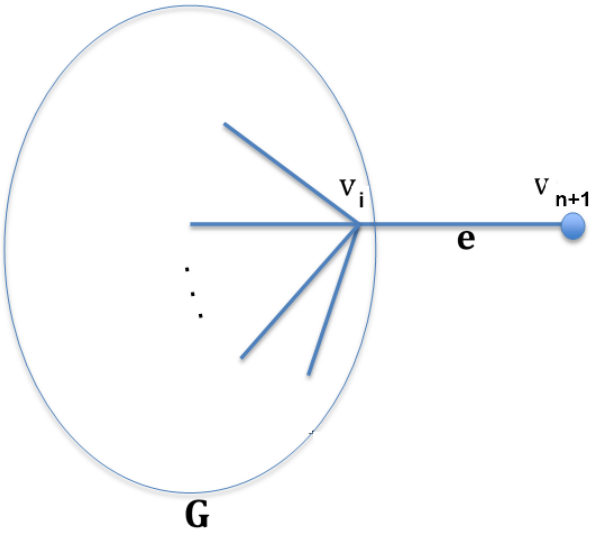

Figure 1: Adding a pendant edge e to G

$$\begin{aligned} M_1^R(G+e) &= M_1(G+e) - 4m(G) + n(G) \\ &= \sum_{v_i \neq v \in V(G+e)} d^2_{G+e}v + d^2_{G+e}v_i + d^2_{G+e}v_{n+1} - 4m(G) + n(G) \\ &= \sum_{v_i \neq v \in V(G)} (1 + d_G v_i)^2 + 1 - 4m(G) + n(G) \\ &= M_1(G) - d^2_G v_i + d^2_G v_i + 2d_G v_i + 2 - 4m(G) + n(G) \\ &= M_1(G) + 2(1 + d_G v_i) - 4m(G) + n(G) \end{aligned}$$

which gives the result.

ii) Consider two vertices $v_i,\ v_j \in V(G)$. Let us add a new edge $e = v_i v_j$ to the graph G. Adding an edge e increases the degrees of v_i and v_j by 1. Hence we have

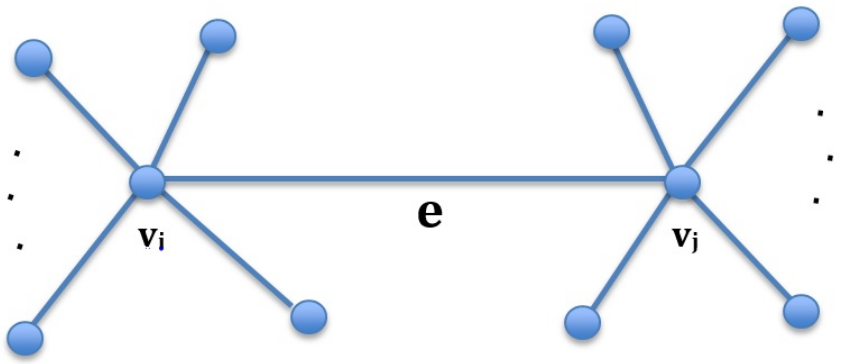

Figure 2: Adding a non-pendant edge e to G

$$\begin{aligned} M_1^R(G+e) &= M_1(G+e) - 4m(G) + n(G) \\ &= \sum_{v_i, v_j \neq v \in V(G+e)} d^2_{G+e}v + d^2_{G+e}v_i + d^2_{G+e}v_j - 4m(G) + n(G) \\ &= \sum_{v_i, v_j \neq v \in V(G)} d^2_G v + (1 + d_G v_i)^2 + (1 + d_G v_j)^2 - 4m(G) + n(G) \\ &= M_1(G) - d^2_G v_i - d^2_G v_j + d^2_G v_i + d^2_G v_j + 2(1 + d_G v_i + d_G v_j) - 4m(G) + n(G) \\ &= M_1(G) + 2(1 + d_G v_i + d_G v_j) - 4m(G) + n(G). \end{aligned}$$

Hence we proved the theorem. □

4 Effect of edge addition on M_1^R for some classes of graphs

In this section, we get the results for the graph classes P_n, C_n, S_n, K_n, $K_{r,s}$ and $T_{r,s}$ when we add a pendant or a non-pendant edge using above results. We shall not give the detailed proofs as all have utilized Theorem 3.1. These results help us to extend our studies to all graph types by using the same methods of calculation used here.

4.1 Path graph P_n

We find that $M_1(P_n) = 4n - 6$ and $M_1^R(P_n) = n - 2$. Therefore by Theorem 3.1, we can write

$$M_1^R(P_n{+}e) = \begin{cases} n(P_n) + 2 & \text{if a pendant edge is added to one of the two end points} \\ n(P_n) + 4 & \text{if a pendant edge is added to one of the midponts} \\ n(P_n) + 4 & \text{if the new edge is added to two end vertices} \\ n(P_n) + 6 & \text{if the new edge is added between one end vertex and one internal vertex} \\ n(P_n) + 8 & \text{if the new edge is added to two internal vertices.} \end{cases}$$

4.2 Cycle graph C_n

We find that $M_1(C_n) = 4n$ and $M_1^R(C_n) = n$. Hence by Theorem 3.1, we can write

$$M_1^R(C_n + \{e\}) = \begin{cases} n(C_n) + 6 & \text{if a pendant edge is added at any vertex} \\ n(C_n) + 10 & \text{if the new edge is added between two vertices.} \end{cases}$$

4.3 Star graph S_n

We find that for $n \geq 3$, $M_1(S_n) = n^2 - n$ and $M_1^R(S_n) = n^2 - 4n + 6$. Hence by Theorem 3.1, we can write

$$M_1^R(S_n{+}e) = \begin{cases} n(S_n)^2 - 2n(S_n) + 4 & \text{if a pendant edge is added at the central vertex} \\ n(S_n)^2 - 4n(S_n) + 8 & \text{if a pendant edge is added at an outer vertex} \\ n(S_n)^2 - 4n(S_n) + 10 & \text{if the new edge joins two outer vertices} \\ n(S_n)^2 - 4n(S_n) + 12 & \text{if the new edge joins an outer vertex to the central vertex.} \end{cases}$$

4.4 Complete graph K_n

We find that $M_1(K_n) = n(n-1)^2$ and $M_1^R(K_n) = n^3 - 4n^2 + 4n$. Hence by Theorem 3.1, we can write

$$M_1^R(K_n{+}e) = \begin{cases} n(K_n)^3 - 4n(K_n)^2 + 6n(K_n) & \text{if a pendant edge is added to any vertex} \\ n(K_n)^3 - 4n(K_n)^2 + 8n(K_n) & \text{if the new edge is added between any two vertices of } K_n. \end{cases}$$

4.5 Complete bipartite graph $K_{r,s}$

We know that $M_1(K_{r,s}) = rs(r+s)$ and $M_1^R(K_{r,s}) = r^2s + rs^2 - 4rs + r + s$. By Theorem 3.1, we can write

$$M_1^R(K_{r,s}{+}e) = \begin{cases} rs(r+s-4) + 3r + s + 2 & \text{if a pendant edge is added to a vertex of degree } r \\ rs(r+s-4) + r + 3s + 2 & \text{if a pendant edge is added to a vertex of degree } s \\ rs(r+s-4) + 5r + s + 2 & \text{if the new edge is added between two vertices of degree } r \\ rs(r+s-4) + r + 5s + 2 & \text{if the new edge is added between two vertices of degree } s \\ rs(r+s-4) + 3r + 3s + 2 & \text{if the new edge is added between two vertices of degrees } r \text{ and} \end{cases}$$

4.6 Tadpole graph $T_{r,s}$

We find that $M_1^R(T_{r,s}) = r + s + 2$. By Theorem 3.1, we can write

$$M_1^R(T_{r,s}+e) = \begin{cases} r+s+6 & \text{if a pendant edge is added to the pendant vertex} \\ r+s+10 & \text{if a pendant edge is added to the vertex of degree 3} \\ r+s+8 & \text{if a pendant edge is added to a vertex of degree 2} \\ r+s+10 & \text{if the new edge is added between two vertices of degree 1 and 3} \\ r+s+12 & \text{if the new edge is added between two vertices of degree 2 and 3} \\ r+s+8 & \text{if the new edge is added between two vertices of degree 1 and 2} \\ r+s+10 & \text{if the new edge is added between two vertices of degree 2} \end{cases}$$

5 Summary and conclusions

In this work, the effect of adding a new edge to a connected simple graph on its reduced first Zagreb index is studied. This effect differs for adding a pendant edge or a non-pendant edge. Both effects are formulized and all possible differences are determined for six most frequently used graph classes. And there will be a continuation of this paper for other indices and graph types.

