Acadlore Transactions on Applied Mathematics and Statistics
https://www.acadlore.com/journals/ATAMS

Neighbourhood Degree-Based Graph Descriptors: A Comprehensive Analysis of Connectivity Patterns in Diverse Graph Families and Their Applicapability

Abdu Alameri[1], Abid Mahboob[2*], Emad Toma Karash[3]

[1] Department of Biomedical Engineering, University of Science and Technology, 15201 Sana'a, Yemen
[2] Department of Mathematics, University of Education Lahore, Vehari Campus, 61170 Vehari, Pakistan
[3] Mechanical Technology Department, Mosul Technical Institute, Northern Technical University, 41000 Mosul, Iraq

[*] Correspondence: Abid Mahboob (abid.mahboob@ue.edu.pk)

Received: 12-12-2023 **Revised:** 01-17-2024 **Accepted:** 01-25-2024

Citation: A. Alameri, A. Mahboob, and E. T. Karash, "Neighbourhood degree-based graph descriptors: A comprehensive analysis of connectivity patterns in diverse graph families and their applicapability," *Acadlore Trans. Appl Math. Stat.*, vol. 2, no. 1, pp. 52–63, 2024. https://doi.org/10.56578/atams020105.

Abstract: In the field of graph theory, the exploration of connectivity patterns within various graph families is paramount. This study is dedicated to the examination of the neighbourhood degree-based topological index, a quantitative measure devised to elucidate the structural complexities inherent in diverse graph families. An initial overview of existing topological indices sets the stage for the introduction of the mathematical formulation and theoretical underpinnings of the neighbourhood degree-based index. Through meticulous analysis, the efficacy of this index in delineating unique connectivity patterns and structural characteristics across graph families is demonstrated. The utility of the neighbourhood degree-based index extends beyond theoretical graph theory, finding applicability in network science, chemistry, and social network analysis, thereby underscoring its interdisciplinary relevance. By offering a novel perspective on topological indices and their role in deciphering complex network structures, this research makes a significant contribution to the advancement of graph theory. The findings not only underscore the versatility of the neighbourhood degree-based topological index but also highlight its potential as a tool for understanding connectivity patterns in a wide array of contexts. This comprehensive analysis not only enriches the theoretical landscape of graph descriptors but also paves the way for practical applications in various scientific domains, illustrating the profound impact of graph theoretical studies on understanding the intricacies of networked systems.

Keywords: Neighbourhood degree-based index; Graph theory; Connectivity patterns; Topological index; Network analysis

1 Introduction and Preliminaries

Graph theory, a branch of discrete mathematics, has found extensive applications across diverse scientific and technological domains. In bioinformatics, the analysis of biological networks, including protein-protein interaction networks, has significantly benefited from graph theory methodologies [1]. Graph-based algorithms play a crucial role in identifying functional modules and predicting protein functions [2]. Moreover, in epidemiology, graph models are employed to study the spread of infectious diseases, where nodes represent individuals and edges represent potential transmission pathways [3]. The applications of graph theory extend into social network analysis, a field where the structure of relationships between individuals or entities is of paramount importance. Graph algorithms aid in identifying influential nodes, detecting communities, and understanding the dynamics of information propagation in online social networks [4, 5]. In the realm of transportation engineering, graph theory is essential for modeling and optimizing transportation networks. Algorithms such as Dijkstra's algorithm and the Minimum Spanning Tree algorithm contribute to route optimization, traffic flow analysis, and infrastructure planning [6]. Similarly, in telecommunication networks, graph theory provides tools for designing efficient communication networks, optimizing data routing, and ensuring robust connectivity [7].

The applications of graph theory are not limited to traditional scientific disciplines. In cybersecurity, graph-based models are employed for detecting and analyzing network vulnerabilities, identifying potential threats, and devising strategies for securing information systems [8]. Additionally, in recommendation systems, graph-based collaborative filtering algorithms are used to provide personalized suggestions by modeling user-item interactions as a graph structure [9]. In chemistry and molecular biology, graph theory is applied to represent molecular structures, with topological indices serving as descriptors in quantitative structure-activity relationship (QSAR) studies [10]. The analysis of chemical compounds as graphs enables the identification of structural features influencing biological activities, which is essential in drug discovery and design. The interdisciplinary nature of graph theory is evident in its applications across various scientific and technological fields, ranging from biology and epidemiology to transportation, telecommunications, cybersecurity, and beyond. As new challenges emerge, the versatility of graph theory continues to contribute valuable insights and solutions across a spectrum of domains.

In the quantitative structure-property relationship (QSPR) and QSAR studies, an integral term widely acknowledged is that of topological indices (TIs). TIs are numeric invariants considered as transformations that convert graphical structures into real numbers, expressed as $f : G \to \mathbb{R}^+$. Functioning as both predictor parameters and molecular descriptors, TIs play a crucial role in narrating molecular structures. Topological indices, derived from the structural connectivity of molecules, play a vital role in various scientific disciplines, offering a quantitative representation of molecular topology. In the field of chemoinformatics, these indices find extensive application in QSAR studies, aiding in the prediction of the biological activities of chemical compounds based on their molecular structures [11]. Also, topological indices play a big role in drug discovery and design. For example, it's important to understand how molecular structure affects pharmacological effects in order to find the best drug candidates [12]. In environmental chemistry, topological indices are employed to assess the toxicity and environmental impact of chemical substances, assisting in the identification of environmentally friendly compounds [13]. Additionally, in material science, topological indices play a role in predicting various physicochemical properties, contributing to the development of novel materials with tailored characteristics [14]. The usefulness of topological indices can be seen in bioinformatics, where they are used to study molecular networks and figure out how living things are connected [15–17].

Among the distance-based topological indices, the Weiner index [18] stands out as the oldest and most extensively studied. Its significance in elucidating molecular structures has been well established. Recent advancements in the field have been marked by the introduction of novel distance-based TIs known as status neighborhood indices, as inaugurated by Kulli [19]. This development adds to the evolving landscape of topological indices, opening new avenues for understanding and predicting molecular properties. The continuous exploration and application of these indices underscore their pivotal role in advancing the field of chemical informatics. To study research work on these graph topology descriptors, we refer to the studies [20–23].

