BAREKENG: Journal of Mathematics and Its Applications
June 2026 Volume 20 Issue 2 Page 0971–0980
P-ISSN: 1978-7227 E-ISSN: 2615-3017
https://doi.org/10.30598/barekengvol20iss2pp0971-0980

SOME CHEMICAL TOPOLOGICAL INDICES FOR THE COPRIME GRAPH OF THE INTEGERS MODULO GROUP

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Article Info

Article History:

Received: 25th April 2025
Revised: 27th May 2025
Accepted: 8th September 2025
Available online: 26th January 2026

Keywords:

Coprime graph;
First Zagreb index;
Second Zagreb index;
Wiener index.

ABSTRACT

This paper delves into the exploration of the coprime graph of a finite group G, a graph with vertices representing all group elements. Vertices x and y are considered adjacent in Γ_G if their orders are relatively prime. Specifically, our focus lies in determining essential topological indices: the first Zagreb index, the second Zagreb index, and the Wiener index of the coprime graph associated with the group of integers modulo n. The groups under consideration in this study are those of integers modulo n, where n takes the form of prime power and multiplication of two prime powers, with p and q representing distinct prime numbers and r and s representing natural numbers. This investigation aims to provide a comprehensive understanding of the structural and numerical properties of the coprime graph within the context of finite groups, shedding light on the intricate relationships between group elements and their algebraic properties.

How to cite this article:

G. Elfiyanti, M. N. Sari, I. G. A. W. Wardhana, A. Candra and G. Semil @ Ismail., "SOME CHEMICAL TOPOLOGICAL INDICES FOR THE COPRIME GRAPH OF THE INTEGERS MODULO GROUP", *BAREKENG: J. Math. & App.*, vol. 20, no. 2, pp. 0969-0978, Jun, 2026.

1. INTRODUCTION

In the digital era, studying mathematical structures is becoming increasingly important, especially in the field of graph theory, which models interactions between objects as vertices and their relationships as edges [1], [2]. Graph theory serves as a foundation for analyzing complex networks and has broad applications across disciplines, including chemistry. In chemical graph theory, molecules are represented as graphs, and from these, numerical descriptors known as topological indices are calculated [3], [4]. These indices, also called graph invariants, remain identical for isomorphic graphs, and one of the main objectives is to identify those that can predict chemical properties based on a molecule's structure [5]. In addition to topological indices, recent studies have also emphasized the concept of graph energy, which measures structural properties of graphs through the eigenvalues of associated matrices. Several variants, such as Sombor energy and degree sum energy, have been investigated in algebraic graph contexts—for instance, the Sombor energy of the nilpotent graph of the ring of integers modulo ε and the degree sum energy of non-coprime graphs on dihedral groups—highlighting the growing role of graph energy in advancing chemical and algebraic graph theory [6], [7], [8].

Several notable topological indices are explored, including both Zagreb Indices (first and second), as well as the Wiener Index [9]. The Zagreb Indices focus on the degree of atoms in a molecular graph, highlighting how individual atoms contribute to the overall structure. On the other hand, the Wiener Index measures the total size of a molecule by summing the shortest paths between every pair of atoms. These indices are crucial for understanding the link between molecular structure and various chemical and biological processes, playing a key role in fields like materials science, environmental chemistry, and drug development [10].

Topological indices can also be applied to finite groups by representing them as graphs, providing a powerful way to capture the structural relationships within the group. In this approach, elements of the finite group are connected through graphs like the coprime and non-coprime graphs, where vertices represent group elements, and edges link pairs of elements according to its algebraics properties [11], [12], [13]. This abstraction as well as the unit graph and the nilpoten graph allows mathematicians to visually explore the complex interactions among group elements [14], [15], [16]. By applying topological indices to these graphs, we gain deeper insights into the group's algebraic properties and the relationships between its elements.

