

DOI: <https://doi.org/10.21123/bsj.2023.8178>

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

Abid Mahboob*¹ 
Jalal Hatem Hussein Bayati² 

Muhammad Waheed Rasheed¹ 
Iqra Hanif¹  Sajid Mahboob Alam³ 

¹Department of Mathematics, Division of Science and Technology, University of Education, Lahore Pakistan.

²Department of Mathematics, College of Science for Women, University of Baghdad, Baghdad, Iraq.

³Department of Mathematics, Minhaj University Lahore, Pakistan.

*Corresponding author: abid.mahboob@ue.edu.pk

E-mail addresses: waheedrasheed461@gmail.com, Jalalhh_math@csw.uobaghdad.edu.iq, iqrahanif955@gmail.com, sajid.mehboob@gmail.com

Received 29/11/2022, Revised 28/2/2023, Accepted 1/3/2023, Published Online First 20/5/2023,
Published 01/1/2024



This work is licensed under a [Creative Commons Attribution 4.0 International License](https://creativecommons.org/licenses/by/4.0/).

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, $\text{Si}_2\text{C}_3-1[t, h]$. 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 $\text{Si}_2\text{C}_3-1[t, h]$, 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 ².

According to the IUPAC terminology³, 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 pharmaceuticals⁴⁻⁷.

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 composition⁸.

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 graphs⁹. He used the additive and multiplicative topological versions of topology to learn more about SiC. Pan used the degree-related Banhatti and Revan indices¹⁰ 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 carbide¹¹. Sadia Akhter¹² 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)¹³. 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 Trinajstić in 1972¹⁴. 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:

$$M_1(G) = \sum_{uv \in E(G)} (d_u + d_v) Z_2(G) \\ = \sum_{uv \in E(G)} (d_u \times d_v)$$

Horoldagva used these indices for various classes of graphs¹⁵. 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 Product¹⁶.

• 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 $PM_2(G)$ ¹⁷. The multiplicative version of the classical degree-related Zagreb indices are defined as:

$$PM_1(G) = \prod_{uv \in E(G)} (d_u + d_v) PM_2(G) \\ = \prod_{uv \in E(G)} (d_u \times d_v)$$

The multiplicative form of the Zagreb indices is used to investigate the other silicon carbide isomers^{18,19}. The properties of unicycle graphs and graphs with bridges are investigated using multiplicative M-indices²⁰.

• First and Second Zagreb Polynomials:

Fath-Tabar introduced Zagreb polynomials in 2009²¹. The Zagreb index is calculated using polynomials. These polynomials are denoted by $M_1(G, K)$ and $M_2(G, K)$ are defined as:

$$M_1(G, K) = \sum_{uv \in E(G)} K^{(d_u + d_v)} M_2(G, K) \\ = \sum_{uv \in E(G)} K^{(d_u \times d_v)}$$

The Isaac graph is a very important graph; hence, these polynomials are a useful tool for studying Isaac graphs in depth²².

• Hyper-Zagreb Index:

The Hyper-Zagreb index is a modified Zagreb index that was proposed by Shirdel, Rezapour, and Sayadi²³ 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:

$$HM(G) = \sum_{uv \in E(G)} (\delta_u + \delta_v)^2$$

• **Second Modified Zagreb Index:**

The modified versions of the Zagreb indices are inspired by the usefulness of the classical Zagreb indices. The $M_2(G)$ is determined as:

$$M_2(G) = \sum_{uv \in E(G)} \frac{1}{(\delta_u \times \delta_v)}$$

• **Reduced Second Zagreb Index:**

Furtula, Gutman, and Ediz²⁴ 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:

$$RM_2(G) = \sum_{uv \in E(G)} (\delta_u - 1 \times \delta_v - 1)$$

To study further information about all Zagreb indices see²⁵.

• **Atom Bond Connectivity Index:**

In 1998, Ernesto Estrada and Fernando Torres proposed the ABC- index after being inspired by Milan Randić's work²⁶. It is used to simulate the thermal properties of organic substances.

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{\delta_u + \delta_v - 2}{\delta_u \times \delta_v}}$$

• **Randić Index:**

Millan Randić suggested the first degree-based index in 1975 to understand the branching structure of carbon atoms in organic compounds²⁷. The Randić The index is defined as:

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{\delta_u \delta_v}}$$

• **General Randić Connectivity Index:**

In 1998, Bollob and Erdos generalized Milan's index by replacing $\frac{1}{\sqrt{2}}$ with any general number α ²⁸.

$$R_\alpha(G) = \sum_{uv \in E(G)} (\delta_u \delta_v)^\alpha$$

• **Reciprocal Randić Index:**

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

$$RR(G) = \sum_{uv \in E(G)} \sqrt{\delta_u \times \delta_v}$$

• **Reduced Reciprocal Randić Index:**

It is the advanced form of the R-index and its mathematical definition is:

$$RRR(G) = \sum_{uv \in E(G)} \sqrt{(\delta_u - 1)(\delta_v - 1)}$$

• **Geometric Arithmetic Index:**

Vukicevic and Furtula suggested the GA-index in 2009²⁹ which is described as:

$$GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{\delta_u \times \delta_v}}{\delta_u + \delta_v}$$

• **Forgotten Index:**

Gutman and Furtula published this index in 2015³⁰, and it is represented as $F(G)$ which is described as:

$$F(G) = \sum_{uv \in E(G)} (\delta_u^2 + \delta_v^2)$$

• **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:

$$X_\alpha(G) = \sum_{uv \in E(G)} (\delta_u + \delta_v)^\alpha$$

• **Symmetric Division Index:**

The degree based symmetric division index was introduced by Vukicević and Furtula.

$$SD(G) = \sum_{uv \in E(G)} \frac{\delta_u^2 + \delta_v^2}{(\delta_u \times \delta_v)}$$

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 index³¹. It's written like this:

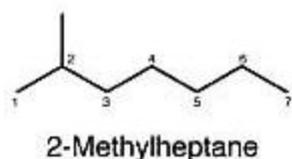
$$H(G) = \sum_{uv \in E(G)} \frac{2}{(\delta_u + \delta_v)}$$

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 SiC³²⁻³⁵. Graph theory defines broad and advanced ideas to facilitate the understanding of many problems in different fields³⁶⁻³⁹.

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.