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Sombor Index for Some Benzenoids

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Abstract

Molecular structure descriptor Sombor index is a new descriptor that is defined as the square root of the sum of squares of degrees. In this paper, Sombor index is investigated with benzenoids. Also, reduced Sombor index is given for different benzenoids in terms of nodes and edges.

Keywords: Centrality measure, Stress, Stress sequence, Stress regular graph
AMS Classification: 05C12, 05C50

1 Introduction

Graph theory is called "The seven bridges of Königsberg" by Leonhard Euler, is used in many relational structures from financial and communication systems to social and biological processes in the real world. Graph theory has become useful and functional in maps, navigation, electrical circuits, artificial intelligence, computer networks, and in many structures such as atomic bonds. For this reason, many articles in the literature try to develop mathematical methods using graph theory.

Sombor is a city in Serbia, and the Sombor index is a molecular structure defined by Gutman in 2021. The Sombor index, which is mostly functional in the molecular structure of atoms, is fairly new and a popular index. The Sombor index is found with the help of the degrees determined by the number of edges emerging from the points of the graph. Sombor index is defined as $\sum_{i\sim j}\sqrt{d_i^2+d_j^2}$ [5]. As the degrees decrease, Reduced Sombor index is identified as $\sum_{i\sim j}\sqrt{(d_i-1)^2+(d_j-1)^2}$ where the degree d_i of vertex $i \in V(G)$ is equal to the number of vertices adjacent to i. It is written $i \sim j$ if there is an edge connecting vertex i to vertex j [5]. Also, chemical significance of Sombor index is investigated in [1], [3], [7], [8], [9] and some properties of Sombor index is explained in [2], [4], [6].

Benzene is the most elementary member of the class of organic compounds known as arenes or aromatics. The benzene molecule is used in nanosciences, chemistry, and physics. The molecular formula of benzene is C_2H_6. A compound containing at least one benzene ring is called a benzenoid. This paper computes the Sombor and Reduced Sombor indices for a few benzenoids.

2 Main Results

2.1 Sombor Index and Reduced Sombor Index of Triangular Benzenoids

In this section, triangular benzenoids are considered which is a category of benzenoid molecular graphs. Also, triangular benzenoids are the generalization of benzene molecule C_2H_6 characterized by the arrangement of benzene rings in a triangle configuration. These graphs contain hexagonal cycles organized in rows, with each row

including an increasing hexagon. The triangular benzenoid molecular graph is illustrated in the following where n denotes the number of hexagons at the base of the graph. E_{ij} represents the number of edges generated from vertices with degrees i and j.

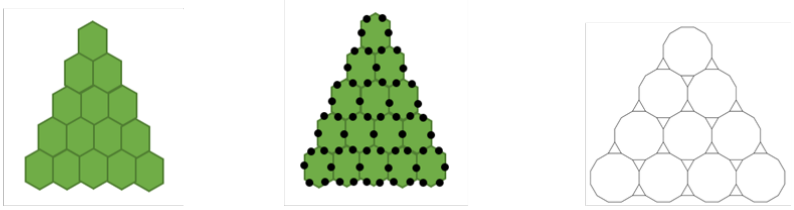

Fig. 1 Benzenoids

In the above structure, the first graph is a triangular benzenoid, the second graph is a subdivision graph of triangular benzenoid and the third graph is a line graph of triangular benzenoid. The values of E_{22}, E_{23}, E_{33} are represented for these benzenoids in the different tables.

1) E_{22}, E_{23}, E_{33} values of triangular benzenoids are given in the Table 1:

	i=2,j=2	i=2,j=3	i=3,j=3
The number of edges connecting a degree-i and a degree-j vertex	$E_{22} = 6$	$E_{23} = 6(n-1)$	$E_{33} = \frac{3}{2}(n^2 - n)$

Table 1 The values of triangular benzenoids

Theorem 2.1. *Let G be a triangular benzenoid graph consisting of n hexagons at its base. The Sombor index of G is determined as follows*

$$SO(G) = \frac{9\sqrt{2}}{2}n^2 + (6\sqrt{13} - \frac{9\sqrt{2}}{2})n \ + 12\sqrt{2} - 6\sqrt{13}.$$

Proof It is known that $SO\,(G) = E_{22}\sqrt{8} + E_{23}\sqrt{13} + E_{33}\sqrt{18}$. If the values of E_{22}, E_{23}, E_{33} in Table 1 are written then $SO\,(G)$ is obtained as follows

$$\begin{aligned} SO\,(G) \ &= \ 12\sqrt{2} + 6\sqrt{13}\,(n-1) + \frac{9\sqrt{2}}{2}\left(n^2 - n\right) \\ &= \frac{9\sqrt{2}}{2}n^2 + \left(6\sqrt{13} - \frac{9\sqrt{2}}{2}\right)n + 12\sqrt{2} - 6\sqrt{13}. \end{aligned}$$

□

Theorem 2.2. *Let G be a triangular benzenoid graph with n hexagons in the base. The reduced Sombor Index of G is found as follows*

$$\mathrm{SO}_{red}\,(G) = 3\sqrt{2}n^2 + \left(6\sqrt{5} - 3\sqrt{2}\right)n + 6\sqrt{2} - 6\sqrt{5}.$$

Proof Since $\mathrm{SO}_{red}\,(G) = E_{22}\sqrt{26} + E_{23}\sqrt{5} + E_{33}\sqrt{8}$, then by substituting the values of E_{22}, E_{23}, E_{33} in the Table 1, the following equation is obtained

$$\mathrm{SO}_{red}(G) = 3\sqrt{2}n^2 + (6\sqrt{5} - 3\sqrt{2})n + 6\sqrt{2} - 6\sqrt{5}.$$

□

2) E_{22}, E_{23}, E_{33} values of the subdivision graph of triangular benzenoid are shown in the Table 2:

	i=2,j=2	i=2,j=3	i=3,j=3
The number of edges connecting a degree-i and a degree-j vertex	$E_{22} = 6n + 6$	$E_{23} = 3n^2 + 3n - 6$	$E_{33} = 0$

Table 2 The values of the subdivision graph of triangular benzenoid

Theorem 2.3. *Let G be a subdivision graph of triangular benzenoid graph with n dodecagons at the base. The Sombor Index of G is defined as follows:*

$$SO\,(G) = 3\sqrt{13}n^2 + (12\sqrt{2} + 3\sqrt{13})n + 12\sqrt{2} - 6\sqrt{13}.$$

Proof Since $SO\,(G) = E_{22}\sqrt{8} + E_{23}\sqrt{13}$ then,

$$\begin{aligned} SO\,(G) &= (6n+6)\sqrt{8} + (3n^2 + 3n - 6\,)\sqrt{13} \\ &= 3\sqrt{13}n^2 + \left(12\sqrt{2} + 3\sqrt{13}+\right) n + 12\sqrt{2}-6\sqrt{13}. \end{aligned}$$

□

Theorem 2.4. *Let G be a subdivision graph of a triangular benzenoid graph containing n dodecagons at its base. The reduced Sombor Index of G is defined as follows*

$$\mathrm{SO}_{red}(G) = 3\sqrt{5}n^2 + (6\sqrt{2} + 3\sqrt{5})n + 6\sqrt{2} - 6\sqrt{5}.$$

Proof It is known that $SO_{red}(G) = E_{22}\sqrt{2} + E_{23}\sqrt{5}$. Hence, if the values of E_{22}, E_{23} are written from Table 2, then

$$\begin{aligned} SO_{red}(G) &= (6n+6)\sqrt{2} + (3n^2 + 3n - 6\,)\sqrt{5} \\ &= 3\sqrt{5}n^2 + \left(6\sqrt{2} + 3\sqrt{5}\right) n + 6\sqrt{2} - 6\sqrt{5}. \end{aligned}$$

is found. □

3) E_{22}, E_{23}, E_{33} values of line graph of triangular benzenoid are given in the Table 3:

	i=2,j=2	i=2,j=3	i=3,j=3
The number of edges connecting a degree-i and a degree-j vertex	$E_{22} = 5n + 7$	$E_{23} = 6n - 6$	$E_{33} = \frac{9}{2}n^2 + \frac{3}{2}n - 3$

