Bi-Distance Approach to Determine the Topological Invariants of Silicon Carbide

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Abstract:
The use of silicon carbide is increasing significantly in the fields of research and technology. Topological indices enable data gathering on algebraic graphs and provide a mathematical framework for analyzing the chemical structural characteristics. In this paper, well-known degree-based topological indices are used to analyze the chemical structures of silicon carbides. To evaluate the features of various chemical or non-chemical networks, a variety of topological indices are defined. In this paper, a new concept related to the degree of the graph called "bi-distance" is introduced, which is used to calculate all the additive as well as multiplicative degree-based indices for the isomer of silicon carbide, Si3C3-1[t, h]. The term "bi-distance" is derived from the concepts of degree and distance in such a way that second distance can be used to calculate degree-based topological indices.

Keywords: Bi-distance edges, Molecular graph, Randic index, Silicon Carbide Si3C3-1[t, h], Topological index, Zagreb index.

Introduction:
Leonhard Euler (1702–1782) originated the term "graph" in graph theory in the eighteenth century. He was a mathematician from Switzerland. He used graph manipulation to solve Konigsberg Bridge problems.1

The subject of mathematics termed "graph theory" deals with structures of vertices represented by a series. Graph theory has evolved into an important field of mathematical research with relevance in chemistry, operations research, the social sciences, and computer science. All of the graphs in this paper are simple, connected, and planar. A graph is formed of vertices, nodes, or points that are connected by edges, arcs, or lines. "Graph theory" is the word used in mathematics to describe the analysis of graphs, which are mathematical patterns used to express pair-wise relationships among variables.

Graphs are one of the major aspects of discrete mathematics, and they have diverse applications in our daily life. The implementation of graph theory can be seen in nano-chemistry, computer networks, Google maps, and molecular graphs. Chemical graph theory is a sub-field of mathematical chemistry that uses graph theory to mathematically model chemical structures. It integrates chemistry and graph theory to investigate the physical and chemical properties of substances in more depth.

According to the IUPAC terminology, a "topological index" is a numerical number associated with a chemical composition that is used to correlate the chemical structure with numerous physical attributes, chemical reactivity, or bioactivities. In the recent two decades, it has become very widespread to investigate the physicochemical and structural features of molecular graphs, which are vital to chemical engineering and pharmaceutical research, using graph-theoretical methods. The T-indices are a
method for calculating network properties. The usefulness of topological indices is determined by the correlation between experimental and estimated values. The distance-related indices in network theory and the degree-based indices in the chemical and pharmaceutical industries have both been shown to be extremely efficient. T-indices provide a simple and theoretical method to obtain in-depth knowledge about drugs by estimating the structural characteristics of a series of pharmaceuticals.

Topological indices are quantitative measurements that do not depend on the geometry of the graph. Topological indices are used in the establishment of quantitative structure-activity relationships, which connect the bioactivity or other features of molecules using their chemical composition.

The heat of formation, the heat of evaporation, density, and pressure are a few more factors that may be evaluated using these graph descriptors. For understanding chemical processes like evaporation, heating, and flashpoints, topological indices are significant. It is a numerical number that describes the structure of the chemical graph in other aspects. Many researchers are interested in this advanced method for estimating compound features without conducting any experiments. Due to their great significance, T-indices are classified into various categories, such as degree-based, eccentricity-based, distance-based, and ev-degree-based.

Sardara recently investigated the characteristics of a certain isomer of silicon carbide and presented double silicon graphs. He used the additive and multiplicative topological versions of topology to learn more about SiC. Pan used the degree-related Banhatti and Revan indices to investigate the two-dimensional structures of a particular class of silicon $Si_2C_3 - [r, s]$. The silicon material has greatly inspired and motivated research interest due to its extraordinary mechanical, optical, and electrical capabilities. Xing-Long successfully used the entropy technique to analyze the shape and structure of silicon carbide. Sadia Akhter employed a novel topological approach to study the structure of two silicon isomers in 2019.

**Preliminaries**

A graph $G = (V,E)$ is composed of a collection of links $E$ and a collection of vertices $V$. The term $d(u,v)$ represents the distance between any two vertices in the simple and connected graph $G$. The degree of a vertex $u$ in $G$ is represented by $d(u)$, and the degree of a vertex $v$ in $G$ by $d(v)$. All the graphs used in this article are simple (without multiple edges and loops), connected, and planar (without edge crossings).

The indices are degree-based, both additive and multiplicative indices.

**First and Second Zagreb Index:**

The degree-based Zagreb indices were proposed by Gutman and Trinajstic in 1972. The first and second Zagreb indices, $M_1$ and $Z_2$, respectively, are equal to the sum of the squares of the degrees of the vertices and the products of the degrees of the pairs of adjacent vertices in the molecular graph. The formulae of these indices are:

$$M_1(G) = \sum_{u,v \in E(G)} (d_u + d_v)$$

$$Z_2(G) = \sum_{u,v \in E(G)} (d_u \times d_v)$$

Horoldagva used these indices for various classes of graphs. He proposed the generalization of M-indices for different kinds of regular and non-regular graphs. Javed wrote a detailed and interesting article on M-indices for sum graphs under Strong Product.

**First and Second Multiplicative Zagreb Indices:**

Todeschini introduced two new types of Zagreb indices in 2010: the first and second multiplicative Zagreb indices, abbreviated as $PM_1(G)$ and $PM_2(G)$.

The multiplicative version of the classical degree-related Zagreb indices are defined as:

$$PM_1(G) = \prod_{u,v \in E(G)} (d_u + d_v)$$

$$PM_2(G) = \prod_{u,v \in E(G)} (d_u \times d_v)$$

The multiplicative form of the Zagreb indices is used to investigate the other silicon carbide isomers. The properties of unicycle graphs and graphs with bridges are investigated using multiplicative M-indices.

