

A Mathematical Study of Irregularity Indices for the Silicon Carbide Lattice $Si_2C_3[p, q]$

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Abstract

Graph theory provides a powerful mathematical framework for analyzing and representing molecular structures, where atoms and chemical bonds are modeled as vertices and edges, respectively. In this study, we investigate the two-dimensional (2D) silicon carbide network Si_2C_3 using graph-theoretic techniques. In particular, we focus on irregularity-based topological indices, which quantify the degree of structural irregularity within molecular graphs and provide valuable insights into their structural and physicochemical characteristics. Sixteen irregularity-related topological indices are computed for the Si_2C_3 network, including the First Zagreb Index, Second Zagreb Index, Randić Index, Degree Variance, Albertson Irregularity Index, and several other related indices. The obtained results provide a comprehensive mathematical characterization of the structural properties of the silicon carbide network and may contribute to a better understanding of its potential applications in chemical and material sciences.

Keywords: Topological index, irregularity indices, Zagreb index, (2-D) Silicon Carbon $Si_2C_3 - I$, $Si_2C_3 - II$ and $Si_2C_3 - III$

1 Introduction

Graphs are mathematical structures used to model pairwise relationships between objects. They are one of the principal objects of study in discrete mathematics. A graph consists of vertices that are connected by edges. Graphs can be used to model various types of relationships and processes in physical, biological, chemical, social, and information systems. Consequently, many practical problems can be represented using graphs.

Mathematical chemistry is a modern field of chemistry in which mathematical techniques are used to describe and analyze chemical structures and their properties. In recent years, numerous studies have been conducted in the field of graph theory and its applications to chemistry. Chemical compounds or molecules represented by structural formulas can be modeled as graphs, which are referred to as molecular graphs. Graph theory provides effective tools for enumerating molecular structures, organizing complex chemical information, developing computational procedures, and representing the relationships between atoms and chemical bonds. These graph-theoretical tools are particularly important in chemistry because of the prevalence of isomerism, which arises from different arrangements of atoms within molecular structures. The study of molecular structures according to well-defined principles is therefore an essential aspect of mathematical chemistry.

This concept plays an important role in the field of chemical sciences. Graph theory can be used to represent a chemical structure, where the vertices represent atoms and the edges represent chemical bonds. Chemical graph theory is a branch of mathematical chemistry that establishes a connection between mathematics, graph theory, and chemistry and provides mathematical approaches for solving chemical problems [1–4]. Many chemical compounds possess unique mathematical structures with numerous applications in industrial, medicinal, research, and commercial chemistry. The arrangement of atoms within a chemical molecule follows specific structural principles that contain useful underlying information. Therefore, analyzing these structural characteristics using mathematical tools, computational techniques, and topological methods plays an important role in applied research.

Silicon is distinguished from many other semiconductor materials by several important properties, including its low cost, relatively low toxicity, abundant availability, and the extensive research conducted on its purification, processing, and device

fabrication. It is widely used in modern technological devices and electronic applications. Topological indices are numerical graph invariants that remain unchanged under graph isomorphism. They play an important role in quantitative structure–activity relationship (QSAR) and quantitative structure–property relationship (QSPR) studies [5, 6].

In this study, we analyze the two-dimensional (2D) silicon carbide structures Si_2C_3 -I, Si_2C_3 -II, and Si_2C_3 -III, which correspond to the first, second, and third lowest-energy structures, respectively. Considerable efforts have been devoted to predicting the most stable configurations of the Si_2C_3 sheet.

Let G be a molecular graph, where $V(G)$ represents the set of vertices corresponding to atoms and $E(G)$ represents the set of edges corresponding to chemical bonds. The degree of a vertex u is denoted by d_u and represents the number of edges incident to u . Similarly, the degree of a vertex v is denoted by d_v . There are several classes of topological indices, including eccentricity-based, degree-based, and distance-based indices, among others. In this paper, we focus on degree-based topological indices.

The numerical parameters used to characterize the structural properties of a graph are known as topological indices. In 1947, Harry Wiener introduced the Wiener index, which is generally regarded as the first topological index. Subsequently, the systematic development of topological indices and their applications in chemistry was significantly advanced by researchers such as Gutman and Trinajstić.

The Zagreb indices were first introduced by Gutman in 1970 [9], they are important molecular descriptors and have been closely correlated with many chemical properties [10–12] and defined as: In fact, one can rewrite the first Zagreb index as

$$M_1(G) = \sum_{st \in E(G)} [d_s + d_t]. \quad (1)$$

The second zagreb index is defined as

$$M_2(G) = \sum_{st \in E(G)} d_s d_t \quad (2)$$

Among widely used graph invariants One such type is the degree-variance proposed by Bell defined as.

$$VAR(G) = \frac{M_1(G)}{n} - \left(\frac{2m}{n}\right)^2 \quad (3)$$

The Albertson irregularity index is defined as [13]

$$AL(G) = \sum_{st \in E(G)} |d_s - d_t| \quad (4)$$

$$IR1(G) = \sum_{s \in t} d_s^3 - \frac{2m}{n} \sum_{s \in t} d_s^2 \quad (5)$$

$$IR2(G) = \sqrt{\frac{M_2(G)}{m}} - \frac{2m}{n} \quad (6)$$

The irregularity index $IRF(G)$ introduced by Gutman in 2018 [14] be defined as

$$IRF(G) = \sum_{st \in E(G)} (d_s - d_t)^2 \quad (7)$$

$$IRFW(G) = \frac{IRF(G)}{M_2(G)} \quad (8)$$

The Randic index $IRA(G)$ was described as by Li and Gutman in 2006 [15] defined as

$$IRA(G) = \sum_{st \in E(G)} \left(d_s^{-\frac{1}{2}} - d_t^{-\frac{1}{2}}\right)^2 \quad (9)$$

$$IRB(G) = \sum_{st \in E(G)} \left(d_s^{\frac{1}{2}} - d_t^{\frac{1}{2}}\right)^2 \quad (10)$$

$$IRC(G) = \sum_{st \in E(G)} \frac{\sqrt{d_s d_t}}{m} - \frac{2m}{n} \quad (11)$$

$$IRDIF(G) = \sum_{st \in E(G)} \left| \frac{d_s}{d_t} - \frac{d_t}{d_s} \right| \quad (12)$$

The irregularity index $IRL(G)$ and $IRLU(G)$ introduced by Vukicevic and Gasparov in (2004) [16] defined as

$$IRL(G) = \sum_{st \in E(G)} |lnd_s - lnd_t| \quad (13)$$

$$IRLU(G) = \sum_{st \in E(G)} \frac{|d_s - d_t|}{\min(d_s, d_t)} \quad (14)$$

$$IRLF(G) = \sum_{st \in E(G)} \frac{|d_s - d_t|}{\sqrt{(d_s, d_t)}} \quad (15)$$

$$IRLA(G) = 2 \sum_{st \in E(G)} \frac{|d_s - d_t|}{(d_s + d_t)} \quad (16)$$

$$IRDI(G) = \sum_{st \in E(G)} \ln(1 + |d_s - d_t|) \quad (17)$$

$$IRGA(G) = \sum_{st \in E(G)} \ln \left(\frac{d_s + d_t}{2\sqrt{d_s d_t}} \right) \quad (18)$$

2 Irregularity indices of Silicon Carbide $Si_2C_3 - I[p, q]$

We will discuss the graph of silicon carbide network $Si_2C_3 - I$ in the given figure 1 and computing the irregularity index of the given graph. In figure 1 the graph (a) is denoted the single unit cell of a molecular graph silicon carbide $Si_2C_3 - I$ and (b) denoted the multi-unit cell. The number of a unit cell is connected in rows, or column and is denoted by p and q respectively, in 1 to demonstrate how the unit cell is joined and how one row is connected to another row. The total number of vertices and edges in a graph depends on $[p, q]$. In silicon carbide network $Si_2C_3 - I$, the number of vertices is $10pq$ and the total number of edges is $15pq - 2p - 3q$.

