OPEN ACCESS

Kashf Journal of Multidisciplinary Research
Vol: 02 - Issue 2 (2025)
P-ISSN: 3007-1992 E-ISSN: 3007-200X
https://kjmr.com.pk

BI-DISTANCE PROCEDURE FOR EVALUATING THE TOPOLOGICAL INDICES FOR RHOMBUS OXIDE NETWORK

Muhammad Imran
Faculty of Sciences, The Superior University Lahore, Pakistan.
Muhammad Rizwan Wahala
Faculty of Sciences, The Superior University Lahore, Pakistan.
Muhammad Nawazish Zaman
Faculty of Sciences, The Superior University Lahore, Pakistan.
Saima Mushtaq*
Faculty of Sciences, The Superior University Lahore, Pakistan.
Zunera Shoukat
Faculty of Sciences, The Superior University Lahore, Pakistan.
****Corresponding author: Saima Mushtaq** (saimamushtaq.fsd@superior.edu.pk)*
DOI: https://doi.org/10.71146/kjmr291

Article Info

This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license https://creativecommons.org/licenses/by/4.0

Abstract

This study explores the fractal nature of rhombus oxide network, leveraging molecular structure descriptors to correlate chemical structure with biological activity in pharmacology. By translating networks into graphical forms and utilizing degree-based topological indices, we calculate various indices (Randić, geometric arithmetic, atom bond connectivity, and more) and their polynomials for rhombus graphs using Mathematica. This computational approach enables the estimation of fractal, thermodynamic, and physicochemical aspects of chemical structures, informing configuration, impact resistance, and design in technical and scientific advancements. Our results provide a comprehensive understanding of chemical graph theory, facilitating the correlation of chemical structure with biological activity and contributing to significant advancements in pharmacology and materials science.

Keywords:
bi-distance edges; edge computing, molecular structure; rhombus oxide network; topological index; Randic index; harmonic index; geometric arithmetic index; forgotten index; symmetric division index; atom bond connectivity index, structure analysis.

Introduction

In the eighteenth century, the mathematician Leonhard Euler (1702–1782) of Switzerland is credited with introducing the term "graph" within the field of graph theory. The Königsberg Bridge Puzzle presented a challenge of crossing seven bridges over a divided river near an island without traversing any bridge more than once [1].

Euler's analysis concluded that there exists no path that can traverse all bridges exactly once and return to the starting point. Though Euler's proof specifically addressed the physical arrangement of bridges, it essentially validated the foundational theorem of graph theory [2].

The mathematical discipline known as "graph theory" focuses on the study of structures composed of vertices connected by edges. Over time, graph theory has developed into a significant area of mathematical inquiry, finding applications in diverse fields. It's worth noting that all graphs discussed in this paper adhere to the criteria of being simple, connected, and planar. "Graph theory" is the mathematical term employed to examine graphs, which are mathematical representations utilized to depict pairwise connections between variables [3].

Graph Theory [4] offers an excellent mathematical foundation for handling a wide range of practical problems in genetics, psychology, sociology, and linguistics. Moreover, it boasts significant intersections with various other mathematical domains like topology, group theory, probability theory, and matrix theory, rendering it an adaptable and broad.

A graph is a mathematical structure made up of vertices (also known as nodes or points) and edges (also known as links or arcs), which connect pairs of vertices. A graph G can be defined as a collection of vertices V and edges E, with each edge in E connecting two vertices in V. Graphs can be used to model item interactions, communication networks, physical structures, and much more. They are fundamental to many branches of mathematics, computer science, and other disciplines [5, 6].

Chemical graph theory is a branch of theoretical chemistry that uses GT to model chemical patterns quantitatively. By merging principles from chemistry and graph theory, it delves deeper into the exploration of the physical and chemical characteristics of substances. In this field, atoms are represented as vertices in a graph, while bonds between atoms are represented as edges. Chemical graph theory plays a crucial role in drug design, materials science, and computational chemistry, offering powerful tools for understanding and predicting the behavior of molecules [7].

The connectivity of molecular graph is an essential aspect. They are required to be connected graphs because each atom in a molecule needs to be bonded to at least one other atom. This ensures that the molecule is a cohesive structure with no isolated atoms. By examining the molecular graph, scientists can gain insights into the molecular characteristics, like shape, extent, and chemical reactivity. Furthermore, various algorithms and techniques can be applied to analyze molecular graphs and predict the behavior of molecules, including their stability, reactivity, and physical properties [8].

Molecular topology plays a crucial role in various scientific fields and research areas that involve the study of molecular structures. One of the key components of molecular topology is the classification of molecules. By categorizing molecules based on their structural characteristics and properties, researchers can gain insights into their behavior and interactions. The use of molecular topology extends to the investigation of the physical occurrence of molecules. Researchers utilize statistical tools and models to analyze and understand the distribution, occurrence, and patterns of molecules in different environments or systems. These **statistical approaches** enable the discovery of new relationships, correlations, and trends in molecular behavior. Overall, molecular topology provides a framework for organizing and

studying molecular structures, and its applications are diverse and interdisciplinary. It contributes to advancements in fields such as chemistry, biochemistry, pharmaceutical sciences, materials science, and more, enabling researchers to uncover new knowledge and make significant discoveries in various areas of science and research [9, 10].

A Topological Index which is represented by TI (T-index) is a graph-based molecular description. The topological index, also referred to as the graph measure, is a set of data on algebraic graphs that provides a methodological framework for evaluating the basic features of chemical compounds. The concept of a TI was first initiated by Wiener in 1947 when he used it to investigate paraffin's boiling temperature [11].

