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Determining Topological Indices of Sheet Oxide Network Using Bi-Distance Technique

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Abstract
Topological indices are numerical invariants that capture the structural properties of graphs, playing a crucial role in quantitative structure-activity relationships (QSARs) by linking molecular structures to their biological activities. This research investigates Bi-distance degree-based topological descriptors, such as the Bi-distance atom bond connectivity index, Randić index, geometric arithmetic index, hyper Zagreb index, forgotten index, first and second Zagreb indices, Zagreb augmented index, and redefined Zagreb indices, applied to sheet oxide network. By partitioning edge sets based on degree and cardinality, these indices are computed using combinatorial methods. The findings reveal that the Zagreb indices, atom bond connectivity index, and forgotten index can be effectively determined using the Bi-distance approach, offering a novel perspective for analyzing molecular structures. This research aims to provide insights into the biological activities and physical properties of oxide molecule, with potential applications in pharmaceutical and biological networks. The study highlights the significance of topological indices in graph theory for examining the structural characteristics of chemical compounds, contributing to a deeper understanding of their properties and behaviors.

Keywords: bi-distance edges; molecular structure; topological index; Randić index; Zagreb index; forgotten index; sheet oxide; structure analysis

Introduction

Leonhard Euler [1], a prominent Swiss scientist, is credited with founding graph theory through his solution to the "Königsberg Bridge Problem" [2] in 1735. This

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problem involved seven bridges over a river, making it impossible to cross each bridge only once. Euler modeled the land masses as vertices and the bridges as edges, analyzing the graph's properties to solve the problem, which became the first theorem in graph theory [3]. Although the first formal text on graph theory was published much later in 1936, the field has since become a vital area of mathematics, applied across diverse disciplines such as computer science, chemistry, and logistics. Graphs, represented as points (vertices) connected by lines (edges), are widely used to model real-world scenarios, such as social networks or communication systems [4].

A graph is defined by two sets: vertices and edges, where each edge connects one or two vertices. The distance between vertices in a simple, connected graph is denoted by d, and the degree of a vertex v is represented by deg(v). This article focuses on simple, connected, and planar graphs [5].

Graph theory has extensive applications, including nano-chemistry, computer networks, navigation systems like Google Maps, and molecular structure analysis. In mathematical chemistry, chemical graph theory uses graphs to represent chemical compounds, combining chemistry and graph theory to study the physical and chemical properties of substances [7]. Biological networks also utilize graph theory to identify therapeutic targets by analyzing protein or gene interactions [8]. Additionally, graph theory aids in studying RNA and DNA structures and is a growing tool in operational research, logistics, and economics [9].

Chemical graph theory [10] examines graphs as mathematical tools to represent relationships between elements, with vertices (nodes) and edges (connections). These graphs can be directed or undirected, forming a key part of discrete mathematics. Topological indices (TIs) [11] are numerical values derived from graph structures, used to correlate chemical properties with molecular graphs. These indices are crucial in fields like chemical engineering and pharmaceutical research, as they predict physicochemical properties without extensive experimentation. TIs are categorized into degree-based, eccentricity-based, distance-based, and ev-degree-based indices [13].

Molecular graphs represent chemical compounds, with vertices as atoms and edges as bonds. Topological indices provide numerical descriptors for chemical, biological, and physical properties, aiding in Quantitative Structure-Property Relationships (QSPR) and Quantitative Structure-Activity Relationships (QSAR) [14,15]. Traditional degree-based TIs focus on single distances, but newer methodologies, such as distance-based and eccentricity-based indices, have expanded their applications. This article introduces a novel "Bi-distance" strategy [16], combining two edges to form a bi-distance edge, enhancing the utility of TIs like the Wiener index.

Materials and Methods

Randić Index

The Randić index [17,18], initially introduced by Milan Randić, is a degree-based index used to measure the branching characteristics of a graph. It was once known as the molecular connectivity index, but it is now commonly known as the Randić index. By using the Randić index, this index is utilized to assess how much a molecule's carbon atom skeleton has been stretched.