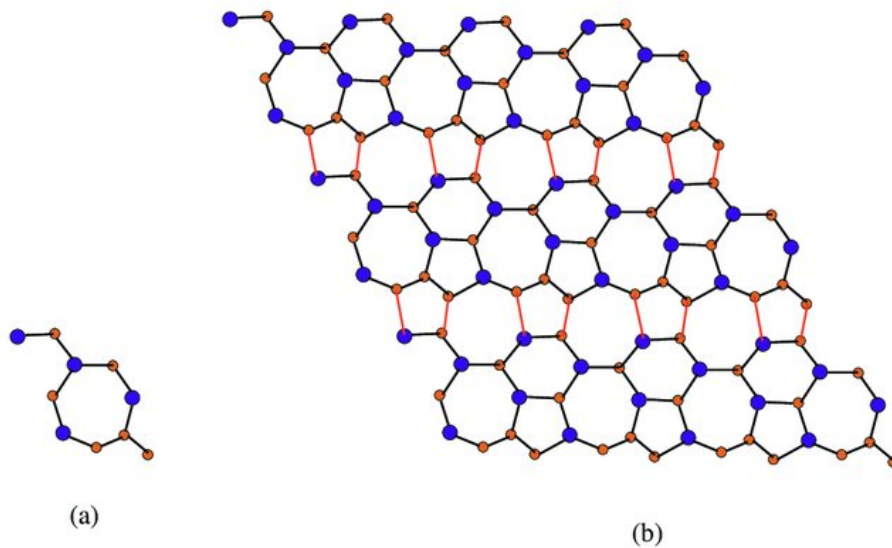


Figure 1: 2D structure of $Si_2C_3 - I$

This table show the edge partition of *Silicon carbied* network $Si_2C_2 - I$

(d_s, d_t) where $st \in E(G)$	Frequency
(2,1)	1
(3,1)	1
(2,2)	$p+2q$
(3,2)	$6p-1+8(q-1)$
(3,3)	$15pq-9p-13q+7$

Table 1: Edge partition of $Si_2C_3 - I$

First and second Zagreb index

$Si_2C_3 - I$ be the graph of Silicon Carbide network Si_2C_3 . By using table 1 we have 1st and 2nd Zagreb indices.

$$M_1(Si_2C_3 - I) = 90pq - 20p - 30q + 4$$

$$M_2(Si_2C_3 - I) = 135pq - 41p - 61q + 14$$

Theorem 1. $Si_2C_3 - I$ be the graph of Silicon-Carbide Network of 2-D structure.

Similarly, the remaining topological indices are derived using the same procedure, as shown below.

$$1. \text{VAR}(Si_2C_3 - I) = \frac{10p^2q - 4p^2 + 15pq^2 - 2pq - 9q^2}{25p^2q^2}$$

$$2. \text{AL}(Si_2C_3 - I) = 6p + 8q - 6$$

$$3. \text{IR1}(Si_2C_3 - I) = \frac{8450pq + 338p + 507q}{5pq}$$

$$4. \text{IR2}(Si_2C_3 - I) = \sqrt{\frac{135pq - 41p - 61q + 4}{15pq - 2p - 3q}} - \frac{(15pq - 2p - 3q)}{5pq}$$

$$5. \text{IRF}(Si_2C_3 - I) = 6p + 8q - 4$$

$$6. \text{IRFW}(Si_2C_3 - I) = \frac{6p + 8q - 4}{135pq - 41p - 61q + 14}$$

Proof. 1. Now used the value of 1st zagreb index, m and n in equation 1. We have

Proof. We compute the irregularity indices of the silicon carbide $Si_2C_3 - I$ by using equation (3-8) and edge partition of degree base end vertices in table 1.

Let $G = Si_2C_3 - I$, From the edge partition of G , we have

The total number of edges is given by

$$\begin{aligned} |E(G)| &= 1 + 1 + (p + 2q) + (6p + 8q - 9) \\ &\quad + (15pq - 9p - 13q + 7) \\ &= 15pq - 2p - 3q. \end{aligned}$$

Hence,

$$|E(G)| = 15pq - 2p - 3q.$$

The degree variance of a graph G is defined as

$$\text{VAR}(G) = \frac{1}{|V(G)|} \sum_{u \in V(G)} d_u^2 - \left(\frac{1}{|V(G)|} \sum_{u \in V(G)} d_u \right)^2.$$

From the edge partition, the numbers of vertices of degree 1, 2, and 3 are

$$|V_1| = 2,$$

$$|V_2| = 4p + 6q - 4,$$

and

$$|V_3| = 10pq - 4p - 6q + 2.$$

Therefore,

$$\begin{aligned} |V(G)| &= |V_1| + |V_2| + |V_3| \\ &= 2 + (4p + 6q - 4) + (10pq - 4p - 6q + 2) \\ &= 10pq. \end{aligned}$$

Thus,

$$|V(G)| = 10pq.$$

By the Handshaking Lemma,

$$\sum_{u \in V(G)} d_u = 2|E(G)|.$$

Hence,

$$\begin{aligned}\sum_{u \in V(G)} d_u &= 2(15pq - 2p - 3q) \\ &= 30pq - 4p - 6q.\end{aligned}$$

Next, we calculate $\sum_{u \in V(G)} d_u^2$. Using the degree distribution, we obtain

$$\begin{aligned}\sum_{u \in V(G)} d_u^2 &= 1^2|V_1| + 2^2|V_2| + 3^2|V_3| \\ &= 1^2(2) + 2^2(4p + 6q - 4) \\ &\quad + 3^2(10pq - 4p - 6q + 2) \\ &= 2 + 4(4p + 6q - 4) \\ &\quad + 9(10pq - 4p - 6q + 2) \\ &= 2 + 16p + 24q - 16 \\ &\quad + 90pq - 36p - 54q + 18 \\ &= 90pq - 20p - 30q + 4.\end{aligned}$$

Therefore,

$$\sum_{u \in V(G)} d_u^2 = 90pq - 20p - 30q + 4.$$

Substituting the above results into the definition of degree variance, we have

$$\begin{aligned}VAR(G) &= \frac{90pq - 20p - 30q + 4}{10pq} \\ &\quad - \left(\frac{30pq - 4p - 6q}{10pq} \right)^2.\end{aligned}$$

Since

$$\frac{30pq - 4p - 6q}{10pq} = \frac{15pq - 2p - 3q}{5pq},$$

we obtain

$$\begin{aligned}VAR(G) &= \frac{90pq - 20p - 30q + 4}{10pq} \\ &\quad - \frac{(15pq - 2p - 3q)^2}{25p^2q^2}.\end{aligned}$$

Taking the common denominator $50p^2q^2$, we get

$$\begin{aligned}VAR(G) &= \frac{5pq(90pq - 20p - 30q + 4)}{50p^2q^2} \\ &\quad - \frac{2(15pq - 2p - 3q)^2}{50p^2q^2}.\end{aligned}$$

Expanding the first numerator gives

$$\begin{aligned}5pq(90pq - 20p - 30q + 4) &= 450p^2q^2 - 100p^2q \\ &\quad - 150pq^2 + 20pq.\end{aligned}$$

Furthermore,

$$\begin{aligned}2(15pq - 2p - 3q)^2 &= 450p^2q^2 + 8p^2 + 18q^2 \\ &\quad - 120p^2q - 180pq^2 + 48pq.\end{aligned}$$

Therefore,

$$\begin{aligned} VAR(G) &= \frac{450p^2q^2 - 100p^2q - 150pq^2 + 20pq}{50p^2q^2} \\ &\quad - \frac{450p^2q^2 + 8p^2 + 18q^2 - 120p^2q - 180pq^2 + 48pq}{50p^2q^2} \\ &= \frac{20p^2q - 8p^2 + 30pq^2 - 4pq - 18q^2}{50p^2q^2}. \end{aligned}$$

Dividing the numerator and denominator by 2, we finally obtain

$$VAR(Si_2C_3 - I) = \frac{10p^2q - 4p^2 + 15pq^2 - 2pq - 9q^2}{25p^2q^2}.$$

□

2.