The adoption of topological indices is a suitable way for expressing chemical components into data variables that can be associated with physical traits in quantitative structure-activity relationships and quantitative structure-property relationships research. TI value helps in understanding the relationship between the chemical structure and various physical properties, chemical reactions, or biological activities. Over the past twenty years, there has been a significant increase in the use of graph-theoretical methods to analyze the physicochemical and structural characteristics of molecular graphs. This trend is crucial for advancements in chemical engineering and pharmaceutical research [12].

In the Quantitative Structure-Activity Relationship (QSAR) or Quantitative Structure Property Relationship (QSPR) assessment, a statistical method is employed to establish a connection between the configuration of a molecule and its related biological activity or characteristic. The objective of this type of study is to quantitatively link the two variables using analytical tools [13, 14].

T-indices offer a way to calculate network properties, particularly in understanding the structural characteristics of pharmaceuticals. The effectiveness of topological indices relies on how well they correlate experimental data with estimated values. TIs serve as an accessible and theoretical technique to acquiring extensive knowledge into medications by evaluating the structural features of distinct pharmaceutical compounds. The abbreviation "Top" refers to the topological index function, which maps a simple finite graph (denoted by Σ), to a real number (denoted by R). Based on a graph's topological characteristics, the TI function assigns an index to it. Notably, if two graphs G_1 and G_2 are isomorphic (meaning they have the same connectivity pattern but may differ in the labeling of vertices or edges), their topological indices will be equal. This can be expressed as

$$Top\ (G_1) = Top(G_2)\,. \qquad (1)$$

Topological indices have been utilized to discover anticancer and anti-HIV drugs. Fortunately, mathematicians have effectively contributed by studying pharmaceutical action using graph theory. There are some major classes of topological indices such as distance based, degree based, eccentricity-based, and ev-degree-based indices [15].

In this paper, a bi-distance approach is used to compute all additive degree-based indices for Rhombus Oxide Network (RHOX).

2 Materials and Methods

In this paper, consider all graphs are simple (without loops and multiple edges), finite connected (exist at least one path between any pair of vertices), undirected (no direction in edges) and planer (without crossing edges). Let G be a graph with vertex set V (G) and edge set E (G). This paper use degree-based indices, encompassing additive variations.

2.1 Randić Index

In 1975 [16], Milan Randić, a chemist, introduced a topological index known as the "branching index", but soon it was re-named to “connectivity index”. Nowadays, most authors refer to it as to the “Randić index” denoted as R (R_{-1} & $R_{-\frac{1}{2}}$). This index was specifically crafted to measure the level of branching in saturated hydrocarbons' carbon-atom structure. This index is one of the oldest topological indices with the most widespread degree structures. It is a mathematical measure that quantifies the structural characteristics of a graph G based on the degrees of its vertices [17, 18].

The Randić Index is defined as

$$R(G) = \sum_{\alpha\beta \in E(G)} \frac{1}{\sqrt{d_\alpha \times d_\beta}} = \sum_{\alpha\beta \in E(G)} \left(d_\alpha \times d_\beta\right)^{-1/2}, \qquad (2)$$

where $\alpha\beta$ represents an edge in the graph.

2.2 General Randić Index

Bollobás, a highly esteemed mathematician, along with Erdős, recognized the intricate mathematical depth concealed within the Randić index. They collaborated on this topic, publishing their initial paper around 1998, though it had been circulating among mathematicians for several years prior [19]. For a (chemical) graph G = (V, E), the general Randić index $R_n(G)$ of G is defined as the sum of $\left(d(\alpha)d(\beta)\right)^n$ overall edges $\alpha\beta$ of G, where $d(\alpha)$ denotes the degree of a vertex α of G,

$$R_n(G) = \sum_{\alpha\beta \in E(G)} \left(d_\alpha \times d_\beta\right)^n, \qquad (3)$$

where n is an arbitrary real number.

2.3 Reciprocal Randić Index

The reciprocal Randic index, introduced by Favaron, Maheó, and Saclé in their research, is another variation derived from the Randic index [20].

$$RR(G) = \sum_{\alpha\beta \in E(G)} \sqrt{d_\alpha \times d_\beta}. \qquad (4)$$

2.4 Atom Bond Connectivity Index

In 1998, Estrada and Torres introduced a new topological index known as the "atom-bond connectivity index [21]" abbreviated as ABC. The Atom Bond Connectivity (ABC) index is a topological index used to quantify the structural properties of a graph [22].

For a graph G with vertex set $V(G)$ and edge set $E(G)$, the ABC index is defined as:

$$ABC(G) = \sum_{\alpha\beta \in E(G)} \sqrt{\frac{d_\alpha + d_\beta - 2}{d_\alpha \times d_\beta}}, \qquad (5)$$

where d_α and d_β are the degrees of vertices α and β, respectively, in the graph G.

2.5 Geometric-Arithmetic Index

Geometric-Arithmetic (GA) index is another well-known topological index. In 2009, Vukicevic and Furtula [23] proposed the GA Index.

The name 'geometric–arithmetic [24]' comes from the fact that $\sqrt{d_\alpha d_\beta}$ and $\frac{1}{2}(d_\alpha + d_\beta)$ are the geometric and arithmetic means, respectively, of the numbers d_α and d_β. Mathematically GA index for a graph G is given by.

$$GA(G) = \sum_{\alpha\beta \in E(G)} \frac{2\sqrt{d_\alpha \times d_\beta}}{(d_\alpha + d_\beta)}. \qquad (6)$$

2.5 Forgotten Index

Followed by the first and second Zagreb indices, Furtula and Gutman (2015) introduced forgotten topological index. This is also called F-index [25] which was defined as

$$F(G) = \sum_{\alpha\beta \in E(G)} (d^2{}_\alpha + d^2{}_\beta). \qquad (7)$$

2.6 Symmetric Division Index

Among the latest developments is the symmetric division index [26]. Vukicević and Furtula introduced the degree-based symmetric division index.