• 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 consist 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

Edges	(d_u, d_v)	Frequency
E_1	(1,3)	2
E_2	(3,2)	1
E_3	(2,2)	3
E_4	(2,1)	1

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

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

$$\begin{aligned} &= \sum_{uv \in E_1(G)} (d_u + d_v) + \sum_{uv \in E_2(G)} (d_u + d_v) + \sum_{uv \in E_3(G)} (d_u + d_v) + \sum_{uv \in E_4(G)} (d_u + d_v) \\ &= |E_1(G)|4 + |E_2(G)|5 + |E_3(G)|4 + |E_4(G)|3 \\ &= 2(4) + 1(5) + 3(4) + 1(3) = 28 \end{aligned}$$

• 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

Edges	(d_u, d_v)	Frequency
E_1	(1, 2)	3
E_2	(3, 2)	1
E_3	(2, 2)	2
E_4	(1, 1)	1

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

$$\begin{aligned} M_1(G) &= \sum_{uv \in E(G)} (d_u + d_v) \\ &= \sum_{uv \in E_1(G)} (d_u + d_v) + \sum_{uv \in E_2(G)} (d_u + d_v) + \sum_{uv \in E_3(G)} (d_u + d_v) + \sum_{uv \in E_4(G)} (d_u + d_v) \\ &= |E_1(G)|3 + |E_2(G)|5 + |E_3(G)|4 + |E_4(G)|2 \\ &= 3(3) + 1(5) + 2(4) + 1(2) \\ &= 24 \end{aligned}$$

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 Si₂C₃-I [t, h]. ChemDraw can also be used for drawing chemical structures in an easy way.

2D Structure and Importance of Silicon Carbide Si₂C₃-I[t, h]

Fig 1 shows the 2D molecular graph of silicon carbide, Si₂C₃-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 component of cutting tools, grinding wheels, and sandpaper since the late 19th century. In 1891, the American inventor Edward G. Acheson discovered silicon carbide while attempting to make an

artificial diamond. Today, silicon carbide elements are used in the melting of glass and nonferrous metals, the heat treatment of metals, float glass manufacture, ceramics, and electronic component production, igniters in pilot lights for gas heaters, and other applications. The unit cell is the basic cell 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.

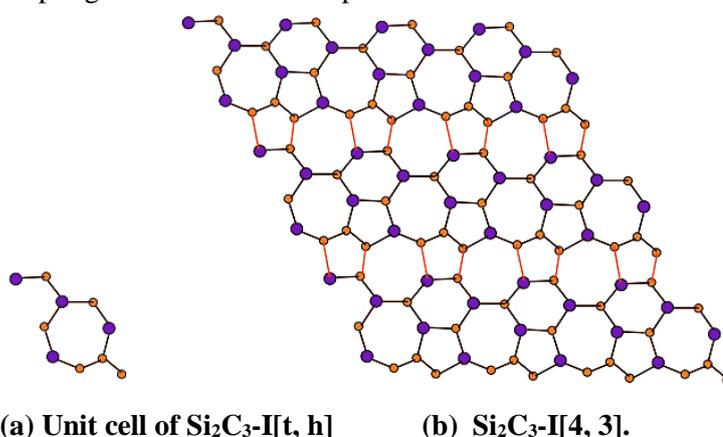


Figure 1. 2D structure of $\text{Si}_2\text{C}_3\text{-I}[t, h]$. (a) A chemical unit cell of $\text{Si}_2\text{C}_3\text{-I}[t, h]$. $\text{Si}_2\text{C}_3\text{-I}[4, 3]$. The carbon atom C is brown, while the silicon atom Si is blue

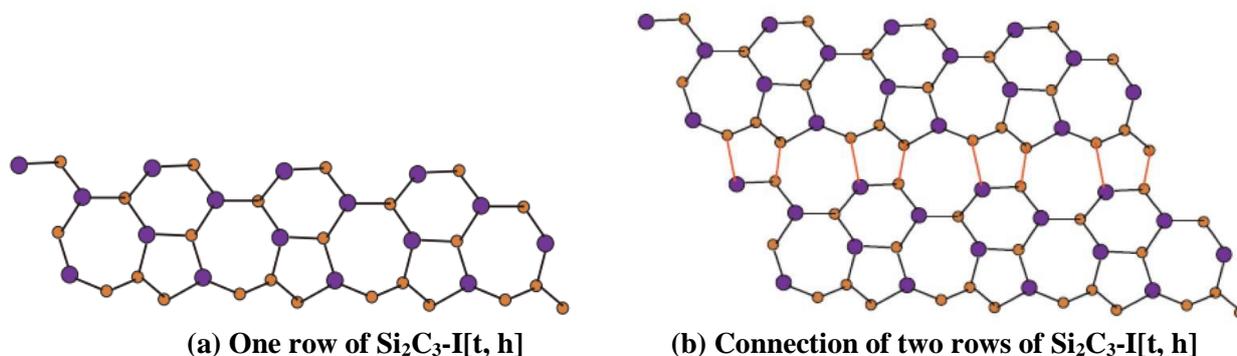


Figure 2. 2D structure of $\text{Si}_2\text{C}_3\text{-I}[t, h]$. (a) $\text{Si}_2\text{C}_3\text{-I}[t, h]$, one row with $t = 4$ and $h = 1$; (b) $\text{Si}_2\text{C}_3\text{-I}[4, 2]$, two rows are being joined together. The upper and lower rows are interlinked by red lines (edges).

There are two major ways to partition a simple, connected, and planar graph. A graph can be partitioned into groups by using vertex degree and edge degree. The edge separation technique can be used to partition the $\text{Si}_2\text{C}_3\text{-I}[t, h]$. There are five different edge bundles of $\text{Si}_2\text{C}_3\text{-I}[t, h]$ given in Table 3. The bundle E_1 is made up of 2 edges, where $d_u = 1$ and $d_v = 2$. The bundle E_2 consist of only one edge, where $d_u = 1$ and $d_v = 3$. Parcel 3, composed of $2h + 2t$ edges, where $d_u = 2$ and $d_v = 2$. The packet E_4 , consist $10h + 16t - 20$ edges, where $d_u = 2$ and $d_v = 3$. The pack E_5 has $30th - 20h - 30t + 19$ edges, where $d_u = 3$ and $d_v = 3$. The partition of edges:

$$E_1 = \{e = uv \in |E(\text{Si}_2\text{C}_3 - \text{I}[t, h])|, d_u = 1 \text{ and } d_v = 2 \}$$

$$E_2 = \{e = uv \in |E(\text{Si}_2\text{C}_3 - \text{I}[t, h])|, d_u = 1 \text{ and } d_v = 3 \}$$

$$E_3 = \{e = uv \in |E(\text{Si}_2\text{C}_3 - \text{I}[t, h])|, d_u = 2 \text{ and } d_v = 2 \}$$

$$E_4 = \{e = uv \in |E(\text{Si}_2\text{C}_3 - \text{I}[t, h])|, d_u = 2 \text{ and } d_v = 3 \}$$

$$E_5 = \{e = uv \in |E(\text{Si}_2\text{C}_3 - \text{I}[t, h])|, d_u = 3 \text{ and } d_v = 3 \}$$

Table 3. Degree-based partition of edges of $\text{Si}_2\text{C}_3\text{-I}[t, h]$

Edges	(d_u, d_v)	Frequency
E_1	(1,2)	2
E_2	(1,3)	1
E_3	(2,2)	$2h + 2t$
E_4	(2,3)	$10h + 16t - 20$
E_5	(3,3)	$30th - 20h - 30t + 19$

Theorem 1: Consider $G \cong \text{Si}_2\text{C}_3 - \text{I}[t, h]$ 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 $\text{Si}_2\text{C}_3 - \text{I}[t, h]$. 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.