In 2022, Zahidah and colleagues explored six different connectivity indices on the coprime graph of the general quaternion group. These indices included the Zagreb indices (first and second), the Wiener indices (regular and hyper), the Harary index, and the Szeged index [17], [18]. Around the same time, Husni and his team focused on the harmonic and Gutman indices, applying them to the coprime graph of the group $\mathbb{Z}_n$ [19], [20]. Building on these studies, the authors are eager to explore the Zagreb indices (first and second), and Wiener Index as applied to the coprime graph of the group of $\mathbb{Z}_n$ of specific order of n.

2. RESEARCH METHODS

To find gaps and areas that need more research, the research methodology starts with a thorough review of the literature on topological indices of graphs. After that, the graphs are arranged in a particular order (n), and a group is established according to their shared attributes. For every graph in the group, a case-by-case analysis is conducted, during which topological indices are examined, and the graph's structure is built. A conjecture concerning the general structure of graphs within the selected group is formulated from these individual cases, with particular emphasis on recurrent patterns. Next, a deductive argument is constructed to verify the conjectured general structure and give a mathematical foundation for the patterns observed in different circumstances. A general formula for the topological indices of graphs inside a given order can be found using the established general structure.

3. RESULTS AND DISCUSSION

Within this segment, we revisit fundamental concepts crucial for the subsequent sections. A prerequisite for a comprehensive understanding includes familiarity with the definition of the order of an element in a group and an understanding of Lagrange's theorem.

Definition 1 [21]. Let G be a group with the identity e. The order of an element a of G is the smallest natural number n such that $a^n = e$. The order of a is denoted by $|a|$. If no such n exists, then a is said to have infinite order.

Theorem 1 [22]. *Let S be a subgroup of a finite group G. Then the order of subgroup S divides the order of the group G.*

Prior to computing the initial Zagreb index, the secondary Zagreb index, and the Wiener index for a linked graph, it is essential to comprehend the definitions of vertex degree and the distance between two vertices within a connected graph.

Definition 2 [3]. The degree of a vertex v in a graph Γ, denoted by $deg(v)$, is the number of vertices that are adjacent to v in Γ.

Definition 3 [3].Suppose that u and v are two distinct vertices in a connected graph Γ. The distance $d(u,v)$ from vertice u to vertice v in graph Γ is the minimum length of the path (u,v) in Γ.

The following are definitions of the topological indices that are used in this research, including the first Zagreb index, the second Zagreb index, and the Wiener index.

Definition 4 [23]. Let Γ be a connected graph. The first Zagreb index of graph Γ is denoted as $M_1(\Gamma)$, defined as follows:

$$M_1(\Gamma) = \sum_{v \in V(\Gamma)} (deg(v))^2.$$

The second Zagreb index of Γ is denoted as $M_2(\Gamma)$, defined as follows:

$$M_2(\Gamma) = \sum_{u,v \in E(\Gamma)} deg(u) \,.\, deg\,(v).$$

Definition 5 [24]. Let Γ be a connected graph. The Wiener index of graph Γ, denoted as $W(\Gamma)$, is defined as follows:

$$W(\Gamma) = \sum_{u,v \in V(H)} d(u,v).$$

Theorem 2 [25]. *If $n = {p_1}^{k_1} {p_2}^{k_2} \dots {p_j}^{k_j}$, where $p_1, p_2, \dots, p_j$ are distinct prime numbers, and $k_1, k_2, \dots, k_j$ are natural numbers, then the coprime graph of $\Gamma_{\mathbb{Z}_n}$ is a $(j+1)$ −partite graph.*

Example 1. The coprime graphs for the groups $\mathbb{Z}_3, \mathbb{Z}_5$, and $\mathbb{Z}_7$ are shown in the following figure.