$$SD(G_1) = \sum_{\alpha\beta \in E(G)} \frac{d^2{}_\alpha + d^2{}_\beta}{d_\alpha \times d_\beta}. \qquad (8)$$

2.7 Harmonic Index

Siemion Fajtlowicz created a computer application in 1990 that produces its own theories in the field of GT. He discovered a vertex-degree-based measure while completing this project. In 2012, Zhong made a new discovery about these unidentified criteria and named it the harmonic index [27].

$$H(G_1) = \sum_{\alpha\beta \in E(G)} \frac{2}{d_\alpha + d_\beta}. \qquad (9)$$

2.8 General Sum Connectivity Index

The sum connectivity indices [28] general form was proposed by Zhou and Trinajstić. The $X_n(G)$-index is mathematically written as

$$X_n(G) = \sum_{\alpha\beta \in E(G)} (d_\alpha + d_\beta)^n, \qquad (10)$$

where n is an arbitrary real number.

2.9 Bi-distance Edge Partitions

The edge partition technique is utilized to divide the bi-distance edges [29] of rhombus oxide network into three categories, as presented in Tables 1. For rhombus oxide network, the frequency of E_1 is 2, where $(d_\alpha, d_\beta) = (2,2)$. The frequency of E_2 is 16n+4, where $(d_\alpha, d_\beta) = (2,4)$. And the frequency of E_3 is $12n^2 - 2$, where $(d_\alpha, d_\beta) = (4,4)$. This study employs various methods and techniques, including vertex degree analysis, edge partitioning, graph analytical approaches, and numerical comparisons, to generate results. MATLAB is used for computations and cross-validation, while Mathematica aids in comparing topological indices. Additionally, ChemDraw provides an efficient platform for drawing chemical structures. In the following section, several degree-based topological descriptors are applied to the rhombus oxide network.

3 Results and Discussion

In this paper, the results of the several topological indices for rhombus oxide network $RHOX(n)$ is discussed.

3.1 Results of Rhombus Oxide Network $RHOX(n)$

TI including the Randić index $R(G)$, reciprocal Randić index $RR(G)$, geometric arithmetic index $GA(G)$, atom-bond connectivity index $ABC(G)$, forgotten index $F(G)$, general sum connectivity index $X_g(G)$, symmetric division index $SD(G)$, harmonic index $H(G)$, are computed in this paper.

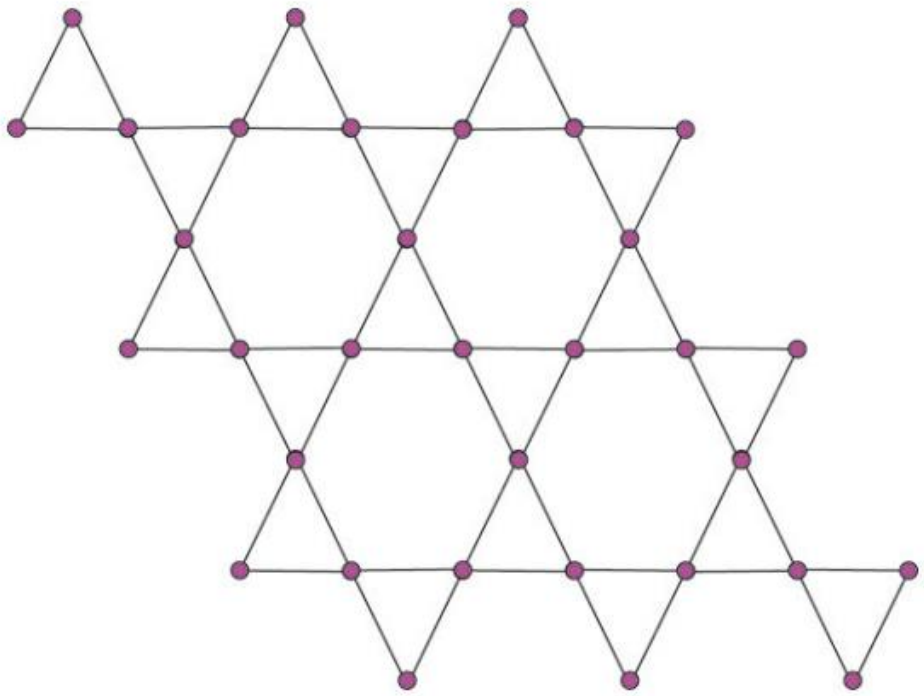

Figure 1: Rhombus Oxide Network $RHOX(n)$

Theorem 3.1.1: *Consider* G_1 *be a simple Rhombus Oxide Network* $RHOX(n)$, *then its Randić index and its general Randić indices are equal to,*

$$R_n(G_1)=\begin{cases}8\left(24n^2+16n+1\right), n=1;\\ \frac{3n^2}{4}+2n+\frac{7}{8}, n=-1;\\ 48n^2+32\sqrt{2}n+8\sqrt{2}-4, n=\frac{1}{2};\\ 3n^2+4\sqrt{2}n+\sqrt{2}+\frac{1}{2}, n=-\frac{1}{2}.\end{cases}$$

Proof:

Let G_1 be a simple, connected rhombus oxide network. The edge collection is divided into three distinct groups. The value of general Randić indices can be determined with the help of Table 1 of the edge partitions.