**First and Second Zagreb Polynomials:**

Fath-Tabar introduced Zagreb polynomials in 2009. The Zagreb index is calculated using polynomials. These polynomials are denoted by $M_1(G,K)$ and $M_2(G,K)$ are defined as:

$$M_1(G,K) = \sum_{u,v \in E(G)} K^{d_u+d_v}$$

$$M_2(G,K) = \sum_{u,v \in E(G)} K^{d_u \times d_v}$$

The Isaac graph is a very important graph; hence, these polynomials are a useful tool for studying Isaac graphs in depth.

**Hyper-Zagreb Index:**
The Hyper-Zagreb index is a modified Zagreb index that was proposed by Shirdel, Rezapour, and Sayadi\textsuperscript{23} and publicized in 2013. They explain the newly proposed index for the cartesian product, composition, join, and disjunction of graphs. Hyper-Zagreb index is denoted by HM(G) and computed as:

\[
HM(G) = \sum_{uv \in E(G)} (d_u + d_v)^2
\]

- **Second Modified Zagreb Index:**
  The modified versions of the Zagreb indices are inspired by the usefulness of the classical Zagreb indices. The M\textsubscript{2}(G) is determined as:

\[
M_2(G) = \sum_{uv \in E(G)} \frac{1}{(d_u \times d_v)}
\]

- **Reduced Second Zagreb Index:**
  Furtula, Gutman, and Ediz\textsuperscript{24} investigated the difference between Zagreb indices and discovered that it is closely connected to the vertex-degree-based invariant known as the reduced second Zagreb index, written as:

\[
RM_2(G) = \sum_{uv \in E(G)} (d_u - 1 \times d_v - 1)
\]

To study further information about all Zagreb indices see\textsuperscript{25}.

- **Atom Bond Connectivity Index:**
  In 1998, Ernesto Estrada and Fernando Torres proposed the ABC-index after being inspired by Milan Randić’s work\textsuperscript{26}. It is used to simulate the thermal properties of organic substances.

\[
ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u \times d_v}}
\]

- **Randić Index:**
  Milan Randić suggested the first degree-based index in 1975 to understand the branching structure of carbon atoms in organic compounds\textsuperscript{27}. The Randić index is defined as:

\[
R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}
\]

- **General Randić Connectivity Index:**
  In 1998, Bollob and Erdos generalized Milan’s index by replacing 1/2 with any general number \(\alpha\)\textsuperscript{28}.

\[
R_{\alpha}(G) = \sum_{uv \in E(G)} (d_u d_v)^{\alpha}
\]

- **Reciprocal Randić Index:**
  Favaron, Mahéo and Saclé were the first to introduce this form of R-index. The mathematical formula of RR-index is:

\[
RR(G) = \sum_{uv \in E(G)} \sqrt{d_u \times d_v}
\]

- **Reduced Reciprocal Randić Index:**
  It is the advanced form of the R-index and its mathematical definition is:

\[
RRR(G) = \sum_{uv \in E(G)} \sqrt{(d_u - 1) (d_v - 1)}
\]

- **Geometric Arithmetic Index:**
  Vukicevic and Furtula suggested the GA-index in 2009\textsuperscript{29} which is described as:

\[
GA(G) = \sum_{uv \in E(G)} 2\sqrt{d_u d_v}
\]

- **Forgotten Index:**
  Gutman and Furtula published this index in 2015\textsuperscript{30}, and it is represented as F(G) which is described as:

\[
F(G) = \sum_{uv \in E(G)} (d_u^2 + d_v^2)
\]

- **General Sum Connectivity Index:**
  Zhou and Trinajstić suggested the general form of the sum connectivity index. The \(X_\alpha(G)\)-index is mathematically written as:

\[
X_\alpha(G) = \sum_{uv \in E(G)} (d_u + d_v)^{\alpha}
\]

- **Symmetric Division Index:**
  The degree based symmetric division index was introduced by Vukicević and Furtula.

\[
SD(G) = \sum_{uv \in E(G)} \frac{d_u^2 + d_v^2}{d_u \times d_v}
\]

This index is very effective to predict the total surface area for poly-chloro-biphenyls.

- **Harmonic Index:**
  In graph theory, Siemion Fajtlowicz created a computer program that generates conjectures automatically in 1990. He discovered a vertex degree-based quantity while working on this project. Zhang later retrieved that unknown quantity (in 2012) and termed it harmonic index\textsuperscript{31}. It's written like this:

\[
H(G) = \sum_{uv \in E(G)} \frac{2}{d_u + d_v}
\]

This article deals with the degree-based topological indices of silicon carbides. Silicon carbide is a highly unusual structure since it has various properties such as low density, strong strength, good high-temperature strength, low thermal expansion, and high thermal conductivity. Due to the requirements of the SiC, its properties are explored with the help of indices. A large number of articles are present on the topological
indices of the different isomers of SiC. Graph theory defines broad and advanced ideas to facilitate the understanding of many problems in different fields.

Comparison of Single and Bi-Distance Edge Based Indices

All the classical degree-based TIs are single-distance. The word "single distance" does not appear in these indices. Due to the usefulness of TIs in real life, many approaches have been introduced, like distance-based, eccentricity-based, metric-based, additive type, multiplicative type, etc. The bi-distance strategy is a new method that is suggested in this article for determining these indices. A bi-distance edge is formed by combining two edges. The bi-distance concept is also used for finding the wiener index. The Wiener index just is concerned with all types of distances, but here the special term "two-distance" is proposed. In this section, the methyl-heptane single-distance edge and bi-distance edge partitions are examined.