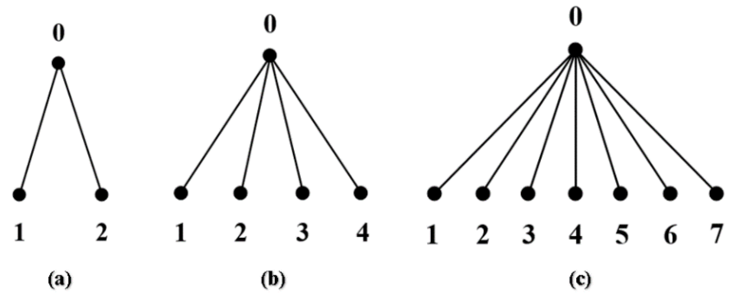

Figure 1. (a) $\Gamma_{\mathbb{Z}_3}$ (b) Γ_5 (c) $\Gamma_{\mathbb{Z}_7}$

Example 2. The coprime graphs for the groups $\mathbb{Z}_{12}, \mathbb{Z}_{20}$, and $\mathbb{Z}_{48}$ are illustrated in the following figure.

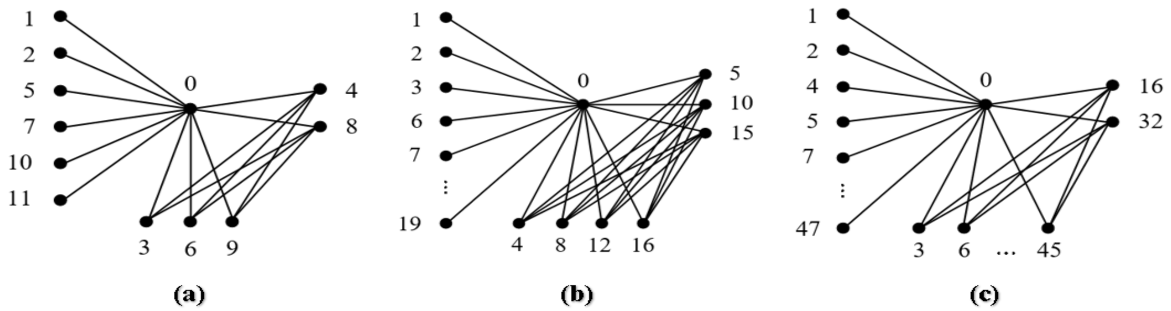

Figure 2. (a) $\Gamma_{\mathbb{Z}_{12}}$ (b) $\Gamma_{\mathbb{Z}_{20}}$ (c) $\Gamma_{\mathbb{Z}_{48}}$

This research aims to determine the Zagreb indices (first and second), and the Wiener index of the coprime graph of the group of integers modulo n, denoted as $\Gamma_{\mathbb{Z}_n}$. Research findings obtained in several theorems are presented in the following.

3.1 The Coprime Graph $\Gamma_{\mathbb{Z}_n}$ of $\mathbb{Z}_n$, $\Gamma_{\mathbb{Z}_n}$ for $n = p^r$

We begin by *examining the structure of the coprime graph* for integers modulo a prime power. This forms the basis for calculating the topological indices presented in the next results.

Lemma 1. *Let $\Gamma_{\mathbb{Z}_n}$ be the coprime graph of $\mathbb{Z}_n$, for n is the power of prime number p, then the degrees of vertices are given in the following:*

$$deg(0) = n - 1,$$
$$deg(u) = 1, \forall u \in V(\Gamma_{\mathbb{Z}_n})\backslash\{0\},$$

and the distance between two vertices of $\Gamma_{\mathbb{Z}_n}$ are

$$d(0, v) = 1,$$
$$d(u, v) = 2, \forall u, v \in V(\Gamma_{\mathbb{Z}_n})\backslash\{0\}.$$