$$AL(Si_2C_3 - I) = \sum_{st \in E(Si_2C_3 - I)} |d_s - d_t|$$

$$\begin{aligned} AL(Si_2C_3 - I) &= 1|2 - 1| + 1|3 - 1| + (p + 2q)|2 - 2| + (6p - 1 + 8(q - 1))|3 - 2| + (15pq - 9p - 13q + 7)|3 - 3| \\ AL(Si_2C_3 - I) &= 1 + 2 + 0 + 6p + 8q - 9 + 0 \\ AL(Si_2C_3 - I) &= 6p + 8q - 6 \end{aligned}$$

3.

$$IR1(Si_2C_3 - I) = \sum_{s \in t} d_s^3 - \frac{2m}{n} \sum_{s \in t} d_s^2$$

$$\begin{aligned} IR1(Si_2C_3 - I) &= (2 + 3 + 2 + 3 + 3)^3 - \frac{2(15pq - 2p - 3q)}{10pq} (2 + 3 + 2 + 3 + 3)^2 \\ IR1(Si_2C_3 - I) &= 2197 - \frac{15pq - 2p - 3q}{5pq} (169) = \frac{10985pq - 2535p + 507q + 507q}{5pq} = \frac{8450pq + 338p + 507q}{5pq} \\ IR1(Si_2C_3 - I) &= \frac{8450pq + 338p + 507q}{5pq} \end{aligned}$$

$$4. IR2(Si_2C_3 - I) = \sqrt{\frac{M_2(Si_2C_3 - I)}{m}} - \frac{2m}{n}$$

$$IR2(Si_2C_3 - I) = \sqrt{\frac{135pq - 41p - 61q + 4}{15pq - 2p - 3q}} - \frac{2(15pq - 2p - 3q)}{10pq}$$

$$IR2(Si_2C_3 - I) = \sqrt{\frac{135pq - 41p - 61q + 4}{15pq - 2p - 3q}} - \frac{(15pq - 2p - 3q)}{5pq} \quad IR2(Si_2C_3 - I) = \frac{5(\sqrt{\frac{135pq - 61p - 61q + 22}{15pq - 3p - 3q}}) - 15pq + 3p + 3q}{5pq}$$

5.

$$IRF(Si_2C_3 - I) = \sum_{st \in E(Si_2C_3 - I)} (d_s - d_t)^2$$

$$\begin{aligned} IRF(Si_2C_3 - I) &= (2 - 1)^2(1) + (3 - 1)^2(1) + (2 - 2)^2(p + 2q) + (3 - 2)^2(6p + 8q - 1 - 8) + (3 - 3)^2(15pq - 13p - 13q + 11) \\ IRF(Si_2C_3 - I) &= 1 + 4 + 6p - 1 + 8q - 8 \quad IRF(Si_2C_3 - I) = 6p + 8q - 4 \end{aligned}$$

$$\begin{aligned} 6. IRFW(Si_2C_3 - I) &= \frac{IRF(Si_2C_3 - I)}{M_2(Si_2C_3 - I)} \\ IRFW(Si_2C_3 - I) &= \frac{6p + 8q - 4}{135pq - 41p - 61q + 14} \end{aligned}$$

□

Theorem 2. Let $Si_2C_3 - I$ be the graph of Silicon-Carbide Network of 2 - D structure.

$$1. IRA(Si_2C_3 - I) = 0.1010p + 0.1344q + 0.1131$$

$$2. IRB(Si_2C_3 - I) = 0.6060p + 0.8080q - 0.2017$$

$$3. IRC(Si_2C_3 - I) = \frac{225p^2q^2 - 60p^2q - 90pq^2 + 4p^2 - 9q^2 + 57pq - 15.4041q - 10.3030p + 2.1008}{75p^2q^2 - 10p^2q - 15pq^2}$$

$$4. IRDIF(Si_2C_3 - I) = 5p + 6.6664q - 3.333$$

$$5. IRL(Si_2C_3 - I) = 2.4327p + 3.2437q - 1.8574$$

Proof. We compute the irregularity indices of the silicon carbide $Si_2C_3 - I$ by using equation (9-13) and edge partition of degree base end vertices in table 1.

1.

$$IRA(Si_2C_3 - I) = \sum_{st \in E(Si_2C_3 - I)} \left(d_s^{-\frac{1}{2}} - d_t^{-\frac{1}{2}} \right)$$

$$\begin{aligned} IRA(Si_2C_3 - I) &= \left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{1}} \right)^2 (1) + \left(\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{1}} \right)^2 (1) + 0 + \left(\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{2}} \right)^2 (6p - 1 + 8q - 8) + 0 \\ IRA(Si_2C_3 - I) &= 0.0857 + 0.1786 + 0.1010p - 0.0168 + 0.1344q - 0.1344 \\ IRA(Si_2C_3 - I) &= 0.1010p + 0.1344q - 0.1131 \end{aligned}$$

2.

$$IRB(Si_2C_3 - I) = \sum_{st \in E(Si_2C_3 - I)} (d_s^{\frac{1}{2}} - d_t^{\frac{1}{2}})^2$$

$$\begin{aligned} IRB(Si_2C_3 - I) &= (\sqrt{2} - \sqrt{1})^2 (1) + (\sqrt{3} - \sqrt{1})^2 (1) + 0 + (\sqrt{3} - \sqrt{2})^2 (6p - 1 + 8q - 8) + 0 \\ IRB(Si_2C_3 - I) &= 0.1715 + 0.5358 + (0.1010)(6p - 1 + 8q - 8) \\ IRB(Si_2C_3 - I) &= 0.1715 + 0.5358 + 0.6060p - 0.1010 + 0.8080q - 0.8080 \\ IRB(Si_2C_3 - I) &= 0.6060p + 0.8080q - 0.2017 \end{aligned}$$

3.

$$IRC(Si_2C_3 - I) = \sum_{st \in E(Si_2C_3 - I)} \frac{\sqrt{d_s d_t}}{m} - \frac{2m}{n}$$

$$\begin{aligned} IRC(Si_2C_3 - I) &= \frac{\sqrt{2 \times 1}(1) + \sqrt{3 \times 1}(1) + \sqrt{2 \times 2}(2p + 2q) + \sqrt{3 \times 2}(8p + 8q - 14) + \sqrt{3 \times 3}(15pq - 13p - 13q + 11)}{15pq - 3p - 3q} - \frac{2(15pq - 3p - 3q)}{10pq} IRC(Si_2C_3 - I) \\ &= \frac{45pq - 10.3030p - 15.4041q + 2.1008}{15pq - 2p - 3q} - \frac{15pq - 3p - 3q}{5pq} \\ IRC(Si_2C_3 - I) &= \frac{225p^2q^2 - 60p^2q - 90pq^2 + 4p^2 - 9q^2 + 57pq - 15.4041q - 10.3030p + 2.1008}{75p^2q^2 - 10p^2q - 15pq^2} \end{aligned}$$

4.

$$IRDIF(Si_2C_3 - I) = \sum_{st \in E(Si_2C_3 - I)} \left| \frac{d_s}{d_t} - \frac{d_t}{d_s} \right|$$

$$\begin{aligned} IRDIF(Si_2C_3 - I) &= \left| \frac{2}{1} - \frac{1}{2} \right| (1) + \left| \frac{3}{1} - \frac{1}{3} \right| (1) + 0 + \left| \frac{3}{2} - \frac{2}{3} \right| (6p - 1 + 8q - 8) + 0 \\ IRDIF(D) &= |2 - 0.5| (1) + |3 - 0.333| (1) + |1.5 - 0.666| (6p - 1 + 8q - 8) \\ IRDIF(Si_2C_3 - I) &= 1.5 + 2.667 + 5p - 0.8333 + 6.6664q - 6.6664 \\ IRDIF(Si_2C_3 - I) &= 5p + 6.6664q - 3.333 \end{aligned}$$

5.

$$IRL(Si_2C_3 - I) = \sum_{st \in E(Si_2C_3 - I)} |\ln d_s - \ln d_t|$$

$$\begin{aligned} IRL(Si_2C_3 - I) &= |\ln(2) - \ln(1)| (1) + |\ln(3) - \ln(1)| (1) + 0 + |\ln(3) - \ln(2)| (6p - 1 + 8q - 8) + 0 \\ IRL(Si_2C_3 - I) &= |0.6931 - 0| + |1.0986 - 0| (1) + 0 + |1.0986 - 0.6931| (6p - 1 + 8q - 8) \\ IRL(Si_2C_3 - I) &= 2.4327p + 3.2437q - 1.8574 \end{aligned}$$

□

Theorem 3. Let $Si_2C_3 - I$ be the graph of Silicon-Carbide Network of 2 - D structure.