The universal Randić index, and the Bi-distance Randić index are represented as,

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$$R_{\alpha}(G)=\sum_{\omega\mu\in E(G)}\left(d(\omega)\times d(\mu)\right)^{\alpha},\ \alpha=1,-1,\frac{1}{2},-\frac{1}{2}.$$

$$\mathrm{B}\,R_{\alpha}(G)=\sum_{\omega\mu\in E(G)}\left(\mathrm{B}\,(\omega)\times \mathrm{B}\,(\mu)\right)^{\alpha},\ \alpha=1,-1,\frac{1}{2},-\frac{1}{2}.$$

Atom Bond Connectivity Index

Atom bond connectivity index [19] is presented by Estrada *et al.* and it's Bi-distance Atom Bond Connectivity index are stated as,

$$ABC(G)=\sum_{\omega\mu\in E(G)}\sqrt{\frac{d(\omega)+d(\mu)-2}{d(\omega)\times d(\mu)}}.$$

$$\mathrm{B}\,ABC(G)=\sum_{\omega\mu\in E(G)}\sqrt{\frac{\mathrm{B}\,(\omega)+\mathrm{B}\,(\mu)-2}{\mathrm{B}\,(\omega)\times \mathrm{B}\,(\mu)}}.$$

Geometric Arithmetic Index

Geometric arithmetic index [20] was computed by Furtula and Vukicevic and the Bi-distance Geometric arithmetic index are represented as:

$$GA(G)=\sum_{\omega\mu\in E(G)}\frac{2\sqrt{d(\omega)\times d(\mu)}}{d(\omega)+d(\mu)}.$$

$$\mathrm{B}\,GA(G)=\sum_{\omega\mu\in E(G)}\frac{2\sqrt{\mathrm{B}\,(\omega)\times \mathrm{B}\,(\mu)}}{\mathrm{B}\,(\omega)+\mathrm{B}\,(\mu)}.$$

Due to its comprehensive nature and improved predictive capabilities, the *GA* index has become a valuable tool in the field of cheminformatics. It allows researchers to assess the bioactivity of chemical compounds and make informed predictions based on their structural characteristics.

Second and First Zagreb Index

Second and First Zagreb index [21] was computed by Gutman *et al.* and the Bi-distance second and first Zagreb index is stated as:

$$M_1(G)=\sum_{\omega\mu\in E(G)}\left(d(\omega)+d(\mu)\right).$$

$$M_2(G)=\sum_{\omega\mu\in E(G)}\left(d(\omega)\times d(\mu)\right).$$

$$\mathrm{B}\,M_1(G)=\sum_{\omega\mu\in E(G)}\left(\mathrm{B}\,(\omega)+\mathrm{B}\,(\mu)\right).$$

$$\mathrm{B}\,M_2(G)=\sum_{\omega\mu\in E(G)}\left(\mathrm{B}\,(\omega)\times \mathrm{B}\,(\mu)\right).$$

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Both the indices one and two for Zagreb are part of a family of TI that describe chemical structures and have supplication in various areas of chemistry, bioinformatics, and graph theory [22].

Hyper Zagreb Index

Hyper Zagreb index [23] was computed by Shirdel *et al.* and the Bi-distance Hyper Zagreb index are defined as:

$$HM(G) = \sum_{\omega\mu \in E(\mathbf{G})} \left(d(\omega) + d(\mu)\right)^2.$$

$$\mathrm{B}\,HM(G) = \sum_{\omega\mu \in E(\mathbf{G})} \left(\mathrm{B}(\omega) + \mathrm{B}(\mu)\right)^2.$$

The Zagreb indices are expanded upon by the hyper Zagreb index one that considers the contributions of higher-order neighbors of vertices in a graph. It provides additional information about the connectivity and distances between vertices.

Forgotten Index

Forgotten index [24] were presented by Gutman and Furtula and its Bi-distance forgotten index are defined as,

$$F(G) = \sum_{\omega\mu \in E(\mathbf{G})} \left(\left(d(\omega)\right)^2 + \left(d(\mu)\right)^2\right).$$

$$\mathrm{B}\,F(G) = \sum_{\omega\mu \in E(\mathbf{G})} \left(\left(\mathrm{B}(\omega)\right)^2 + \left(\mathrm{B}(\mu)\right)^2\right).$$

Augmented Zagreb Index

Augmented Zagreb index [25] were introduced by Furtula *et al.* and the Bi-distance (AZ) index are stated as,

$$AZ(G) = \sum_{\omega\mu \in E(\mathbf{G})} \left(\frac{d(\omega) \times d(\mu)}{d(\omega) + d(\mu) - 2}\right)^3.$$

$$\mathrm{B}\,AZI(G) = \sum_{\omega\mu \in E(\mathbf{G})} \left(\frac{\mathrm{B}(\omega) \times \mathrm{B}(\mu)}{\mathrm{B}(\omega) + \mathrm{B}(\mu) - 2}\right)^3$$

The augmented Zagreb index is a graph invariant that extends the concept of the Zagreb indices by incorporating the weights of vertices or edges into the calculation.