Proof. It is clear that $|0| = 1$ and $|u| = p^i$ for $1 \leq i \leq r$. Then we have $gcd(|0|, |v|) = 1$ and $gcd(|u|, |v|) \neq 1$, $\forall u, v \in V(\Gamma_{\mathbb{Z}_n})\backslash\{0\}$. Hence, 0 is adjacent to other vertices in $\Gamma_{\mathbb{Z}_n}$, while the remaining nodes are not adjacent to each other. Therefore, the degrees of vertices are $deg(0) = n - 1$, $deg(u) = 1$, $\forall u \in V(\Gamma_{\mathbb{Z}_n})\backslash\{0\}$. Meanwhile, the distance between two vertices is $d(0, v) = 1$, and $d(u, v) = 2, \forall u, v \in V(\Gamma_{\mathbb{Z}_n})\backslash\{0\}$. ■

Subsequently, the propositions for the Zagreb indices (first and second), and the Wiener index of the coprime graph associated with the group of integers modulo n, where n equals p^r, are established in the following manner:

Theorem 3. *Let $\Gamma_{\mathbb{Z}_n}$ be the coprime graph of $\mathbb{Z}_n$, for $n = p^r$, where p is a prime number and $r \in \mathbb{N}$. Then, the first Zagreb index, the second Zagreb index, and the Wiener index of $\Gamma_{\mathbb{Z}_n}$ are*

$$M_1(\Gamma_{\mathbb{Z}_n}) = n^2 - n,$$
$$M_2(\Gamma_{\mathbb{Z}_n}) = n^2 - 2n + 1,$$
$$W(\Gamma_{\mathbb{Z}_n}) = n^2 - 2n + 1.$$

Proof. According to Lemma 1, it is known that $deg(0) = n - 1$ and $deg(v) = 1, \forall v \in V(\Gamma_{\mathbb{Z}_n})\backslash\{0\}$ hence

1. The First Zagreb Index of $\Gamma_{\mathbb{Z}_n}$

$$\begin{aligned} M_1(\Gamma_{\mathbb{Z}_n}) &= \sum_{v \in V(\Gamma_{\mathbb{Z}_n})} (deg(v))^2, \\ &= (deg(0))^2 + \sum_{v \in V(\Gamma_{\mathbb{Z}_n})\backslash\{0\}} (deg(v))^2, \\ &= (n-1)^2 + (n-1) \cdot 1^2, \\ &= n^2 - n. \end{aligned}$$

2. The Second Zagreb Index of $\Gamma_{\mathbb{Z}_n}$

$$\begin{aligned} M_2(\Gamma_{\mathbb{Z}_n}) &= \sum_{u,v \in E(\Gamma_{\mathbb{Z}_n})} deg(u) \cdot deg(v), \\ &= deg(0) \sum_{v \in E(\Gamma_{\mathbb{Z}_n})} deg(v), \\ &= (n-1) \cdot ((n-1) \cdot 1), \\ &= n^2 - 2n + 1. \end{aligned}$$

And from Lemma 1, it is also known that $d(0,v) = 1$ and $d(u,v) = 2, \forall u, v \in V(\Gamma_{\mathbb{Z}_n}) \backslash \{0\}$, hence

3. The Wiener Index of $\Gamma_{\mathbb{Z}_n}$

The important thing to note before calculating the Wiener index of $\Gamma_{\mathbb{Z}_n}$ is to determine the number of pairs of two distinct non-zero nodes, which is

$$C_2^{n-1} = \frac{(n-1)!}{((n-1)-2)!\,(2)!} = \frac{(n-1)(n-2)}{2}.$$

Then, it can be obtained that

$$\begin{aligned} W(\Gamma_{\mathbb{Z}_n}) &= \sum_{u,v \in V(\Gamma_{\mathbb{Z}_n})} d(u,v), \\ &= \sum_{v \in V(\Gamma_{\mathbb{Z}_n})} d(0,v) + \sum_{u,v \in V(\Gamma_{\mathbb{Z}_n})} d(u,v), \\ &= (n-1) + (n-1)(n-2), \\ &= (n-1) + (n^2 - 3n + 2), \\ &= n^2 - 2n + 1. \end{aligned}$$

■

3.2 The Coprime graph $\Gamma_{\mathbb{Z}_n}$ of $\mathbb{Z}_n$, for $n = p^r q^s$

Next, we extend the analysis to the coprime graph of integers modulo a product of two distinct prime powers. The following result describes the degrees and distances in this case.