Let G be a connected graph with $E(G)$ and $V(G)$ edge and vertex set respectively. Degree of vertex ν is number of vertices adjacent to ν and distance is length of shortest path between two vertices ν_1 and ν_2, denoted by $d(\nu)$ and $d(\nu_1, \nu_2)$ respectively. For vertex ν, sum of all distances of all other vertices is called status of ν denoted by $\sigma_n(\nu)$. We refer the study [24] for undefined notions and terms. Now we define status sum of neighbor vertices:

$$\sigma_n(u) = \sum_{u \in N(\nu)} \sigma(u)$$

where, $N(\nu) = N_G\nu = \{\nu : u\nu \in E(G)\}$. Kulli [25] introduced first and second status neighbouredhood indices of a graph defined as:

$$SNI_1 = \sum_{\nu_1\nu_2 \in E(G)} [\sigma_n(\nu_1) + \sigma_n(\nu_2)] \quad \text{and} \quad SNI_2 = \sum_{\nu_1\nu_2 \in E(G)} [\sigma_n(\nu_1).\sigma_n(\nu_2)]$$

Kulli [19] introduced some new indices defined. Atom bond connectivity (ABC) status neighborhood index, geometric-arithmetic (GA) status neighborhood index and arithmetic-geometric (AG) status neighborhood index for a graph G are defined as:

$$\mathcal{ABCSNI}(G) = \sum_{\nu_1\nu_2 \in E(G)} \sqrt{\frac{\sigma_n(\nu_1) + \sigma_n(\nu_2) - 2}{\sigma_n(\nu_1) \times \sigma_n(\nu_2)}}$$

$$\mathcal{GASNI}(G) = \sum_{\nu_1\nu_2 \in E(G)} \frac{2\sqrt{\sigma_n(\nu_1) \times \sigma_n(\nu_2)}}{\sigma_n(\nu_1) + \sigma_n(\nu_2)}$$

$$\mathcal{AGSNI}(G) = \sum_{\nu_1\nu_2 \in E(G)} \frac{\sigma_n(\nu_1) + \sigma_n(\nu_2)}{2\sqrt{\sigma_n(\nu_1) \times \sigma_n(\nu_2)}}$$

Harmonic status neighborhood index and its polynomial are defined as:

$$\mathcal{HSNI}(G) = \sum_{\nu_1\nu_2 \in E(G)} \frac{2}{\sigma_n(\nu_1) + \sigma_n(\nu_2)}$$

$$\mathcal{HSNI}(G,x)=\sum_{\nu_1\nu_2\in E(G)} x^{\frac{2}{\sigma_n(\nu_1)+\sigma_n(\nu_2)}}$$

Symmetric division status neighborhood index and its polynomial are defined as:

$$\mathcal{SDSNI}(G)=\sum_{\nu_1\nu_2\in E(G)} \frac{\sigma_n(\nu_1)}{\sigma_n(\nu_2)}+\frac{\sigma_n(\nu_1)}{\sigma_n(\nu_2)}$$

$$\mathcal{SDSNI}(G,x)=\sum_{\nu_1\nu_2\in E(G)} x^{\left(\frac{\sigma_n(\nu_1)}{\sigma_n(\nu_2)}+\frac{\sigma_n(\nu_1)}{\sigma_n(\nu_2)}\right)}$$

Inverse sum index status neighborhood index and its polynomial are defined as:

$$\mathcal{ISSNI}(G)=\sum_{\nu_1\nu_2\in E(G_n)} \frac{\sigma_n(\nu_1)\times\sigma_n(\nu_2)}{\sigma_n(\nu_1)+\sigma_n(\nu_2)}$$

$$\mathcal{ISSNI}(G,x)=\sum_{\nu_1\nu_2\in E(G)} x^{\frac{\sigma_n(\nu_1)\times\sigma_n(\nu_2)}{\sigma_n(\nu_1)+\sigma_n(\nu_2)}}$$

The augmented status neighborhood index and its polynomial are defined as:

$$\mathcal{ASNI}(G)=\sum_{\nu_1\nu_2\in E(G)} \left[\frac{\sigma_n(\nu_1)\times\sigma_n(\nu_1)}{\sigma_n(\nu_1)+\sigma_n(\nu_1)-2}\right]^3$$

$$\mathcal{ASNI}(G,x)=\sum_{\nu_1\nu_2\in E(G)} x^{\left[\frac{\sigma_n(\nu_1)\times\sigma_n(\nu_1)}{\sigma_n(\nu_1)+\sigma_n(\nu_1)-2}\right]^3}$$

This article talks about neighborhood degree-based graph descriptors and their M-polynomials as an alternative to traditional valency-based descriptors that can be used to describe chemical structures in more detail. These indices were used on a number of well-known graph families to see how well they worked at capturing changes in the topological features of chemical structures. The results were then presented graphically to enhance clarity and comprehension.

2 Results

In our quest to extract meaningful insights from molecular structures, we employ a diverse array of computational strategies to compute topological indices. Our approach involves leveraging sophisticated techniques such as the vertex partition strategy, where the molecular graph is systematically partitioned into subsets of vertices based on specific criteria. Additionally, we employ edge partition techniques, meticulously categorizing the graph's edges to unveil intricate patterns that contribute to the overall molecular connectivity. We use expository strategies to make the results easier to understand and to capture important structural details. This gives us a full picture of how the different molecular parts are connected. In the pursuit of a thorough analysis, we harness sum of degrees of neighboring techniques, which involves summing the degrees of adjacent vertices to derive valuable information about the molecular environment. Degree checking techniques further refine our computations, allowing us to scrutinize the distribution of vertex degrees and identify pivotal nodes within the molecular structure. Combinatorial techniques, an integral part of our methodology, enable the exploration of combinatorial properties within the molecular graph, providing deeper insights into the graph's topological characteristics. Table 1 delineates the different edge types in the Gear graph, organized based on their neighborhood vertex degrees and respective frequencies. Each set of edges was subjected to the application of the specified index formulas, and the resulting values were determined by multiplying them with the corresponding frequencies. Maple software was utilized for the computation of extensive summations. Similar approaches were employed for Table 2, which presents neighborhood degree-based vertex and edge partitions for the generalized Helm graph. Matlab was subsequently used to assess the numeric values of calculated formulas within the specified range in Tables 3 and 4.