Edges	(d_α, d_β)	**Frequency**
E_1	$(2,2)$	2
E_2	$(2,4)$	$16n+4$
E_3	$(4,4)$	$12n^2-2$

Table 1: Bi-distance Edge Partitions for Rhombus Oxide Network $RHOX(n)$

General Randić indices for the Rhombus Oxide Network can be calculated as

$$R_n(G_1) = \sum_{\alpha\beta\in E(G_1)} \left(d_\alpha \times d_\beta\right)^n.$$

$$R_n(G_1)=|E_1|\left(d_{\alpha_1}\times d_{\beta_1}\right)^n+|E_2|\left(d_{\alpha_2}\times d_{\beta_2}\right)^n+|E_3|\left(d_{\alpha_3}\times d_{\beta_3}\right)^n.$$

For $n=1$,

$$R_1(G_1)=\left[(2)(2\times 2)^1+(16n+4)(2\times 4)^1+\left(12n^2-2\right)(4\times 4)^1\right],$$

$$R_1(G_1)=\left[(2)(4)^1+(16n+4)(8)^1+\left(12n^2-2\right)(16)^1\right],$$

$$R_1(G_1)=\left[8+(16n+4)(8)+\left(12n^2-2\right)(16)\right],$$

$$R_1(G_1)=\left[192n^2+128n+8\right],$$

$$R_1(G_1)=8\left(24n^2+16n+1\right).$$

For $n=-1$,

$$R_{-1}(G_1)=\left[(2)(2\times 2)^{-1}+(16n+4)(2\times 4)^{-1}+(12n^2-2)(4\times 4)^{-1}\right],$$

$$R_{-1}(G_1)=\left[(2)(4)^{-1}+(16n+4)(8)^{-1}+(12n^2-2)(16)^{-1}\right],$$

$$R_{-1}(G_1)=\left[(2)\left(\frac{1}{4}\right)+(16n+4)\left(\frac{1}{8}\right)+(12n^2-2)\left(\frac{1}{16}\right)\right],$$

$$R_{-1}(G_1)=\left[\left(\frac{1}{2}\right)+(16n+4)\left(\frac{1}{8}\right)+(12n^2-2)\left(\frac{1}{16}\right)\right],$$

$$R_{-1}(G_1)=\left[\left(\frac{1}{2}\right)+\left(\frac{16n+4}{8}\right)+\left(\frac{12n^2-2}{16}\right)\right],$$

$$R_{-1}(G_1)=\left[\left(\frac{1}{2}\right)+\left(2n+\frac{1}{2}\right)+\left(\frac{3}{4}n^2-\frac{1}{8}\right)\right],$$

$$R_{-1}(G_1)=\left[\frac{3}{4}n^2+2n+\frac{7}{8}\right].$$

Now, here it is a reciprocal Randić index that can be expressed as

$$RR(G_1)=\sum_{\alpha\beta\in E(G_1)}\sqrt{d_\alpha\times d_\beta}.$$

When $n=\frac{1}{2}$,

$$RR_{\frac{1}{2}}(G_1)=\left[(2)(2\times 2)^{\frac{1}{2}}+(16n+4)(2\times 4)^{\frac{1}{2}}+(12n^2-2)(4\times 4)^{\frac{1}{2}}\right],$$

$$RR_{\frac{1}{2}}(G_1)=\left[(2)(4)^{\frac{1}{2}}+(16n+4)(8)^{\frac{1}{2}}+(12n^2-2)(16)^{\frac{1}{2}}\right],$$

$$RR_{\frac{1}{2}}(G_1)=\left[(2)(2^2)^{\frac{1}{2}}+(16n+4)(2^3)^{\frac{1}{2}}+(12n^2-2)(2^4)^{\frac{1}{2}}\right],$$

$$RR_{\frac{1}{2}}(G_1)=\left[(2)(2)+(16n+4)(2\sqrt{2})+(12n^2-2)(2^2)\right],$$

$$RR_{\frac{1}{2}}(G_1)=\left[(4)+(16n+4)(2\sqrt{2})+(12n^2-2)(4)\right],$$

$$RR_{\frac{1}{2}}(G_1)=\left[(4)+(32n\sqrt{2}+8\sqrt{2})+(48n^2-8)\right],$$

$$RR_{\frac{1}{2}}(G_1)=\left[48n^2+32\sqrt{2}n+8\sqrt{2}-4\right].$$

Randić index is

$$R_{\frac{-1}{2}}(G_1)=\sum_{\alpha\beta\in E(G_1)}\frac{1}{\sqrt{d_\alpha d_\beta}}=\sum_{\alpha\beta\in E(G)}\left(d_\alpha d_\beta\right)^{-½}.$$

When $n=-\frac{1}{2}$,

$$R_{-\frac{1}{2}}(G_1)=\left[(2)(2\times2)^{-\frac{1}{2}}+(16n+4)(2\times4)^{-\frac{1}{2}}+\left(12n^2-2\right)(4\times4)^{-\frac{1}{2}}\right],$$

$$R_{-\frac{1}{2}}(G_1)=\left[(2)(4)^{-\frac{1}{2}}+(16n+4)(8)^{-\frac{1}{2}}+\left(12n^2-2\right)(16)^{-\frac{1}{2}}\right],$$

$$R_{-\frac{1}{2}}(G_1)=\left[(2)\left(\frac{1}{4}\right)^{\frac{1}{2}}+(16n+4)\left(\frac{1}{8}\right)^{\frac{1}{2}}+\left(12n^2-2\right)\left(\frac{1}{16}\right)^{\frac{1}{2}}\right],$$

$$R_{-\frac{1}{2}}(G_1)=\left[(2)\left(\frac{1}{2^2}\right)^{\frac{1}{2}}+(16n+4)\left(\frac{1}{2^3}\right)^{\frac{1}{2}}+\left(12n^2-2\right)\left(\frac{1}{2^4}\right)^{\frac{1}{2}}\right],$$

$$R_{-\frac{1}{2}}(G_1)=\left[(2)\left(\frac{1}{2}\right)+(16n+4)\left(\frac{1}{2\sqrt{2}}\right)+\left(12n^2-2\right)\left(\frac{1}{2^2}\right)\right],$$