1. $IRLU(Si_2C_3 - I) = 3p + 4q - 1.5$
2. $IRLF(Si_2C_3 - I) = 4.8989p + 6.5319q - 5.4865$
3. $IRLA(Si_2C_3 - I) = 4.8p + 6.4q - 5.5333$
4. $IRDI(Si_2C_3 - I) = 4.1588p + 5.5451q - 4.4465$
5. $IRGA(Si_2C_3 - I) = 0.1224p + 0.1632q - 0.019$

Proof. We compute the irregularity indices of the silicon carbide $Si_2C_3 - I$ by using equation (14-18) and edge partition of degree base end vertices in table 1.

1.

$$IRLU(Si_2C_3 - I) = \sum_{st \in E(Si_2C_3 - I)} \frac{|d_s - d_t|}{\min(d_s, d_t)}$$

$$\begin{aligned} IRLU(Si_2C_3 - I) &= \frac{|2-1|(1)}{\min(2,1)} + \frac{|3-1|(1)}{\min(3,1)} + 0 + \frac{|3-2|(6p-1+8q-8)}{\min(2,3)} + 0 \\ IRL(Si_2C_3 - I) &= \frac{1}{1} + \frac{2}{1} + \frac{6p-1+8q-8}{2} \\ IRLU(Si_2C_3 - I) &= 6p + 8q - 6 \end{aligned}$$

2.

$$IRLF(Si_2C_3 - I) = \sum_{st \in E(Si_2C_3 - I)} \frac{|d_s - d_t|}{\sqrt{(d_s, d_t)}}$$

$$\begin{aligned} IRLF(Si_2C_3 - I) &= \frac{|2-1|(1)}{\sqrt{2 \times 1}} + \frac{|3-1|(1)}{\sqrt{3 \times 1}} + 0 + \frac{|3-2|(6p-1+8q-8)}{\sqrt{2 \times 3}} + 0 \\ IRLF(Si_2C_3 - I) &= \frac{1}{\sqrt{2}} + \frac{2}{\sqrt{3}} + \frac{6p-1+8q-8}{\sqrt{6}} \\ IRLF(Si_2C_3 - I) &= 0.7071 + 1.1547 + 4.8989p - 0.8164 + 6.5319q - 6.5319 \\ IRLF(Si_2C_3 - I) &= 4.8989p + 6.5319q - 5.4865 \end{aligned}$$

3.

$$IRLA(Si_2C_3 - I) = 2 \sum_{st \in E(Si_2C_3 - I)} \frac{|d_s - d_t|}{(d_s + d_t)}$$

$$\begin{aligned} IRLA(Si_2C_3 - I) &= \frac{|2-1|(1)}{2+1} + \frac{|3-1|(1)}{3+1} + 0 + \frac{|3-2|(6p-1+8q-8)}{3+2} + 0 \\ &= \frac{4}{3} + \frac{4}{4} + 0 + \frac{16p + 16q - 28}{5} + 0 \end{aligned}$$

$$\begin{aligned} IRLA(Si_2C_3 - I) &= 0.6667 + 1 + 4.8p - 0.8 + 6.4q - 6.4 \\ IRLA(Si_2C_3 - I) &= 4.8p + 6.4q - 5.5333 \end{aligned}$$

4.

$$IRDI(Si_2C_3 - I) = \sum_{st \in E(Si_2C_3 - I)} \ln 1 + |d_s - d_t|$$

$$\begin{aligned} IRDI(Si_2C_3 - I) &= \ln 1 + |2 - 1|(1) + \ln 1 + |3 - 1|(1) + 0 + \ln 1 + |3 - 2|(6p - 1 + 8q - 8) + 0 \\ IRDI(Si_2C_3 - I) &= 4.1588p + 5.5451q - 4.4465 \end{aligned}$$

5.

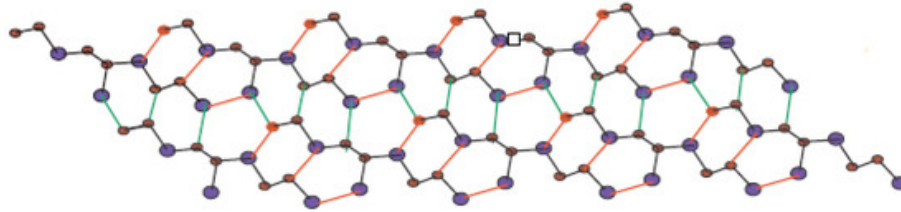
$$IRGA(Si_2C_3 - I) = \sum_{st \in E(Si_2C_3 - I)} \ln \left(\frac{d_s + d_t}{2\sqrt{d_s d_t}} \right)$$

$$\begin{aligned} IRGA(Si_2C_3 - I) &= (1)\ln \left(\frac{2+1}{2\sqrt{2 \times 1}} \right) + (1)\ln \left(\frac{3+1}{2\sqrt{3}} \right) + (p+2q)\ln \left(\frac{2+2}{2\sqrt{2 \times 2}} \right) + (6p+8q-9)\ln \left(\frac{3+2}{2\sqrt{3 \times 2}} \right) + (15pq-9p-13q+7)\ln \left(\frac{3+3}{2\sqrt{3 \times 3}} \right) \\ IRGA(Si_2C_3 - I) &= \ln \left(\frac{3}{\sqrt{2}} \right) + \ln \left(\frac{4}{2\sqrt{3}} \right) + (p+2q)\ln(1) + (6p+8q-9)\ln \left(\frac{5}{2\sqrt{6}} \right) + (15pq-9p-13q+7)\ln \left(\frac{6}{2\sqrt{9}} \right) \\ IRGA(Si_2C_3 - I) &= (0.0588)(1) + (0.1438) + 0 + 0.1224p - 0.0204 + 0.1632q - 0.1632 \\ IRGA(Si_2C_3 - I) &= 0.1224p + 0.1632q - 0.019 \end{aligned}$$

□

3 Irregularity indices of Silicon carbide $Si_2C_3 - II[p, q]$ 2D Structure

We will discuss the graph of silicon carbide network $Si_2C_3 - II$ in the given figure 2 and calculate the irregularity index of the given graph. In figure 2 the graph represents a multi-unit cell that is connected in rows and columns of silicon carbide $Si_2C_3 - II$. The number of a unit cell is connected in rows, or columns, and is denoted by p and q respectively, in 2 to demonstrate how the unit cell is joined and how one row is connected to another row. The total number of vertices and edges in a graph depends on $[p, q]$. The number of vertices in the silicon carbide network $Si_2C_3 - II$ is $10pq$, and the total number of edges is $15pq - 3p - 3q$.