Lemma 2. *Let $\Gamma_{\mathbb{Z}_n}$ be the coprime graph of $\mathbb{Z}_n$, for n is the multiplication of the power of two distinct prime number p and q. Then, the degrees of vertices are given in the following:*

$$\begin{aligned} deg(0) &= n-1, \\ X_1 &= \{u \in V_2 \mid deg(u) = 1\}, \\ X_2 &= \{v \in V_2 \mid deg(v) = q^s\}, \\ X_3 &= \{w \in V_3 \mid deg(w) = p^r\}, \end{aligned}$$

and the distance between two vertices of $\Gamma_{\mathbb{Z}_n}$ are

$$\begin{aligned} d(0,v) &= n-1, v \in V(\Gamma_{\mathbb{Z}_n}) \backslash \{0\}, \\ d(u,v) &= 2, \\ d(u,w) &= 2, \\ d(v,w) &= 1. \end{aligned}$$

Proof. Let $\Gamma_{\mathbb{Z}_n}$ with $n = p^r q^s$, where p and q are distinct prime numbers, and r and s are positive integers, are partitioned into three cases:

$$V_1 = \{0\},$$

$$V_2 = \{u \in V(\Gamma_{\mathbb{Z}_n}); |u| = p^i q^j\} \text{ with } 1 \le i \le r \text{ and } 0 \le j \le s,$$

$$V_3 = \{v \in V(\Gamma_{\mathbb{Z}_n}); |v| = q^j\} \text{ with } 1 \le q \le s.$$

Then we can obtain $gcd(|0|,|u|) = 1$, $gcd(|0|,|v|) = 1$, in if $|u| = p^i q^j$ with $j = 0$ hence $gcd(|u|,|v|) \neq 1$. So that the coprime graph of the group $\mathbb{Z}_n$ for $n = p^r q^s$ is illustrated in Fig. 3.

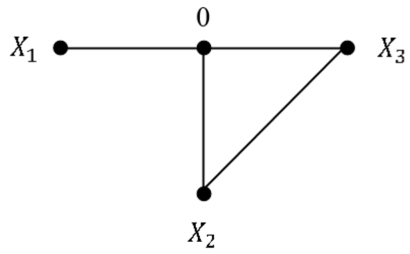

Figure 3. The Coprime Graph of $\mathbb{Z}_n$, $\Gamma_{\mathbb{Z}_n}$ for $n = p^r q^s$

Therefore, the degrees of vertices are given in the following:

$$\begin{aligned} deg(0) &= n - 1, \\ X_1 &= \{u \in V_2 |\, deg(u) = 1\}, \\ X_2 &= \{v \in V_2 |\, deg(v) = q^s\}, \\ X_3 &= \{w \in V_3 |\, deg(w) = p^r\}, \end{aligned}$$

and the distance between two vertices of $\Gamma_{\mathbb{Z}_n}$ are

$$\begin{aligned} d(0,v) &= n - 1, v \in V(\Gamma_{\mathbb{Z}_n})\backslash\{0\}, \\ d(u,v) &= 2, \\ d(u,w) &= 2, \\ d(v,w) &= 1. \end{aligned}$$

■

Then, the Theorem for the first Zagreb index, the second Zagreb index, and the Wiener index will be given for the coprime graph of the group of integers modulo n, for $n = p^r q^s$.