First, Second and Third Redefined Zagreb Index

Redefined Zagreb indices of First, Second, third type were presented by Ranjini *et al.* and its Bi-distance indices is defined as,

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$$RZ_1(G) = \sum_{\omega\mu\in E(\mathbf{G})} \left(\frac{d(\omega)+d(\mu)}{d(\omega)\times d(\mu)} \right).$$

$$RZ_2(G) = \sum_{\omega\mu\in E(\mathbf{G})} \left(\frac{d(\omega)\times d(\mu)}{d(\omega)+d(\mu)} \right).$$

$$RZ_3(G) = \sum_{\omega\mu\in E(\mathbf{G})} \left(\left(d(\omega)+d(\mu) \right) \left(d(\omega)\times d(\mu) \right) \right).$$

$$\mathrm{B}\,RZ_1(G) = \sum_{\omega\mu\in E(\mathbf{G})} \left(\frac{\mathrm{B}(\omega)+\mathrm{B}(\mu)}{\mathrm{B}(\omega)\times \mathrm{B}(\mu)} \right).$$

$$\mathrm{B}\,RZ_2(G) = \sum_{\omega\mu\in E(\mathbf{G})} \left(\frac{\mathrm{B}(\omega)\times \mathrm{B}(\mu)}{\mathrm{B}(\omega)+\mathrm{B}(\mu)} \right).$$

$$\mathrm{B}\,RZ_3(G) = \sum_{\omega\mu\in E(\mathbf{G})} \left(\left(\mathrm{B}(\omega)+\mathrm{B}(\mu) \right) \left(\mathrm{B}(\omega)\times \mathrm{B}(\mu) \right) \right).$$

Bi-distance Edge Partitions

This study employs edge partitioning to divide bi-distance edges of Sheet Oxide and Sheet Silicate into three packets (Tables 1-2). Various methods, including vertex degree, edge partitioning, and graph analytical approaches, are used to analyze the networks. Computational tools, such as MATLAB and Mathematica, facilitate calculations and visualization of results. ChemDraw is utilized for drawing chemical structures. Degree-based topological descriptors [29] are applied to Chain Oxide Molecular Networks in the subsequent section.

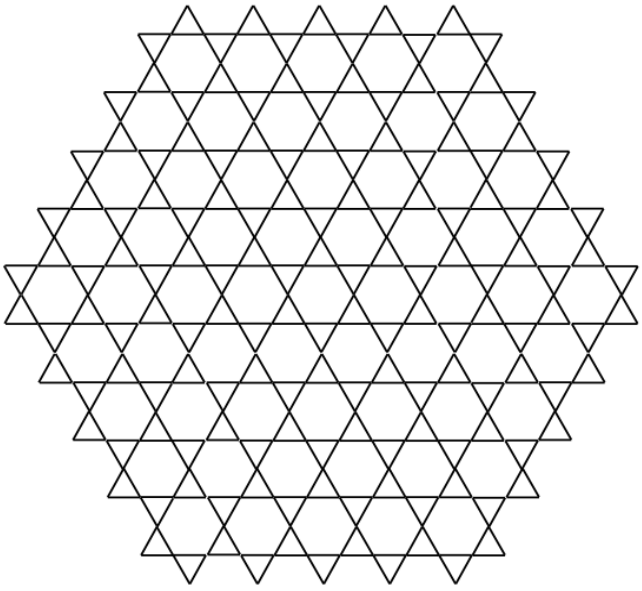

Figure 1: Sheet Oxide Network (OX_5)

Results and Discussion

In this section, the results of the several Bi-distance topological indices of Sheet oxide (OX_n) and Sheet silicate (SL_n) networks have been discussed.

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Results for Sheet Oxide Network (OX_n)

The sum of all edges is $24n^2$, where $n \geq 1$ is also applicable. These indices were computed using the edge partition method, which groups the edges according to the sum of the degrees at which the connected vertices are connected.

Theorem 1: *Consider* G_1 *be the Sheet Oxide network, then its Bi-distance Randić Index is,*

$$\mathrm{B}R_{\alpha}(G_1) = \begin{cases} 24(1-4n)^2, \alpha = 1; \\ \frac{3}{8}(2n+1)^2, \alpha = -1; \\ 12\left(8n^2 + 4\left(\sqrt{2}-2\right)n - 2\sqrt{2} + 3\right), \alpha = \frac{1}{2}; \\ 6n^2 + 6\left(\sqrt{2}-1\right)n - 3\sqrt{2} + \frac{9}{2}, \alpha = -\frac{1}{2}. \end{cases}$$

Proof:

Consider G_1 to be the Sheet Oxide (OX_n) network's Molecular graph.