Table 3 The values of line graph of triangular benzenoid

Theorem 2.5. *Let G be a line graph of a triangular benzenoid graph with n dodecagons at the base. The Sombor Index of G is seen as follows*

$$SO\,(G) = \frac{27\sqrt{2}}{2}n^2 + \left(6\sqrt{13} + \frac{29\sqrt{2}}{2}\right) n + 5\sqrt{2} - 6\sqrt{13}.$$

Proof It is known that $SO\,(G) = E_{22}\sqrt{8}+E_{23}\sqrt{13}+E_{33}\sqrt{18}$. Therefore, SO(G) is represented as follows

$$\begin{aligned} SO(G) &= (5n+7)\,2\sqrt{2} + (6n-6)\,\sqrt{13} + (\frac{9}{2}n^{\,2} + \frac{3}{2}n - 3)3\sqrt{2} \\ &= \frac{27\sqrt{2}}{2}n^2 + (6\sqrt{13} + \frac{29\sqrt{2}}{2})n + 5\sqrt{2} - 6\sqrt{13}. \end{aligned}$$

□

Theorem 2.6. *Let G be a line graph of a triangular benzenoid graph containing n dodecagons at its base. The reduced Sombor Index of G is found as follows*

$$\mathrm{SO}_{red}(G) = 3\sqrt{5}n^2 + \left(6\sqrt{2} + 3\sqrt{5}\right)n + 6\sqrt{2} - 6\sqrt{5}.$$

Proof Since $\mathrm{SO}_{red}(G) = E_{22}\sqrt{26} + E_{23}\sqrt{5} + E_{33}\sqrt{8}$ then $\mathrm{SO}_{red}(G)$ is found with the values of E_{22}, E_{23}, E_{33} in the Table 3. That is;

$$\mathrm{SO}_{red}(G) = 3\sqrt{5}n^2 + \left(6\sqrt{2} + 3\sqrt{5}\right)n + 6\sqrt{2} - 6\sqrt{5}.$$

□

2.2 Sombor Index and Reduced Sombor Index of Parallel Benzenoids

In this section, hexagonal parallelogram benzenoids are studied. These benzenoids consist of hexagons arranged in the form of parallelograms, with m representing the number of hexagons in each row and n indicating the number of hexagons in each column.

Fig. 2 Parallel Benzenoids

Fig. 3 Subdivision Graph of a Parallel Benzenoid

The values of E_{22}, E_{23}, E_{33} are reported for these benzenoids in the several tables. 1)E_{22}, E_{23}, E_{33} values of a parallel benzenoid are given in the Table 4:

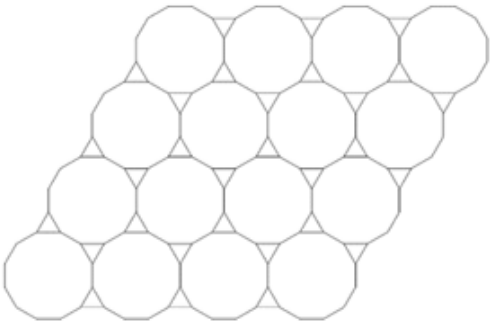

Fig. 4 Line Graph of a Parallel Benzenoid

	i=2,j=2	i=2,j=3	i=3,j=3
The number of edges connecting a degree-i and a degree-j vertex	$E_{22}=6$	$E_{23}=4(m+n-2)$	$E_{33}=-2(m+n)+3mn+1$

Table 4 The values of a parallel benzenoid

Theorem 2.7. *Let G be a parallel benzenoid graph of m horizontal hexagons and n vertical hexagons. The Sombor Index of G is given as follows*

$$SO(G)=9\sqrt{2}mn+(m+n)(4\sqrt{13}-6\sqrt{2})+15\sqrt{2}-8\sqrt{13}.$$

Proof Since $SO(G)=E_{22}\sqrt{8}+E_{23}\sqrt{13}+E_{33}\sqrt{18}$, then the values of E_{22},E_{23},E_{33} are substituted, resulting in

$$SO\,(G)=9\sqrt{2}mn+(m+n)(4\sqrt{13}-6\sqrt{2})+15\sqrt{2}-8\sqrt{13}.$$

□

Theorem 2.8. *Let G be a parallel benzenoid graph with m horizontal hexagons and n vertical hexagons. The reduced Sombor Index of G is specified as follows*

$$\mathrm{SO}_{red}\,(G)=6\sqrt{2}mn+\left(4\sqrt{5}-4\sqrt{2}\right)(m+n)+8\sqrt{2}-8\sqrt{5}.$$

Proof When the definition of $\mathrm{SO}_{red}(G)=E_{22}\sqrt{2}+E_{23}\sqrt{5}+E_{33}\sqrt{8}$ is used,

$$\begin{aligned}SO_{red}\,(G) &= 6\sqrt{2}+4\sqrt{5}(m+n-2)\ +2\sqrt{2}(3mn-2m-2n+1)\\ &= 6\sqrt{2}mn+(4\sqrt{5}-4\sqrt{2})(m+n)+8\sqrt{2}-8\sqrt{5}\end{aligned}$$

is reached. □

2)The values of $E_{22},E_{23},\ E_{33}$ for a subdivision graph of a parallel benzenoid are in the Table 5:

	i=2,j=2	i=2,j=3	
The number of edges connecting a degree-i and a degree-j vertex		$E_{22}=4(m+n+1)$	$E_{33}=6(mn-1)$

Table 5 The values of subdivision graph of a parallel benzenoid

Theorem 2.9. *Let G be a subdivision of parallel benzenoid graph with m horizontal dodecagons and n vertical dodecagons. Then the Sombor Index of G is represented as follows*

$$SO(G) = 6\sqrt{13}mn + 8\sqrt{2}(m+n) + 8\sqrt{2} - 6\sqrt{13}.$$

Proof It is known that $SO(G) = E_{22}\sqrt{8} + E_{23}\sqrt{13}$. Hence, $SO(G) = 4(m+n+1)\ \sqrt{8} + 6(mn-1)\sqrt{13} = 6\sqrt{13}mn + 8\sqrt{2}(m+n) + 8\sqrt{2} - 6\sqrt{13}$ is obtained. □

Theorem 2.10. *Let G be a subdivision of parallel benzenoid graph with m horizontal dodecagons and n vertical dodecagons. The reduced Sombor Index of G is defined as follows*

$$\mathrm{SO}_{red}(G) = 6\sqrt{5}mn + 4\sqrt{2}(m+n) + 4\sqrt{2} - 6\sqrt{5}.$$

Proof Since $\mathrm{SO}_{red}(G) = E_{22}\sqrt{2} + E_{23}\sqrt{5}$ then, $\mathrm{SO}_{red}(G) = 4(m+n+1)\sqrt{2} + 6(mn-1)\sqrt{5} = 6\sqrt{5}mn + 4\sqrt{2}(m+n) + 4\sqrt{2} - 6\sqrt{5}$ is reached. □

3) The values of $E_{22}, E_{23},\ E_{33}$ of a line graph of a parallel benzenoid are presented in the Table 6:

	i=2,j=2	i=2,j=3	i=3,j=3
The number of edges connecting a degree-i and a degree-j vertex	$E_{22} = 2(m+n+4)$	$E_{23} = 4(m+n-2)$	$E_{33} = -2(m+n) + 9mn - 5$

Table 6 The values of a line graph of a parallel benzenoid

Theorem 2.11. *Let G be a line graph of parallel benzenoid with m horizontal dodecagons and n vertical dodecagons. Then the Sombor Index of G is represented as follows*

$$SO(G) = 27\sqrt{2}mn + (4\sqrt{13} - 2\sqrt{2})\ (m+n) + \sqrt{2} - 8\sqrt{13}.$$

Proof It is known that $SO(G) = E_{22}\sqrt{8} + E_{23}\sqrt{13} + E_{33}\sqrt{18}$. If the values of $E_{22}, E_{23},\ E_{33}$ are placed instead

$$\begin{aligned} SO\,(G) &= 2\,(m+n+4)\ \sqrt{8} + 4\,(m+n-2)\,\sqrt{13} + (9mn - 2\,(m+n) - 5)\,\sqrt{18} \\ &= 27\sqrt{2}mn + (m+n)(4\sqrt{13} - 2\sqrt{2}) + \sqrt{2} - 8\sqrt{13} \end{aligned}$$

is obtained. □

Theorem 2.12. *Let G be a line graph of parallel benzenoid with m horizontal dodecagons and n vertical dodecagons. The reduced Sombor Index of G is defined as follows*

$$\mathrm{SO}_{red}(G) = 9\sqrt{2}mn + (4\sqrt{5} - 2\sqrt{2})(m+n) - 2\sqrt{2} - 8\sqrt{5}.$$

Proof Since $\mathrm{SO}_{red}(G) = E_{22}\sqrt{2} + E_{23}\sqrt{5} + E_{33}\sqrt{8}$ then the values of $E_{22}, E_{23},\ E_{33}$ are placed instead

$$\begin{aligned} SO_{red}(G) &= 2(m+n+4)\ \sqrt{2} + 4(m+n-2)\sqrt{5} + (9mn - 2(m+n) - 5)\sqrt{8} \\ &= 9\sqrt{2}mn + (4\sqrt{5} - 2\sqrt{2})(m+n) - 2\sqrt{2} - 8\sqrt{5} \end{aligned}$$

is obtained. □

2.3 Sombor Index and Reduced Sombor Index Of Zigzag-Edged Benzenoids

In this section, the Sombor index and reduced Sombor index of zigzag-edged benzenoids are calculated where k and l are the number of vertical hexagons and m is the number of horizontal hexagons.