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

$$= \sum_{uv \in E_1(G)} (d_u + d_v) + \sum_{uv \in E_2(G)} (d_u + d_v) + \sum_{uv \in E_3(G)} (d_u + d_v) + \sum_{uv \in E_4(G)} (d_u + d_v) + \sum_{uv \in E_5(G)} (d_u + d_v)$$

$$= |E_1(G)|3 + |E_2(G)|4 + |E_3(G)|4 + |E_4(G)|5 + |E_5(G)|6$$

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

$$M_1(G) = 180ht - 62h - 92t + 24$$

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

$$Z_2(G) = \sum_{uv \in E(G)} (d_u \times d_v)$$

$$Z_2(G) = \sum_{uv \in E_1(G)} (d_u \times d_v) + \sum_{uv \in E_2(G)} (d_u \times d_v) + \sum_{uv \in E_3(G)} (d_u \times d_v) + \sum_{uv \in E_4(G)} (d_u \times d_v) + \sum_{uv \in E_5(G)} (d_u \times d_v)$$

$$= |E_1(G)|2 + |E_2(G)|3 + |E_3(G)|4 + |E_4(G)|8 + |E_5(G)|9$$

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

$$= 270th - 112h - 166t + 58$$

Theorem 2: Consider $G \cong \text{Si}_2\text{C}_3 - \text{I}[t, h]$ be the graph of a special isomer of silicon carbide, then the multiplicative version of Zagreb indices are:

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

$$PM_2(G) = 12 \times 4^{2h+2t} \times 4^{10h+16t-20} \times 9^{30th-20h-30t+19}$$

Proof: Assume that G is a simple graph of $\text{Si}_2\text{C}_3 - \text{I}[t, h]$ 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.

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

$$= \prod_{uv \in E_1(G)} (d_u + d_v) \times \prod_{uv \in E_2(G)} (d_u + d_v) \times \prod_{uv \in E_3(G)} (d_u + d_v) \times \prod_{uv \in E_4(G)} (d_u + d_v) \times \prod_{uv \in E_5(G)} (d_u + d_v)$$

$$= 3^{|E_1(G)|} \times 4^{|E_2(G)|} \times 4^{|E_3(G)|} \times 5^{|E_4(G)|} \times 6^{|E_5(G)|}$$

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

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

The $PM_2(G)$ -index is determined as:

$$PM_2(G) = \prod_{uv \in E(G)} (d_u \times d_v)$$

$$= \prod_{uv \in E_1(G)} (d_u \times d_v) \times \prod_{uv \in E_2(G)} (d_u \times d_v) \times \prod_{uv \in E_3(G)} (d_u \times d_v) \times \prod_{uv \in E_4(G)} (d_u \times d_v) \times \prod_{uv \in E_5(G)} (d_u \times d_v)$$

$$= 2^{|E_1(G)|} \times 3^{|E_2(G)|} \times 4^{|E_3(G)|} \times 6^{|E_4(G)|} \times 9^{|E_5(G)|}$$

$$= 12 \times 4^{2h+2t} \times 6^{10h+16t-20} \times 9^{30th-20h-30t+19}$$

Theorem 3: Suppose $G \cong \text{Si}_2\text{C}_3 - \text{I}[t, h]$ is the graph of silicon carbide, then the outcomes of both the Zagreb polynomials are:

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

$$M_2(G, K) = 2K^2 + K^3 + (2h + 2t)K^4 + (10h + 16t - 20)K^6 + (30th - 20h - 30t + 19)K^9$$

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:

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

$$= \sum_{uv \in E_1(G)} K^{(d_u+d_v)} + \sum_{uv \in E_2(G)} K^{(d_u+d_v)} + \sum_{uv \in E_3(G)} K^{(d_u+d_v)} + \sum_{uv \in E_4(G)} K^{(d_u+d_v)} + \sum_{uv \in E_5(G)} K^{(d_u+d_v)}$$

$$= \sum_{uv \in E_1(G)} K^3 + \sum_{uv \in E_2(G)} K^4 + \sum_{uv \in E_3(G)} K^4 + \sum_{uv \in E_4(G)} K^5 + \sum_{uv \in E_5(G)} K^6$$

$$= |E_1(G)|K^3 + |E_2(G)|K^4 + |E_3(G)|K^4 + |E_4(G)|K^5 + |E_5(G)|K^6$$

$$= 2K^3 + K^4 + (2h+2t)K^4 + (10h+16t-20)K^5 + (30th-20h-30t+19)K^6$$

The $M_2(G, K)$ -polynomial for $\text{Si}_2\text{C}_3 - \text{I}[t, h]$ is calculated as bellow:

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

$$= \sum_{uv \in E_1(G)} K^{(d_u \times d_v)} + \sum_{uv \in E_2(G)} K^{(d_u \times d_v)} + \sum_{uv \in E_3(G)} K^{(d_u \times d_v)} + \sum_{uv \in E_4(G)} K^{(d_u \times d_v)} + \sum_{uv \in E_5(G)} K^{(d_u \times d_v)}$$

$$= \sum_{uv \in E_1(G)} K^2 + \sum_{uv \in E_2(G)} K^3 + \sum_{uv \in E_3(G)} K^4 + \sum_{uv \in E_4(G)} K^6 + \sum_{uv \in E_5(G)} K^9$$

$$= |E_1(G)|K^2 + |E_2(G)|K^3 + |E_3(G)|K^4 + |E_4(G)|K^6 + |E_5(G)|K^9$$

$$= 2K^2 + K^3 + (2h + 2t)K^4 + (10h + 16t - 20)K^6 + (30th - 20h - 30t + 19)K^9$$

Theorem 4: Let $G \cong \text{Si}_2\text{C}_3\text{-I}[t, h]$ be the graph of silicon carbide, then two different forms of Z-indices are computed as:

$$HM(G) = 1080th - 438h - 648t + 218$$

$$M_2(G) = \frac{10}{3}ht - \frac{h}{18} - \frac{t}{6} + \frac{1}{9}$$

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.

$$\begin{aligned} HM(G) &= \sum_{uv \in E(G)} (d_u + d_v)^2 \\ &= \sum_{uv \in E_1(G)} (d_u + d_v)^2 + \sum_{uv \in E_2(G)} (d_u + d_v)^2 + \sum_{uv \in E_3(G)} (d_u + d_v)^2 + \sum_{uv \in E_4(G)} (d_u + d_v)^2 \\ &\quad + \sum_{uv \in E_5(G)} (d_u + d_v)^2 \\ &= |E_1(G)|9 + |E_2(G)|16 + |E_3(G)|16 + |E_4(G)|25 + |E_5(G)|36 \\ &= 9(2) + 16(1) + 16(2h + 2t) + 25(10h + 16t - 20) + 36(30th - 20h - 30t + 19) \\ &= 1080th - 438h - 648t + 218 \end{aligned}$$