Table 1: Bi-distance Edge Partitions for Sheet Oxide (OX_n) Network

(d_{ω}, d_{μ}), **where** $\omega\mu \in E(G)$	$E_1 = [2,2]$	$E_2 = [2,4]$	$E_3 = [4,4]$
Number of Edges	6	$(24n-12)$	$\left(24n^2 - 24n + 6\right)$

Bi-distance Randić Index is,

$$\mathrm{B}R_{\alpha}(G) = \sum_{\omega\mu \in E(\mathbf{G})} \left(\mathrm{B}(\omega) \times \mathrm{B}(\mu)\right)^{\alpha}, \alpha = 1, -1, \frac{1}{2}, -\frac{1}{2}.$$

Bi-distance Randić Index of the Chain Oxide network can be calculated as,

$$\mathrm{B}R_{\alpha}(G_1) = \left(\mathrm{B}(\omega_1) \times \mathrm{B}(\mu_1)\right)^{\alpha} + \left(\mathrm{B}(\omega_2) \times \mathrm{B}(\mu_2)\right)^{\alpha} + \left(\mathrm{B}(\omega_3) \times \mathrm{B}(\mu_3)\right)^{\alpha},$$

For $\alpha = 1$,

$$\mathrm{B}R_1(G_1) = \left(\mathrm{B}(\omega_1) \times \mathrm{B}(\mu_1)\right)^1 + \left(\mathrm{B}(\omega_2) \times \mathrm{B}(\mu_2)\right)^1 + \left(\mathrm{B}(\omega_3) \times \mathrm{B}(\mu_3)\right)^1,$$

$$\mathrm{B}R_1(G_1) = (6)(2\times 2)^1 + (24n-12)(2\times 4)^1 + \left(24n^2 - 24n + 6\right)(4\times 4)^1$$

$$= (6)(4) + (24n-12)(8) + \left(24n^2 - 24n + 6\right)(16)$$

$$= 24(1-4n)^2.$$

For $\alpha = -1$,

$$\mathrm{B}R_{-1}(G_1) = \left(\mathrm{B}(\omega_1) \times \mathrm{B}(\mu_1)\right)^{-1} + \left(\mathrm{B}(\omega_2) \times \mathrm{B}(\mu_2)\right)^{-1} + \left(\mathrm{B}(\omega_3) \times \mathrm{B}(\mu_3)\right)^{-1},$$

$$\mathrm{B}R_{-1}(G_1) = (6)(2\times 2)^{-1} + (24n-12)(2\times 4)^{-1} + \left(24n^2 - 24n + 6\right)(4\times 4)^{-1}$$

$$= (6)\left(\frac{1}{4}\right) + (24n-12)\left(\frac{1}{8}\right) + \left(24n^2 - 24n + 6\right)\left(\frac{1}{16}\right)$$

$$= \frac{3}{8}(2n+1)^2.$$

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For $\alpha = \frac{1}{2}$,

$$\mathrm{B}\,R_{\frac{1}{2}}(G_1) = \left(\mathrm{B}(\omega_1)\times\mathrm{B}(\mu_1)\right)^{\frac{1}{2}} + \left(\mathrm{B}(\omega_2)\times\mathrm{B}(\mu_2)\right)^{\frac{1}{2}} + \left(\mathrm{B}(\omega_3)\times\mathrm{B}(\mu_3)\right)^{\frac{1}{2}},$$

$$\mathrm{B}\,R_{\frac{1}{2}}(G_1) = (6)(2\times 2)^{\frac{1}{2}} + (24n-12)(2\times 4)^{\frac{1}{2}} + \left(24n^2-24n+6\right)(4\times 4)^{\frac{1}{2}}$$

$$= (6)(2) + (24n-12)\left(2\sqrt{2}\right) + \left(24n^2-24n+6\right)(4)$$

$$= 12\left(8n^2 + 4\left(\sqrt{2}-2\right)n - 2\sqrt{2} + 3\right)$$

For $\alpha = -\frac{1}{2}$,

$$\mathrm{B}\,R_{-\frac{1}{2}}(G_1) = \left(\mathrm{B}(\omega_1)\times\mathrm{B}(\mu_1)\right)^{-\frac{1}{2}} + \left(\mathrm{B}(\omega_2)\times\mathrm{B}(\mu_2)\right)^{-\frac{1}{2}} + \left(\mathrm{B}(\omega_3)\times\mathrm{B}(\mu_3)\right)^{-\frac{1}{2}},$$

$$\mathrm{B}\,R_{-\frac{1}{2}}(G_1) = (6)(2\times 2)^{-\frac{1}{2}} + (24n-12)(2\times 4)^{-\frac{1}{2}} + \left(24n^2-24n+6\right)(4\times 4)^{-\frac{1}{2}}$$

$$= (6)\left(\frac{1}{2}\right) + (24n-12)\left(\frac{1}{2\sqrt{2}}\right) + \left(24n^2-24n+6\right)\left(\frac{1}{4}\right)$$

$$= 6n^2 + 6\left(\sqrt{2}-1\right)n - 3\sqrt{2} + \frac{9}{2}.$$

Theorem 2: *If G_1 be the Sheet Oxide network, then its Bi-distance atom bond (ABC)index is,*