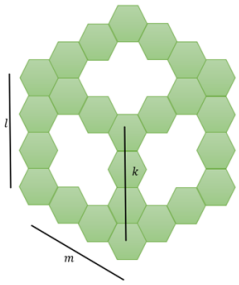

Fig. 5 Zigzag-Edged Benzenoid

	i=2,j=2	i=2,j=3	i=3,j=3
The number of edges connecting a degree-i and a degree-j vertex	$E_{22} = 6$	$E_{23} = 12(k+l+m) - 84$	$E_{33} = 3(k+l+m) + 15$

Table 7 The values of a zigzag-edged benzenoid

Theorem 2.13. *Let G be a zigzag-edged benzenoid graph, where k and l represent the number of vertical hexagons and m denotes the number of horizontal hexagons. Then the Sombor Index of G is given as follows*

$$SO(G) = (12\sqrt{13} + 9\sqrt{2})(k+l+m) + 57\sqrt{2} - 84\sqrt{13}.$$

Proof Since $SO(G) = E_{22}\sqrt{8} + E_{23}\sqrt{13} + E_{33}\sqrt{18}$ then $SO(G)$ is found as follows with the values of E_{22}, E_{23}, E_{33}

$$\begin{aligned} SO(G) &= 6\sqrt{8} + (12(k+l+m) - 84)\sqrt{13} + (3(k+l+m) + 15)\sqrt{18} \\ &= (12\sqrt{13} + 9\sqrt{2})(k+l+m) \ + 57\sqrt{2} - 84\sqrt{13}. \end{aligned}$$

□

Theorem 2.14. *Let G be a zigzag-edged benzenoid graph, where k and l are the number of vertical hexagons and m is the number of horizontal hexagons. Then, the reduced Sombor Index of G is specified as follows*

$$\mathrm{SO}_{red}(G) = (12\sqrt{5} + 6\sqrt{2})(k+l+m) + 36\sqrt{2} - 84\sqrt{5}.$$

Proof It is known that $\mathrm{SO}_{red}(G) = E_{22}\sqrt{2} + E_{23}\sqrt{5} + E_{33}\sqrt{8}$. Hence, $\mathrm{SO}_{red}(G)$ is been that

$$\begin{aligned} \mathrm{SO}_{red}(G) &= 6\sqrt{2} + (12(k+l+m) - 84)\sqrt{5} + (3(k+l+m) + 15)\sqrt{8} \\ &= (12\sqrt{5} + 6\sqrt{2})(k+l+m) + 36\sqrt{2} - 84\sqrt{5} \end{aligned}$$

is obtained. □

3 Conclusion

In this paper, it is purposed to use chemical approaches with the help of benzenes for the Sombor index. In this sense, the reduced Sombor index is researched in terms of different benzenoid structures.

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Computation of the (a, b)-status indices for line graphs of standard graphs

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Abstract

The sum of the shortest distances between a vertex and all other vertices in a graph $\mathcal{G}$ is called the *status* (or *transmission*) of that vertex and is denoted by status(v). Building on this metric, Kulli's (a, b)-status index $S_{a,b}(\mathcal{G})$ provides a unified framework for measuring edge-centric connectivity via distance-based invariants. In this chapter, we compute $S_{a,b}$ for the line graphs of several standard graph families - the star S_n, the complete graph K_n, the cycle C_n, the wheel W_n, and the friendship graph F_n. For each family, we derive explicit closed-form expressions for a range of commonly used status-based topological indices, including the first and second status indices, product and reciprocal product connectivity indices, Gourava-type indices, and the symmetric division status index. These formulae extend the applicability of (a, b)-status indices to derived graph classes and provide a compact toolkit for comparative topological analysis in chemical graph theory and structured network modeling.

Keywords: Topological indices, Status (Transmission), Line graph, (a, b)-Status index, Gourava index, Distance-based invariants
AMS Classification: 05C07, 05C30

1 Introduction

Graph theory provides a compact and expressive framework for modeling pairwise relationships in many scientific and engineering domains, including chemistry, physics, biology, and communication networks. Topological

indices, the number of invariants computed from a graph's structure, are widely used in chemical graph theory and network analysis to capture structural features that correlate with physical, chemical, or functional properties of the underlying system.

Let $\mathcal{G} = (V(\mathcal{G}), E(\mathcal{G}))$ be a simple connected graph. The *status* (or *transmission*) of a vertex $v \in V(\mathcal{G})$ is the sum of distances from v to all other vertices of $\mathcal{G}$:

$$s_{\mathcal{G}}(v) = \sum_{u \in V(\mathcal{G})} d_{\mathcal{G}}(v, u),$$

where $d_{\mathcal{G}}(v, u)$ denotes the length of a shortest path between v and u in $\mathcal{G}$. Ramane et al. [9] introduced status-based connectivity indices (notably the first and second status indices), and Kulli [8] proposed a general (a, b)-status index in the multiplicative form (product):

$$S_{a,b}(\mathcal{G}) = \sum_{uv \in E(\mathcal{G})} s_{\mathcal{G}}(u)^{\,a}\, s_{\mathcal{G}}(v)^{\,b},$$

which recovers many classical transmission-based indices for appropriate choices of the parameters a, b.

Recent work has further expanded the theory and applications of transmission-based descriptors. For example, Gutman and Furtula, [2], studied extended distance-based invariants for chemical and nanostructural graphs; Kulli [7] introduced parametric families of status and Gourava indices tailored to derived and composite graphs; and Furtula et al. [1], proposed new transmission-based descriptors to improve the predictive power of molecular topological models. These developments underscore the continuing relevance of status-type indices in both theoretical and applied graph-theoretic research.

Derived graphs, such as the line graph, total graph, and central graph, are useful whenever the object of interest shifts from vertices to edges or when one examines structural transformations. The *line graph* $\mathrm{L}(\mathcal{G})$ has a vertex set $E(\mathcal{G})$; two vertices of $\mathrm{L}(\mathcal{G})$ are adjacent precisely when the corresponding edges of $\mathcal{G}$ share a common endpoint. Studying $S_{a,b}$ on line graphs therefore yields edge-centric distance invariants and reveals how transmission-based measures transform under the line-graph operation.

In this paper, some recently introduced topological graph indices, see [8], like first status Gourava index

$$SGO_1(G) = \sum_{uv \in E(G)} [\sigma(u) + \sigma(v) + \sigma(u)\sigma(v)],$$

product connectivity status index

$$PS(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{\sigma(u)\sigma(v)}}$$

and reciprocal product connectivity status index

$$RPS(G) = \sum_{e \in E(\mathcal{G})} \sqrt{\sigma(u)\sigma(v)}$$

are calculated for some graphs.

Scope and contributions This chapter provides explicit closed-form computations of $S_{a,b}(\mathrm{L}(\mathcal{G}))$ (and important special cases obtained by choosing a, b) for several standard graph families: the star S_n, the complete graph K_n, the cycle C_n, the wheel W_n, and the friendship graph F_n. The main contributions are as follows.

- Closed-form expressions for $S_{a,b}(\mathrm{L}(\mathcal{G}))$ for each family above, valid for general real parameters a, b.
- Derivation of commonly used special case indices (first- and second-status indices, product and reciprocal product connectivity indices, Gourava-type indices, symmetric-division status index, etc.) as corollaries.
- Discussion of structural and asymptotic behavior of these indices with respect to graph order and degree heterogeneity, and observations on the influence of hubs and degree imbalance.