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

$$\begin{aligned} M_2(G) &= \sum_{uv \in E(G)} \frac{1}{(d_u \times d_v)} \\ &= \frac{1}{2}|E_1(G)| + \frac{1}{3}|E_2(G)| + \frac{1}{4}|E_3(G)| + \frac{1}{6}|E_4(G)| + \frac{1}{9}|E_5(G)| \\ &= \frac{2}{2} + \frac{1}{3} + \frac{2h+2t}{4} + \frac{10h+16t-20}{6} + \frac{30th-20h-30t+19}{9} \\ &= \frac{10th}{3} - \frac{h}{18} - \frac{t}{6} + \frac{1}{9} \end{aligned}$$

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

$$RM_2(G) = 120th - 58h - 86t + 36$$

$$\begin{aligned} ABC(G) &= \frac{1}{\sqrt{2}}(12h + 18t - 18) + \frac{\sqrt{2}}{\sqrt{3}} + 20th \\ &\quad - \frac{40h}{3} - 20t + \frac{38}{3} \end{aligned}$$

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:

$$\begin{aligned} RM_2(G) &= \sum_{uv \in E(G)} (d_u - 1 \times d_v - 1) \\ &= |E_1(G)|(1-1 \times 2-1) + |E_2(G)|(1-1 \times 3-1) + |E_3(G)|(2-1 \times 2-1) + |E_4(G)|(2-1 \times 3-1) + |E_5(G)|(3-1 \times 3-1) \\ &= 2(0 \times 1) + 1(0 \times 2) + 1(2h+2t) + (10h+16t-20)(1 \times 2) + (30th-20h-30t+19)(4) \\ &= 120th - 58h - 86t + 36 \end{aligned}$$

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

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

$$\begin{aligned} &= |E_1(G)|\frac{1}{\sqrt{2}} + |E_2(G)|\frac{\sqrt{2}}{\sqrt{3}} + |E_3(G)|\frac{1}{\sqrt{2}} + |E_4(G)|\frac{1}{\sqrt{2}} + |E_5(G)|\frac{2}{3} \\ &= 2\left(\frac{1}{2}\right) + \sqrt{\frac{2}{3}} + (2h + 2t)\frac{1}{\sqrt{2}} + (10h + 16t - 20)\frac{1}{\sqrt{2}} + (30th - 20h - 30t + 19)\frac{2}{3} \\ &= \frac{1}{\sqrt{2}}(12h + 18t - 18) + \sqrt{\frac{2}{3}} + 20th - \frac{40}{3}h - 20t + \frac{38}{3} \end{aligned}$$

Theorem 6: Consider $G \cong \text{Si}_2\text{C}_3\text{-I}[t, h]$ to be the two-dimensional graph of SiC, then the results of two different forms of R-index are given below.

$$R_\alpha(G) = 270th - 112h - 166t + 58$$

$$R(G) = 10.02th - 1.5980h - 2.489t + 0.1736$$

Proof: The R-index is the most common and significant index. The values of the R-index and its generalized form can be easily calculated by using Table 3.

$$\begin{aligned} R_\alpha(G) &= \sum_{uv \in E(G)} (d_u d_v)^\alpha \\ &= \sum_{uv \in E_1(G)} (d_u d_v)^\alpha + \sum_{uv \in E_2(G)} (d_u d_v)^\alpha + \sum_{uv \in E_3(G)} (d_u d_v)^\alpha + \sum_{uv \in E_4(G)} (d_u d_v)^\alpha + \sum_{uv \in E_5(G)} (d_u d_v)^\alpha \\ &= |E_1(G)|2 + |E_2(G)|3 + |E_3(G)|4 + |E_4(G)|6 + |E_5(G)|2 \\ &= 2(2) + 3(1) + 4(2h+2t) + 6(10h+16t-20) + (30th - 20h - 30t + 19) \\ &= 270th - 112h - 166t + 58 \end{aligned}$$

The $R(G)$ -index is determined as:

$$\begin{aligned} R(G) &= \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}} \\ &= \sum_{uv \in E_1(G)} \frac{1}{\sqrt{d_u d_v}} + \sum_{uv \in E_2(G)} \frac{1}{\sqrt{d_u d_v}} + \sum_{uv \in E_3(G)} \frac{1}{\sqrt{d_u d_v}} + \sum_{uv \in E_4(G)} \frac{1}{\sqrt{d_u d_v}} + \sum_{uv \in E_5(G)} \frac{1}{\sqrt{d_u d_v}} \\ &= 0.7071(2) + 0.5774(1) + 0.5(2h + 2t) + 0.4082(10h + 16t - 20) + 0.334(30th - 20h - 30t + 19) \\ &= 10.02th - 1.5980h - 2.489t + 0.1736 \end{aligned}$$

Theorem 7: Suppose $G \cong \text{Si}_2\text{C}_3\text{-I}[t, h]$ is the planar graph of an isomer of SiC, then the results related to the Randic type indices are determined below.

$$RR(G) = 90th - 31.50h - 46.808t + 12.5705$$

$$RRR(G) = 60th - 38h - 58t + 38 + \sqrt{2}(10h + 16t - 20)$$

Proof: The collection of edges of $\text{Si}_2\text{C}_3\text{-I}[t, h]$ are split into five different groups according to the degree and written as $E(G) = E_1(G) \cup E_2(G) \cup E_3(G) \cup E_4(G) \cup E_5(G)$. By using the definition of $RR(G)$:

$$\begin{aligned} RR(G) &= \sum_{uv \in E(G)} \sqrt{d_u d_v} \\ &= \sum_{uv \in E_1(G)} \sqrt{d_u d_v} + \sum_{uv \in E_2(G)} \sqrt{d_u d_v} + \\ &\sum_{uv \in E_3(G)} \sqrt{d_u d_v} + \sum_{uv \in E_4(G)} \sqrt{d_u d_v} \\ &\quad + \sum_{uv \in E_5(G)} \sqrt{d_u d_v} \\ &= 1.4142(2) + 1.7321(1) + 2(2h + 2t) + \\ &\quad 2.4495(10h + 16t - 20) + \\ &\quad 3(30th - 20h - 30t + 19) \\ &= 90th - 31.50h - 46.808t + 12.5705 \end{aligned}$$

The RRR(G)-index is computed as:

$$\begin{aligned} RRR(G) &= \sum_{uv \in E(G)} \sqrt{(d_u - 1)(d_v - 1)} \\ &= \sum_{uv \in E_1(G)} \sqrt{(d_u - 1)(d_v - 1)} + \\ &\sum_{uv \in E_2(G)} \sqrt{(d_u - 1)(d_v - 1)} + \sum_{uv \in E_3(G)} \sqrt{(d_u - 1)(d_v - 1)} \\ &\quad + \sum_{uv \in E_4(G)} \sqrt{(d_u - 1)(d_v - 1)} + \\ &\sum_{uv \in E_5(G)} \sqrt{(d_u - 1)(d_v - 1)} \\ &= |E_1(G)|0 + |E_2(G)|0 + |E_3(G)|1 + \\ &\quad |E_4(G)|\sqrt{2} + |E_5(G)|2 \\ &= 60th - 38h - 58t + 38 + \sqrt{2}(10h + \\ &\quad 16t - 20) \end{aligned}$$

Theorem 8: Let $G \cong Si_2C_3-I[t, h]$ be the graph of silicon carbide.