2.1 Results for Generalized Gear Graph

A Gear graph is obtained by replacing each edge on the perimeter of wheel graph W_n by a path of length 2 and denoted by G_n. The Gear graph contains $3n$ edges and $2n+1$ vertices. In this graph, there are two tyoes of edges as given below:

$$E_1=\{\nu_1\nu_2\in E(G_n)|d_{G_n}(\nu_1)=2 \quad d_{G_n}(\nu_2)=3\} \qquad |E_1=2n|$$

$$E_2 = \{\nu_1\nu_2 \in E(G_n) | d_{G_n}(\nu_1) = 3 \quad d_{G_n}(\nu_2) = n\} \qquad |E_2 = n|$$

Therefore by calculation, there are two types of status edges as follows:

$$E_1 = \{\nu_1\nu_2 \in E(G_n) | \sigma(\nu_1) = 5n-5 \quad \sigma(\nu_2) = 7n-10\} \qquad |E_1 = 2n|$$

$$E_2 = \{\nu_1\nu_2 \in E(G_n) | \sigma(\nu_1) = 5n-5 \qquad \sigma(\nu_2) = 3n\} \qquad |E_2 = n|$$

By calculation, there are two types of status neighborhood edges given in Table 1.

Table 1. Status neighborhood edge partition of G_n

$\boldsymbol{\sigma_n(\nu_1), \sigma_n(\nu_1)}$	**Number of Edges**
$(10(n-1), 17n-20)$	$2n$
$(17n-20, n(5n-5))$	n

By using status neighborhood edge partition of Gear graph G_n given in Table 1, we compute the following:

• Atom bond vonnectivity (ABC) status neighborhood index:

$$\begin{aligned}
\mathcal{ABCSNI}(G_n) &= \sum_{\nu_1\nu_2 \in E(G_n)} \sqrt{\frac{\sigma_n(\nu_1) + \sigma_n(\nu_2) - 2}{\sigma_n(\nu_1) \times \sigma_n(\nu_2)}} \\
&= 2n\left(\frac{10(n-1) + (17n-20) - 2}{10(n-1)(17n-20)}\right)^{\frac{1}{2}} + n\left(\frac{(17n-20) + 5n(n-1) - 2}{(17n-20).5n(n-1)}\right)^{\frac{1}{2}} \\
&= 2n\left(\frac{27n-32}{170n^2 - 370n + 200}\right)^{\frac{1}{2}} + n\left(\frac{5n^2 + 12n - 22}{85n^3 - 185n^2 + 100n}\right)^{\frac{1}{2}}
\end{aligned}$$

• Geometric-arithmetic (GA) status neighborhood index:

$$\begin{aligned}
\mathcal{GASNI}(G_n) &= \sum_{\nu_1\nu_2 \in E(G_n)} \frac{2\sqrt{\sigma_n(\nu_1) \times \sigma_n(\nu_2)}}{\sigma_n(\nu_1) + \sigma_n(\nu_2)} \\
&= 2n.\frac{2\sqrt{10(n-1)(17n-20)}}{10(n-1) + (17n-20)} + n.\frac{2\sqrt{(17n-20).5n(n-1)}}{(17n-20) + 5n(n-1)} \\
&= 4n\frac{\sqrt{170n^2 - 370n + 200}}{27n-30} + 2n\frac{\sqrt{85n^3 - 185n^2 + 100n}}{5n^2 + 12n - 20}
\end{aligned}$$

• Arithmetic-geometric (AG) status neighborhood index:

$$\begin{aligned}
\mathcal{AGSNI}(G_n) &= \sum_{\nu_1\nu_2 \in E(G_n)} \frac{\sigma_n(\nu_1) + \sigma_n(\nu_2)}{2\sqrt{\sigma_n(\nu_1) \times \sigma_n(\nu_2)}} \\
&= 2n.\frac{10(n-1) + (17n-20)}{2\sqrt{10(n-1)(17n-20)}} + n.\frac{(17n-20) + 5n(n-1)}{2\sqrt{(17n-20).5n(n-1)}} \\
&= n\frac{27n-30}{\sqrt{170n^2 - 370n + 200}} + n\frac{5n^2 + 12n - 20}{2\sqrt{85n^3 - 185n^2 + 100n}}
\end{aligned}$$

• Harmonic status neighborhood index and its polynomial:

$$\begin{aligned}
\mathcal{HSN}(G_n) &= \sum_{\nu_1\nu_2 \in E(G_n)} \frac{2}{\sigma_n(\nu_1) + \sigma_n(\nu_2)} \\
&= 2n\left(\frac{2}{10(n-1) + (17n-20)}\right) + n\left(\frac{2}{(17n-20) + 5n(n-1)}\right) \\
&= \frac{4n}{27n-30} + \frac{2n}{5n^2 + 12n - 20}
\end{aligned}$$

$$\begin{aligned}
\mathcal{HSN}(G_n, x) &= \sum_{\nu_1\nu_2 \in E(G)} x^{\frac{2}{\sigma_n(\nu_1) + \sigma_n(\nu_2)}} \\
&= 2n.x^{\frac{2}{(10n-10) + (17n-20)}} + n.x^{\frac{2}{(17n-20) + (5n^2 - 5n)}} \\
&= 2n.x^{\frac{2}{27n-30}} + n.x^{\frac{2}{5n^2 + 12n - 20}}
\end{aligned}$$

• Symmetric division status neighborhood index and its polynomial:

$$\begin{aligned}
\mathcal{SDSNI}(G_n) &= \sum_{\nu_1\nu_2\in E(G)} \frac{\sigma_n(\nu_1)}{\sigma_n(\nu_2)} + \frac{\sigma_n(\nu_1)}{\sigma_n(\nu_2)} \\
&= 2n\left(\frac{10n-10}{17n-20} + \frac{17n-20}{10n-10}\right) + n\left(\frac{17n-20}{5n^2-5n} + \frac{5n^2-5n}{17n-20}\right) \\
&= 2n\left(\frac{389n^2-880n+500}{170n^2-370n+200}\right) + n\left(\frac{25n^4-50n^3+314n^2-680n+400}{85n^3-185n^2+100n}\right)
\end{aligned}$$

$$\begin{aligned}
\mathcal{SDSNI}(G_n,x) &= \sum_{uv\in E(G_n)} x^{\left(\frac{\sigma_n(\nu_1)}{\sigma_n(\nu_2)} + \frac{\sigma_n(\nu_1)}{\sigma_n(\nu_2)}\right)} \\
&= 2nx^{\left(\frac{10n-10}{17n-20}+\frac{17n-20}{10n-10}\right)} + nx^{\left(\frac{17n-20}{5n^2-5n}+\frac{5n^2-5n}{17n-20}\right)} \\
&= 2nx^{\left(\frac{389n^2-880n+500}{170n^2-370n+200}\right)} + nx^{\left(\frac{25n^4-50n^3+314n^2-680n+400}{85n^3-185n^2+100n}\right)}
\end{aligned}$$