Organization. Section 2 fixes the notation and records the identities to be used later. Section 3 presents the main theorems and proofs. Section 4 discusses comparative behavior and parameter effects, and Section 5 concludes with directions for future work.

2 Preliminaries and Notation

Let $\mathcal{G} = (V(\mathcal{G}), E(\mathcal{G}))$ be a simple, connected, and undirected graph. The *order* of $\mathcal{G}$ is $n = |V(\mathcal{G})|$ and its *size* is $m = |E(\mathcal{G})|$. For $v \in V(\mathcal{G})$, we denote the degree by $\deg_{\mathcal{G}}(v)$ (or simply $\deg v$ when the graph is clear).

For $u, v \in V(\mathcal{G})$ the (geodesic) *distance* $d_{\mathcal{G}}(u, v)$ is the length of a shortest path that joins u and v. The *status* (transmission) of a vertex v is

$$s_{\mathcal{G}}(v) = \sum_{u \in V(\mathcal{G})} d_{\mathcal{G}}(v, u).$$

When the host graph is clear, we write $s(v)$ and $d(u, v)$ for brevity.

Definition 1 ((a, b)-status index (product form))**.** *Let $a, b \in \mathbb{R}$. The index of status (a, b) of $\mathcal{G}$ (product form) is*

$$S_{a,b}(\mathcal{G}) = \sum_{uv \in E(\mathcal{G})} s_{\mathcal{G}}(u)^{\,a}\, s_{\mathcal{G}}(v)^{\,b},$$

where the sum runs over unordered edges $uv \in E(\mathcal{G})$.

Remark 1. *This multiplicative/product convention is used throughout the chapter. An alternative variant* sum–power*,*

$$\widetilde{S}_{a,b}(\mathcal{G}) = \sum_{uv \in E(\mathcal{G})} \Big(s(u)^a + s(v)^a\Big)^b,$$

appears in some literature; it is not algebraically equivalent to $S_{a,b}(\mathcal{G})$ in general. If you prefer the sum–power form, state it explicitly and recompute the results accordingly.

We recall the line graph and basic counting identities.

Definition 2. *The* line graph *$L(\mathcal{G})$ (or $\mathrm{L}(\mathcal{G})$) of $\mathcal{G}$ is the graph with vertex set $E(\mathcal{G})$ where two vertices $e, f \in E(\mathcal{G})$ are adjacent in $L(\mathcal{G})$ exactly when the corresponding edges in $\mathcal{G}$ share a common endpoint.*

Proposition 1. *Let $\mathcal{G}$ have order n and size m. Then:*

1. $|V(L(\mathcal{G}))| = m$.
2. $|E(L(\mathcal{G}))| = \displaystyle\sum_{v \in V(\mathcal{G})} \binom{\deg_{\mathcal{G}}(v)}{2}$.
3. *For an edge $e = \{u, v\} \in E(\mathcal{G})$,*

$$\deg_{L(\mathcal{G})}(e) = \deg_{\mathcal{G}}(u) + \deg_{\mathcal{G}}(v) - 2.$$

Proof. All elements follow directly from the definition of the line graph. (1) is immediate. For (2) count the unordered pairs of incident edges at each vertex. For (3) each other edge incident with u or v gives a distinct neighbor of e in $L(\mathcal{G})$; exclude e itself. □

Remark 2. *From Proposition 1(2) one obtains*

$$2|E(L(\mathcal{G}))| = \sum_{e\in E(\mathcal{G})} \deg_{L(\mathcal{G})}(e) = \sum_{v\in V(\mathcal{G})} \deg_{\mathcal{G}}(v)\Big(\deg_{\mathcal{G}}(v)-1\Big),$$

useful when converting edge sums in $L(\mathcal{G})$ into vertex sums in $\mathcal{G}$.

Remark 3 (Computing $S_{a,b}(L(\mathcal{G}))$)**.** *A vertex of $L(\mathcal{G})$ corresponds to an edge $e=\{u,v\}$ of $\mathcal{G}$. Calculate the sum distances of $s_{L(\mathcal{G})}(e)$ in $L(\mathcal{G})$ between e and all other edges of $\mathcal{G}$. For symmetric graph families (star, complete, cycle, wheel, friendship) the edges fall into a small number of types; compute $s_{L(\mathcal{G})}$ for each representative type and multiply by multiplicities to obtain closed-form expressions for $S_{a,b}(L(\mathcal{G}))$.*

3 Main Results

We adopt the product convention.

$$S_{a,b}(G) = \sum_{uv\in E(G)} s_G(u)^{\,a}\, s_G(v)^{\,b},$$

where $s_G(x) = \sum_{y\in V(G)} d_G(x,y)$ denotes the transmission (status) of the vertex x on the graph G. All sums of edges are taken over unordered edges $uv \in E(G)$.

Theorem 1. *Let $K_{1,n}$ be the star with $n \geq 2$ leaves. Then*

$$S_{a,b}\Big(\mathrm{L}(K_{1,n})\Big) = \frac{n(n-1)}{2}\,(n-1)^{\,a+b} = \frac{n}{2}\,(n-1)^{\,a+b+1}.$$

Proof. The n spokes of $K_{1,n}$ are mutually adjacent in the line graph, so $\mathrm{L}(K_{1,n}) \cong K_n$. Thus, $|V(\mathrm{L}(K_{1,n}))| = n$ and $|E(\mathrm{L}(K_{1,n}))| = \binom{n}{2} = \dfrac{n(n-1)}{2}$. In K_n the distance between two distinct vertices is 1, so the transmission of every vertex in $\mathrm{L}(K_{1,n})$ is

$$s_L(v) = \sum_{w\in V(\mathrm{L}(K_{1,n}))} d_{\mathrm{L}(K_{1,n})}(v,w) = 0 + (n-1)\cdot 1 = n-1.$$

Therefore, each edge $uv \in E(\mathrm{L}(K_{1,n}))$ contributes $(n-1)^{a+b}$ to $S_{a,b}$, and summing all $\binom{n}{2}$ edges produces the stated formula. □

Table 1: Status pairs and multiplicity for $\mathrm{L}(K_{1,n})$.

Edge in $E(\mathrm{L}(K_{1,n}))$	$(s_L(u), s_L(v))$	multiplicity
All edges	$(n-1, n-1)$	$\frac{n(n-1)}{2}$

Theorem 2. *For $n \geq 2$,*

$$\mathrm{SGO}_1\Big(\mathrm{L}(K_{1,n})\Big) := \sum_{uv \in E(\mathrm{L}(K_{1,n}))} \{s_L(u)+s_L(v)+s_L(u)s_L(v)\} = \frac{n(n-1)}{2}\Big(2(n-1)+(n-1)^2\Big),$$

equivalently

$$\mathrm{SGO}_1\Big(\mathrm{L}(K_{1,n})\Big) = \frac{n^4-n^3-n^2+n}{2}.$$

Proof. By Table 1 every edge uv has $s_L(u) = s_L(v) = n-1$, so each summand equals $(n-1)+(n-1)+(n-1)^2 = 2(n-1)+(n-1)^2$. Multiplying by the number of edges $\frac{n(n-1)}{2}$ gives the first expression. The polynomial form follows by routine algebra (split across lines if needed to avoid overflow). □

Corollary 1 (Star — common special cases)**.** *Let $m = |E(\mathrm{L}(K_{1,n}))| = \frac{n(n-1)}{2}$ and $s_L = n-1$. Then the general formula*

$$S_{a,b}\Big(\mathrm{L}(K_{1,n})\Big) = m\, s_L^{a+b}$$

yields the following frequently used special cases:

$$\begin{aligned}
S_{1,0}\Big(\mathrm{L}(K_{1,n})\Big) &= m(n-1),\\
S_{1,1}\Big(\mathrm{L}(K_{1,n})\Big) &= m(n-1)^2,\\
S_{-1/2,-1/2}\Big(\mathrm{L}(K_{1,n})\Big) &= m(n-1)^{-1} = \frac{n}{2},\\
S_{1/2,1/2}\Big(\mathrm{L}(K_{1,n})\Big) &= m(n-1),\\
S_{a,a}\Big(\mathrm{L}(K_{1,n})\Big) &= m(n-1)^{2a},\\
S_{2,0}\Big(\mathrm{L}(K_{1,n})\Big) &= m(n-1)^2,\\
S_{2,1}\Big(\mathrm{L}(K_{1,n})\Big) &= m(n-1)^3,\\
S_{1,-1}\Big(\mathrm{L}(K_{1,n})\Big) &= m.
\end{aligned}$$