$$GA(G) = 30th - 28t - 18h + \frac{1}{3\sqrt{3}}(4\sqrt{6} + 63) + \frac{2\sqrt{6}}{5}(10h + 16t - 20)$$

$$SD(G) = 60th - \frac{43}{3}h - 64t - 5$$

Proof: By using Table 3 and the definition of GA-index, it can be easily computed as:

$$\begin{aligned} GA(G) &= \sum_{uv \in E(G)} 2 \frac{\sqrt{d_u d_v}}{d_u + d_v} \\ &= \sum_{uv \in E_1(G)} 2 \frac{\sqrt{d_u d_v}}{d_u + d_v} + \sum_{uv \in E_2(G)} 2 \frac{\sqrt{d_u d_v}}{d_u + d_v} + \\ &\quad \sum_{uv \in E_3(G)} 2 \frac{\sqrt{d_u d_v}}{d_u + d_v} + \\ &\quad \sum_{uv \in E_4(G)} 2 \frac{\sqrt{d_u d_v}}{d_u + d_v} + \\ &\quad \sum_{uv \in E_5(G)} 2 \frac{\sqrt{d_u d_v}}{d_u + d_v} \\ &= \frac{2\sqrt{2}}{3} |E_1(G)| + \frac{2}{\sqrt{3}} |E_2(G)| + 1|E_3(G)| + \\ &\quad \frac{2\sqrt{6}}{5} |E_4(G)| + 1|E_5(G)| \\ &= \frac{2\sqrt{2}}{3} (2) + \frac{2}{\sqrt{3}} (1) + 1(2h + 2t) + \frac{2\sqrt{6}}{5} \\ &\quad (10h + 16t - 20) + 1(30th - \\ &\quad 20h - 30t + 19) \\ &= 30ht - 28t - 18h + \frac{1}{3\sqrt{3}}(4\sqrt{6} + 63) + \\ &\quad \frac{2\sqrt{6}}{5} (10h + 16t - 20) \end{aligned}$$

The SD(G)-index can be identified as:

$$\begin{aligned} SD(G) &= \sum_{uv \in E(G)} \frac{d_u^2 + d_v^2}{(d_u + d_v)} \\ &= \sum_{uv \in E_1(G)} \frac{d_u^2 + d_v^2}{(d_u + d_v)} + \\ &\quad \sum_{uv \in E_2(G)} \frac{d_u^2 + d_v^2}{(d_u + d_v)} + \\ &\quad \sum_{uv \in E_3(G)} \frac{d_u^2 + d_v^2}{(d_u + d_v)} + \\ &\quad \sum_{uv \in E_4(G)} \frac{d_u^2 + d_v^2}{(d_u + d_v)} + \\ &\quad \sum_{uv \in E_5(G)} \frac{d_u^2 + d_v^2}{(d_u + d_v)} \end{aligned}$$

$$\begin{aligned} &= \frac{5}{2} |E_1(G)| + \frac{10}{3} |E_2(G)| + \frac{8}{4} |E_3(G)| + \\ &\quad \frac{13}{6} |E_4(G)| + \frac{18}{9} |E_5(G)| \\ &= \frac{5}{2} (2) + \frac{10}{3} (1) + \frac{8}{4} (2h + 2t) + \\ &\quad \frac{13}{6} (10h + 16t - 20) + \frac{18}{9} (30ht - \\ &\quad 20h - 30t + 19) \\ &= 60ht - \frac{43}{3}h - 64t - 5 \end{aligned}$$

Theorem 9: Consider $G \cong Si_2C_3-I[t, h]$ be the graph of a particular isomer of SiC, then resultant values of F-index and H-index are given below:

$$F(G) = 540ht - 86h - 316t + 9$$

$$H(G) = 10ht - \frac{5}{3}h - \frac{13}{5}t + \frac{1}{6}$$

Proof: The 2D general structure of $Si_2C_3-I[t, h]$ 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:

$$\begin{aligned} F(G) &= \sum_{uv \in E(G)} (d_u^2 + d_v^2) \\ &= \sum_{uv \in E_1(G)} (d_u^2 + d_v^2) + \\ &\quad \sum_{uv \in E_2(G)} (d_u^2 + d_v^2) + \\ &\quad \sum_{uv \in E_3(G)} (d_u^2 + d_v^2) + \\ &\quad \sum_{uv \in E_4(G)} (d_u^2 + d_v^2) + \\ &\quad \sum_{uv \in E_5(G)} (d_u^2 + d_v^2) \\ &= |E_1(G)|5 + |E_2(G)|10 + |E_3(G)|8 + \\ &\quad |E_4(G)|13 + |E_5(G)|18 \\ &= 5(1) + 10(1) + 8(2h + 2t) + \\ &\quad 13(10h + 16t - 20) + 18(30ht - \\ &\quad 20h - 30t + 19) \\ &= 540ht - 86h - 316t + 97 \end{aligned}$$

The H(G)-index is calculated as:

$$\begin{aligned} H(G) &= \sum_{uv \in E(G)} \frac{2}{(d_u + d_v)} \\ &= \sum_{uv \in E_1(G)} \frac{2}{(d_u + d_v)} + \sum_{uv \in E_2(G)} \frac{2}{(d_u + d_v)} \\ &\quad + \sum_{uv \in E_3(G)} \frac{2}{(d_u + d_v)} + \sum_{uv \in E_4(G)} \frac{2}{(d_u + d_v)} \\ &\quad + \sum_{uv \in E_5(G)} \frac{2}{(d_u + d_v)} \\ &= |E_1(G)|\frac{2}{3} + |E_2(G)|\frac{2}{4} + |E_3(G)|\frac{2}{4} + \\ &\quad |E_4(G)|\frac{2}{5} + |E_5(G)|\frac{2}{6} \\ &= \frac{2}{3} (2) + \frac{1}{2} (1) + \frac{1}{2} (2h + 2t) + \\ &\quad \frac{2}{5} (10h + 16t - 20) + \frac{1}{3} (30th - \\ &\quad 20h - 30t + 19) \\ &= 10ht - \frac{5}{3}h - \frac{13}{5}t + \frac{1}{6} \end{aligned}$$

Theorem 10: Let $G \cong Si_2C_3-I[t, h]$ be the graph of silicon carbide without loops and multiple edges than the values of $X_\alpha(G)$ are:

$$X_\alpha(G) = 180ht - 62h - 92t + 24$$

Proof: The edges collection $E(G)$ splits into 5 different edges which can be written as $E(G) = E_1(G) \cup E_2(G) \cup E_3(G) \cup E_4(G) \cup E_5(G)$. According to Table 3, the outcome of $X_\alpha(G)$ is calculated as:

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

$$\begin{aligned}
 &= \sum_{uv \in E_1(G)} (\delta_u + \delta_v)^\alpha + \sum_{uv \in E_2(G)} (\delta_u + \delta_v)^\alpha + \sum_{uv \in E_3(G)} (\delta_u + \delta_v)^\alpha + \sum_{uv \in E_4(G)} (\delta_u + \delta_v)^\alpha + \sum_{uv \in E_5(G)} (\delta_u + \delta_v)^\alpha \\
 &= |E_1(G)|(3)^\alpha + |E_2(G)|(4)^\alpha + |E_3(G)|(4)^\alpha + |E_4(G)|(5)^\alpha + |E_5(G)|(6)^\alpha \\
 &= (3)^\alpha(2) + (4)^\alpha + (4)^\alpha(2h+2t) + (5)^\alpha(10h+16t-20) + (6)^\alpha(30th-20h-30t+19)
 \end{aligned}$$

If $\alpha=1$ then,

$$= 180th - 62h - 92t + 24$$

Numerical Analysis

This section represents the numerical calculation of silicon carbide, $Si_2C_3-I[t, h]$. 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.