$$R_{-\frac{1}{2}}(G_1)=\left[(1)+(16n+4)\left(\frac{1}{2\sqrt{2}}\right)+\left(12n^2-2\right)\left(\frac{1}{4}\right)\right],$$

$$R_{-\frac{1}{2}}(G_1)=\left[(1)+\left(\frac{16n+4}{2\sqrt{2}}\right)+\left(\frac{12n^2-2}{4}\right)\right],$$

$$R_{-\frac{1}{2}}(G_1)=\left[(1)+\left(4\sqrt{2}n+\sqrt{2}\right)+\left(3n^2-\frac{1}{2}\right)\right],$$

$$R_{-\frac{1}{2}}(G_1)=\left[3n^2+4\sqrt{2}n+\sqrt{2}+1-\frac{1}{2}\right],$$

$$R_{-\frac{1}{2}}(G_1)=\left[3n^2+4\sqrt{2}n+\sqrt{2}+\frac{1}{2}\right].$$

Theorem 3.1.2: *Suppose* G_1 *be the Rhombus Oxide Network* $RHOX(n)$, *then general sum connectivity index is equal to,*

$$X_n(G_1)=\begin{cases}16\left(6n^2+6n+1\right), n=1;\\ \frac{1}{12}\left(18n^2+32n+11\right), n=-1.\end{cases}$$

Proof:

For rhombus oxide graph, the general sum connectivity index is

$$X_n\left(G_1\right)=\sum_{\alpha\beta\in E(G_1)}\left(d_\alpha+d_\beta\right)^n.$$

This gives that

$$X_n(G_1)=|E_1|\left(d_{\alpha_1}+d_{\beta_1}\right)^n+|E_2|\left(d_{\alpha_2}+d_{\beta_2}\right)^n+|E_3|\left(d_{\alpha_3}+d_{\beta_3}\right)^n.$$

For $n=1$,

$$X_1\left(G_1\right)=\sum_{\alpha\beta\in E(G_1)}\left(d_\alpha+d_\beta\right)^1.$$

$$X_1(G_1)=\left[(2)(2+2)^1+(16n+4)(2+4)^1+\left(12n^2-2\right)(4+4)^1\right],$$

$$X_1(G_1)=\left[(2)(4)+(16n+4)(6)+\left(12n^2-2\right)(8)\right],$$

$$X_1(G_1)=\left[8+(96n+24)+\left(96n^2-16\right)\right],$$

$$X_1(G_1)=96n^2+96n+16$$

$$X_1\left(G\right)=16\left(6n^2+6n+1\right).$$

For $n=-1$,

$$X_{-1}\left(G_1\right)=\sum_{\alpha\beta\in E(G_1)}\left(d_\alpha+d_\beta\right)^{-1}.$$

After calculations the final result is obtained.

$$X_{-1}(G_1)=\left[(2)(2+2)^{-1}+(16n+4)(2+4)^{-1}+\left(12n^2-2\right)(4+4)^{-1}\right],$$

$$X_{-1}(G_1)=\left[(2)(4)^{-1}+(16n+4)(6)^{-1}+\left(12n^2-2\right)(8)^{-1}\right],$$

$$X_{-1}(G_1)=\left[(2)\left(\frac{1}{4}\right)+(16n+4)\left(\frac{1}{6}\right)+\left(12n^2-2\right)\left(\frac{1}{8}\right)\right],$$

$$X_{-1}(G_1)=\left[\left(\frac{1}{2}\right)+4(4n+1)\left(\frac{1}{6}\right)+2\left(6n^2-1\right)\left(\frac{1}{8}\right)\right],$$

$$X_{-1}(G_1)=\frac{1}{12}\left[\left(\frac{1}{2}\times 12\right)+2(4n+1)\left(\frac{1}{3}\times 12\right)+\left(6n^2-1\right)\left(\frac{1}{4}\times 12\right)\right],$$

$$X_{-1}(G_1)=\frac{1}{12}\left[(6)+2(4n+1)(4)+\left(6n^2-1\right)(3)\right],$$

$$X_{-1}(G_1)=\frac{1}{12}\left[(6)+(32n+8)+\left(18n^2-3\right)\right],$$

$$X_{-1}(G_1)=\frac{1}{12}\left(18n^2+32n+11\right).$$

Theorem 3.1 3: *Let* G_1 *be the Rhombus Oxide Network* $RHOX(n)$*, then ABC index is equal to,*

$$ABC(G_1)=\frac{6\sqrt{3}n^2+16n-\sqrt{3}+6}{\sqrt{2}}.$$

Proof:

By utilizing the edge partition of the graph, the ABC index is written as

$$ABC\left(G_1\right)=\sum_{\alpha\beta\in E(G_1)}\sqrt{\frac{d_\alpha+d_\beta-2}{d_\alpha\times d_\beta}}.$$

This implies that

$$ABC(G_1)=|E_1|\sqrt{\frac{d_{\alpha_1}+d_{\beta_1}-2}{d_{\alpha_1}\times d_{\beta_1}}}+|E_2|\sqrt{\frac{d_{\alpha_2}+d_{\beta_2}-2}{d_{\alpha_2}\times d_{\beta_2}}}+|E_3|\sqrt{\frac{d_{\alpha_3}+d_{\beta_3}-2}{d_{\alpha_3}\times d_{\beta_3}}}.$$

Now,

$$ABC(G_1)=(2)\sqrt{\frac{2+2-2}{2\times 2}}+(16n+4)\sqrt{\frac{2+4-2}{2\times 4}}+\left(12n^2-2\right)\sqrt{\frac{4+4-2}{4\times 4}}.$$