• Inverse sum indeg status neighborhood index and its polynomial:

$$\begin{aligned}
\mathcal{ISSNI}(G_n) &= \sum_{\nu_1\nu_2\in E(G_n)} \frac{\sigma_n(\nu_1)\times\sigma_n(\nu_2)}{\sigma_n(\nu_1)+\sigma_n(\nu_2)} \\
&= 2n\frac{(10n-10)(17n-20)}{10n-10+17n-20} + n\frac{(17n-20)(5n^2-5n)}{17n-20+5n^2-5n} \\
&= 2n\left(\frac{170n^2-370n+200}{27n-30}\right) + n\left(\frac{85n^3-185n^2+100n}{5n^2+12n-20}\right)
\end{aligned}$$

$$\begin{aligned}
\mathcal{ISSN}(G_n,x) &= \sum_{\nu_1\nu_2\in E(G_n)} x^{\frac{\sigma_n(\nu_1)\times\sigma_n(\nu_2)}{\sigma_n(\nu_1)+\sigma_n(\nu_2)}} \\
&= 2nx^{\frac{(10n-10)(17n-20)}{10n-10+17n-20}} + nx^{\frac{(17n-20)(5n^2-5n)}{17n-20+5n^2-5n}} \\
&= 2nx^{\left(\frac{170n^2-370n+200}{27n-30}\right)} + nx^{\left(\frac{85n^3-185n^2+100n}{5n^2+12n-20}\right)}
\end{aligned}$$

• Augmented status neighborhood index and its polynomial:

$$\begin{aligned}
\mathcal{ASNI}(G_n) &= \sum_{\nu_1\nu_2\in E(G)} \left[\frac{\sigma_n(\nu_1)\times\sigma_n(\nu_1)}{\sigma_n(\nu_1)+\sigma_n(\nu_1)-2}\right]^3 \\
&= 2n\left[\frac{(10n-10)(17n-20)}{10n-10+17n-20-2}\right]^3 + n\left[\frac{(17n-20)(5n^2-5n)}{17n-20+5n^2-5n-2}\right]^3 \\
&= 2n\left[\frac{170n^2-370n+200}{27n-32}\right]^3 + n\left[\frac{85n^3-185n^2+100n}{5n^2+12n-22}\right]
\end{aligned}$$

$$\begin{aligned}
\mathcal{ASNI}(G_n,x) &= \sum_{\nu_1\nu_2\in E(G)} x^{\left[\frac{\sigma_n(\nu_1)\times\sigma_n(\nu_1)}{\sigma_n(\nu_1)+\sigma_n(\nu_1)-2}\right]^3} \\
&= 2nx^{\left[\frac{(10n-10)(17n-20)}{10n-10+17n-20-2}\right]^3} + nx^{\left[\frac{(17n-20)(5n^2-5n)}{17n-20+5n^2-5n-2}\right]^3} \\
&= 2nx^{\left[\frac{170n^2-370n+200}{27n-32}\right]^3} + nx^{\left[\frac{85n^3-185n^2+100n}{5n^2+12n-22}\right]^3}
\end{aligned}$$

2.2 Results for Helm Graph

A graph obtained by adjoining a pendant edge at each vertex of cycle of wheel graph is called the Helm graph and denoted by H_n. The Helm graph contains $3n$ edges and $2n+1$ vertices. In this graph, there are three tyoes of edges as given below:

$$E_1 = \{\nu_1\nu_2 \in E(H_n) | d_{H_n}(\nu_1) = 1 \quad d_{H_n}(\nu_2) = 4\} \qquad |E_1 = n|$$

$$E_2 = \{\nu_1\nu_2 \in E(H_n) | d_{H_n}(\nu_1) = 4 \quad d_{H_n}(\nu_2) = 4\} \quad |E_2 = n|$$
$$E_3 = \{\nu_1\nu_2 \in E(H_n) | d_{H_n}(\nu_1) = 4 \quad d_{H_n}(\nu_2) = 5\} \quad |E_3 = n|$$

Therefore by calculation, there are three types of status edges as follows:

$$E_1 = \left\{\nu_1\nu_2 \in E(H_n) | \sigma(\nu_1) = 10n^2 - 63n + 112 \quad \sigma(\nu_2) = 5n - 7\right\} \quad |E_1 = n|$$
$$E_2 = \{\nu_1\nu_2 \in E(H_n) | \sigma(\nu_1) = 5n - 7 \quad \sigma(\nu_2) = 5n - 7\} \quad |E_2 = n|$$
$$E_3 = \{\nu_1\nu_2 \in E(H_n) | \sigma(\nu_1) = 5n - 7 \quad \sigma(\nu_2) = 3n\} \quad |E_3 = n|$$

By calculation, there are three types of status neighborhood edges given in Table 2.

Table 2. Status neighborhood edge partition of H_n

$\boldsymbol{\sigma_n(\nu_1), \sigma_n(\nu_1)}$	**Number of Edges**
$(5n - 7, 5n^2 - 15n + 38)$	n
$(5n^2 - 15n + 38, 5n^2 - 15n + 38)$	n
$(5n^2 - 15n + 38, n(5n - 7))$	n

By using status neighborhood edge partition of Helm graph H_n given in Table 2, we compute the following:
• Atom bond connectivity (ABC) status neighborhood index:

$$\begin{aligned}
\mathcal{ABCSNI}(H_n) &= \sum_{\nu_1\nu_2 \in E(H_n)} \sqrt{\frac{\sigma_n(\nu_1) + \sigma_n(\nu_2) - 2}{\sigma_n(\nu_1) \times \sigma_n(\nu_2)}} \\
&= n\left(\frac{(5n-7) + (5n^2 - 15n + 38) - 2}{(5n-7)(5n^2 - 15n + 38)}\right)^{\frac{1}{2}} \\
&+ n\left(\frac{(5n^2 - 15n + 38) + (5n^2 - 15n + 38) - 2}{(5n^2 - 15n + 38)(5n^2 - 15n + 38)}\right)^{\frac{1}{2}} \\
&+ n\left(\frac{(5n^2 - 15n + 38) + (5n^2 - 7n - 2) - 2}{(5n^2 - 15n + 38)(5n^2 - 7n - 2)}\right)^{\frac{1}{2}} \\
&= n\left(\frac{5n^2 - 10n + 29}{25n^3 - 110n^2 + 295n - 266}\right)^{\frac{1}{2}} \\
&+ n\left(\frac{10n^2 - 30n + 74}{25n^4 - 150n^3 + 605n^2 - 1140n + 1444}\right)^{\frac{1}{2}} \\
&+ n\left(\frac{10n^2 - 22n + 36}{25n^4 - 110n^3 + 295n^2 - 266n}\right)^{\frac{1}{2}}
\end{aligned}$$