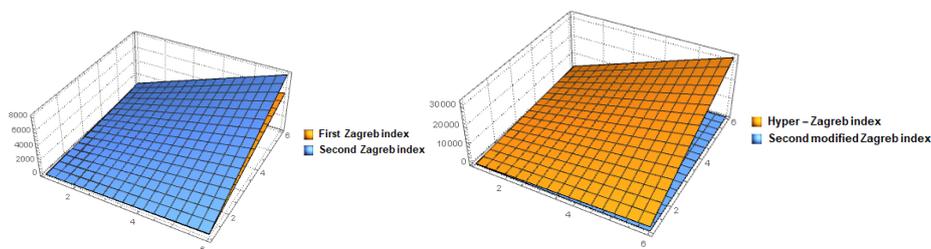
Table 4. Numerical Analysis for $Si_2C_3-I[t, h]$

Topological indices	(t, h)=[1, 1]	(t, h)=[2, 2]	(t, h)=[3, 3]	(t, h)=[4, 4]	(t, h)=[5, 5]
$M_2(G)$	50	436	1182	2288	3754
$Z_2(G)$	50	582	1654	3266	5418
$PM_1(G)$	1.247×10^{39}	4.074×10^{43}	3.520×10^{46}	2.136×10^{49}	1.068×10^{52}
$PM_2(G)$	4.972×10^{44}	1.612×10^{49}	1.393×10^{52}	1.290×10^{50}	4.031×10^{51}
$HM(G)$	212	2366	6680	13154	21788
$M_2(G)$	3.23	13	29.45	52.56	82.34
$RM_2(G)$	12	228	684	1380	2316
$ABC(G)$	8.6321	56.52	144.399	272.28	440.16
$R_\alpha(G)$	50	582	1654	3266	5418
$R(G)$	6.1066	32.08	78.093	144.15	230.24
$RR(G)$	24.27	215.96	587.65	1139.34	1871.04
$RRR(G)$	10.49	131.26	372.03	732.794	1213.57
$GA(G)$	23.89	113.37	263.42	460.56	741.79
$SD(G)$	-23.34	78.34	300	641.67	1103.34
$F(G)$	235	1453	3751	7129	11587
$H(G)$	5.9	31.64	77.37	143.1	228.84
$X_\alpha(G)$	50	436	1182	2288	3754

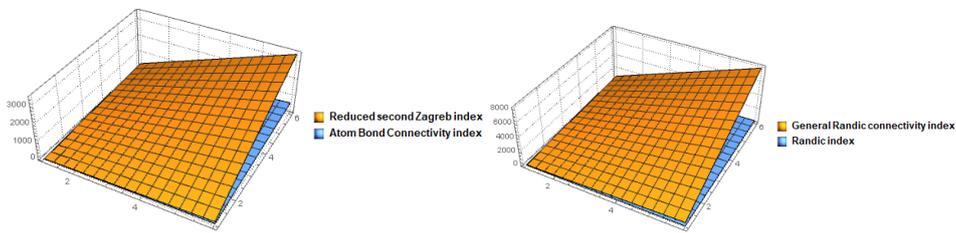
Graphical Analysis of Data

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

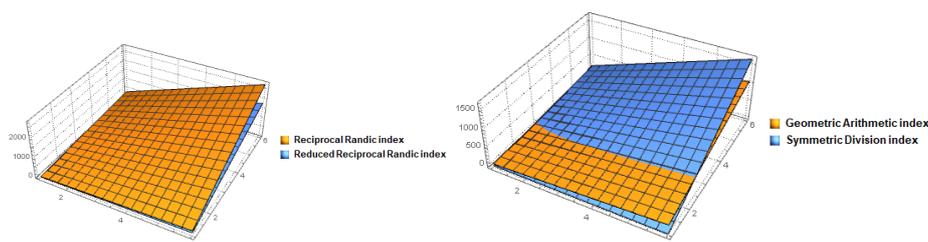
key ideas simply and effectively. According to the type of data, there are several graph types, including bar charts, line graphs, area graphs, scatter plots, pie charts, pictographs, column charts, and bubble charts. The 3D axis graphs are used here to understand the relationship between the T-indices 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.



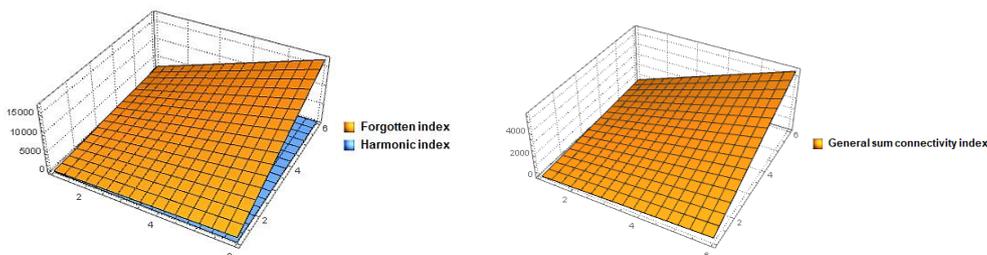
(a) The first and second Zagreb indices (b) The HM and second modified Zagreb indices



(c) The RM_2 and ABC indices (d) The general R-index and R-index



(e) The RR-index and RRR-index (f) The GA-index and SD-index



(g) The F-index and H-index (h) The SC-index

Figure 3. All the 3D graphs of degree based indices

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 $Si_2C_3-1[t, h]$ 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 carbide³⁵.

- 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 $t = h = 1, 2, 3, 4,$ and 5 .

Table 5. Numerical Analysis for $Si_2C_3-1[t, h]$

Topological indices	(t, h)=[1, 1]	(t, h)=[2, 2]	(t, h)=[3, 3]	(t, h)=[4, 4]	(t, h)=[5, 5]
$M_1(G)$	44	264	664	1244	2004
$Z_2(G)$	47	350	923	1766	2879

- Fig 4 illustrates the graphical representations of the first and second Zagreb indices for the isomer of SiC.