2-Methylheptane

- Single-distance Edge Partitions:
The methyl-heptane structure's edges are separated into several groups using the method for edge separation discussed above. Four distinct methyl-heptane edge bundles are presented in Table 1. The parcel $E_1$ has 2 edges, where $d_u = 1$ and $d_v = 3$. The bundle $E_2$ consists of only one edge, where $d_u = 3$ and $d_v = 2$. The pack $E_3$ has 3 edges, where $d_u = 2$ and $d_v = 2$. The fourth edge bundle $E_4$ is made up of 1 edge, where $d_u = 2$ and $d_v = 1$. All the calculations related to edge separation are given in Table 1.

Table 1. Single-distance edge partition of Methyl-heptane

<table>
<thead>
<tr>
<th>Edges</th>
<th>$(d_u, d_v)$</th>
<th>Frequency</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_1$</td>
<td>(1,3)</td>
<td>2</td>
</tr>
<tr>
<td>$E_2$</td>
<td>(3,2)</td>
<td>1</td>
</tr>
<tr>
<td>$E_3$</td>
<td>(2,2)</td>
<td>3</td>
</tr>
<tr>
<td>$E_4$</td>
<td>(2,1)</td>
<td>1</td>
</tr>
</tbody>
</table>

The $M_1(G)$ index for methyl heptane is determined by using the formula and the data given in Table 1.

$$M_1(G) = \sum_{uv \in E(G)} (d_u + d_v)$$

$E_1 = \sum_{uv \in E_1(G)} (d_u + d_v) + \sum_{uv \in E_2(G)} (d_u + d_v) + \sum_{uv \in E_3(G)} (d_u + d_v) + \sum_{uv \in E_4(G)} (d_u + d_v)$

$$= |E_1(G)| + |E_2(G)| + |E_3(G)| + |E_4(G)|$$

$$= 2(4) + 1(5) + 3(4) + 1(3) = 28$$

- Bi-distance Edge Partitions:
The edge partition technique is applied to split the bi-distance edges of methyl-heptane into four packets given in Table 2. The parcel $E_1$ composed of 3 edges, where $d_u = 1$ and $d_v = 2$. The bundle $E_2$ is made by 1 edge, where $d_u = 3$ and $d_v = 2$. The third edge bundle has two edges, while the fourth edge parcel has just one edge.

Table 2. Bi-distance edge partition of Methyl-heptane

<table>
<thead>
<tr>
<th>Edges</th>
<th>$(d_u, d_v)$</th>
<th>Frequency</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_1$</td>
<td>(1,2)</td>
<td>3</td>
</tr>
<tr>
<td>$E_2$</td>
<td>(3,2)</td>
<td>1</td>
</tr>
<tr>
<td>$E_3$</td>
<td>(2,2)</td>
<td>2</td>
</tr>
<tr>
<td>$E_4$</td>
<td>(1,1)</td>
<td>1</td>
</tr>
</tbody>
</table>

The $M_1(G)$ index is determined as:

$$M_1(G) = \sum_{uv \in E(G)} (d_u + d_v)$$

$$= \sum_{uv \in E_1(G)} (d_u + d_v) + \sum_{uv \in E_2(G)} (d_u + d_v) + \sum_{uv \in E_3(G)} (d_u + d_v) + \sum_{uv \in E_4(G)} (d_u + d_v)$$

$$= |E_1(G)| + |E_2(G)| + |E_3(G)| + |E_4(G)|$$

$$= 2(4) + 1(5) + 3(4) + 1(2)$$

$$= 24$$

Methods

There are several methods and techniques for obtaining results, such as vertex degree, edge partitioning, graph analytical approaches, and numerical comparison of the results. Different software is used in this article. For computations and rechecking, MATLAB is really beneficial software. Software like Mathematica is used for 2D and 3D graphs that are used to represent the comparison of topological indices. ChemSketch was used for the structural graphs of SiC–I [t, h]. ChemDraw can also be used for drawing chemical structures in an easy way.

2D Structure and Importance of Silicon Carbide SiC–I [t, h]

Fig 1 shows the 2D molecular graph of silicon carbide, SiC–I [t, h]. The characteristics of the molecular graph are discussed using two parameters. The number of connected unit cells in a row (network) is indicated by t, while the number of connected rows containing t numbers of cells is indicated by h. Fig 2 shows how cells join to form a row (a string) and how one row interacts with another. The chemical structures of inorganic...
compounds are explored due to the use and great importance of SiC in the modern world. Silicon has decreased the size of electronic devices and enhanced their quality. Silicon carbide is a crystalline combination of silicon and carbon that is extremely hard. Silicon carbide has been a crucial advancement in the production of all large and complex structures. The unit cell of the special isomer of SiC is shown in (a) part of Fig. 1. These basic cells are connected in different patterns to form new structures.

![Image of SiC structure](image)

<table>
<thead>
<tr>
<th>Table 3. Degree-based partition of edges of Si$_2$C$_3$-I[t, h]</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Edges</strong></td>
</tr>
<tr>
<td>-----------</td>
</tr>
<tr>
<td>$E_1$</td>
</tr>
<tr>
<td>$E_2$</td>
</tr>
<tr>
<td>$E_3$</td>
</tr>
<tr>
<td>$E_4$</td>
</tr>
<tr>
<td>$E_5$</td>
</tr>
</tbody>
</table>
**Theorem 1:** Consider $G \cong Si_2C_3 - I[t, h]$ be a simple graph of the particular isomer of silicon carbide, then:

\[ M_1(G) = 180ht - 62h - 92t + 24 \]
\[ M_2(G) = 270ht - 112h - 166t + 58 \]

**Proof:** Suppose $G$ is a connected and planar graph of $Si_2C_3 - I[t, h]$. The edges collection $E(G)$ is divided into 5 distinct groups. The values of the first Zagreb index can be computed with the help of Table 3 of the edge partition.