• Geometric-arithmetic (GA) status neighborhood index:

$$\begin{aligned}
\mathcal{GASNI}(H_n) &= \sum_{\nu_1\nu_2 \in E(H_n)} \frac{2\sqrt{\sigma_n(\nu_1) \times \sigma_n(\nu_2)}}{\sigma_n(\nu_1) + \sigma_n(\nu_2)} \\
&= n.\frac{2\sqrt{(5n-7)(5n^2 - 15n + 38)}}{(5n-7) + (5n^2 - 15n + 38)} \\
&+ n.\frac{2\sqrt{(5n^2 - 15n + 38)(5n^2 - 15n + 38)}}{(5n^2 - 15n + 38) + (5n^2 - 15n + 38)} \\
&+ n.\frac{2\sqrt{(5n^2 - 15n + 38)(5n^2 - 7n)}}{(5n^2 - 15n + 38) + (5n^2 - 7n)} \\
&= n + n\frac{\sqrt{25n^4 - 110n^3 + 295n^2 - 266n}}{5n^2 - 11n + 19} \\
&+ 2n\frac{\sqrt{25n^3 - 110n^2 + 295n - 266}}{5n^2 - 10n + 31}
\end{aligned}$$

• Arithmetic-geometric (AG) status neighborhood index:

$$\begin{aligned}
\mathcal{AGSNI}(H_n) &= \sum_{\nu_1\nu_2\in E(H_n)} \frac{\sigma_n(\nu_1)+\sigma_n(\nu_2)}{2\sqrt{\sigma_n(\nu_1)\times\sigma_n(\nu_2)}} \\
&= 2n.\,\frac{(5n-7)+(5n^2-15n+38)}{2\sqrt{(5n-7)(5n^2-15n+38)}} + n.\,\frac{(5n^2-15n+38)+(5n^2-15n+38)}{2\sqrt{(5n^2-15n+38)(5n^2-15n+38)}} \\
&+ n.\,\frac{(5n^2-15n+38)+(5n^2-7n)}{2\sqrt{(5n^2-15n+38)(5n^2-7n)}} \\
&= n + n\,\frac{5n^2-10n+31}{\sqrt{25n^3-110n^2+295n-266}} + n\,\frac{5n^2-11n+19}{2\sqrt{25n^4-110n^3+295n^2-266n}}
\end{aligned}$$

• Harmonic status neighborhood index and its polynomial:

$$\begin{aligned}
\mathcal{HSNI}(H_n) &= \sum_{\nu_1\nu_2\in E(H_n)} \frac{2}{\sigma_n(\nu_1)+\sigma_n(\nu_2)} \\
&= n\left(\frac{2}{(5n-7)+(5n^2-15n+38)}\right) + n\left(\frac{2}{(5n^2-15n+38)+(5n^2-15n+38)}\right) \\
&+ n\left(\frac{2}{(5n^2-15n+38)+(5n^2-7n)}\right) \\
&= \frac{2n}{5n^2-10n+31} + \frac{n}{5n^2-15n+38} + \frac{n}{5n^2-11n+19}
\end{aligned}$$

$$\begin{aligned}
\mathcal{HSNI}(H_n,x) &= \sum_{\nu_1\nu_2\in E(H_n)} x^{\frac{2}{\sigma_n(\nu_1)+\sigma_n(\nu_2)}} \\
&= n.x^{\frac{2}{(5n-7)+(5n^2-15n+38)}} + n.x^{\frac{2}{(5n^2-15n+38)+(5n^2-15n+38)}} \\
&+ n.x^{\frac{2}{(5n^2-15n+38)+(5n^2-7n)}} \\
&= n.x^{\frac{2}{5n^2-10n+31}} + n.x^{\frac{2}{5n^2-15n+38}} + n.x^{\frac{2}{5n^2-11n+19}}
\end{aligned}$$

• Symmetric division status neighborhood index and its polynomial:

$$\begin{aligned}
\mathcal{SDSNI}(H_n) &= \sum_{\nu_1\nu_2\in E(H_n)} \frac{\sigma_n(\nu_1)}{\sigma_n(\nu_2)} + \frac{\sigma_n(\nu_1)}{\sigma_n(\nu_2)} \\
&= n\left(\frac{5n-7}{5n^2-15n+38} + \frac{5n^2-15n+38}{5n-7}\right) + n\left(\frac{5n^2-15n+38}{5n^2-15n+38} + \frac{5n^2-15n+38}{5n^2-15n+38}\right) \\
&+ n\left(\frac{5n^2-15n+38}{5n^2-7n} + \frac{5n^2-7n}{5n^2-15n+38}\right) \\
&= 2n + n\left(\frac{25n^4-150n^3+630n^2-1210n+1493}{25n^3-110n^2+295n-266}\right) \\
&+ n\left(\frac{50n^4-220n^3+654n^2-1140n+1444}{25n^4-110n^3+295n^2-266n}\right)
\end{aligned}$$

$$\begin{aligned}
\mathcal{SDSNI}(H_n,x) &= \sum_{\nu_1\nu_2\in E(H_n)} x^{\frac{\sigma_n(\nu_1)}{\sigma_n(\nu_2)}+\frac{\sigma_n(\nu_1)}{\sigma_n(\nu_2)}} \\
&= nx^{\left(\frac{5n-7}{5n^2-15n+38}+\frac{5n^2-15n+38}{5n-7}\right)} + nx^{\left(\frac{5n^2-15n+38}{5n^2-15n+38}+\frac{5n^2-15n+38}{5n^2-15n+38}\right)} \\
&+ nx^{\left(\frac{5n^2-15n+38}{5n^2-7n}+\frac{5n^2-7n}{5n^2-15n+38}\right)} \\
&= nx^2 + nx^{\left(\frac{25n^4-150n^3+630n^2-1210n+1493}{25n^3-110n^2+295n-266}\right)} + nx^{\left(\frac{50n^4-220n^3+654n^2-1140n+1444}{25n^4-110n^3+295n^2-266n}\right)}
\end{aligned}$$