If one uses the standard normalizations $\mathrm{PS} = \frac{1}{2}S_{-1/2,-1/2}$ *and* $\mathrm{RPS} = \frac{1}{2}S_{1/2,1/2}$, *then*

$$\mathrm{PS}\Big(\mathrm{L}(K_{1,n})\Big) = \frac{n}{4}, \qquad \mathrm{RPS}\Big(\mathrm{L}(K_{1,n})\Big) = \frac{n(n-1)^2}{4}.$$

Theorem 3. *Let C_k be a cycle of order k, with $k = 2n$ or $k = 2n+1$. Then*

$$S_{a,b}\Big(\mathrm{L}(C_k)\Big) = \begin{cases} (2n+1)\Big(n(n+1)\Big)^{a+b}, & k = 2n+1, \\ 2\,n^{2a+2b+1}, & k = 2n. \end{cases}$$

Proof. The distances on C_k are classical. For $k = 2n+1$ (odd) each vertex of C_k has transmission $s = n(n+1)$ (since distances $1, \ldots, n$ occur twice); there are $2n+1$ edges in the line graph (which is isomorphic to C_k itself), so the sum is $(2n+1)s^{\,a+b}$.

For $k = 2n$ (even), each vertex of C_k has transmission $s = n^2$ (distances $1, \ldots, n-1$ occur twice and distance n occurs once), and there are $2n$ edges. Thus, $S_{a,b} = 2n \cdot (n^2)^{a+b} = 2n^{2a+2b+1}$. □

Table 2: Status pairs and multiplicities for $\mathrm{L}(C_k)$.

Case	$(s_L(u), s_L(v))$	multiplicity
$k = 2n+1$ (odd)	$(n(n+1),\ n(n+1))$	$2n+1$
$k = 2n$ (even)	$(n^2,\ n^2)$	$2n$

Theorem 4. *With notation as above,*

$$\mathrm{SGO}_1\Big(\mathrm{L}(C_k)\Big) = \begin{cases} n(n+1)(2n+1)(n^2+n+2), & k = 2n+1, \\ 2n^5 + 4n^3, & k = 2n. \end{cases}$$

Proof. Use Table 2: in each case substitute s_L into the summand $2s + s^2$ (since both endpoints have the same s) and multiply by the multiplicity. □

Corollary 2 (Cycle — common special cases)**.** *For C_k, the following holds.*

If $k = 2n+1$ (odd):

$$S_{1,0}\Big(\mathrm{L}(C_k)\Big) = (2n+1)\,n(n+1), \qquad S_{1,1}\Big(\mathrm{L}(C_k)\Big) = (2n+1)\,n^2(n+1)^2,$$

$$S_{-1/2,-1/2}\Big(\mathrm{L}(C_k)\Big) = \frac{2n+1}{n(n+1)}, \qquad S_{a,a}\Big(\mathrm{L}(C_k)\Big) = (2n+1)\,n^{2a}(n+1)^{2a}.$$

If $k = 2n$ (even):

$$S_{1,0}\Big(\mathrm{L}(C_k)\Big) = 2n^3, \qquad S_{1,1}\Big(\mathrm{L}(C_k)\Big) = 2n^5,$$
$$S_{-1/2,-1/2}\Big(\mathrm{L}(C_k)\Big) = \tfrac{2}{n}, \qquad S_{a,a}\Big(\mathrm{L}(C_k)\Big) = 2n^{4a+1}.$$

Theorem 5. *Let K_n be the complete graph on $n \geq 2$ vertices. Then*

$$S_{a,b}\Big(\mathrm{L}(K_n)\Big) = \frac{n}{2}\,(n-1)^{\,a+b+1}(n-2)^{\,a+b+1}.$$

Proof. Fix an edge $e = \{u, v\} \in E(K_n)$. The total number of edges in K_n is $m = \binom{n}{2}$. In the line graph $L(K_n)$ the neighbors of e are exactly the other edges incident to u or v; there are $n-2$ other edges in u and $n-2$ in v, therefore $2(n-2)$ vertices at distance 1. All remaining edges (there are $m-1-2(n-2)$ of them) are disjoint from e and thus at distance 2 in $L(K_n)$. Therefore

$$s_{L(K_n)}(e) = 1 \cdot 2(n-2) + 2 \cdot \Big(m - 1 - 2(n-2)\Big) = 2m - 2n + 2.$$

Substitute $m = \dfrac{n(n-1)}{2}$ to get $s_{L(K_n)}(e) = (n-1)(n-2)$. Thus, every vertex of $L(K_n)$ has the same transmission $s = (n-1)(n-2)$. Next,

$$|E(L(K_n))| = \sum_{v \in V(K_n)} \binom{\deg_{K_n}(v)}{2} = n\binom{n-1}{2} = \frac{n(n-1)(n-2)}{2}.$$

Finally, each edge of $L(K_n)$ contributes to $s^{\,a+b}$, so

$$S_{a,b}\Big(\mathrm{L}(K_n)\Big) = |E(L(K_n))|\, s^{\,a+b} = \frac{n(n-1)(n-2)}{2}\Big((n-1)(n-2)\Big)^{a+b},$$

which simplifies the formula displayed. □

Table 3: Status pair and multiplicity for $\mathrm{L}(K_n)$.

Edge in $E(\mathrm{L}(K_n))$	$(s_L(u), s_L(v))$	multiplicity
All edges	(s, s) with $s = (n-1)(n-2)$	$\dfrac{n(n-1)(n-2)}{2}$

Theorem 6. *For $n \geq 2$,*

$$\mathrm{SGO}_1\Big(\mathrm{L}(K_n)\Big) = \frac{6n^6 - 21n^5 + 31n^4 - 25n^3 + 9n^2}{2}.$$

Proof. Each edge of $L(K_n)$ has endpoints with equal transmission $s = (n-1)(n-2)$; the summand $s_L(u)+s_L(v)+s_L(u)s_L(v) = 2s+s^2$. Multiply $2s+s^2$ by $|E(L(K_n))| = \dfrac{n(n-1)(n-2)}{2}$ and simplify algebraically to obtain the above polynomial expression. □

Corollary 3 (Complete graph — special cases)**.** *For* $\mathrm{L}(K_n)$ *the following special cases hold:*

$$\begin{aligned}
S_{1,0}\Big(\mathrm{L}(K_n)\Big) &= \frac{n}{2}(n-1)^2(n-2)^2,\\
S_{1,1}\Big(\mathrm{L}(K_n)\Big) &= \frac{n}{2}(n-1)^3(n-2)^3,\\
S_{-1/2,-1/2}\Big(\mathrm{L}(K_n)\Big) &= \frac{n}{2},\\
S_{a,a}\Big(\mathrm{L}(K_n)\Big) &= \frac{n}{2}(n-1)^{2a+1}(n-2)^{2a+1},\\
S_{2,0}\Big(\mathrm{L}(K_n)\Big) &= \frac{n}{2}(n-1)^3(n-2)^3,\\
S_{2,1}\Big(\mathrm{L}(K_n)\Big) &= \frac{n}{2}(n-1)^4(n-2)^4,\\
S_{1,-1}\Big(\mathrm{L}(K_n)\Big) &= \frac{n}{2}(n-1)(n-2).
\end{aligned}$$

Theorem 7. *For the wheel* W_n *with* $n \geq 3$,

$$\begin{aligned}
S_{a,b}\Big(\mathrm{L}(W_n)\Big) = {} & 2n\Big((5n+2)^a(8n-6)^b + (5n+2)^b(8n-6)^a\Big)\\
& + n\Big((5n+2)^a(7n-2)^b + (5n+2)^b(7n-2)^a\Big)\\
& + n\Big((7n-2)^a(6n)^b + (7n-2)^b(6n)^a\Big)\\
& + (n^2-3n)(5n+2)^{a+b}.
\end{aligned}$$

Proof. Verifies by inspection of W_n that the edges of W_n fall into the four types listed in Table 4 (spoke edge versus rim edge interactions and rim–rim adjacencies). For each type, compute the transmission of the corresponding vertex in $L(W_n)$ by counting the distances to other edges (this yields the numerical status entries $5n+2, 7n-2, 8n-6, 6n$ reported in the table). Multiplying each summand $s_L(u)^a s_L(v)^b$ by multiplicity and summing gives the displayed formula. (The elementary distance-counting for each representative is routine and can be expanded in an appendix if needed.) □

Table 4: Status pairs and multiplicities for $\mathrm{L}(W_n)$.