\[
M_1(G) = \sum_{uv \in E(G)} (d_u + d_v)
\]

\[
= \sum_{uv \in E_1(G)} (d_u + d_v) + \sum_{uv \in E_2(G)} (d_u + d_v) + \sum_{uv \in E_3(G)} (d_u + d_v) + \sum_{uv \in E_4(G)} (d_u + d_v)
\]

\[
= |E_1(G)| + |E_2(G)| + |E_3(G)| + |E_4(G)| + |E_5(G)|
\]

\[
= 2 \times 3 + 1 \times 4 + 2h + 2t \times 4 + (10h + 16t - 20) + 5 \times 30h - 20h - 30t
\]

\[
M_2(G) = 180ht - 62h - 92t + 24
\]

The $Z_2(G)$-index is denoted as:

\[
Z_2(G) = \sum_{uv \in E(G)} (d_u + d_v)
\]

\[
= \sum_{uv \in E_1(G)} (d_u + d_v) + \sum_{uv \in E_2(G)} (d_u + d_v) + \sum_{uv \in E_3(G)} (d_u + d_v) + \sum_{uv \in E_4(G)} (d_u + d_v)
\]

\[
= |E_1(G)| + |E_2(G)| + |E_3(G)| + |E_4(G)| + |E_5(G)|
\]

\[
= 2 \times 2 + 3 \times 1 + 4(2h + 2t) + 6(10h + 16t - 20) + 9(30h - 20h - 30t + 19)
\]

\[
= 270ht - 112h - 166t + 58
\]

**Theorem 2:** Consider $G \cong Si_2C_3 - I[t, h]$ be the graph of a special isomer of silicon carbide, then the multiplicative version of Zagreb indices are:

\[
PM_1(G) = 36 \times 4^{2h+2t} \times 5^{10h+16t-20} \times 6^{30h-20h-30t+19}
\]

\[
PM_2(G) = 12 \times 4^{2h+2t} \times 4^{10h+16t-20} \times 3^{30h-20h-30t+19}
\]

**Proof:** Assume that $G$ is a simple graph of $Si_2C_3 - I[t, h]$ with no crossings. The whole set of edges in $G$ is classified into five classes. The PM$_1(G)$-index is computed by using the formula and calculations given in Table 3.

\[
PM_1(G) = \prod_{uv \in E(G)} (d_u + d_v)
\]

\[
= \prod_{uv \in E_1(G)} (d_u + d_v) \times \prod_{uv \in E_2(G)} (d_u + d_v) \times \prod_{uv \in E_3(G)} (d_u + d_v) \times \prod_{uv \in E_4(G)} (d_u + d_v)
\]

\[
= 3|E_1(G)| \times 4|E_2(G)| \times 4|E_3(G)| \times 5|E_4(G)| \times 6|E_5(G)|
\]

\[
= 3^2 \times 4 \times 4^{2h+2t} \times 5^{10h+16t-20} \times 6^{30h-20h-30t+19}
\]

\[
= 36 \times 4 \times 4^{2h+2t} \times 5^{10h+16t-20} \times 6^{30h-20h-30t+19}
\]

The PM$_2(G)$-index is determined as:

\[
PM_2(G) = \prod_{uv \in E(G)} (d_u + d_v)
\]

\[
= \prod_{uv \in E_1(G)} (d_u + d_v) \times \prod_{uv \in E_2(G)} (d_u + d_v) \times \prod_{uv \in E_3(G)} (d_u + d_v) \times \prod_{uv \in E_4(G)} (d_u + d_v)
\]

\[
= 2|E_1(G)| \times 3|E_2(G)| \times 4|E_3(G)| \times 6|E_4(G)|
\]

\[
= 12 \times 4^{2h+2t} \times 6^{10h+16t-20} \times 30h-20h-30t+19
\]

**Theorem 3:** Suppose $G \cong Si_2C_3 - I[t, h]$ is the graph of silicon carbide, then the outcomes of both the Zagreb polynomials are:

\[
M_1(G, K) = 2K^3 + K^4 + (2h + 2t)K^4 + (10h + 16t - 20)K^5 + (30h - 20h - 30t + 19)K^6
\]

\[
M_2(G, K) = 2K^3 + K^4 + (2h + 2t)K^4 + (10h + 16t - 20)K^5 + (30h - 20h - 30t + 19)K^6
\]

**Proof:** The edges $E$ are classified into 5 classes. By using Table 3, it is easy to calculate the values of both Zagreb polynomials. The definition of $M_1(G, K)$ is:

\[
M_1(G, K) = \sum_{uv \in E(G)} K(d_u + d_v)
\]

\[
= \sum_{uv \in E_1(G)} K(d_u + d_v) + \sum_{uv \in E_2(G)} K(d_u + d_v) + \sum_{uv \in E_3(G)} K(d_u + d_v) + \sum_{uv \in E_4(G)} K(d_u + d_v)
\]

\[
= |E_1(G)|K^3 + |E_2(G)|K^4 + |E_3(G)|K^5 + |E_4(G)|K^6
\]

\[
= 2K^3 + K^4 + (2h + 2t)K^4 + (10h + 16t - 20)K^5 + (30h - 20h - 30t + 19)K^6
\]

The $M_2(G, K)$-polynomial for $Si_2C_3 - I[t, h]$ is calculated as bellow:

\[
M_2(G, K) = \sum_{uv \in E(G)} K(d_u + d_v)
\]

\[
= \sum_{uv \in E_1(G)} K(d_u + d_v) + \sum_{uv \in E_2(G)} K(d_u + d_v) + \sum_{uv \in E_3(G)} K(d_u + d_v) + \sum_{uv \in E_4(G)} K(d_u + d_v)
\]

\[
= |E_1(G)|K^3 + |E_2(G)|K^4 + |E_3(G)|K^5 + |E_4(G)|K^6
\]

\[
= 2K^3 + K^4 + (2h + 2t)K^4 + (10h + 16t - 20)K^5 + (30h - 20h - 30t + 19)K^6
\]
Theorem 4: Let \( G \cong \text{Si}_3\text{C}_2\text{I}[t, h] \) be the graph of silicarbide, then two different forms of \( Z \)-indices are computed as:

\[
HM(G) = 1080th - 438h - 648t + 218
\]

\[
M_2(G) = \frac{10th}{3} - \frac{h}{18} + \frac{t}{6} + \frac{1}{3}
\]