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

Proof:

Consider G_1 to be the Sheet Oxide (OX_n) network's Molecular graph. Bi-distance (ABC) Index is,

$$\mathrm{B}\,ABC(G) = \sum_{\omega\mu\in\mathrm{E}(\mathbf{G})}\sqrt{\frac{\mathrm{B}(\omega)+\mathrm{B}(\mu)-2}{\mathrm{B}(\omega)\times\mathrm{B}(\mu)}}.$$

Bi-distance Atom Bond Connectivity Index of the Chain Oxide Network can be calculated as,

$$\mathrm{B}\,ABC(G_1) = \sqrt{\frac{\mathrm{B}(\omega_1)+\mathrm{B}(\mu_1)-2}{\mathrm{B}(\omega_1)\times\mathrm{B}(\mu_1)}} + \sqrt{\frac{\mathrm{B}(\omega_2)+\mathrm{B}(\mu_2)-2}{\mathrm{B}(\omega_2)\times\mathrm{B}(\mu_2)}} + \sqrt{\frac{\mathrm{B}(\omega_3)+\mathrm{B}(\mu_3)-2}{\mathrm{B}(\omega_3)\times\mathrm{B}(\mu_3)}},$$

$$\mathrm{B}\,ABC(G_1) = (6)\left(\sqrt{\frac{2+2-2}{2\times 2}}\right) + (24n-12)\left(\sqrt{\frac{2+4-2}{2\times 4}}\right) + \left(24n^2-24n+6\right)\left(\sqrt{\frac{4+4-2}{4\times 4}}\right),$$

$$= (6)\left(\frac{1}{\sqrt{2}}\right) + (24n-12)\left(\frac{1}{\sqrt{2}}\right) + \left(24n^2-24n+6\right)\left(\frac{\sqrt{3}}{2\sqrt{2}}\right),$$

$$= \frac{3\left(4\sqrt{3}n^2 - 4\left(\sqrt{3}-2\right)n + \sqrt{3}-2\right)}{\sqrt{2}}.$$

Theorem 3: *The Bi-distance Geometric Arithmetic Index for Sheet Oxide*

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network, if G_1 be the graph is,

$$\mathrm{B}\,GA(G_1) = 4\left(6n^2 + \left(4\sqrt{2}-6\right)n - 2\sqrt{2} + 3\right).$$

Proof:

Consider G_1 to be the Sheet Oxide (OX_n) network's Molecular graph. Bi-distance Geometric Arithmetic Index is,

$$\mathrm{B}\,GA(G) = \sum_{\omega\mu\in E(\mathbf{G})} \frac{2\sqrt{\mathrm{B}(\omega)\times\mathrm{B}(\mu)}}{\mathrm{B}(\omega)+\mathrm{B}(\mu)}.$$

Bi-distance Geometric Arithmetic Index of the Chain Oxide Network can be calculated as,

$$\mathrm{B}\,GA(G_1) = \frac{2\sqrt{\mathrm{B}(\omega_1)\times\mathrm{B}(\mu_1)}}{\mathrm{B}(\omega_1)+\mathrm{B}(\mu_1)} + \frac{2\sqrt{\mathrm{B}(\omega_2)\times\mathrm{B}(\mu_2)}}{\mathrm{B}(\omega_2)+\mathrm{B}(\mu_2)} + \frac{2\sqrt{\mathrm{B}(\omega_3)\times\mathrm{B}(\mu_3)}}{\mathrm{B}(\omega_3)+\mathrm{B}(\mu_3)},$$

$$\mathrm{B}\,GA(G_1) = (6)\left(\frac{2\sqrt{2\times 2}}{2+2}\right) + (24n-12)\left(\frac{2\sqrt{2\times 4}}{2+4}\right) + \left(24n^2-24n+6\right)\left(\frac{2\sqrt{4\times 4}}{4+4}\right),$$

$$= (6)(1) + (24n-12)\left(\frac{2\sqrt{2}}{3}\right) + \left(24n^2-24n+6\right)(1),$$

$$= 4\left(6n^2 + \left(4\sqrt{2}-6\right)n - 2\sqrt{2} + 3\right).$$

Theorem 4: *If G_1 be the Sheet Oxide network, then its Bi-distance first and second Zagreb indices are,*

$$\mathrm{B}\,M_1(G_1) = 48n(4n-1).$$

$$\mathrm{B}\,M_2(G_1) = 24(1-4n)^2.$$

Proof:

Consider G_1 to be the Sheet Oxide (OX_n) network's Molecular graph. Bi-distance first Zagreb Index is,

$$\mathrm{B}\,M_1(G) = \sum_{\omega\mu\in E(\mathbf{G})} \left(\mathrm{B}(\omega)+\mathrm{B}(\mu)\right).$$

Bi-distance First Zagreb Index of the Sheet Oxide Network can be calculated as,

$$\mathrm{B}\,M_1(G_1) = \left(\mathrm{B}(\omega_1)+\mathrm{B}(\mu_1)\right) + \left(\mathrm{B}(\omega_2)+\mathrm{B}(\mu_2)\right) + \left(\mathrm{B}(\omega_3)+\mathrm{B}(\mu_3)\right),$$

$$\mathrm{B}\,M_1(G_1) = (6)(2+2) + (24n-12)(2+4) + \left(24n^2-24n+6\right)(4+4),$$

$$= (6)(4) + (24n-12)(6) + \left(24n^2-24n+6\right)(8),$$

$$= 48n(4n-1).$$

Bi-distance second Zagreb Index is

$$\mathrm{B}\,M_2(G) = \sum_{\omega\mu\in E(\mathbf{G})} \left(\mathrm{B}(\omega)\times\mathrm{B}(\mu)\right).$$

Bi-distance second Zagreb Index of the Sheet Oxide Network can be calculated as,

$$\mathrm{B}\,M_2(G_1) = \left(\mathrm{B}(\omega_1)\times\mathrm{B}(\mu_1)\right) + \left(\mathrm{B}(\omega_2)\times\mathrm{B}(\mu_2)\right) + \left(\mathrm{B}(\omega_3)\times\mathrm{B}(\mu_3)\right),$$

$$\mathrm{B}\,M_2(G_1) = (6)(2\times 2) + (24n-12)(2\times 4) + \left(24n^2-24n+6\right)(4\times 4),$$

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$$= (6)(4) + (24n-12)(8) + (24n^2 - 24n + 6)(16),$$

$$= 24(1-4n)^2.$$

Theorem 5: *Consider G_1 be the Sheet Oxide network, then its Bi-distance Hyper Zagreb Index is,*

$$\mathrm{B}\,HM(G_1) = 48(32n^2 - 14n + 1).$$

Proof:

Consider G_1 to be the Sheet Oxide (OX_n) network's Molecular graph. Bi-distance Hyper Zagreb Index *is*,

$$\mathrm{B}\,HM(G) = \sum_{\omega\mu \in E(\mathbf{G})} (\mathrm{B}(\omega) + \mathrm{B}(\mu))^2.$$

Bi-distance Hyper Zagreb Index of the Sheet Oxide Network can be calculated as,

$$\mathrm{B}\,HM(G_1) = (\mathrm{B}(\omega_1) + \mathrm{B}(\mu_1))^2 + (\mathrm{B}(\omega_2) + \mathrm{B}(\mu_2))^2 + (\mathrm{B}(\omega_3) + \mathrm{B}(\mu_3))^2,$$

$$\mathrm{B}\,HM(G_1) = (6)((2+2)^2) + (24n-12)((2+4)^2) + (24n^2 - 24n + 6)((4+4)^2),$$

$$= (6)(16) + (24n-12)(36) + (24n^2 - 24n + 6)(64),$$

$$= 48(32n^2 - 14n + 1).$$

Theorem 6: *Consider G_1 be the Sheet Oxide network, then its Bi-distance Forgotten Index is,*

$$\mathrm{B}\,F(G_1) = 96n(8n-3).$$

Proof:

Consider G_1 to be the Sheet Oxide (OX_n) network's Molecular graph. Bi-distance Forgotten Index *is*,

$$\mathrm{B}\,F(G) = \sum_{\omega\mu \in E(\mathbf{G})} \left((\mathrm{B}(\omega))^2 + (\mathrm{B}(\mu))^2\right).$$

Bi-distance Forgotten Index of the Sheet Oxide Network can be calculated as,

$$\mathrm{B}\,F(G_1) = \left((\mathrm{B}(\omega_1))^2 + (\mathrm{B}(\mu_1))^2\right) + \left((\mathrm{B}(\omega_2))^2 + (\mathrm{B}(\mu_2))^2\right) + \left((\mathrm{B}(\omega_3))^2 + (\mathrm{B}(\mu_3))^2\right),$$

$$\mathrm{B}\,F(G_1) = \left((6)((2)^2 + (2)^2) + (24n-12)((2)^2 + (4)^2) + (24n^2 - 24n + 6)((4)^2 + (4)^2)\right),$$

$$= \left((6)(8) + (24n-12)(20) + (24n^2 - 24n + 6)(32)\right),$$

$$= 96n(8n-3).$$

Theorem 7: *The Bi-distance Augmented Zagreb Index for Sheet Oxide network, if G_1 be the graph is,*

$$\mathrm{B}\,AZI(G_1) = \frac{16}{9}(256n^2 - 148n + 37).$$

Proof:

Consider G_1 to be the Sheet Oxide (OX_n) network's Molecular graph. Bi-distance Augmented Zagreb Index is,

$$\mathrm{B}\,AZI(G) = \sum_{\omega\mu \in E(\mathbf{G})} \left(\frac{\mathrm{B}(\omega) \times \mathrm{B}(\mu)}{\mathrm{B}(\omega) + \mathrm{B}(\mu) - 2}\right)^3$$

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Bi-distance Forgotten Index of the Sheet Oxide Network can be calculated as,

$$\mathrm{B}\,AZI(G)=\left(\frac{\mathrm{B}(\omega_1)\times\mathrm{B}(\mu_1)}{\mathrm{B}(\omega_1)+\mathrm{B}(\mu_1)-2}\right)^3+\left(\frac{\mathrm{B}(\omega_2)\times\mathrm{B}(\mu_2)}{\mathrm{B}(\omega_2)+\mathrm{B}(\mu_2)-2}\right)^3+\left(\frac{\mathrm{B}(\omega_3)\times\mathrm{B}(\mu_3)}{\mathrm{B}(\omega_3)+\mathrm{B}(\mu_3)-2}\right)^3,$$

$$\mathrm{B}\,AZI(G_1)=(6)\left(\frac{2\times2}{2+2-2}\right)^3+(24n-12)\left(\frac{2\times4}{2+4-2}\right)^3+(24n^2-24n+6)\left(\frac{4\times4}{4+4-2}\right)^3,$$

$$=(6)(8)+(24n-12)(8)+(24n^2-24n+6)\left(\frac{512}{27}\right),$$

$$=\frac{16}{9}(256n^2-148n+37).$$

Theorem 8: *Suppose G_1 be the Sheet Oxide network then its Bi-distance First, Second and third Redefined Zagreb Indices are,*

$$\mathrm{B}\,RZ_1(G_1)=6n(2n+1).$$

$$\mathrm{B}\,RZ_2(G_1)=48n^2-16n+2.$$

$$\mathrm{B}\,RZ_3(G_1)=96(32n^2-20n+3).$$

Proof:

Consider G_1 to be the Sheet Oxide (OX_n) network's Molecular graph. Bi-distance First, Second and third Redefined Zagreb Indices are,

$$\mathrm{B}\,RZ_1(G)=\sum_{\omega\mu\in E(\mathbf{G})}\left(\frac{\mathrm{B}(\omega)+\mathrm{B}(\mu)}{\mathrm{B}(\omega)\times\mathrm{B}(\mu)}\right).$$

$$\mathrm{B}\,RZ_2(G)=\sum_{\omega\mu\in E(\mathbf{G})}\left(\frac{\mathrm{B}(\omega)\times\mathrm{B}(\mu)}{\mathrm{B}(\omega)+\mathrm{B}(\mu)}\right).$$

$$\mathrm{B}\,RZ_3(G)=\sum_{\omega\mu\in E(\mathbf{G})}\left((\mathrm{B}(\omega)+\mathrm{B}(\mu))(\mathrm{B}(\omega)\times\mathrm{B}(\mu))\right).$$

Bi-distance First, Second and third Redefined Zagreb Indices of the Sheet Oxide Network can be calculated as,

$$\mathrm{B}\,RZ_1(G_1)=\left(\frac{\mathrm{B}(\omega_1)+\mathrm{B}(\mu_1)}{\mathrm{B}(\omega_1)\times\mathrm{B}(\mu_1)}\right)+\left(\frac{\mathrm{B}(\omega_2)+\mathrm{B}(\mu_2)}{\Re(\omega_2)\times\mathrm{B}(\mu_2)}\right)+\left(\frac{\mathrm{B}(\omega_3)+\mathrm{B}(\mu_3)}{\mathrm{B}(\omega_3)\times\mathrm{B}(\mu_3)}\right),$$

$$\mathrm{B}\,RZ_1(G_1)=(6)\left(\frac{2+2}{2\times2}\right)+(24n-12)\left(\frac{2+4}{2\times4}\right)+(24n^2-24n+6)\left(\frac{4+4}{4\times4}\right),$$