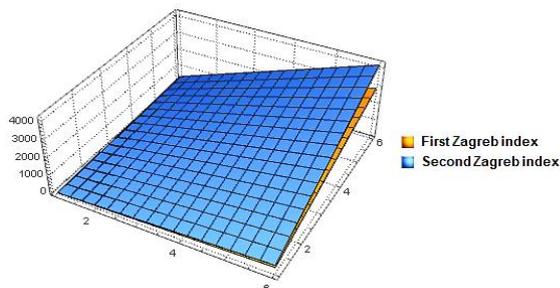


Figure 4. First and second Zagreb indices for $\text{Si}_2\text{C}_3-1[t, h]$

Table 6. Numerical Analysis for $\text{Si}_2\text{C}_3-1[t, h]$

Topological indices	(t, h)=[1, 1]	(t, h)=[2, 2]	(t, h)=[3, 3]	(t, h)=[4, 4]	(t, h)=[5, 5]
$M_1(G)$	50	436	1182	2288	3754
$Z_1(G)$	50	582	1654	3266	5418

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

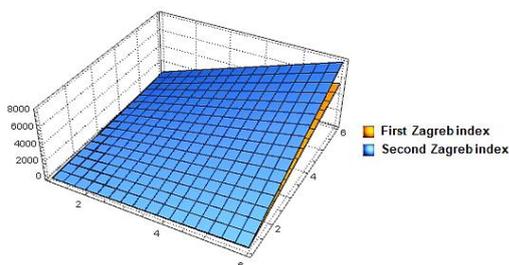


Figure 5. The bi-distance M_1 and M_2 -indices of $\text{Si}_2\text{C}_3-I[t, h]$

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 above, which analyzed fixed variables connected to chemical structure graphs. In chemistry, silicon carbide, $\text{Si}_2\text{C}_3-I[t, h]$, plays a crucial role, especially in manufacturing techniques and host-guest collisions. Silicon carbide is often used in protective jackets, automobile clutches, vehicle brake pads, LED bulbs, and sensors. The effect of various multiplicative implementations of degree-based topological invariants of silicon carbide, $\text{Si}_2\text{C}_3-I[t, h]$ was explored. The results of this study can be used to better understand the biological activities and physical characteristics of silicon carbide.

Bi- distance Topological Index

The bi-distance first and second Zagreb indices for $\text{Si}_2\text{C}_3-1[t, h]$ 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.

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 $\text{Si}_2\text{C}_3-I[t, h]$.

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.

Funding Statement

This research received no funding.

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. H. B. All authors read and agreed to the published version of the manuscript.

References:

1. Rätz T. Euler's Königsberg: The Explanatory Power of Mathematics. *Eur J Philos Sci.* 2018; 8(3): 331-346. https://doi.org/10.1007/978-1-4419-0594-9_8
2. Liu JB. Novel Applications of Graph Theory in Chemistry and Drug Designing. *Comb Chem High Throughput Screen.* 2022 Mar 1; 25(3): 439-40. <https://doi.org/10.2174/1386207325666220104223136>
3. Malik MYH, Binyamin MA, Hayat S. Correlation Ability of Degree-Based Topological Indices for Physicochemical Properties of Polycyclic Aromatic Hydrocarbons with Applications. *Polycycl Aromat Compd.* 2022 Oct 21; 42(9): 6267-6281. DOI: <https://doi.org/10.1080/10406638.2021.1977349>
4. Mondal S, De N, Pal A. Topological Indices of Some Chemical Structures Applied for the Treatment of COVID-19 patients. *Polycycl Aromat Compd.* 2022 Apr 21; 42(4): 1220-34. <https://doi.org/10.1080/10406638.2020.1770306>
5. Bokhary SAU, Adnan, Siddiqui MK, Cancan M. On Topological Indices and QSPR Analysis of Drugs Used for the Treatment of Breast Cancer. *Polycycl Aromat Compd.* 2022 Oct 21; 42(9): 6233-6253. <https://doi.org/10.1080/10406638.2021.1977353>
6. Nicolaou CA, Apostolakis J, Pattichis CS. De Novo Drug Design Using Multi Objective Evolutionary Graphs. *J Chem Inf Model.* 2009 Jan 26; 49(2): 295-307. <https://doi.org/10.1021/ci800308h>
7. Ibrahim M, Zahra N, Siddiqui MK. On Ve-Degree and Ev-Degree Based Topological Indices for the Series of Benzenoid Graphs. *Polycycl Aromat Compd.* 2022 Aug 9; 42(7): 4726-4735. <https://doi.org/10.1080/10406638.2021.1926294>
8. Shao Z, Jahanbani A, Sheikholeslami SM. Multiplicative Topological Indices of Molecular Structure in Anticancer Drugs. *Polycycl Aromat Compd.* 2022 Feb 14; 42(2): 475-488. <https://doi.org/10.1080/10406638.2020.1743329>
9. Sardara MS, Alia MA, Ashrafa F, Cancanb M. On Topological Indices of Double and Strong Double Graph of Silicon Carbide Si₂C₃-I [p, q]. *Eurasian Chem. Commun.* 2023; 5: 37-49. <https://doi.org/10.22034/ecc.2023.356160.1519>
10. Pan Y-H, Khalid A, Ali P, Rehman AU, Siddiqui MK, Ishtiaq M, et. al. Topological Study of Polycyclic Silicon Carbide Structure. *Polycycl Aromat Compd.* 2022 Jan 1; 43(2): 1-2. <https://doi.org/10.1080/10406638.2021.2024861>
11. Wang XL, Siddiqui MK, Kirmani SA, Manzoor S, Ahmad S, Dhlamini M. On Topological Analysis of Entropy Measures for Silicon Carbides Networks. *Complexity.* 2021 Nov 5; 2021(2): 1-26. DOI: <https://doi.org/10.1155/2021/4178503>
12. Akhter S, Ashraf R. Harmonic Polynomial and Harmonic Index of Silicon Carbide Graphs SiC₃-I and SiC₃-II. *Int J Fuzzy Math Arch.* 2019 October 22; 17(2): 83-89. <http://dx.doi.org/10.22457/204ijfma.v17n2a3>
13. Cioabă SM, Murty MR. A First Course in Graph Theory and Combinatorics. 2nd edition. Texts and Readings in Mathematics 55. Springer; 2022 July 8. p. 252. <https://link.springer.com/book/10.1007/978-981-19-0957-3>
14. Gutman I, Trinajstić N. Graph Theory and Molecular Orbitals. Total ϕ -electron Energy of Alternant Hydrocarbons. *Chem Phys Lett.* 1972 Dec 15; 17(4): 535-8. [https://doi.org/10.1016/0009-2614\(72\)85099-6](https://doi.org/10.1016/0009-2614(72)85099-6)
15. Horoldagva B, Das KC. On Zagreb Indices of Graphs. *MATCH Commun. Math Comput Chem.* 2021; 85(2): 295-301. https://match.pmf.kg.ac.rs/electronic_versions/Match85/n2/match85n2_295-301.pdf
16. Javaid M, Javed S, Alanazi AM, Alotaibi MR. Computing analysis of Zagreb Indices for Generalized Sum Graphs Under Strong Product. *J Chem.* 2021 Jan 9; 2021: 1-20. <https://doi.org/10.1155/2021/6663624>
17. Todeschini R, Ballabio D, Consonni V. Novel Molecular Descriptors Based on Functions of New Vertex Degrees. In Gutman I, Furtula B, editors. *Novel Molecular Structure Descriptors - Theory and Applications I.* Serbia: Kragujevac J Math; 2010. p. 73-100.
18. Mondal S, De N, Pal A. Multiplicative Degree Based Topological Indices of Nanostar Dendrimers. *Biointerface Res Appl Chem.* 2021 Jul; 11(1): 7700-11.
19. Alam SM, Jarad F, Mahboob A, Siddique I, Altunok T, Rasheed MW. A Survey on Generalized Topological Indices for Silicon Carbide Structure. *J Chem.* 2022 Jun 2; 2022: 1-11. <https://doi.org/10.1155/2022/7311404>
20. Alfuraidan MR, Imran M, Jamil MK, Vetrík T. General Multiplicative Zagreb Indices of Graphs with Bridges. *IEEE Access.* 2020 Jun 25; 8: 118725-31.
21. Fath-Tabar G. Zagreb Polynomial and PI Indices of Some Nano Structures. *Dig J Nanomater Biostructures.* 2009 Mar 1; 4(1): 189 – 191.
22. Poojary P, Raghavendra A, Shenoy BG, Farahani MR, Sooryanarayana B. Certain Topological Indices and Polynomials for the Isaac graphs. *J Discrete Math. Sci Cryptogr.* 2021 Feb 17; 24(2): 511-25.