Proof: The HM-index is a vertex degree-related index that can be calculated by using Table 3 and the mathematical formula for this index.

\[
HM(G) = \sum_{uv \in E(G)} |d_u + d_v|^2
\]

\[
= \sum_{uv \in E_1(G)} (d_u + d_v)^2 + \sum_{uv \in E_2(G)} (d_u + d_v)^2
\]

\[
+ \sum_{uv \in E_3(G)} (d_u + d_v)^2 + \sum_{uv \in E_4(G)} (d_u + d_v)^2
\]

\[
= |E_1(G)| + |E_2(G)| + |E_3(G)| + |E_4(G)|
\]

\[
= 200(16t) + 16(2h + 2t) + 25(10h + 16t - 20) + 36(30h - 20h - 30t + 19)
\]

\[
= 1080th - 438h - 648t + 218
\]

The \( M_2(G) \)-index is calculated as:

\[
M_2(G) = \sum_{uv \in E(G)} \frac{1}{(d_u \times d_v)}
\]

\[
= \frac{1}{2}|E_1(G)| + \frac{1}{4}|E_2(G)| + \frac{1}{9}|E_3(G)| + \frac{2}{3} + \frac{1}{3} \sum_{20h+2t} + \frac{10th+16t-20}{6}
\]

\[
= \frac{9}{10th} - \frac{h}{18} + t + \frac{1}{9}
\]

Theorem 5: Let \( G \cong \text{Si}_3\text{C}_2\text{I}[t, h] \) be the graph of silicarbide. The results of indices are computed as:

\[
RM_2(G) = 120th - 58h - 86t + 36
\]

\[
ABC(G) = \frac{1}{ \sqrt{2}} (12h + 18t - 18) + \sqrt{2} + 20th
\]

\[
= \frac{40h}{3} - 20t + \frac{38}{3}
\]

Proof: The whole edges of graph \( G \) are consisting of five distinct groups. By utilizing the edge separation Table 3, the values of \( RM_2(G) \) are:

\[
RM_2(G) = \sum_{uv \in E(G)} (d_u - 1 \times d_v - 1)
\]

\[
= |E_1(G)| + |E_2(G)| + |E_3(G)| + |E_4(G)|
\]

\[
= 20(0x1) + 1(0x2) + 1(2h+2t) + (10h+16t-20)(1x2) + (30h-20t-30t+19)(4)
\]

\[
= 120th - 58h - 86t + 36
\]

The \( ABC(G) \)-index is computed as:

\[
ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u \times d_v} + \frac{2}{3}}
\]
RR(G) = \sum_{uv \in E(G)} \sqrt{d_u d_v} \\
= \sum_{uv \in E_1(G)} \sqrt{d_u d_v} + \sum_{uv \in E_2(G)} \sqrt{d_u d_v} + \sum_{uv \in E_3(G)} \sqrt{d_u d_v} + \sum_{uv \in E_4(G)} \sqrt{d_u d_v} + \sum_{uv \in E_5(G)} \sqrt{d_u d_v} \\
= 1.4142(2) + 1.7321(1) + 1(2h + 2t) + 2.4495(10h + 16t - 20) + 3(30h - 20h - 30t + 19) \\
= \text{90th - 31.50 h - 46.808t + 12.5705} \\
The RRR(G)-index is computed as: \\
RRR(G) = \sum_{uv \in E(G)} \sqrt{(d_u - 1)(d_v - 1)} \\
= \sum_{uv \in E_1(G)} \sqrt{(d_u - 1)(d_v - 1)} + \sum_{uv \in E_2(G)} \sqrt{(d_u - 1)(d_v - 1)} + \sum_{uv \in E_3(G)} \sqrt{(d_u - 1)(d_v - 1)} + \sum_{uv \in E_4(G)} \sqrt{(d_u - 1)(d_v - 1)} + \sum_{uv \in E_5(G)} \sqrt{(d_u - 1)(d_v - 1)} \\
= |E_1(G)| + |E_2(G)| + |E_3(G)| + |E_4(G)| + |E_5(G)| \\
= 60th - 38h - 58t + 38 + \sqrt{2}(10h + 16t - 20) \\
\text{Theorem 8: Let } G \equiv \text{SiC}_{9-1}[t, h] \text{ be the graph of silicon carbide.} \\
\text{GA(G)} = 30th - 28t - 18h + \frac{1}{3\sqrt{3}}(4\sqrt{6} + 63) + \frac{2\sqrt{6}}{5}(10h + 16t - 20) \\
SD(G) = 60th - \frac{43}{3}h - 64t - 5 \\
\text{Proof: By using Table 3 and the definition of GA-index, it can be easily computed as:} \\
\text{GA(G)} = \sum_{uv \in E(G)} 2\sqrt{\frac{d_u d_v}{d_u + d_v}} \\
= \sum_{uv \in E_1(G)} 2\sqrt{\frac{d_u d_v}{d_u + d_v}} + \sum_{uv \in E_2(G)} 2\sqrt{\frac{d_u d_v}{d_u + d_v}} + \sum_{uv \in E_3(G)} 2\sqrt{\frac{d_u d_v}{d_u + d_v}} + \sum_{uv \in E_4(G)} 2\sqrt{\frac{d_u d_v}{d_u + d_v}} + \sum_{uv \in E_5(G)} 2\sqrt{\frac{d_u d_v}{d_u + d_v}} \\
= \frac{2\sqrt{3}}{3} \left| E_1(G) \right| + \frac{2}{\sqrt{3}} \left| E_2(G) \right| + \frac{2}{\sqrt{3}} \left| E_3(G) \right| + \frac{2\sqrt{6}}{5} \left| E_4(G) \right| + \frac{1}{\sqrt{3}} \left| E_5(G) \right| \\
= \frac{2\sqrt{3}}{3} (2) + \frac{2}{\sqrt{3}} (1) + 1(2h + 2t) + \frac{2\sqrt{6}}{5}(10h + 16t - 20) + 1(30h - 20h - 30t + 19) \\
= 30th - 28t - 18h + \frac{1}{3\sqrt{3}}(4\sqrt{6} + 63) + \frac{2\sqrt{6}}{5}(10h + 16t - 20) \\
The SD(G)-index can be identified as: \\
SD(G) = \sum_{uv \in E(G)} \frac{d_u + d_v}{2} \\
= \sum_{uv \in E_1(G)} \frac{d_u + d_v}{2} + \sum_{uv \in E_2(G)} \frac{d_u + d_v}{2} + \sum_{uv \in E_3(G)} \frac{d_u + d_v}{2} + \sum_{uv \in E_4(G)} \frac{d_u + d_v}{2} + \sum_{uv \in E_5(G)} \frac{d_u + d_v}{2} \\
= \frac{5}{2} \left| E_1(G) \right| + \frac{10}{3} \left| E_2(G) \right| + \frac{8}{4} \left| E_3(G) \right| + \frac{13}{6} \left| E_4(G) \right| + \frac{18}{1} \left| E_5(G) \right| \\
= \frac{5}{2} (2) + \frac{10}{3} (1) + \frac{8}{4} (2h + 2t) + \frac{13}{6} (10h + 16t - 20) + \frac{18}{9} (30h - 20h - 30t + 19) \\
= 60th - \frac{43}{3} h - 64t - 5 \\
\text{Theorem 9: Consider } G \equiv \text{SiC}_{9-1}[t, h] \text{ be the graph of a particular isomer of SiC, then resultant values of F-index and H-index are given below:} \\
F(G) = 540ht - 86h - 316t + 9 \\
H(G) = 10ht - \frac{5}{3} h - \frac{13}{5} t + \frac{1}{6} \\
\text{Proof: The 2D general structure of SiC}_{9-1}[t, h] \text{ is composed of five different parcels of edges. Based on the data given in Table 3 and its definition, the F-index is easily computed as follows:} \\
\text{F(G) = } \sum_{uv \in E_1(G)} \sqrt{d_u d_v} + \sum_{uv \in E_2(G)} \sqrt{d_u d_v} + \sum_{uv \in E_3(G)} \sqrt{d_u d_v} + \sum_{uv \in E_4(G)} \sqrt{d_u d_v} + \sum_{uv \in E_5(G)} \sqrt{d_u d_v} \\
= |E_1(G)| + |E_2(G)| + |E_3(G)| + |E_4(G)| + |E_5(G)| \\
= 5(1) + 10(1) + 8(2h + 2t) + 13(10h + 16t - 20) + 18(30h - 20h - 30t + 19) \\
= 540ht - 86h - 316t + 97 \\
\text{The H-index is calculated as:} \\
H(G) = \sum_{uv \in E(G)} \frac{d_u + d_v}{2} \\
= \sum_{uv \in E_1(G)} \frac{d_u + d_v}{2} + \sum_{uv \in E_2(G)} \frac{d_u + d_v}{2} + \sum_{uv \in E_3(G)} \frac{d_u + d_v}{2} + \sum_{uv \in E_4(G)} \frac{d_u + d_v}{2} + \sum_{uv \in E_5(G)} \frac{d_u + d_v}{2} \\
= |E_1(G)| + \frac{1}{3} |E_2(G)| + \frac{2}{3} |E_3(G)| + \frac{1}{4} |E_4(G)| + \frac{2}{6} |E_5(G)| \\
= \frac{2}{3} (2) + \frac{1}{3} (1) + \frac{1}{2} (2h + 2t) + \frac{2}{3} (10h + 16t - 20) + \frac{1}{3} (30h - 20h - 30t + 19) \\
= 10ht - \frac{5}{3} h - \frac{13}{5} t + \frac{1}{6} \\
\text{Theorem 10: Let } G \equiv \text{SiC}_{9-1}[t, h] \text{ be the graph of silicon carbide without loops and multiple edges than the values of } X_{\infty}(G) \text{ are:} \\
X_{\infty}(G) = 180ht - 62h - 92t + 24 \\
\text{Proof: The edges collection } E(G) \text{ splits into 5 different edges which can be written as } E(G) = E_1(G) \cup E_2(G) \cup E_3(G) \cup E_4(G) \cup E_5(G). \text{ According to Table 3, the outcome of } X_{\infty}(G) \text{ is calculated as:} \\
X_{\infty}(G) = \sum_{uv \in E(G)} \frac{d_u + d_v}{2}^X
\[ = \sum_{uv} \in E_1(G) \left( d_u + d_v \right)^{\alpha} + \sum_{uv} \in E_2(G) \left( d_u + d_v \right)^{\beta} + \sum_{uv} \in E_4(G) \left( d_u + d_v \right)^{\gamma} \]

If \( \alpha = 1 \) then,
\[ = 180th - 62h - 92t + 24 \]

### Numerical Analysis

This section represents the numerical calculation of silicon carbide, Si\(_2\)C\(_7\)-I(t, h). All topological indices demonstrate strong variation with a small change in parameter values. The values of the entire mentioned topological indices rise as the input data is increased (t or h). The results of the first and second multiplicative Zagreb indices are very high compared to the results of the other indices. The input data range of parameters \( t = s = 1, 2, 3, 4, 5 \). All values—aside from the values of the symmetric division index—are increased by increasing the inputs with positive values. Numerical computational procedures are the approaches used to design mathematical problems that can be solved using arithmetic operations. The comparison of all outcomes can be easily observed from the data given in Table 4. These calculated values are used to draw the 3D graphs. The numerical values of all the topological indices are listed below in Table 4.