Figure 2: 2D structur of $Si_2C_3-II[p,q]$

This table show the edge partition of *Silicon carbied* network of $Si_2C_3 - II$

(d_s, d_t) where $st \in E(G)$	Frequency
(2,1)	2
(3,1)	1
(2,2)	$2p+2q$
(3,2)	$8p+8q-14$
(3,3)	$15pq-13p-13q+11$

Table 2: Edge partition of $Si_2C_3 - II$

First and second Zagreb index

Let $Si_2C_3 - II$ be the graph of *Silicon Carbide* network Si_2C_3 . By using table 2 we have 1st and 2nd Zagreb indices's.

$$M_1(Si_2C_3 - II) = 90pq - 30p - 30q + 6$$

$$M_2(Si_2C_3 - II) = 135pq - 61p - 61q + 22$$

Theorem 4. Let $Si_2C_3 - II$ be the graph of *Silicon-Carbide Network* of 2 - D structure.

$$1. \text{VAR}(Si_2C_3 - II) = \frac{15p^2q - 9p^2 + 15pq^2 - 3pq - 9q^2}{25p^2q^2}$$

$$2. \text{AL}(Si_2C_3 - II) = 8p + 8q - 10$$

$$3. \text{IR1}(Si_2C_3 - II) = \frac{8450pq + 507p + 507q}{5pq}$$

$$4. \text{IR2}(Si_2C_3 - II) = \sqrt{\frac{135pq - 61p - 61q + 22}{15pq - 3p - 3q}} - \frac{2(15pq - 3p - 3q)}{10pq}$$

$$5. \text{IRF}(Si_2C_3 - II) = 8p - 8q - 8$$

$$6. \text{IRFW}(Si_2C_3 - II) = \frac{8p - 8q - 8}{135pq - 61p - 61q + 22}$$

Proof. We compute the irregularity indices of the silicon carbide $Si_2C_3 - II$ by using equation (3-8) and edge partition of degree base end vertices in table 2.

Now used the value of 1st zagreb index, m and n in equation 1. We have

1.

$$\text{VAR}(Si_2C_3 - II) = \frac{M_1(Si_2C_3 - II)}{n} - \left(\frac{2m}{n}\right)^2$$

$$\text{VAR}(Si_2C_3 - II) = \frac{90pq - 30p - 30q + 6}{10pq} - \left(\frac{15pq - 3p - 3q}{5pq}\right)^2$$

$$\text{VAR}(Si_2C_3 - II) = \frac{90pq - 30p - 30q + 6}{10pq} - \left(\frac{225p^2q^2 + 9p^2 + 9q^2 - 90p^2q - 90pq^2 + 18pq}{25p^2q^2}\right)$$

$$\text{VAR}(Si_2C_3 - II) = \frac{15p^2q - 9p^2 + 15pq^2 - 3pq - 9q^2}{25p^2q^2}$$

2.

$$\text{AL}(Si_2C_3 - II) = \sum_{st \in E(Si_2C_3 - II)} |d_s - d_t|$$

$$\text{AL}(Si_2C_3 - II) = 2|2 - 1| + 1|3 - 1| + (2p + 2q)|2 - 2| + (8p + 8q - 14)|3 - 2| + (15pq - 13p - 13q + 11)|3 - 3|$$

$$\text{AL}(Si_2C_3 - II) = 2 + 2 + 0 + 8p + 8q - 14 + 0$$

$$\text{AL}(Si_2C_3 - II) = 8p + 8q - 10$$

3.

$$IR1(Si_2C_3 - II) = \sum_{s \in t} d_s^3 - \frac{2m}{n} \sum_{s \in t} d_s^2$$

$$\begin{aligned} IRI(Si_2C_3 - II) &= (2 + 3 + 2 + 3 + 3)^3 - \frac{2(15p-3p-3q)}{10pq} (2 + 3 + 2 + 3 + 3)^2 \\ IR1(Si_2C_3 - II) &= 2197 - \frac{15pq-3p-3q}{5pq} (169) = \frac{10985pq-2535pq+507p+507q}{5pq} = \frac{8450pq+507p+507q}{5pq} \\ IR1(Si_2C_3 - II) &= \frac{8450pq+507p+507q}{5pq} \end{aligned}$$

4.

$$IR2(Si_2C_3 - II) = \sqrt{\frac{M_2(Si_2C_3 - II)}{m}} - \frac{2m}{n}$$

$$\begin{aligned} IR2(Si_2C_3 - II) &= \sqrt{\frac{135pq-61p-61q+22}{15pq-3p-3q}} - \frac{2(15pq-3p-3q)}{10pq} = \sqrt{\frac{135pq-61p-61q+22}{15pq-3p-3q}} - \frac{(15pq-3p-3q)}{5pq} \\ IR2(Si_2C_3 - II) &= \frac{5\left(\sqrt{\frac{135pq-61p-61q+22}{15pq-3p-3q}}\right) - 15pq+3p+3q}{5pq} \end{aligned}$$

5.

$$IRF(Si_2C_3 - II) = \sum_{st \in E(Si_2C_3 - II)} (d_s - d_t)^2$$

$$\begin{aligned} &= (2-1)^2(2) + (3-1)^2(1) + (2-2)^2(2p+2q) + (3-2)^2(8p+8q-14) + (3-3)^2(15pq-13p-13q+11) \\ IRF(Si_2C_3 - II) &= 2 + 4 + 8p + 8q - 14 \\ IRF(Si_2C_3 - II) &= 8p - 8q - 8 \end{aligned}$$

6.

$$IRFW(Si_2C_3 - II) = \frac{IRF(Si_2C_3 - II)}{M_2(Si_2C_3 - II)}$$

$$IRFW(Si_2C_3 - II) = \frac{8p-8q-8}{135pq-61p-61q+22}$$

□

Theorem 5. Let $Si_2C_3 - II$ be the graph of Silicon-Carbide Network of 2 - D structure.

1. $IRA(Si_2C_3 - II) = 0.1346p + 0.1346q + 0.1144$
2. $IRB(Si_2C_3 - II) = 0.808p + 0.808q - 0.5351$
3. $IRC(Si_2C_3 - II) = \frac{12.9795p^2q+12.9795pq^2-9p^2-9q^2-1.662pq}{75p^2q^2-15p^2q-15pq^2}$
4. $IRDIF(Si_2C_3 - II) = 6.6672p + 6.6672q - 6$
5. $IRL(Si_2C_3 - II) = 3.244p + 3.244q - 3.1922$

Proof. We compute the irregularity indices of the silicon carbide $Si_2C_3 - II$ by using equation (9-13) and edge partition of degree base end vertices in table 2

1.

$$IRA(Si_2C_3 - II) = \sum_{st \in E(Si_2C_3 - II)} \left(d_s^{-\frac{1}{2}} - d_t^{-\frac{1}{2}} \right)$$

$$\begin{aligned} IRA(Si_2C_3 - II) &= \left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{1}} \right)^2 (2) + \left(\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{1}} \right)^2 (1) + 0 + \left(\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{2}} \right)^2 (8p+8q-14) + 0 \\ IRA(Si_2C_3 - II) &= 0.1715 + 0.1786 + 0.1346p + 0.1346q - 0.2357 \\ IRA(Si_2C_3 - II) &= 0.1346p + 0.1346q + 0.1144 \end{aligned}$$

2.

$$IRB(Si_2C_3 - II) = \sum_{st \in E(Si_2C_3 - II)} (d_s^{\frac{1}{2}} - d_t^{\frac{1}{2}})^2$$

$$\begin{aligned} IRB(Si_2C_3 - II) &= (\sqrt{2} - \sqrt{1})^2(2) + (\sqrt{3} - \sqrt{1})^2(1) + 0 + (\sqrt{3} - \sqrt{2})^2(8p+8q-14) + 0 \\ IRB(Si_2C_3 - II) &= 0.1715(2) + 0.5358 + (0.1010)(8p+8q-14) \\ IRB(Si_2C_3 - II) &= 0.3431 + 0.5358 + 0.808p + 0.808q - 1.414 \\ IRB(Si_2C_3 - II) &= 0.808p + 0.808q - 0.5351 \end{aligned}$$

3.

$$IRC(Si_2C_3 - II) = \sum_{st \in E(Si_2C_3 - II)} \frac{\sqrt{d_s d_t}}{m} - \frac{2m}{n}$$

$$IRC(Si_2C_3 - II) = \frac{\sqrt{2 \times 1}(2) + \sqrt{3 \times 1}(1) + \sqrt{2 \times 2}(2p+2q) + \sqrt{3 \times 2}(8p+8q-14) + \sqrt{3 \times 3}(15pq-13p-13q+11)}{15pq-3p-3q} - \frac{2(15pq-3p-3q)}{10pq}$$

$$IRC(Si_2C_3 - II) = \frac{45pq-15.4041p-15.4041q+3.2676}{15pq-3p-3q} - \frac{15pq-3p-3q}{5pq}$$

$$IRC(Si_2C_3 - II) = \frac{12.9795p^2q+12.9795pq^2-9p^2-9q^2-1.662pq}{75p^2q^2-15p^2q-15pq^2}$$