• Inverse sum indeg status neighborhood index and its polynomial:

$$\begin{aligned}
\mathcal{ISSNI}(H_n) &= \sum_{\nu_1\nu_2\in E(H_n)} \frac{\sigma_n(\nu_1)\times\sigma_n(\nu_2)}{\sigma_n(\nu_1)+\sigma_n(\nu_2)} \\
&= n\frac{(5n-7)(5n^2-15n+38)}{(5n-7)+(5n^2-15n+38)} + n\frac{(5n^2-15n+38)(5n^2-15n+38)}{(5n^2-15n+38)+(5n^2-15n+38)} \\
&+ n\frac{(5n^2-15n+38)(5n^2-7n)}{(5n^2-15n+38)+(5n^2-7n)} \\
&= n\left(\frac{25n^3-110n^2+295n-266}{5n^2-10n+31}\right) + \frac{1}{2}n(5n^2-15n+38) \\
&+ \frac{n}{2}\left(\frac{25n^4-110n^3+295n^2-266n}{5n^2-11n+19}\right)
\end{aligned}$$

$$\begin{aligned}
\mathcal{ISSNI}(H_n,x) &= \sum_{\nu_1\nu_2\in E(H_n)} x^{\frac{\sigma_n(\nu_1)\times\sigma_n(\nu_2)}{\sigma_n(\nu_1)+\sigma_n(\nu_2)}} \\
&= nx^{\frac{(5n-7)(5n^2-15n+38)}{(5n-7)+(5n^2-15n+38)}} + nx^{\frac{(5n^2-15n+38)(5n^2-15n+38)}{(5n^2-15n+38)+(5n^2-15n+38)}} \\
&+ nx^{\frac{(5n^2-15n+38)(5n^2-7n)}{(5n^2-15n+38)+(5n^2-7n)}} \\
&= nx^{\left(\frac{25n^3-110n^2+295n-266}{5n^2-10n+31}\right)} + nx^{\frac{1}{2}\left(5n^2-15n+38\right)} \\
&+ nx^{\frac{1}{2}\left(\frac{25n^4-110n^3+295n^2-266n}{5n^2-11n+19}\right)}
\end{aligned}$$

• Augmented status neighborhood index and its polynomial:

$$\begin{aligned}
\mathcal{ASNI}(H_n) &= \sum_{\nu_1\nu_2\in E(G_n)} \left[\frac{\sigma_n(\nu_1)\times\sigma_n(\nu_1)}{\sigma_n(\nu_1)+\sigma_n(\nu_1)-2}\right]^3 \\
&= n\left[\frac{(5n-7)(5n^2-15n+38)}{(5n-7)+(5n^2-15n+38)-2}\right]^3 + n\left[\frac{(5n^2-15n+38)(5n^2-15n+38)}{(5n^2-15n+38)+(5n^2-15n+38)-2}\right]^3 \\
&+ n\left[\frac{(5n^2-15n+38)(5n^2-7n)}{(5n^2-15n+38)+(5n^2-7n)-2}\right]^3 \\
&= n\left[\frac{25n^3-110n^2+295n-266}{5n^2-10n+29}\right]^3 + n\left[\frac{25n^4-150n^3+605n^2-1140n+1444}{10n^2-30n+74}\right]^3 \\
&+ n\left[\frac{25n^4-110n^3+295n^2-266n}{10n^2-22n+36}\right]^3
\end{aligned}$$

$$\begin{aligned}
\mathcal{ASNI}(H_n,x) &= \sum_{\nu_1\nu_2\in E(H_n)} x^{\left[\frac{\sigma_n(\nu_1)\times\sigma_n(\nu_1)}{\sigma_n(\nu_1)+\sigma_n(\nu_1)-2}\right]^3} \\
&= nx^{\left[\frac{(5n-7)(5n^2-15n+38)}{(5n-7)+(5n^2-15n+38)-2}\right]^3} + nx^{\left[\frac{25n^4-150n^3+605n^2-1140n+1444}{10n^2-30n+74}\right]^3} \\
&+ nx^{\left[\frac{(5n^2-15n+38)(5n^2-7n)}{(5n^2-15n+38)+(5n^2-7n)-2}\right]^3} \\
&= nx^{\left[\frac{25n^3-110n^2+295n-266}{5n^2-10n+29}\right]^3} + nx^{\left[\frac{25n^4-150n^3+605n^2-1140n+1444}{10n^2-30n+74}\right]^3} \\
&+ nx^{\left[\frac{(5n^2-15n+38)(5n^2-7n)}{(5n^2-15n+38)+(5n^2-7n)-2}\right]^3}
\end{aligned}$$

3 Graphical Analysis

In this dedicated section of our research, we conducted a systematic generation of two comprehensive tables specifically tailored for the generalized Gear and Helm graphs. These tables were derived from the indices meticulously evaluated in the preceding section, employing sophisticated MATLAB algorithms designed to ensure accuracy and efficiency in the computational processes. For the convenience and transparency of interested researchers, the detailed MATLAB algorithms utilized in the calculations have been made publicly accessible on our GitHub repository [https://github.com/alleerazza786/MASNI]. The first table intricately lays out the numeric values corresponding to the generalized Gear graph, denoted as G_n, as the variable n systematically varies from 3 to 15. This comprehensive representation serves as a valuable resource for elucidating the numerical patterns and variations inherent in G_n across different values of n. In the same way, the second table shows in detail the numerical values that go with the Helm graph, which is written as H_n. These values help us understand how it behaves when the variable n changes within the given range. Together, these meticulously crafted tables and the accompanying MATLAB algorithms form a robust foundation for further analysis, fostering both transparency and reproducibility in our research endeavors.