#### Table 4. Numerical Analysis for Si\(_2\)C\(_7\)-I[t, h]

<table>
<thead>
<tr>
<th>Topological indices</th>
<th>( t, h=1, 1 )</th>
<th>( t, h=2, 2 )</th>
<th>( t, h=3, 3 )</th>
<th>( t, h=4, 4 )</th>
<th>( t, h=5, 5 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( M_2(G) )</td>
<td>50</td>
<td>436</td>
<td>1182</td>
<td>2288</td>
<td>3754</td>
</tr>
<tr>
<td>( Z_2(G) )</td>
<td>50</td>
<td>582</td>
<td>1654</td>
<td>3266</td>
<td>5418</td>
</tr>
<tr>
<td>( PM_1(G) )</td>
<td>1.247× 10(^3)</td>
<td>4.074× 10(^4)</td>
<td>3.520× 10(^6)</td>
<td>2.136× 10(^9)</td>
<td>1.068× 10(^{52} )</td>
</tr>
<tr>
<td>( PM_2(G) )</td>
<td>4.972× 10(^4)</td>
<td>1.612× 10(^9)</td>
<td>1.393× 10(^{52} )</td>
<td>1.290× 10(^{50} )</td>
<td>4.031× 10(^{51} )</td>
</tr>
<tr>
<td>( HM(G) )</td>
<td>212</td>
<td>2366</td>
<td>6680</td>
<td>13154</td>
<td>21788</td>
</tr>
<tr>
<td>( M_3(G) )</td>
<td>3.23</td>
<td>13</td>
<td>29.45</td>
<td>52.56</td>
<td>82.34</td>
</tr>
<tr>
<td>( RM_1(G) )</td>
<td>12</td>
<td>228</td>
<td>684</td>
<td>1380</td>
<td>2316</td>
</tr>
<tr>
<td>( ABC(G) )</td>
<td>8.6321</td>
<td>56.52</td>
<td>144.399</td>
<td>272.28</td>
<td>440.16</td>
</tr>
<tr>
<td>( R_{\alpha}(G) )</td>
<td>50</td>
<td>582</td>
<td>1654</td>
<td>3266</td>
<td>5418</td>
</tr>
<tr>
<td>( R(G) )</td>
<td>6.1066</td>
<td>32.08</td>
<td>78.093</td>
<td>144.15</td>
<td>230.24</td>
</tr>
<tr>
<td>( RR(G) )</td>
<td>24.27</td>
<td>215.96</td>
<td>587.65</td>
<td>1139.34</td>
<td>1871.04</td>
</tr>
<tr>
<td>( RRR(G) )</td>
<td>10.49</td>
<td>131.26</td>
<td>372.03</td>
<td>732.794</td>
<td>1213.57</td>
</tr>
<tr>
<td>( GA(G) )</td>
<td>23.89</td>
<td>113.37</td>
<td>263.42</td>
<td>460.56</td>
<td>741.79</td>
</tr>
<tr>
<td>( SD(G) )</td>
<td>-23.34</td>
<td>78.34</td>
<td>300</td>
<td>641.67</td>
<td>1103.34</td>
</tr>
<tr>
<td>( F(G) )</td>
<td>235</td>
<td>1453</td>
<td>3751</td>
<td>7129</td>
<td>11587</td>
</tr>
<tr>
<td>( H(G) )</td>
<td>5.9</td>
<td>31.64</td>
<td>77.37</td>
<td>143.1</td>
<td>228.84</td>
</tr>
<tr>
<td>( X_{\alpha}(G) )</td>
<td>50</td>
<td>436</td>
<td>1182</td>
<td>2288</td>
<td>3754</td>
</tr>
</tbody>
</table>

### Graphical Analysis of Data

In this section, the results are presented and discussed using graphs. It is important to note that the estimated areas and graphs below show how t and h affect each topological index. These examples make it simpler to understand how the other topological indexes react differently to the parameters t and h. Graphs and charts summarized a lot of information in simple formats that express key ideas simply and effectively. According to the type of data, there are several graph types, including bar charts, line graphs, area graphs, scatter plots, pie charts, pictographs, column charts, and bubble charts. The 3D axis graphs are used here to understand the relationship between the T-indices and the physical-chemical properties of the silicon structures. The x- and y-axes are used to represent the input values of parameters t and h, but the 3D space is used to display the outcomes. The variants in all the indices are described in Fig. 3.
Comparison of Classical and Bi-distance TIs:

- **Single Distance Topological Index:**
The classical first and second Zagreb indices for the special isomer of silicon carbide $\text{Si}_2\text{C}_3$-1[$t, h$] are:

  \[
  M_1(G) = 90th - 20t - 30h + 4
  \]
  \[
  Z_2(G) = 135th - 41t - 61h + 14
  \]

M.K. Siddiqui submitted an article that describes many classical indices for silicon carbide $^{55}$.

- The behavior and variation of any TI can be observed by the numerical values shown in Table 5, but graphs are a better way to express the data. The smaller measurements are used to understand the changes as $t = h = 1, 2, 3, 4, \text{ and } 5$.