4.

$$IRDIF(Si_2C_3 - II) = \sum_{st \in E(Si_2C_3 - II)} \left| \frac{d_s}{d_t} - \frac{d_t}{d_s} \right|$$

$$IRDIF(Si_2C_3 - II) = \left| \frac{2}{1} - \frac{1}{2} \right|(2) + \left| \frac{3}{1} - \frac{1}{3} \right|(1) + 0 + \left| \frac{3}{2} - \frac{2}{3} \right|(8p+8q-14) + 0$$

$$IRDIF(Si_2C_3 - II) = |2 - 0.5|(2) + |3 - 0.333|(1) + |1.5 - 0.666|(8p-8q-14)$$

$$IRDIF(Si_2C_3 - II) = 6.6672p + 6.6672q - 6$$

5.

$$IRL(Si_2C_3 - II) = \sum_{st \in E(Si_2C_3 - II)} |lnd_s - lnd_t|$$

$$IRL(Si_2C_3 - II) = |ln(2) - ln(1)|(2) + |ln(3) - ln(1)|(1) + 0 + |ln(3) - ln(2)|(8p-8q-14) + 0$$

$$IRL(Si_2C_3 - II) = |0.6931 - 0|(2) + |1.0986 - 0|(1) + 0 + |1.0986 - 0.6931|(8p-8q-14)$$

$$IRL(Si_2C_3 - II) = 3.244p + 3.244q - 3.1922$$

□

Theorem 6. Let $Si_2C_3 - II$ be the graph of Silicon-Carbide Network of 2 - D structure.

1. $IRLU(Si_2C_3 - II) = 4p + 4q - 3$
2. $IRLF(Si_2C_3 - II) = 3.2659p + 3.2659q - 3.1465$
3. $IRLA(Si_2C_3 - II) = 3.22p + 3.22q - 3.2667$
4. $IRDI(Si_2C_3 - II) = 5.5451p + 5.5451q - 7.2192$
5. $IRGA(Si_2C_3 - II) = 0.1632p + 0.1632q - 0.0242$

Proof. We compute the irregularity indices of the silicon carbide $Si_2C_3 - II$ by using equation (14-18) and edge partition of degree base end vertices in table 2.

1.

$$IRLU(Si_2C_3 - II) = \sum_{st \in E(Si_2C_3 - II)} \frac{|d_s - d_t|}{\min(d_s, d_t)}$$

$$IRLU(Si_2C_3 - II) = \frac{|2-1|(2)}{\min(2,1)} + \frac{|3-1|(1)}{\min(3,1)} + 0 + \frac{|3-2|(8p-8q-14)}{\min(2,3)} + 0$$

$$IRLU(Si_2C_3 - II) = \frac{2}{1} + \frac{2}{1} + \frac{8p+8q-14}{2}$$

$$IRLU(Si_2C_3 - II) = 4p + 4q - 3$$

2.

$$IRLF(Si_2C_3 - II) = \sum_{st \in E(Si_2C_3 - II)} \frac{|d_s - d_t|}{\sqrt{(d_s, d_t)}}$$

$$IRLF(Si_2C_3 - II) = \frac{|2-1|(2)}{\sqrt{2 \times 1}} + \frac{|3-1|(1)}{\sqrt{3 \times 1}} + 0 + \frac{|3-2|(8p+8q-14)}{\sqrt{2 \times 3}} + 0$$

$$IRLF(Si_2C_3 - II) = \frac{2}{\sqrt{2}} + \frac{2}{\sqrt{3}} + \frac{8p+8q-14}{\sqrt{6}}$$

$$IRLF(Si_2C_3 - II) = 3.2659p + 3.2659q - 3.1465$$

3.

$$IRLA(Si_2C_3 - II) = 2 \sum_{st \in E(Si_2C_3 - II)} \frac{|d_s - d_t|}{(d_s + d_t)}$$

$$IRLA(Si_2C_3 - II) = (2) \frac{|2-1|(2)}{2+1} + (2) \frac{|3-1|(1)}{3+1} + 0 + (2) \frac{|3-3-2|(8p+8q-14)}{2+3} + 0$$

$$IRLA(Si_2C_3 - II) = \frac{4}{3} + \frac{4}{4} + 0 + \frac{16p+16q-28}{5} + 0$$

$$IRLA(Si_2C_3 - II) = 3.22p + 3.22q - 3.2667$$

4.

$$IRDI(Si_2C_3 - II) = \sum_{st \in E(Si_2C_3 - II)} \ln 1 + |d_s - d_t|$$

$$IRDI(Si_2C_3 - II) = \ln 1 + |2 - 1|(2) + \ln 1 + |3 - 1|(1) + 0 + \ln 1 + |3 - 2|(8p + 8q - 14) + 0$$

$$IRDI(Si_2C_3 - II) = 5.5451p + 5.5451q - 7.2192$$

5.

$$IRGA(Si_2C_3 - II) = \sum_{st \in E(Si_2C_3 - II)} \ln \left(\frac{d_s + d_t}{2\sqrt{d_s d_t}} \right)$$

$$IRGA(Si_2C_3 - II) = (2)\ln \left(\frac{2+1}{2\sqrt{2 \times 1}} \right) + (1)\ln \left(\frac{3+1}{2\sqrt{3}} \right) + (2p+2q)\ln \left(\frac{2+2}{2\sqrt{2 \times 2}} \right) + (8p+8q-14)\ln \left(\frac{3+2}{2\sqrt{3 \times 2}} \right) + (15pq-13p-13q+11)\ln \left(\frac{3+3}{2\sqrt{3 \times 3}} \right)$$

$$IRGA(Si_2C_3 - II) = (2)\ln \left(\frac{3}{\sqrt{2}} \right) + (1)\ln \left(\frac{4}{2\sqrt{3}} \right) + (2p+2q)\ln \left(\frac{4}{2\sqrt{4}} \right) + (8p+8q-14)\ln \left(\frac{5}{2\sqrt{6}} \right) + (15pq-13p-13q+11)\ln \left(\frac{6}{2\sqrt{9}} \right)$$

$$IRGA(Si_2C_3 - II) = (0.0588)(2) + (0.1438) + 0 + (0.0204)(8p+8q-14) + 0$$

$$IRGA(Si_2C_3 - II) = 0.1632p + 0.1632q - 0.0242$$

□

4 Irregularity Indices of Silicon Carbide $Si_2C_3 - III[p, q]$

We will discuss the graph of silicon carbide network $Si_2C_3 - III$ in the given figure 3 and calculated the irregularity index of the given graph. In figure 3 the graph represents a multi-unit cell that is connected in rows and columns of silicon carbide $Si_2C_3 - III$. The number of a unit cell is connected in rows, or columns, and is denoted by p and q respectively, in 3 to demonstrate how the unit cell is joined and how one row is connected to another row. The total number of vertices and edges in a graph depends on $[p, q]$. The number of vertices in the silicon carbide network $Si_2C_3 - III$ is $10pq$, and the total number of edges is $15pq - 2p - 3q$.