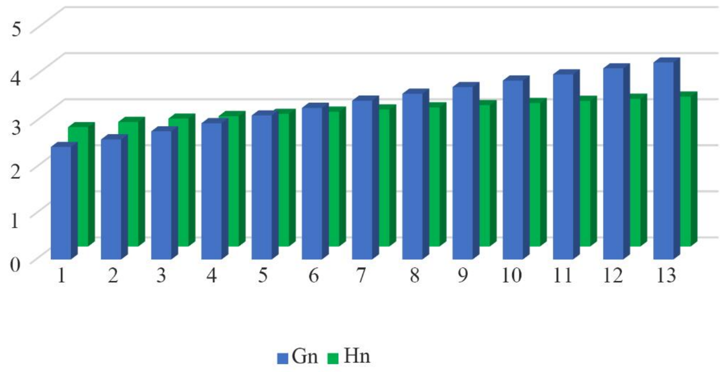

Figure 1. $\mathcal{ABCSNI}$ for generalized Gear and Helm graphs

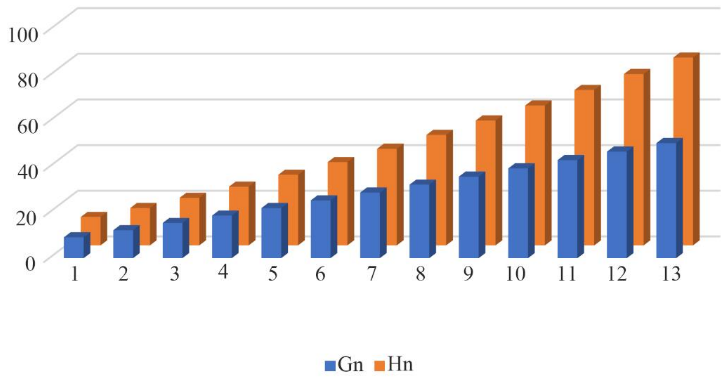

Figure 2. $\mathcal{AGSNI}$ for generalized Gear and Helm graphs

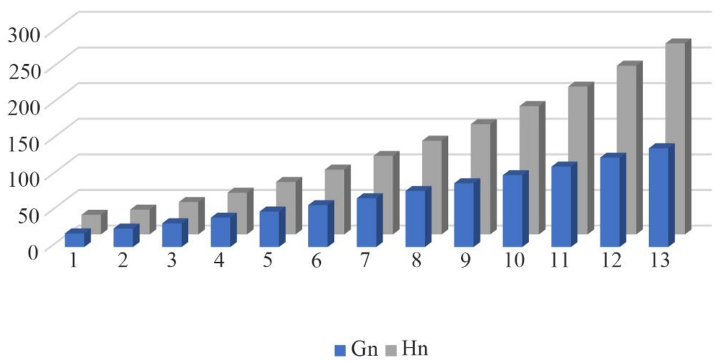

Figure 3. $\mathcal{SDSNI}$ for generalized Gear and Helm graphs

In Figures 1, 2, and 3, we present a visual representation elucidating the atom bond connectivity index (ABCI), arithmetic geometric index (AGI), and symmetric division status neighborhood index (SDSNI) for both graphs, all meticulously derived from the data encapsulated in Tables 3 and 4. These pictures are very helpful for figuring out the complicated details in the atom bond connectivity, arithmetic geometric, and symmetric division status neighborhood parts of the graphs we're looking at. As the graphs unfold, a discernible trend emerges, highlighting the dynamic relationship between these TIs and the graph's size and order. Notably, the numeric values of these descriptors exhibit a consistent increase with each incremental change in the graph size and order. This pattern accurately shows the natural connection between the topological indices and the changing complexity of the graphs' structures. It also gives us useful information about how TIs and graph structure work together. Based on the information in Tables 3 and 4, the graphs are very helpful for not only understanding but also visually interpreting the complex relationships between ABCI, AGI, and SDSNI in the context of the graphs that were looked at. The correlation between the indices and the structure of the mentioned graphs serves as a fundamental tool for QSPR and QSAR analyses. This connection is particularly significant for chemistry researchers, as it significantly reduces the cost and time involved in predicting the physicochemical properties of numerous chemical compounds. The insights gained from studying these indices and their relationship with graph structures contribute to more efficient and economical approaches in the field of chemical research, facilitating quicker and more accurate predictions of properties crucial for various applications.

Table 3. The evaluated degree based descriptors values for numerous generalized Gear graph

G_n	$\mathcal{ABCSNI}$	$\mathcal{AGSNI}$	$\mathcal{GASNI}$	$\mathcal{HSNI}$	$\mathcal{SDSNI}$	$\mathcal{ISSNI}$
3	2.4424	9.145	8.8584	0.33365	19.174	118.68
4	2.6053	12.247	11.759	0.2792	26.000	254.36
5	2.7821	15.413	14.599	0.25108	33.346	444.59
6	2.9573	18.645	17.379	0.23354	41.253	690.83
7	3.1267	21.942	20.105	0.22141	49.733	993.99
8	3.2896	25.302	22.785	0.21245	58.794	1354.7
9	3.4462	28.723	25.423	0.20553	68.438	1773.2
10	3.5968	32.203	28.025	0.2000	78.667	2250
11	3.7418	35.739	30.595	0.19548	89.481	2785.2
12	3.8819	39.33	33.137	0.1917	100.88	3378.9
13	4.0173	42.974	35.653	0.1885	112.87	4031.3
14	4.1486	46.669	38.146	0.18574	125.45	4742.4
15	4.2759	50.413	40.618	0.18335	138.61	5512.4

Table 4. The evaluated degree based descriptors values for numerous generalized Helm graph

H_n	$\mathcal{ABCSNI}$	$\mathcal{AGSNI}$	$\mathcal{GASNI}$	$\mathcal{HSNI}$	$\mathcal{SDSNI}$	$\mathcal{ISSNI}$
3	2.5899	12.455	8.1967	0.30616	27.526	120.96
4	2.7033	16.346	11.088	0.25437	34.79	268.15
5	2.776	20.817	13.754	0.20734	45.47	517.19
6	2.8304	25.7	16.308	0.17146	58.503	899.42
7	2.8789	30.93	18.79	0.14472	73.666	1445.3
8	2.926	36.469	21.222	0.12453	90.892	2185.2
9	2.9729	42.29	23.616	0.10894	110.16	3148.9
10	3.0199	48.374	25.981	0.096627	131.45	4366.7
11	3.0669	54.705	28.322	0.086706	154.76	5868.5
12	3.1138	61.269	30.643	0.078565	180.08	7684.3
13	3.1604	68.055	32.949	0.071778	207.41	9844.1
14	3.2067	75.054	35.24	0.066042	236.75	12378
15	3.2524	82.256	37.518	0.061134	268.1	15316

4 Conclusions

In conclusion, our study focused on formulating and evaluating general formulas for newly introduced graph descriptors for the generalized Gear and Helm graphs, well-known families in graph theory. Leveraging MATLAB algorithms, we computed the numeric values of these indices, allowing for a quantitative analysis of their behavior concerning graph size and order. The graphical analysis presented in the previous section, based on the calculated values and corresponding tables, revealed a consistent increase in descriptor values with the growth of graph size and order. This visual exploration provided valuable insights into the relationship between topological indices and the evolving structural complexities of the studied graphs, offering a comprehensive understanding of their interplay. Our findings contribute both theoretically and practically to the field, establishing a robust framework for further investigations into the application and interpretation of graph descriptors within diverse graph families.