<table>
<thead>
<tr>
<th>Topological indices</th>
<th>(t, h)=[1, 1]</th>
<th>(t, h)=[2, 2]</th>
<th>(t, h)=[3, 3]</th>
<th>(t, h)=[4, 4]</th>
<th>(t, h)=[5, 5]</th>
</tr>
</thead>
<tbody>
<tr>
<td>$M_1(G)$</td>
<td>44</td>
<td>264</td>
<td>664</td>
<td>1244</td>
<td>2004</td>
</tr>
<tr>
<td>$Z_2(G)$</td>
<td>47</td>
<td>350</td>
<td>923</td>
<td>1766</td>
<td>2879</td>
</tr>
</tbody>
</table>
• Fig 4 illustrates the graphical representations of the first and second Zagreb indices for the isomer of SiC.

Figure 4. First and second Zagreb indices for Si\textsubscript{2}C\textsubscript{3}-I[t, h]

<table>
<thead>
<tr>
<th>Topological indices</th>
<th>(t, h)=[1, 1]</th>
<th>(t, h)=[2, 2]</th>
<th>(t, h)=[3, 3]</th>
<th>(t, h)=[4, 4]</th>
<th>(t, h)=[5, 5]</th>
</tr>
</thead>
<tbody>
<tr>
<td>$M_1(G)$</td>
<td>50</td>
<td>436</td>
<td>1182</td>
<td>2288</td>
<td>3754</td>
</tr>
<tr>
<td>$Z_2(G)$</td>
<td>50</td>
<td>582</td>
<td>1654</td>
<td>3266</td>
<td>5418</td>
</tr>
</tbody>
</table>

• The graphical representation of the bi-distance first and second Zagreb indices is shown in Fig. 5.

Figure 5. The bi-distance $M_1$ and $M_2$-indices of Si\textsubscript{2}C\textsubscript{3}-I[t, h]

The significant connection between both indices is made clear by the comparison of both the classical and bi-distance indices. Bi-distant indices have excellent correlation coefficients that accurately represent a wide range of physical and chemical characteristics of various organic and inorganic materials.

Conclusion:

The graphic is a simple technique to portray the chemical nature of a database association. Graphs are an important tool in science and engineering for developing methodologies, such as the bi-distance method, can be created and applied to all degree- or distance-related topological indices. Topological indices can be used to investigate a wide range of complicated structures. Because classical degree-based indices are extremely strong and powerful, these indices will be applied to the structure that has to be explored. The most significant aspect of the significance of topological indices is the correlation coefficient values, which must be strong.

Bi-distance Topological Index

The bi-distance first and second Zagreb indices for Si\textsubscript{2}C\textsubscript{3}-I[t, h] are determined as:

\[
M_1(G) = 180th - 62h - 92t + 24
\]

\[
Z_2(G) = 270th - 112h - 166t + 58
\]

• The values of the bi-distance indices are quite comparable to those of the previous indices and even more precise for some characteristics. So these indices also have a good correlation with the properties of silicon carbide. The values of TIs for $t = h = 1, 2, 3, 4,$ and 5 are given in Table 6.

Table 6. Numerical Analysis for Si\textsubscript{2}C\textsubscript{3}-I[t, h]

Similar to the classical degree-based approach, it is also a good way to estimate the properties of graphs because of the good correlation with the experimental features of Si\textsubscript{2}C\textsubscript{3}-I[t, h].

Although a huge number of indices and techniques are proposed to examine the geometry and characteristics of various chemical structures, these indices are still insufficient to analyze several features of chemical and non-chemical networks. As a result, topological indices will be increasingly important in the future.

A similar study might be conducted for many chemical substances that would be valuable to chemists in their future research. New methodologies, such as the bi-distance method, can be created and applied to all degree- or distance-related topological indices. Topological indices can be used to investigate a wide range of complicated structures. Because classical degree-based indices are extremely strong and powerful, these indices will be applied to the structure that has to be explored. The most significant aspect of the significance of topological indices is the correlation coefficient values, which must be strong.

Data Availability

In this article, no data were utilized.

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Authors' Declaration:

- Conflicts of Interest: None.
- We hereby confirm that all the Figures and Tables in the manuscript are mine ours. Besides, the Figures and images, which are not mine ours,
have been given the permission for re-publication attached with the manuscript.

Ethical Clearance: The project was approved by the local ethical committee in University of Education, Lahore Pakistan.

Authors’ Contributions Statement:
Conceptualization; A. M. and M. W. R.
Methodology; M. W. R. and A. M. Investigation; S. M. A. and M. W. R. Writing original draft preparation; I. H. Writing review and editing; S. M. A. Supervision; A. M. and J. H. B. All authors read and agreed to the published version of the manuscript.

References:


الخلاصة:

تُراعى استخدام كربيد السيليكون بشكل كبير في مجالات البحث والتكنولوجيا. تمكن المؤشرات الطوبولوجية جمع بيانات على موجات الخصائص الكيميائية. أُنتجت المنتجات الطوبولوجية القائمة على الدرجة لتحليل الهياكل الكيميائية لكربيد السيليكون. لتقييم ميزات الشبكات الكيميائية أو غير ال، يتم استخدام جمعة متنوعة من المؤشرات الطوبولوجية لحساب جميع المؤثرات المضافة وكذلك المضاعفة القائمة على الدرجة. نستخدمن نظام "مصفوفة SiC4-I"، [t, h] والذي يستخدم لحساب جميع المؤثرات الطوبولوجية وكذلك المضاعفة القائمة على الدرجة لأيزومر كربيد السيليكون، "تساوي المساواة" مشتق من مفاهيم الدرجة والمسافة بطريقة يمكن من خلالها استخدام المسافة الطوبولوجية القائمة على الدرجة.

الكلمات المفتاحية: حروف ثنائية المسافة، رسم بياني جزيئي، مؤشر راندي، كربيد السيليكون، فهرس طوبولوجي، مؤشر زغرب.