$$=(6)(1)+(24n-12)\left(\frac{3}{4}\right)+(24n^2-24n+6)\left(\frac{(1)}{2}\right),$$

$$=6n(2n+1)$$

$$\mathrm{B}\,RZ_2(G_1)=\left(\frac{\mathrm{B}(\omega_1)\times\mathrm{B}(\mu_1)}{\mathrm{B}(\omega_1)+\mathrm{B}(\mu_1)}\right)+\left(\frac{\mathrm{B}(\omega_2)\times\mathrm{B}(\mu_2)}{\mathrm{B}(\omega_2)+\mathrm{B}(\mu_2)}\right)+\left(\frac{\mathrm{B}(\omega_3)\times\mathrm{B}(\mu_3)}{\mathrm{B}(\omega_3)+\mathrm{B}(\mu_3)}\right),$$

$$\mathrm{B}\,RZ_2(G_1)=(6)\left(\frac{2\times2}{2+2}\right)+(24n-12)\left(\frac{2\times4}{2+4}\right)+(24n^2-24n+6)\left(\frac{4\times4}{4+4}\right),$$

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$$= (6)(1) + (24n-12)\left(\frac{4}{3}\right) + \left(24n^2 - 24n + 6\right)(2),$$

$$= 48n^2 - 16n + 2.$$

$$\mathrm{B}\,Z_3(G_1) = \left((\mathrm{B}(\omega_1) + \mathrm{B}(\mu_1))(\mathrm{B}(\omega_1) \times \mathrm{B}(\mu_1))\right) + \left((\mathrm{B}(\omega_2) + \mathrm{B}(\mu_2))(\mathrm{B}(\omega_2) \times \mathrm{B}(\mu_2))\right)$$
$$+ \left((\mathrm{B}(\omega_3) + \mathrm{B}(\mu_3))(\mathrm{B}(\omega_3) \times \mathrm{B}(\mu_3))\right),$$
$$\mathrm{B}\,RZ_3(G_1) = (6)\left((2+2)(2\times 2)\right) + (24n-12)\left((2+4)(2\times 4)\right) + \left(24n^2 - 24n + 6\right)\left((4+4)(4\times 4)\right),$$

$$= (6)(16) + (24n-12)(48) + \left(24n^2 - 24n + 6\right)(128),$$

$$= 96\left(32n^2 - 20n + 3\right).$$

Table 3: Comparison of Topological Indices for Sheet Oxide Molecular Structure

N	$\mathrm{B}\,R_1(G_1)$	$\mathrm{B}\,R_{-1}(G_1)$	$\mathrm{B}\,R_{\frac{1}{2}}(G_1)$	$\mathrm{B}\,R_{-\frac{1}{2}}(G_1)$
1	216	3.375	69.941	8.743
2	1176	9.375	329.823	29.228
3	2904	18.375	781.706	61.713
4	5400	30.375	1425.588	106.198
5	8664	45.375	2261.470	162.684
6	12696	63.375	3289.352	231.169
7	17496	84.375	4509.235	311.654
8	23064	108.375	5921.117	404.140
9	29400	135.375	7525.000	508.625
10	36504	165.375	9320.881	625.110

Table 4: Comparison of Topological Indices for Sheet Oxide Molecular Structure

N	$\mathrm{B}\,ABC(G_1)$	$\mathrm{B}\,GA(G_1)$	$\mathrm{B}\,M_1(G_1)$	$\mathrm{B}\,HM(G_1)$	$\mathrm{B}\,F(G_1)$	$\mathrm{B}\,AZI(G_1)$	$\mathrm{B}\,RZ_1(G_1)$
1	16.402	23.314	144	912	480	257.778	18
2	62.767	93.941	672	4848	2496	1360	60
3	138.525	212.569	1584	11856	6048	3372.444	126
4	243.677	379.196	2880	21936	11136	6295.111	216
5	378.223	593.823	4560	35088	17760	10128	330
6	542.163	856.451	6624	51312	25920	14871.111	468
7	735.497	1167.08	9072	70608	35616	20524.444	630
8	958.225	1525.71	11904	92976	46848	27088	816
9	1210.346	1932.333	15120	118416	59616	34561.778	1026

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10	1491.862	2386.960	18720	146928	73920	42945.778	1260

Conclusion

Graphics effectively illustrate chemical composition and database relationships. Graphs are a crucial tool in science and engineering for visualizing complex phenomena. This study explores topological indices, examining variables linked to chemical structure graphs. Focusing on sheet Oxide network, it investigates how different formulations of degree-based topological invariants impact results. The findings can enhance understanding of biological activities and physical characteristics in these molecular structures, with applications in materials science, environmental remediation, and medicine.

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