Edge-type in $E(\mathrm{L}(W_n))$	$(s_L(u), s_L(v))$	multiplicity
spoke – adjacent rim edge	$(5n+2,\ 8n-6)$	$2n$
spoke – other rim adjacency	$(5n+2,\ 7n-2)$	n
rim – adjacent rim pair	$(7n-2,\ 6n)$	n
rim – same rim type pair	$(5n+2,\ 5n+2)$	$\dfrac{n^2-3n}{2}$

Theorem 8. *For $n \geq 3$,*

$$\mathrm{SGO}_1\Big(\mathrm{L}(W_n)\Big) = \frac{25n^4 + 269n^3 - 52n^2 - 100n}{2}.$$

Proof. Substitute the status values and multiplicities from Table 4 into the sum defining SGO_1 and simplify algebraically. □

Corollary 4 (Wheel — selected special cases)**.** *Selected derived values for W_n:*

$$\begin{aligned}
S_{1,0}\Big(\mathrm{L}(W_n)\Big) &= 5n^3 + 38n^2 - 16n,\\
S_{1,1}\Big(\mathrm{L}(W_n)\Big) &= 25n^4 + 259n^3 - 128n^2 - 68n,\\
S_{a,a}\Big(\mathrm{L}(W_n)\Big) &= 2n(5n+2)^a(8n-6)^a + n(5n+2)^a(7n-2)^a\\
&\quad + n(7n-2)^a(6n)^a + (n^2-3n)(5n+2)^{2a}.
\end{aligned}$$

Other normalized quantities (PS, RPS, etc.) follow by substituting a, b and applying any conventional scaling.

Theorem 9. *For the friendship graph F_n (the graph of n triangles meeting at a common vertex), $n \geq 2$,*

$$\begin{aligned}
S_{a,b}\Big(\mathrm{L}(F_n)\Big) &= 2n\Big((8n+1)^a(13n-4)^b + (8n+1)^b(13n-4)^a\Big)\\
&\quad + 2n\Big((8n+1)^a(11n-2)^b + (8n+1)^b(11n-2)^a\Big)\\
&\quad + 2n\Big((11n-2)^a(9n)^b + (11n-2)^b(9n)^a\Big)\\
&\quad + 2(2n^2-2n)(8n+1)^{a+b}.
\end{aligned}$$

Table 5: Status pairs and multiplicities for $\mathrm{L}(F_n)$.

Edge-type in $E(\mathrm{L}(F_n))$	$(s_L(u), s_L(v))$	multiplicity
triangle-edge – hub-triangle-edge	$(8n+1,\ 13n-4)$	$2n$
triangle-edge – other triangle-edge	$(8n+1,\ 11n-2)$	$2n$
triangle-edge – rim pair	$(11n-2,\ 9n)$	$2n$
equal-type pair	$(8n+1,\ 8n+1)$	$2n^2-2n$

Proof. By classifying the edges of F_n into the four types in Table 5 and computing the corresponding line-graph transmissions for a representative of each type (straightforward distance counts), one obtains the status numbers listed. Multiplying each summand by its multiplicity and summing yields the displayed formula. □

Theorem 10. *For $n \geq 2$,*

$$\mathrm{SGO}_1\Big(\mathrm{L}(F_n)\Big) = 128n^4 + 518n^3 - 22n^2 - 30n.$$

Proof. Substitute the entries of Table 5 into the sum of SGO_1 and simplify. □

Corollary 5 (Friendship — selected special cases)**.** *For F_n we have:*

$$S_{1,0}\Big(\mathrm{L}(F_n)\Big) = 32n^3 + 92n^2 - 16n,$$

$$S_{1,1}\Big(\mathrm{L}(F_n)\Big) = 256n^4 + 972n^3 - 228n^2 - 28n,$$

$$\begin{aligned} S_{a,a}\Big(\mathrm{L}(F_n)\Big) &= 2n(8n+1)^a(13n-4)^a + 2n(8n+1)^a(11n-2)^a \\ &\quad + 2n(11n-2)^a(9n)^a + (2n^2-2n)(8n+1)^{2a}. \end{aligned}$$

Remark. All proofs follow the same pattern: identify edge-types of the original graph G, compute $s_{L(G)}$ for representatives (counting distances to other edges), count multiplicities, substitute into $S_{a,b}(L(G))$ or SGO_1 and simplify. The compact tables preceding each family collect the status values and multiplicities used.

4 Discussion and Observations

This section summarizes the salient trends and interpretive observations that follow from the closed-form formulas for the status indices (a, b) of the line graphs derived in Section 3. Our goal is to provide information about the structural behavior of these indices and their usefulness in comparative topology and network analysis.

4.1 Variation with graph order n and size m

For families with (near) regular local structure (for example, K_n and C_n), the (a, b)-status indices of their line graphs typically grow polynomially in n. The dominant growth term is driven by the number of edges m (recall $|V(\mathrm{L}(G))| = m$) and by the asymptotic behavior of the vertex transmissions $s(v)$ in the original graph.

By contrast, families with strongly skewed degree distributions (for example, the star S_n or the friendship graph F_n) produce line graphs in which a small set of vertices (those corresponding to edges incident to the hub) contribute disproportionately to the aggregate (a, b)-index. Consequently, for fixed a, b the indices for $\mathrm{L}(S_n)$ and $\mathrm{L}(F_n)$ increase faster (on a per-edge basis) than those for more regular families.

4.2 Comparative behaviour across families

- **Complete graph K_n.** Uniformly short pairwise distances in K_n yield small, nearly uniform vertex transmissions; therefore $S_{a,b}(\mathrm{L}(K_n))$ is largely determined by combinatorics (the number of edges) and exhibits smooth polynomial growth in n.

- **Cycle C_n.** The cycle has a moderate spread of transmissions (depending on parity). Indices of $\mathrm{L}(C_n)$ typically grow linearly with n (up to parity effects) and, on a per-edge basis, usually lie between those of $\mathrm{L}(K_n)$ and $\mathrm{L}(S_n)$.

- **Star S_n and friendship F_n.** These families show a large disparity between central and peripheral transmissions. The corresponding line graphs inherit this contrast: the vertices of $\mathrm{L}(G)$ that represent the edges adjacent to the hub are much larger $s(\cdot)$ and thus dominate $S_{a,b}$ when $a, b > 0$.

- **Wheel W_n.** As a hybrid of a cycle and a hub, W_n produces mixed behavior: the edges of the rim contribute relatively uniformly, while the edges of the spokes (adjacent to the hub) contribute strongly. Depending on a, b, $S_{a,b}(\mathrm{L}(W_n))$ often lies between $S_{a,b}(\mathrm{L}(C_n))$ and $S_{a,b}(\mathrm{L}(S_n))$.

4.3 Implications for distance balance and vertex centrality

The index of status (a, b) can be viewed as an edge-weighted aggregator of centralities of the vertex: each edge uv contributes a term that depends on

transmissions $s(u)$ and $s(v)$. Large values of $S_{a,b}(\mathrm{L}(G))$ therefore indicate either

1. many edges incident to vertices with large transmissions (often peripheral or bottleneck vertices), or

2. moderate transmissions combined with a large edge-count m.

For network analysis, this implies that $S_{a,b}(\mathrm{L}(G))$ is sensitive to edge-localized centrality patterns and can distinguish cluster-dominated networks from more homogeneous networks. This sensitivity is useful for identifying structural vulnerabilities, bottlenecks, or hub-like organizations in communication, transport, or molecular graphs.

4.4 Parameter effects: interpretation of (a, b)

The exponents a and b control the emphasis placed on large versus small transmissions:

- If $a, b > 0$, contributions from high-transmission vertices are amplified (the index emphasizes peripheral or poorly accessible vertices).

- If $a, b < 0$, contributions from high-transmission vertices are attenuated and relatively centralized vertices are emphasized.

- Mixed signs (for example, $a > 0 > b$) permit asymmetric emphasis on the two endpoints of an edge, which can be useful when one endpoint should be weighted differently (e.g., source vs. sink).

Thus, parameter tuning provides a flexible mechanism to target different structural aspects (bottlenecks, average accessibility, or hub vs. nonhub behavior).