Theorem 4. *Let $\Gamma_{\mathbb{Z}_n}$ is a coprime graph of $\mathbb{Z}_n$, for n is the multiplication of the power of two distinct prime number p and q. Then the first Zagreb, the second Zagreb index, and the Wiener Index of $\Gamma_{\mathbb{Z}_n}$ are*

$$\begin{aligned} M_1(\Gamma_{\mathbb{Z}_n}) &= n^2 + (p^r + q^s - 1)n - p^r(p^r + 1) - q^s(q^s + 1) + 2, \\ M_2(\Gamma_{\mathbb{Z}_n}) &= n(4n - 3p^r - 3q^s - 1) + 2(p^r + q^s) - 1, \\ W(\Gamma_{\mathbb{Z}_n}) &= n^2 - 3n + p^r + q^s. \end{aligned}$$

Proof. Let $\Gamma_{\mathbb{Z}_n}$ be the coprime graph of the group $\mathbb{Z}_n$ for $n = p^r q^s$ where p and q are distinct prime numbers, and r and s are positive integers. Then, let $a = p^r$ and $b = q^s$ so according to Lemma 2, it is known that $deg(0) = n - 1$, $deg(u) = 1$, $deg(v) = b$, and $deg(w) = a$ hence

1. The first Zagreb index of $\Gamma_{\mathbb{Z}_n}$ P

$$\begin{aligned} M_1(\Gamma_{\mathbb{Z}_n}) &= \sum_{v \in V(\Gamma_{\mathbb{Z}_n})} (deg(v))^2, \\ &= (deg(0))^2 + \sum_{u \in X_1\backslash\{0\}} (deg(u))^2 + \sum_{v \in X_2\backslash\{0\}} (deg(v))^2 + \sum_{w \in X_3\backslash\{0\}} (deg(w))^2, \\ &= (n-1)^2 + (n - a - b + 1)\cdot(1)^2 + (a-1)\cdot(b)^2 + (b-1)\cdot(a)^2, \\ &= n^2 + (p^r + q^s - 1)n - p^r(p^r + 1) - q^s(q^s + 1) + 2. \end{aligned}$$

2. The first Zagreb index of $\Gamma_{\mathbb{Z}_n}$

$$\begin{aligned} M_2(\Gamma_{\mathbb{Z}_n}) &= \sum_{u,v \in E(\Gamma_{\mathbb{Z}_n})} deg(u)\cdot deg(v), \\ &= deg(0)\cdot \sum_{u \in X_1\backslash\{0\}} deg(u) + deg(0)\cdot \sum_{v \in X_2\backslash\{0\}} deg(v) + \sum_{v \in X_2\backslash\{0\}} deg(v)\cdot \sum_{w \in X_3\backslash\{0\}} deg(w) \\ &\quad + deg(0)\cdot \sum_{w \in X_3\backslash\{0\}} deg(w), \end{aligned}$$

$$= (n-1)\cdot(n-a-b+1)+(n-1)\cdot b(a-1)+b(a-1)\cdot a(b-1)+(n-1)\cdot a(b-1),$$
$$= 4n^2-3an-3bn-n+2a+2b-1,$$
$$= n(4n-3p^r-3q^s-1)+2(p^r+q^s)-1.$$

And based on Lemma 2, it is also known that $d(0,v)=n-1, v\in V(\Gamma_{\mathbb{Z}_n})\backslash\{0\}$, $d(u,v)=2$, $d(u,w)=2$, and $d(v,w)=1$ such as

3. The Wiener Index of $\Gamma_{\mathbb{Z}_n}$

$$W(\Gamma_{\mathbb{Z}_n}) = \sum_{u,v\in V(\Gamma_{\mathbb{Z}_n})} d(u,v),$$
$$= \sum_{v\in V(\Gamma_{\mathbb{Z}_n})} d(0,v)+\sum_{u\in X_1,v\in X_2} d(u,v)+\sum_{u\in X_1,v\in X_3} d(u,v)+\sum_{u\in X_2,v\in X_3} d(u,v)+\sum_{u,v\in X_1} d(u,v)+\sum_{u,v\in X_2} d(u,v)+\sum_{u,v\in X_3} d(u,v),$$
$$= (n-1)+2(n-a-b+1)\cdot(a-1)+2(n-a-b+1)\cdot(b-1)+(a-1)\cdot(b-1)+(n-a-b+1)\cdot(n-a-b)+(a-1)\cdot(a-2)+(b-1)\cdot(b-1),$$
$$= n^2-3n+a+b,$$
$$= n^2-3n+p^r+q^s.$$