5 Future Work

The techniques outlined in our article can be applied for the in-depth analysis of the topological aspects of even more complex chemical structures. Additionally, similar methodologies can be employed to analyze distance and eccentricity-based descriptors. By extending these approaches, researchers can gain valuable insights into the structural characteristics and properties of intricate chemical compounds, contributing to a more comprehensive understanding of their behavior and facilitating advancements in chemical research.

Data Availability

Not applicable.

Conflicts of Interest

The authors declare no conflict of interest.

References

[1] R. Albert, H. Jeong, and A. L. Barabási, "Error and attack tolerance of complex networks," *Nature*, vol. 406, no. 6794, pp. 378–382, 2000. https://doi.org/10.1038/35019019

[2] M. E. J. Newman, "Modularity and community structure in networks," *Proc. Nat. Acad. Sci.*, vol. 103, no. 23, pp. 8577–8582, 2006. https://doi.org/10.1073/pnas.0601602103

[3] R. Pastor-Satorras and A. Vespignani, "Epidemic spreading in scale-free networks," *Phys. Rev. Lett.*, vol. 86, no. 14, pp. 3200–3203, 2001. https://doi.org/10.1103/physrevlett.86.3200

[4] A. L. Barabási, *Network Science*. Cambridge University Press, UK, 2016.

[5] J. Leskovec, J. Kleinberg, and C. Faloutsos, "Graphs over time: Densification laws, shrinking diameters and possible explanations," in *Proceedings of the Eleventh ACM SIGKDD International Conference on Knowledge Discovery and Data Mining, Chicago, IL, USA*, 2005, pp. 177–187. https://doi.org/10.1145/1081870.1081893

[6] J. de Dios Ortúzar and L. G. Willumsen, *Modelling Transport*. John Wiley & Sons, UK, 2011.

[7] D. B. West, *Introduction to Graph Theory*. Prentice Hall, Upper Saddle River, NJ, USA, 2001.

[8] R. Sommer and V. Paxson, "Outside the closed world: On using machine learning for network intrusion detection," in *Proceedings of the 2010 ACM SIGCOMM Conference on Computer Communication, Oakland, CA, USA*, 2010, pp. 305–316. https://doi.org/10.1109/sp.2010.25

[9] G. Adomavicius and A. Tuzhilin, "Toward the next generation of recommender systems: A survey of the state-of-the-art and possible extensions," *IEEE Trans. Knowl. Data Eng.*, vol. 17, no. 6, pp. 734–749, 2005. https://doi.org/10.1109/tkde.2005.99

[10] M. Randić, "Generalized molecular descriptors," *J. Math. Chem.*, vol. 7, pp. 155–168, 1991. https://doi.org/10.1007/BF01200821

[11] R. Todeschini and V. Consonni, *Handbook of Molecular Descriptors*. Wiley-VCH, Germany, 2000.

[12] M. Randić, "Novel shape descriptors for molecular graphs," *J. Chem. Inf. Comput. Sci.*, vol. 41, no. 3, pp. 607–613, 2001. https://doi.org/10.1021/ci0001031

[13] K. Roy and I. Mitra, "Advances in quantitative structure–activity relationship models of antioxidants," *Expert Opin. Drug Discovery*, vol. 4, no. 11, pp. 1157–1175, 2009. https://doi.org/10.1517/17460440903307409

[14] A. T. Balaban, "Topological indices based on topological distances in molecular graphs," *Pure Appl. Chem.*, vol. 55, no. 2, pp. 199–206, 1983. https://doi.org/10.1351/pac198855020199

[15] M. Dehmer, K. Varmuza, S. Borgert, and F. Emmert-Streib, "On entropy-based molecular descriptors: Statistical analysis of real and synthetic chemical structures," *J. Chem. Inf. Model.*, vol. 49, no. 7, pp. 1655–1663, 2009. https://doi.org/10.1021/ci900060x

[16] J. Wei, A. Fahad, A. Raza, P. Shabir, and A. Alameri, "On distance dependent entropy measures of poly propylene imine and zinc porphyrin dendrimers," *Int. J. Quantum Chem.*, vol. 124, no. 1, p. e27322, 2024. https://doi.org/10.1002/qua.27322

[17] A. Raza and M. M. Munir, "Insights into network properties: Spectrum-based analysis with Laplacian and signless Laplacian spectra," *Eur. Phys. J. Plus*, vol. 138, no. 9, 2023. https://doi.org/10.1140/epjp/s13360-023-04441-z

[18] H. Wiener, "Structural determination of paraffin boiling points," *J. Am. Chem. Soc.*, vol. 69, no. 1, pp. 17–20, 1947. https://doi.org/10.1021/ja01193a005

[19] V. R. Kulli, "Some new status neighborhood indices of graphs," *Int. J. Math. Trends Technol.*, vol. 66, no. 6, pp. 139–153, 2020.

[20] A. Raza, M. Munir, T. Abbas, S. M. Eldin, and I. Khan, "Spectrum of prism graph and relation with network related quantities," *AIMS Math.*, vol. 8, no. 2, pp. 2634–2647, 2023. https://doi.org/10.3934/math.2023137

[21] J. R. Lee, A. Hussain, A. Fahad, A. Raza, M. Imran Qureshi, A. Mahboob, and C. Park, "On ev and ve-degree based topological indices of silicon carbides," *Comput. Model. Eng. Sci.*, vol. 130, no. 2, pp. 871–885, 2022. https://doi.org/10.32604/cmes.2022.016836

[22] X. Zhang, A. Raza, A. Fahad, M. K. Jamil, M. A. Chaudhry, and Z. Iqbal, "On face index of silicon carbides," *Discrete Dyn. Nat. Soc.*, vol. 2020, pp. 1–8, 2020. https://doi.org/10.1155/2020/6048438

[23] D. Alghazzawi, A. Raza, U. Munir, and Md. Shajib Ali, "Chemical applicability of newly introduced topological invariants and their relation with polycyclic compounds," *J. Math.*, vol. 2022, pp. 1–16, 2022. https://doi.org/10.1155/2022/5867040

[24] Md. Saidur Rahman, *Basic Graph Theory*. Springer, India, 2017.

[25] V. R. Kulli, "Computation of status neighborhood indices of graphs," *Int. Recent Sci. Res.*, vol. 11, no. 4, pp. 38 079–38 085, 2020. https://doi.org/10.24327/ijrsr.2020.1104.5236