23. Shirdel GH, Rezapour H, Sayadi AM. The Hyper-Zagreb Index of Graph Operations. *Iranian J Math Chem.* 2013 Dec; 4(2): 213-220.
24. Furtula B, Gutman I, Ediz S. On Difference of Zagreb Indices. *Discret Appl Math.* 2014 Dec 11; 178: 83-8.
25. Chu YM, Siddiqui MK, Javed S, Sherin L, Kausar F. On Zagreb Type Molecular Descriptors of Ceria Oxide and their Applications. *J Clust Sci.* 2022 Mar; 33(2): 537-46.
26. Estrada E, Torres L, Rodriguez L, Gutman I. An Atom-Bond Connectivity Index: Modelling the Enthalpy of Formation of Alkanes. *Indian J Chem.* 1998; 37A: 1998; 849-855.
27. Randic M. Characterization of Molecular Branching. *J. Am. Chem. Soc.* 1975 Nov; 97(23): 6609-15.
28. Bollobás B, Erdős P. Graphs of Extremal Weights. *Ars combinatoria.* 1998; 50: 225-233.
29. Vukičević D, Furtula B. Topological Index Based on the Ratios of Geometrical and Arithmetical Means of end-Vertex Degrees of Edges. *J Math Chem.* 2009 Nov; 46(4): 1369-76.
30. Furtula B, Gutman I. A Forgotten Topological Index. *J Math Chem.* 2015 Apr; 53(4): 1184-90.
31. Zhong L. The Harmonic Index for Graphs. *Appl Math Lett.* 2012 Mar 1; 25(3): 561-6.
32. Mahboob A, Alrowaili D, Alam SM, Ali R, Rasheed MW, Siddique I. Topological Attributes of Silicon Carbide $SiC_4-II[i, j]$ Based on Ve-Degree and Ev-Degree. *J Chem.* 2022 April 7; 2022(4): 1-11. <https://doi.org/10.1155/2022/3188993>
33. Mahboob A, Mahboob S, Jaradat MM, Nigar N, Siddique I. On Some Properties of Multiplicative Topological Indices in Silicon-Carbon. *J Math.* 2021 Nov 8; 2021: 1-10. <https://doi.org/10.1155/2021/4611199>
34. Lee JR, Hussain A, Fahad A, Raza A, Qureshi MI, Mahboob A, Park C. On ev and ve-Degree Based Topological Indices of Silicon Carbides. *CMES-Comput Model Eng Sci.* 2022 Jan 1; 130(2): 871-85.
35. Mahboob A, Muhiuddin G, Siddique I, Alam SM. A View of Banhatti and Revan Indices in Chemical Graphs. *J Math.* 2022 Jul 31; 2022: 1-8. <https://doi.org/10.1155/2022/5680712>
36. Ahmed A. Omran, Oda HH. Hn-Domination in Graphs. *Baghdad Sci J.* 2019; 16(1(Suppl.)): 242-247. [https://doi.org/10.21123/bsj.2019.16.1\(Suppl.\).0242](https://doi.org/10.21123/bsj.2019.16.1(Suppl.).0242)
37. Mekala A, Murali R. Topological Indices Polynomials of Domination David Derived Networks. *Baghdad Sci J.* 2022 Nov. 20; 1-12. <https://doi.org/10.21123/bsj.2022.6909>
38. Sporns O. Graph Theory Methods: Applications in Brain Networks. *Dialogues Clin Neurosci.* 2018 Jun; 20(2): 111-121.
39. Alsulami SH, Bayati JH. COVID-19 Infection Structure Analysis Based on Minimum Spanning Tree Visualization in the Kingdom of Saudi Arabia Regions. *J Chem.* 2022 Jul 26; 2022: 1-8. <https://doi.org/10.1155/2022/1726286>

نهج المسافة الثنائية لتحديد الثوابت التوبولوجية لكربيد السيليكون

اقرأ حنيف¹

جلال حاتم حسين البياتي²

محمد وحيد رشيد¹

عابد محبوب¹

ساجد محبوب علام³

¹ قسم الرياضيات، شعبة العلم والتكنولوجيا، جامعة التبرية، لاهور، باكستان.

² قسم الرياضيات، كلية العلوم للبنات، جامعة بغداد، بغداد، العراق.

³ قسم الرياضيات، جامعة مناهج، لاهور، باكستان.

الخلاصة:

يتزايد استخدام كربيد السيليكون بشكل كبير في مجالات البحث والتكنولوجيا. تمكن المؤشرات التوبولوجية جمع البيانات على الرسوم البيانية الجبرية وتوفر إطاراً رياضياً لتحليل الخصائص الهيكلية الكيميائية. في هذه الورقة، يتم استخدام المؤشرات التوبولوجية المعروفة القائمة على الدرجة لتحليل الهياكل الكيميائية لكربيدات السيليكون. لتقييم ميزات الشبكات الكيميائية أو غير الكيميائية المختلفة، يتم تحديد مجموعة متنوعة من المؤشرات التوبولوجية. في هذه الورقة، نقدم مفهوماً جديداً يتعلق بدرجة الرسم البياني يسمى "ثنائية المسافة"، والذي يستخدم لحساب جميع المؤشرات المضافة وكذلك المضاعفة القائمة على الدرجة لأيزومر كربيد السيليكون، $Si_2C_3-1[t, h]$ مصطلح "ثنائية المسافة" مشتق من مفاهيم الدرجة والمسافة بطريقة يمكن من خلالها استخدام المسافة الثنائية لحساب المؤشرات التوبولوجية القائمة على الدرجة.

الكلمات المفتاحية: حواف ثنائية المسافة، رسم بياني جزئي، مؤشر راندي، كربيد السيليكون $Si_2C_3-1[t, h]$ ، فهرس طوبولوجي، مؤشر زغرب.