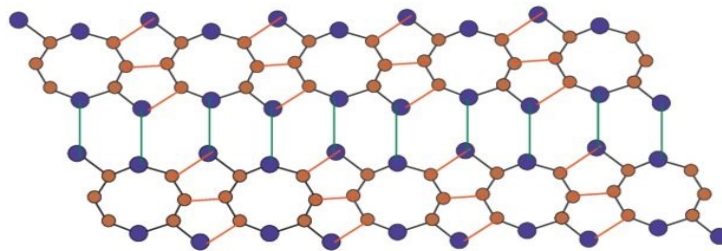


Figure 3: 2D structure of $Si_2C_3 - III[p, q]$

This table show the edge partition of *Silicon carbide* network of $Si_2C_3 - III$

(d_s, d_t) where $st \in E(G)$	Frequency
(1,3)	2
(2,2)	$2q+2$
(2,3)	$8p+8q-12$
(3,3)	$15pq-10p-13q+8$

Table 3: Edge partition of $Si_2C_3 - III$

First and second Zagreb index

Let $Si_2C_3 - III$ be the graph of *Silicon Carbide* network Si_2C_3 . By using table 3 we have 1st and 2nd Zagreb indices's.

$$M_1(Si_2C_3 - III) = 90pq - 30q - 20p + 4$$

$$M_2(Si_2C_3 - III) = 135pq - 61q - 42p + 14$$

Theorem 7. Let $Si_2C_3 - III$ be the graph of *Silicon-Carbide Network* of 2-D structure.

$$1. \text{VAR}(Si_2C_3 - III) = \frac{10p^2q - 4p^2 - 15pq^2 - 2pq - 9q^2}{25p^2q^2}$$

2. $AL(Si_2C_3 - III) = 8p + 8q - 8$
3. $IR1(Si_2C_3 - III) = \frac{1600pq-128p-192q}{5pq}$
4. $IR2(Si_2C_3 - III) = \sqrt{\frac{135-61q-42p+14}{15pq-2p-3q}} - \frac{(15pq-2p-3q)}{5pq}$
5. $IRF(Si_2C_3 - III) = 8p + 8q - 4$
6. $IRFW(Si_2C_3 - III) = \frac{8p+8q-4}{135pq-61q-42p+14}$

Proof. We compute the irregularity indices of the silicon carbide $Si_2C_3 - III$ by using equation (3-8) and edge partition of degree base end vertices in table 3.

1.

$$VAR(Si_2C_3 - III) = \frac{M_1(Si_2C_3 - III)}{n} - \left(\frac{2m}{n}\right)^2$$

$$\begin{aligned} VAR(Si_2C_3 - III) &= \frac{90pq-30-20p+4}{10pq} - \left(\frac{15pq-2p-3q}{5pq}\right)^2 \\ VAR(Si_2C_3 - III) &= \frac{(45pq-10p-15q+2)5-(15pq-2p-3q)^2}{25p^2q^2} \\ VAR(Si_2C_3 - III) &= \frac{10p^2q-4p^2-15pq^2-2pq-9q^2}{25p^2q^2} \end{aligned}$$

2.

$$AL(Si_2C_3 - III) = \sum_{st \in E(Si_2C_3 - III)} |d_s - d_t|$$

$$\begin{aligned} AL(Si_2C_3 - III) &= 4 + 8p + 8q - 12 \\ AL(Si_2C_3 - III) &= 8p + 8q - 8 \end{aligned}$$

3.

$$IR1(Si_2C_3 - III) = \sum_{s \in t} d_s^3 - \frac{2m}{n} \sum_{s \in t} d_s^2$$

$$\begin{aligned} IR1(Si_2C_3 - III) &= (1 + 2 + 2 + 3)^3 - \frac{2(15pq-2p-3q)}{10pq} (1 + 2 + 2 + 3)^2 \\ IR1(Si_2C_3 - III) &= 512 - \frac{15pq-2p-3q}{5pq} (64) = \frac{2560pq-960pq-128p-192q}{5pq} \\ IR1(Si_2C_3 - III) &= \frac{1600pq-128p-192q}{5pq} \\ IR1(Si_2C_3 - III) &= \frac{1600pq-128p-192q}{5pq} \end{aligned}$$

4.

$$IR2(Si_2C_3 - III) = \sqrt{\frac{M_2(Si_2C_3 - III)}{m}} - \frac{2m}{n}$$

$$\begin{aligned} IR2(Si_2C_3 - III) &= \sqrt{\frac{135-61q-42p+14}{15pq-2p-3q}} - \frac{2(15pq-2p-3q)}{10pq} \\ IR2(Si_2C_3 - III) &= \sqrt{\frac{135-61q-42p+14}{15pq-2p-3q}} - \frac{(15pq-2p-3q)}{5pq} \end{aligned}$$

5.

$$IRF(Si_2C_3 - III) = \sum_{st \in E(Si_2C_3 - III)} (d_s - d_t)^2$$

$$\begin{aligned} IRF(Si_2C_3 - III) &= (2)(1-3)^2 + (2q+2)(2-2)^2 + (8p+8q-12)(2-3)^2 + (15pq-10p-13q+8)(3-3)^2 \\ IRF(Si_2C_3 - III) &= 8 + 0 + 8p + 8q - 12 \\ IRF(Si_2C_3 - III) &= 8p + 8q - 4 \end{aligned}$$

6.

$$IRFW(Si_2C_3 - III) = \frac{IRF(Si_2C_3 - III)}{M_2(Si_2C_3 - III)}$$

$$IRFW(Si_2C_3 - III) = \frac{8p+8q-4}{135pq-61q-42p+14}$$

□

Theorem 8. Let $Si_2C_3 - III$ be the graph of Silicon-Carbide Network of 2 - D structure.

1. $IRA(Si_2C_3 - III) = 0.1346p + 0.1346q + 0.1552$
2. $IRB(Si_2C_3 - III) = 0.8081p + 0.8081q - 0.1405$
3. $IRC(Si_2C_3 - III) = \frac{45pq - 15.41q - 15.41p + 2.0703 - 225p^2q^2 + 4p^2 - 9q^2 - 60p^2q - 90pq^2 + 12pq}{75p^2q^2 - 10p^2q - 15pq^2}$
4. $IRDIF(Si_2C_3 - III) = 6.6666p + 6.6666q - 4.6667$
5. $IRL(Si_2C_3 - III) = 3.2437q + 3.2437p - 2.6683$

Proof. We compute the irregularity indices of the silicon carbide $Si_2C_3 - III$ by using equation (9-13) and edge partition of degree base end vertices in table 3.

1.

$$IRA(Si_2C_3 - III) = \sum_{st \in E(Si_2C_3 - III)} \left(d_s^{-\frac{1}{2}} - d_t^{-\frac{1}{2}} \right)$$

$$\begin{aligned} IRA(Si_2C_3 - III) &= \left(\frac{1}{\sqrt{1}} - \frac{1}{\sqrt{3}} \right)^2 (2) + \left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{2}} \right)^2 (2q + 2) + \left(\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{3}} \right)^2 (15pq - 10p - 13q + 8) \\ IRA(Si_2C_3 - III) &= 0.3572 + 0 + 0.1346p + 0.1346q - 0.2020 \\ IRA(Si_2C_3 - III) &= 0.1346p + 0.1346q + 0.1552 \end{aligned}$$

2.

$$IRB(Si_2C_3 - III) = \sum_{st \in E(Si_2C_3 - III)} (d_s^{\frac{1}{2}} - d_t^{\frac{1}{2}})^2$$

$$\begin{aligned} IRB(Si_2C_3 - III) &= (\sqrt{1} - \sqrt{3})^2 (2) + (\sqrt{2} - \sqrt{2})^2 (8pq - 12) + (\sqrt{3} - \sqrt{3})^2 (15pq - 10p - 13q + 8) \\ IRB(Si_2C_3 - III) &= 1.0717 + 0 + 0.8081p + 0.8081q - 1.2122 \\ IRB(Si_2C_3 - III) &= 0.8081p + 0.8081q - 0.1405 \end{aligned}$$

3.

$$IRC(Si_2C_3 - III) = \sum_{st \in E(Si_2C_3 - III)} \frac{\sqrt{d_s d_t}}{m} - \frac{2m}{n}$$

$$\begin{aligned} IRC(Si_2C_3 - III) &= \frac{\sqrt{1 \times 3}(2) + \sqrt{2 \times 2}(2q + 2) + \sqrt{2 \times 3}(8p + 8q - 12) + \sqrt{3 \times 3}(15pq - 10p - 13q + 8)}{15pq - 2p - 3q} - \frac{2(15pq - 2p - 3q)}{10pq} \\ IRC(Si_2C_3 - III) &= \frac{45pq - 15.41q - 15.41p + 2.0703 - (15pq - 2p - 3q)^2}{(15pq - 2p - 3q)5pq} \\ IRC(Si_2C_3 - III) &= \frac{45pq - 15.41q - 15.41p + 2.0703 - 225p^2q^2 + 4p^2 - 9q^2 - 60p^2q - 90pq^2 + 12pq}{75p^2q^2 - 10p^2q - 15pq^2} \end{aligned}$$