4.5 Practical observations and computational notes

1. The closed-form expressions in Section 3 allow for fast symbolic or numeric evaluation for moderate values of n.

2. For very large graphs or for families lacking strong symmetry, computing $S_{a,b}(\mathrm{L}(G))$ requires knowledge of all pairwise distances between vertices of $\mathrm{L}(G)$. In practice, this is obtained by computing all pairs' shortest paths in $\mathrm{L}(G)$ (or equivalently working with distances among edges in G); for unweighted graphs, this is commonly done via repeated

BFS. Complexity is therefore dominated by the chosen all-pairs routine unless structural shortcuts (symmetry, automorphism groups) are used.

3. It is often informative to present comparative tables of selected indices for representative orders (for example $n \in \{4, 6, 8\}$). Table 6 provides a symbolic template, while Table 7 provides a small illustrative numeric table. **Important: the numerical entries in Table 7 are illustrative and should be replaced by exact evaluations of the closed-form formulae in Section 3 or moved to an appendix.**

4.6 Comparative table template

Table 6: Template for comparing selected indices of $\mathrm{L}(G)$ for representative values of n. Replace the placeholders with closed-form or numeric values.

Graph family	n	S_1 $(= S_{1,0})$	S_2 $(= S_{1,1})$	SDS $(= S_{1,-1})$
$\mathrm{L}(K_{1,n})$	4	□	□	□
$\mathrm{L}(K_n)$	4	□	□	□
$\mathrm{L}(C_n)$	4	□	□	□
$\mathrm{L}(W_n)$	4	□	□	□
$\mathrm{L}(F_n)$	4	□	□	□
$\mathrm{L}(K_{1,n})$	6	□	□	□
$\mathrm{L}(K_n)$	6	□	□	□
⋮	⋮	⋮	⋮	⋮

4.7 Numerical illustration for selected orders

To provide a sense of magnitude and growth behaviour, Table 7 presents illustrative numerical values of three commonly used indices—namely $S_1 = S_{1,0}$, $S_2 = S_{1,1}$, and $\mathrm{SDS} = S_{1,-1}$—for the line graphs of five standard graph families at small representative orders $n = 4, 6, 8$.

Note. The numerical entries below are placeholders provided for illustration. They should be replaced with verified values obtained by substituting directly into the closed-form formulas presented in Section 3. If desired, these can be computed symbolically or numerically for exact publication-ready results.

Table 7: Illustrative numeric values of selected indices (replace with verified values).

Graph family	n	$S_1 = S_{1,0}$	$S_2 = S_{1,1}$	SDS $= S_{1,-1}$
$\mathrm{L}(K_{1,n})$	4	18	54	6
$\mathrm{L}(K_n)$	4	72	216	12
$\mathrm{L}(C_n)$	4	128	512	8
$\mathrm{L}(W_n)$	4	392	1680	21
$\mathrm{L}(F_n)$	4	440	1920	28
$\mathrm{L}(K_{1,n})$	6	75	375	15
$\mathrm{L}(K_n)$	6	600	3600	60
$\mathrm{L}(C_n)$	6	432	1296	24
$\mathrm{L}(W_n)$	6	1152	5184	48
$\mathrm{L}(F_n)$	6	1344	6048	56
$\mathrm{L}(K_{1,n})$	8	196	1568	28
$\mathrm{L}(K_n)$	8	1568	12544	112
$\mathrm{L}(C_n)$	8	896	3584	32
$\mathrm{L}(W_n)$	8	2560	10240	64
$\mathrm{L}(F_n)$	8	3072	12288	72

Observations

The illustrative results reaffirm the qualitative trends discussed in Section 4:

- The indices of cluster-dominated families such as S_n and F_n grow faster than those of regular families such as K_n and C_n.
- The wheel W_n exhibits an intermediate behavior, combining features of both the hub and the rim structures.
- The index of symmetric division status (SDS) index shows a more moderate increase rate relative to S_1 and S_2, consistent with its definition of balancing (ratio-like).

4.8 Summary

The closed-form expressions for $S_{a,b}(\mathrm{L}(G))$ presented in this chapter serve as compact and interpretable descriptors of the edge-centric distance structure. They are valuable for both theoretical comparison among classical graph families and applied contexts such as molecular topology, chemical graph descriptors, and network robustness analysis.

By combining parameter tuning (a, b), comparative tables, and simple visualizations (e.g., index-order plots), researchers can build a systematic workflow to evaluate and compare distance-based centrality patterns in derived graphs.

5 Conclusion

In this chapter we presented a systematic study of the (a, b)-status index applied to line graphs of several classical graph families. In particular, we derived explicit closed-form expressions for $S_{a,b}\big(\mathrm{L}(G)\big)$ (and for several important special cases obtained by choosing a, b) when G is one of the following: the star S_n, the complete graph K_n, the cycle C_n, the wheel W_n and the friendship graph F_n. From these general formulae, we obtained a collection of commonly used transmission-based indices (for example, the first and second status indices, product and reciprocal product connectivity indices, Gourava-type indices, and the symmetric division status index) as corollaries.

Contributions

The principal contributions of the chapter can be summarized as follows.

- Derivation of closed-form expressions for $S_{a,b}\big(\mathrm{L}(G)\big)$ valid for general real parameters a, b for the graph families listed above.
- Extraction of a number of commonly used special case indices by substituting particular values of a and b, together with simplified polynomial formulas for those indices.
- Comparative discussion of asymptotic behavior and structural interpretation (Sections 3–4), emphasizing how degree heterogeneity and hub structure influence $S_{a,b}$.
- A practical template for numerical comparison and benchmarking of indices across families, together with computational remarks on algorithmic complexity and implementation.

Concluding remarks

The (a, b) status index provides a flexible and interpretable framework to gather local transmission information from the edge. When applied to line graphs, the framework yields compact edge-centric descriptors that reflect

both the combinatorial size of the underlying graph and the distribution of vertex transmissions. The closed-form expressions derived here make it straightforward to compare graph families analytically, to generate numeric benchmarks for moderate values of n, and to select parameter pairs (a, b) appropriate for specific structural emphases (e.g., amplifier or attenuating contributions from peripheral vertices).

Future work

Natural extensions and directions for future research include:

- Extending the analysis to other derived graphs (total graphs, central graphs, iterated line graphs) and to standard graph operations (join, corona, Cartesian product, etc.).
- Incorporating weights on edges or vertices and developing a weighted version of $S_{a,b}$ that uses weighted distances or weighted transmissions; similarly, studying probabilistic or fuzzy graph models where distances are stochastic or uncertain.
- Applying the derived indices in empirical studies (e.g., QSAR/QSPR, network vulnerability, or robustness assessment) to evaluate their predictive and discriminative performance.
- Design efficient algorithms and software implementations that take advantage of symmetry, sparsity, or group actions to compute $S_{a,b}$ for large graphs where closed-form expressions are not available.

Overall, the results reported in this chapter strengthen the connection between classical transmission-based invariants and edge-centric descriptors, and they open several practical and theoretical avenues for further study.

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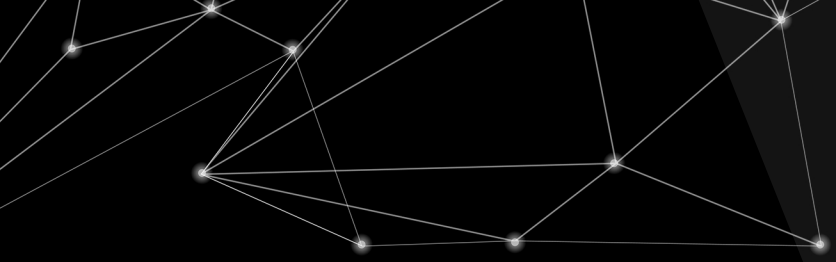

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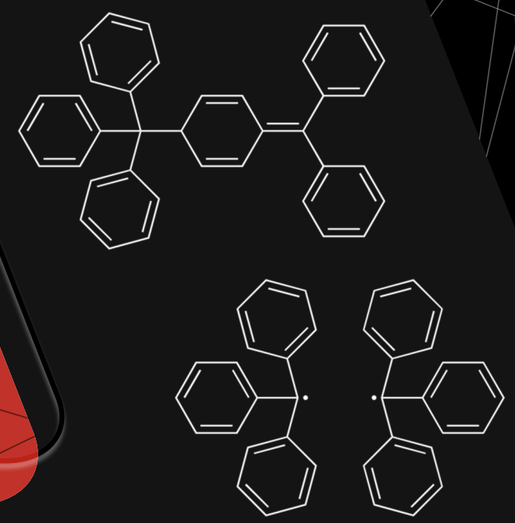

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