After several iterations, the desired result is attained.

$$ABC(G_1)=(2)\sqrt{\frac{2}{4}}+(16n+4)\sqrt{\frac{4}{8}}+\left(12n^2-2\right)\sqrt{\frac{6}{16}},$$

$$ABC(G_1)=(2)\sqrt{\frac{1}{2}}+(16n+4)\sqrt{\frac{1}{2}}+(12n^2-2)\sqrt{\frac{3}{8}},$$

$$ABC(G_1)=\sqrt{2}+\frac{(16n+4)}{\sqrt{2}}+\left(\frac{12n^2-2}{2\sqrt{2}}\times\sqrt{3}\right),$$

$$ABC(G_1)=\sqrt{2}+\frac{(16n+4)}{\sqrt{2}}+\left(\frac{2(6n^2-1)}{2\sqrt{2}}\times\sqrt{3}\right),$$

$$ABC(G_1)=\sqrt{2}+\frac{(16n+4)}{\sqrt{2}}+\left(\frac{6\sqrt{3}n^2-\sqrt{3}}{\sqrt{2}}\right),$$

$$ABC(G_1)=\frac{2+16n+4+6\sqrt{3}n^2-\sqrt{3}}{\sqrt{2}},$$

$$ABC(G_1)=\frac{6\sqrt{3}n^2+16n-\sqrt{3}+6}{\sqrt{2}}.$$

Theorem 3.1.4: *If G_1 be the Rhombus Oxide Network $RHOX(n)$, then GA index is equal to,*

$$GA(G_1)=12n^2+\frac{8}{3}\sqrt{2}(4n+1).$$

Proof:

The geometric arithmetic index is

$$GA(G_1)=\sum_{\alpha\beta\in E(G_1)}\frac{2\sqrt{d_\alpha\times d_\beta}}{d_\alpha+d_\beta}.$$

Geometric arithmetic index for the Rhombus Oxide Network can be expressed as,

$$GA(G_1)=(2)\left(\frac{2\sqrt{2\times 2}}{2+2}\right)+(16n+4)\left(\frac{2\sqrt{2\times 4}}{2+4}\right)+(12n^2-2)\left(\frac{2\sqrt{4\times 4}}{4+4}\right),$$

$$GA(G_1)=(2)\left(\frac{2\sqrt{4}}{4}\right)+(16n+4)\left(\frac{2\sqrt{8}}{6}\right)+(12n^2-2)\left(\frac{2\sqrt{16}}{8}\right),$$

$$GA(G_1)=(2)\left(\frac{2\times 2}{4}\right)+(16n+4)\left(\frac{2\sqrt{2}}{3}\right)+(12n^2-2)\left(\frac{2\times 4}{8}\right),$$

$$GA(G_1) = (2)(1) + (16n+4)\left(\frac{2\sqrt{2}}{3}\right) + (12n^2-2)(1),$$

$$GA(G_1) = (2) + (16n+4)\left(\frac{2\sqrt{2}}{3}\right) + (12n^2-2),$$

$$GA(G_1) = 12n^2 + \frac{32\sqrt{2}}{3}n + \frac{8\sqrt{2}}{3},$$

$$GA(G_1) = 12n^2 + \frac{8}{3}\sqrt{2}(4n+1).$$

Theorem 3.1.5: *For Rhombus Oxide Network* $RHOX(n)$*, the forgotten index will be equal to,*

$$F(G_1) = 32(12n^2+10n+1).$$

Proof:

Let G_1 be the Rhombus Oxide Network. Then, forgotten index is written as

$$F(G_1) = \sum_{\alpha\beta \in E(G_1)} (d^2{}_\alpha + d^2{}_\beta).$$

This suggests that

$$F(G_1) = |E_1|\left(d^2{}_{\alpha_1} + d^2{}_{\beta_1}\right) + |E_2|\left(d^2{}_{\alpha_2} + d^2{}_{\beta_2}\right) + |E_3|\left(d^2{}_{\alpha_3} + d^2{}_{\beta_3}\right),$$

$$F(G_1) = \left[(2)\left((2)^2+(2)^2\right) + (16n+4)\left((2)^2+(4)^2\right) + (12n^2-2)\left((4)^2+(4)^2\right)\right],$$

$$F(G_1) = \left[(2)(4+4) + (16n+4)(4+16) + (12n^2-2)(16+16)\right],$$

$$F(G_1) = \left[(2)(8) + (16n+4)(20) + (12n^2-2)(32)\right],$$

$$F(G_1) = \left[16 + 320n + 80 + 384n^2 - 64\right],$$

$$F(G_1) = 32(12n^2+10n+1).$$

Theorem 3.1.6: *If* G_1 *be the Rhombus Oxide Network* $RHOX(n)$*, then symmetric division index is equal to,*

$$SD(G_1) = 24n^2 + 40n + 10.$$

Proof:

The symmetric division index is

$$SD(G_1) = \sum_{\alpha\beta \in E(G_1)} \frac{d^2{}_\alpha + d^2{}_\beta}{d_\alpha \times d_\beta}.$$

Symmetric division index for the Rhombus Oxide Network can be summarized as,

$$SD(G_1) = (2)\left(\frac{2^2+2^2}{2\times 2}\right) + (16n+4)\left(\frac{2^2+4^2}{2\times 4}\right) + (12n^2-2)\left(\frac{4^2+4^2}{4\times 4}\right),$$

$$SD(G_1) = (2)\left(\frac{4+4}{4}\right) + (16n+4)\left(\frac{4+16}{8}\right) + (12n^2-2)\left(\frac{16+16}{16}\right),$$

$$SD(G_1) = (2)\left(\frac{8}{4}\right) + (16n+4)\left(\frac{20}{8}\right) + (12n^2-2)\left(\frac{32}{16}\right),$$

$$SD(G_1) = 4 + (16n+4)\left(\frac{5}{2}\right) + (12n^2-2)(2),$$

$$SD(G_1) = 4 + \frac{80n+20}{2} + 24n^2 - 4,$$

$$SD(G_1) = 4 + 40n + 10 + 24n^2 - 4,$$

$$SD(G_1) = 24n^2 + 40n + 10.$$

Theorem 3.1.7: *Consider* G_1 *be the Rhombus Oxide Network* $RHOX(n)$, *so harmonic index is equal to,*

$$H(G_1) = 3n^2 + \frac{16n}{3} + \frac{11}{6}.$$

Proof:

The harmonic index is

$$H(G_1) = \sum_{\alpha\beta \in E(G_1)} \frac{2}{d_\alpha + d_\beta}.$$

For rhombus oxide graph, the harmonic index result is attained after several iterations.

$$H(G_1) = (2)\left(\frac{2}{2+2}\right) + (16n+4)\left(\frac{2}{2+4}\right) + (12n^2-2)\left(\frac{2}{4+4}\right),$$

$$H(G_1) = (2)\left(\frac{2}{4}\right) + (16n+4)\left(\frac{2}{6}\right) + (12n^2-2)\left(\frac{2}{8}\right),$$

$$H(G_1) = (2)\left(\frac{1}{2}\right) + (16n+4)\left(\frac{1}{3}\right) + (12n^2-2)\left(\frac{1}{4}\right),$$

$$H(G_1) = 1 + \left(\frac{16n+4}{3}\right) + \left(\frac{12n^2-2}{4}\right),$$

$$H(G_1) = 1 + \frac{16n}{3} + \frac{4}{3} + 3n^2 - \frac{1}{2},$$

$$H(G_1) = 3n^2 + \frac{16n}{3} + \frac{11}{6}.$$

3.3 Numerical Analysis

In this section, the comparison of all above topological indices for rhombus oxide network through tables are discussed.

n	$R_{-\frac{1}{2}}(G_1)$	$RR_{\frac{1}{2}}(G_1)$	$X_1(G_1)$	$X_{-1}(G_1)$	$ABC(G_1)$	$GA(G_1)$	$F(G_1)$	$SD(G_1)$	$H(G_1)$
1	10.57	100.56	208	5.08	21.68	30.85	736	74	10.16
2	25.22	289.82	592	12.25	55.03	81.94	2208	186	24.5
3	45.88	575.07	1168	22.41	103.09	157.02	4448	346	44.83
4	72.54	956.33	1936	35.58	165.84	256.11	7456	554	71.16
5	105.19	1433.59	2896	51.76	243.29	379.19	11232	810	103.5
6	143.85	2006.84	4048	70.91	335.44	526.28	15776	1114	141.83
7	188.51	2676.1	5392	93.08	442.28	697.36	21088	1466	186.16
8	239.16	3441.35	6928	118.25	563.83	892.45	27168	1866	236.5
9	295.82	4302.61	8656	146.41	700.06	1111.54	34016	2314	292.83
10	358.48	5259.86	10576	177.58	851.00	1354.62	41632	2810	355.16

Table 2: Numerical Analysis for rhombus oxide network

3.4 Discussion

The arrangement and connectivity of the atoms in a molecule are described by a topological index, which can also be used to offer information on the characteristics and effects of the chemical substance involved. A molecular graph is a graph-theoretical depiction of the structural formula of a chemical compound, where the vertices are the atoms of the complex and the edges are its chemical bonds. Chemoinformatics is a relatively new discipline that combines chemistry, information science, and mathematics. It examines the relationships between QSAR and QSPR, which are used to forecast physiologically active molecules and chemical compound properties.

Graphs are universal structures that are used to model various relations and processes in different fields of sciences, such as physics, chemistry, biology, and economics. In computer science, graphs are also essential in networking and database applications. In geometry, the structure of points and lines has significant importance, where each point has a geometrical significance, and the slope of each line is particular. To analyze situations modeled by graphs, one must have a better understanding of graph terminologies.

In *CGT* , a number of graph-based indices and descriptors have been created to measure various molecular features. These descriptors comprise topological indices, connection indices, chemical fingerprints, and

the number of vertices. These techniques aid in describing molecular structures and foretelling their chemical, physical, and biological characteristics.

The Wiener, Randi'c, Zagreb, and Balaban indices are examples of biological indicators that are used to predict and investigate the physical and chemical characteristics of chemical compounds.

In mathematical chemistry, the topological index, which can be an integer, polynomial, or other sequence of integers and a matrix that specifies the whole network, is used to describe the molecular structure within each chemical element. A crucial part of graph theory is chemical graph theory. Chemical networks have intrigued researchers since their inception because of their widespread application.

A unique and interesting topic in graph theory is figuring out the equations for topological indices of rhombus graphs. In this study, certain graphs produced by the hexagonal shape are examined, and the precise results for various degree-based topological indices are found. Additionally, a visual comparison of all produced indices is provided. Chemical networks are transformed into a quantity that describes their topology to provide topological indices.

Degree-based topological indices and measuring topological indices are two examples of the numerous topological indices for graphs. The above indices can be used to learn more about the compound's physical-chemical properties, biological functions. The discussion focuses on the results of various indices for two different network types: Rhombus Oxide network.

4 Conclusion

Topological indices, which typically do not depend on graphs, are numerical characteristics that convey a system's topology. To anticipate the biological activities and characteristics of chemical compounds, topological indices offer a mathematical foundation for the development of quantitative structure-activity relationships (QSAR) and quantitative structure-property relationships (QSPR).