Example 3. Given the group $\mathbb{Z}_{36}$, according to Theorem 4, we have $p=2, q=3$, and $r=s=2$, thus the indices are:

$$M_1(\Gamma_{\mathbb{Z}_{36}}) = 36^2+(2^2+3^2-1)36-2^2(2^2+1)-3^2(3^2+1)+2 = 1620,$$
$$M_2(\Gamma_{\mathbb{Z}_{36}}) = 36(4(36)-3(2^2)-3(3^2)-1)+2(2^2+3^2)-1 = 3769,$$
$$W(\Gamma_{\mathbb{Z}_{36}}) = 36^2-3(36)+2^2+3^2 = 1201.$$

4. CONCLUSION

The results for the Zagreb indices (first and second), and the Wiener index on the coprime graph of the group of integers modulo n, for is the power of prime number p, are obtained as follows:

$$M_1(\Gamma_{\mathbb{Z}_n}) = n^2-n,$$
$$M_2(\Gamma_{\mathbb{Z}_n}) = n^2-2n+1,$$
$$W(\Gamma_{\mathbb{Z}_n}) = n^2-2n+1.$$

On the other hand, we have computed the Zagreb indices (first and second), and the Wiener index on the coprime graph of the group of integers modulo n, for n is the multiplication of the power of two distinct prime number p and q, are as follows:

$$M_1(\Gamma_{\mathbb{Z}_n}) = n^2+(p^r+q^s-1)n-p^r(p^r+1)-q^s(q^s+1)+2,$$
$$M_2(\Gamma_{\mathbb{Z}_n}) = n(4n-3p^r-3q^s-1)+2(p^r+q^s)-1,$$
$$W(\Gamma_{\mathbb{Z}_n}) = n^2-3n+p^r+q^s.$$

For example, when $p=2$, $q=3$, $s=2$ and $r=2$ we obtain that the first Zagreb index of the coprime graph is 840, the second Zagreb index is 5040, and the Wiener index is 2065.

Author Contributions

Gustina Elfiyanti: Conceptualization, Methodology, Investigation, Project Administration, Supervision, and Writing - Original Draft. Mutia Novita Sari: Data Curation, Formal Analysis, Resources, and Draft Preparation. I Gede Adhitya Wisnu Wardhana: Conceptualization, Validation, and Writing–Review and Editing. Ade Chandra assisted: Formal Analysis, Validation, and Visualization. Ghazali Semil @ Ismail: Visualization, Computation, and Validation. All authors discussed the results and contributed to the final manuscript.

Funding Statement

The authors thank the Center of Research and Publication UIN Syarif Hidayatullah Jakarta for providing financial support for this research with contract number UN.01/KPA/1165/2023.

Acknowledgment

The authors would like to express their sincere gratitude to Universitas Islam Negeri Syarif Hidayatullah, Universitas Mataram, and Universiti Teknologi Malaysia for providing the academic environment, support, and collaboration that made this research possible. The constructive discussions and valuable insights shared among the research team members from these institutions have greatly contributed to the completion of this work.. We also appreciate the editor's and reviewers' insightful comments, which helped improve the article.

Declarations

The authors declare no competing interest.

Declaration of Generative AI and AI-assisted Technologies

Generative AI tools (e.g., ChatGPT) were used solely for language refinement (grammar, spelling, and clarity). The scientific content, analysis, interpretation, and conclusions were developed entirely by the authors. The authors reviewed and approved all final text.

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