The application of topological polynomials in GT and their significance in representing graph invariants. These polynomials are used to describe the topology of chemical structures and execute a part in quantitative structure-property relationships (QSPR). Distance-based TIs are widely used and studied in CGT. In paper, the main focuses on computing the randić index $R(G)$, general randić index $R_g(G)$, reciprocal randić index $RR(G)$, $GA(G)$, $ABC(G)$, $F(G)$, general sum connectivity index $X_g(G)$, symmetric division index $SD(G)$, harmonic index $H(G)$, along with their corresponding polynomials, for rhombus graphs. Additionally, the study includes a comparison of these indices to analyze their relative properties and relationships.

ETHICS APPROVAL AND CONSENT TO PARTICIPATE

Not applicable.

HUMAN AND ANIMAL RIGHTS

No animals/humans were used for studies that are the basis of this research.

CONSENT FOR PUBLICATION

Not applicable.

FUNDING

None.

AVAILABILITY OF DATA AND MATERIALS

Not applicable.

CONFLICT OF INTEREST

None.

ACKNOWLEDGEMENTS

None declared.

References

[1] Hopkins, B. and R.J. Wilson. 2004. The truth about Königsberg. *Coll. Math. J.* 35:198–207.

[2] Zaytsev, E. 2008. Euler's Problem of Konigsberg Bridges and Leibniz'geometria situs. *Int. Arch. Hist. Sci.* 58:151.

[3] Bondy, J.A. and U.S.R. Murty. 1976. *Graph theory with applications*. Macmillan London.

[4] Zhang, P. and G. Chartrand. 2006. *Introduction to graph theory*. Tata McGraw-Hill.

[5] Erdös, P. 1959. Graph theory and probability. *Can. J. Math.* 11:34–38.

[6] Liu, J.-B., X. Zhang, J. Cao and L. Chen. 2024c. Mean first-passage time and robustness of complex cellular mobile communication network. *IEEE Trans. Netw. Sci. Eng*.

[7] Balaban, A.T. 1985. Applications of graph theory in chemistry. *J. Chem. Inf. Comput. Sci.* 25:334–343.

[8] Gutman, I. and N. Trinajstić. 2005. Graph theory and molecular orbitals. *New Concepts II*. Springer. pp.49–93.

[9] A Tudoran, M. and M. V Putz. 2015. Molecular graph theory: From adjacency information to colored topology by chemical reactivity. *Curr. Org. Chem.* 19:359–386.

[10] Liu, J.-B., Y.-Q. Zheng and C.-C. Lee. 2024d. Statistical analysis of the regional air quality index of Yangtze River Delta based on complex network theory. *Appl. Energy* 357:122529.

[11] Graovac, A. and T. Pisanski. 1991. On the Wiener index of a graph. *J. Math. Chem.* 8:53–62.

[12] Stankevich, M.I., I. V Stankevich and N.S. Zefirov. 1988. Topological indices in organic chemistry. *Russ. Chem. Rev.* 57:191.

[13] Balaban, A.T. and O. Ivanciuc. 2000. Historical development of topological indices. *Topological Indices and Related Descriptors in QSAR and QSPAR*. CRC Press. pp.31–68.

[14] Dearden, J.C. 2017. The use of topological indices in QSAR and QSPR modeling. *Adv. QSAR Model. Appl. Pharm. Chem. Food, Agric. Environ. Sci.* 57–88.

[15] Estrada, E. and E. Uriarte. 2001. Recent advances on the role of topological indices in drug discovery research. *Curr. Med. Chem.* 8:1573–1588.

[16] Randic, M. 1975. Characterization of molecular branching. *J. Am. Chem. Soc.* 97:6609–6615.

[17] Delorme, C., O. Favaron and D. Rautenbach. 2002. On the Randić index. *Discrete Math.* 257:29–38.

[18] Li, X. and Y. Shi. 2008. A survey on the Randić index. *Match* 59:127–156.

[19] Bollobás, B. and P. Erdös. 1998. Graphs of extremal weights. *Ars Comb.* 50:225.

[20] Bilal, A., & Munir, M. M. (2023). Randic and reciprocal randic spectral radii and energies of some graph operations. *Journal of Intelligent & Fuzzy Systems*, 44(4), 5719-5729.

[21] Estrada, E., L. Torres, L. Rodriguez and I. Gutman. 1998. An atom-bond connectivity index: modelling the enthalpy of formation of alkanes *Indian J. Chem*. 37A:849-855.

[22] Liu, J.-B., X. Wang and J. Cao. 2024b. The Coherence and Properties Analysis of Balanced

2 p-Ary Tree Networks. *IEEE Trans. Netw. Sci. Eng*.

[23] Vukičević, D. and B. Furtula. 2009. Topological index based on the ratios of geometrical and arithmetical means of end-vertex degrees of edges. *J. Math. Chem.* 46:1369–137.

[24] Yuan, Y., B. Zhou and N. Trinajstić. 2010. On geometric-arithmetic index. *J. Math. Chem.* 47:833–841.

[25] Furtula, B. and I. Gutman. 2015. A forgotten topological index. *J. Math. Chem.* 53:1184–1190.

[26] Gupta, C.K., V. Lokesha, S.B. Shwetha and P.S. Ranjini. 2016. On the Symmetric Division deg Index of Graph. *Southeast asian Bull. Math.* 40.

[27] Zhong, L. 2012. The harmonic index for graphs. *Appl. Math. Lett.* 25:561–566.

[28] Zhou, B. and N. Trinajstić. 2010. On general sum-connectivity index. *J. Math. Chem*. 47:210–218.

[28] Mahboob, A., M.W. Rasheed, J.H.H. Bayati, I. Hanif and S.M. Alam. 2024. Bi-distance approach to determine the topological invariants of silicon carbide. *Baghdad Sci. J*. 21:174.