4.

$$IRDIF(Si_2C_3 - III) = \sum_{st \in E(Si_2C_3 - III)} \left| \frac{d_s}{d_t} - \frac{d_t}{d_s} \right|$$

$$\begin{aligned} IRDIF(Si_2C_3 - III) &= \left| \frac{1}{3} - \frac{3}{1} \right| (2) + \left| \frac{2}{2} - \frac{2}{2} \right| (2q + 2) + \left| \frac{2}{3} - \frac{3}{2} \right| (8p + 8q - 12) + \left| \frac{3}{3} - \frac{3}{3} \right| (15pq - 10p - 13q + 8) \\ IRDIF(Si_2C_3 - III) &= 5.3333 + 0 + 6.6666p + 6.6666q - 10 \\ IRDIF(Si_2C_3 - III) &= 6.6666p + 6.6666q - 4.6667 \end{aligned}$$

5.

$$IRL(Si_2C_3 - III) = \sum_{st \in E(Si_2C_3 - III)} |\ln d_s - \ln d_t|$$

$$\begin{aligned} IRL(Si_2C_3 - III) &= |\ln(1) - \ln(3)| (2) + |\ln(2) - \ln(2)| (2q + 2) + |\ln(2) - \ln(3)| (8p + 8q - 12) + |\ln(3) - \ln(3)| (15pq - 10p - 13q + 8) \\ IRL(Si_2C_3 - III) &= 2.1972 + 0 + 3.2437p + 3.2437q - 4.8655 \\ IRL(Si_2C_3 - III) &= 3.2437q + 3.2437p - 2.6683 \end{aligned}$$

□

Theorem 9. Let $Si_2C_3 - III$ be the graph of Silicon-Carbide Network of 2 - D structure.

1. $IRLU(Si_2C_3 - III) = 4p + 4q - 2$
2. $IRLF(Si_2C_3 - III) = 3.2659p + 3.2659q - 2.5895$
3. $IRLA(Si_2C_3 - III) = 1.6p + 1.6q - 2.8$
4. $IRDI(Si_2C_3 - III) = 5.5451p + 5.5451q - 6.1205$

$$5. \text{IRGA}(Si_2C_3 - III) = 0.1632p + 0.1632q - 0.0428$$

Proof. We compute the irregularity indices of the silicon carbide $Si_2C_3 - III$ by using equation (14-18) and edge partition of degree base end vertices in table 3.

1.

$$\text{IRLU}(Si_2C_3 - III) = \sum_{st \in E(Si_2C_3 - III)} \frac{|d_s - d_t|}{\min(d_s, d_t)}$$

$$\text{IRLU}(Si_2C_3 - III) = \frac{|1-3|(2)}{\min(1,3)} + \frac{|2-2|(2q+2)}{\min(2,2)} + \frac{|2-3|(8p+8q-12)}{\min(2,3)} + 0$$

$$\text{IRLU}(Si_2C_3 - III) = \frac{4}{1} + 0 + \frac{8p+8q-12}{2} + 0$$

$$\text{IRLU}(Si_2C_3 - III) = 4p + 4q - 2$$

2.

$$\text{IRLF}(Si_2C_3 - III) = \sum_{st \in E(Si_2C_3 - III)} \frac{|d_s - d_t|}{\sqrt{(d_s, d_t)}}$$

$$\text{IRLF}(Si_2C_3 - III) = \frac{|1-3|(2)}{\sqrt{1 \times 3}} + \frac{|2-2|(2q+2)}{\sqrt{2 \times 2}} + \frac{|2-3|(8p+8q-12)}{\sqrt{2 \times 3}} + \frac{|3-3|(15pq-10p-13q+8)}{\sqrt{3 \times 3}}$$

$$\text{IRLF}(Si_2C_3 - III) = \frac{4}{\sqrt{3}} + \frac{8p+8q-12}{\sqrt{6}}$$

$$\text{IRLF}(Si_2C_3 - III) = 3.2659p + 3.2659q - 2.5895$$

3.

$$\text{IRLA}(Si_2C_3 - III) = 2 \sum_{st \in E(Si_2C_3 - III)} \frac{|d_s - d_t|}{(d_s + d_t)}$$

$$\text{IRLA}(Si_2C_3 - III) = 2 \left[\frac{|1-3|(2)}{1+3} + \frac{|2-2|(2q+2)}{2+2} + \frac{|2-3|(8p+8q-12)}{2+3} + \frac{|3-3|(15pq-10p-13q+8)}{3+3} \right]$$

$$\text{IRLA}(G = 2[1 + 0 + 1.6p + 1.6q - 2.4])$$

$$\text{IRLA}(Si_2C_3 - III) = 1.6p + 1.6q - 2.8$$

4.

$$\text{IRDI}(Si_2C_3 - III) = \sum_{st \in E(Si_2C_3 - III)} \ln 1 + |d_s - d_t|$$

$$\text{IRDI}(Si_2C_3 - III) = \ln 1 + |1-3|(2) + \ln 1 + |2-2|(2q+2) + \ln 1 + |2-3|(8p+8q-12) + \ln(1) + |3-3|(15pq-10p-13q+8)$$

$$\text{IRDI}(Si_2C_3 - III) = 0 + 4 + 0 + 0 + 8p + 8q - 12$$

$$\text{IRDI}(Si_2C_3 - III) = 5.5451p + 5.5451q - 6.1205$$

5.

$$\text{IRGA}(Si_2C_3 - III) = \sum_{st \in E(Si_2C_3 - III)} \ln \left(\frac{d_s + d_t}{2\sqrt{d_s d_t}} \right)$$

$$\text{IRGA}(Si_2C_3 - III) = (2)\ln \left(\frac{1+3}{2\sqrt{1 \times 3}} \right) + (2q+2)\ln \left(\frac{2+2}{2\sqrt{2}} \right) + (8p+8q-12)\ln \left(\frac{2+3}{2\sqrt{2 \times 3}} \right) + (15pq-10p-13q+8)\ln \left(\frac{3+3}{2\sqrt{3 \times 3}} \right)$$

$$\text{IRGA}(Si_2C_3 - III) = 0.2876 + 0 + 0 + (0.0204)(8p + 8q - 12) + 0$$

$$\text{IRGA}(Si_2C_3 - III) = 0.2876 + 0.1632p + 0.1632q - 0.244$$

$$\text{IRGA}(Si_2C_3 - III) = 0.1632p + 0.1632q - 0.0428$$

□

5 Graphical Comparison of Irregular Indices Si_2C_3

In this section, we show the graphical comparison of the above calculated irregular topological indices of the *Silicon Carbide* network $Si_2C_3 - I, Si_2C_3 - II$ and $Si_2C_3 - III$. Figure 4, figure 5, and figure 6 contain the graphical value of irregular topological indices of Albertson index ($AL(Si_2C_3)$), irregularity index $IRF(Si_2C_3)$, Randic index $IRA(Si_2C_3)$, irregularity index $IRB(Si_2C_3)$ and irregularity index $IRC(Si_2C_3)$. $IRDIF(Si_2C_3)$ indices, irregularity index $IRL(Si_2C_3)$, irregularity index $IRLU(Si_2C_3)$, irregularity index $IRLF(Si_2C_3)$, irregularity index $IRLA(Si_2C_3)$, irregularity index $IRDI(Si_2C_3)$ and irregularity index $IRGA(Si_2C_3)$. In figure 4 three different graphs show where in the graph the irregularity index IRF is most irregular as compared to others, and IRA is the least irregular. In the next graph, $IRDIF$ is the most irregular as compared to others, and the maximum value is shown in the graph. In the next graph, $IRLF$ is the most irregular as compared to the others, and $IRGA$ is the least irregular. Most of the irregularity indices behave mostly similarly, as shown in the following figures.

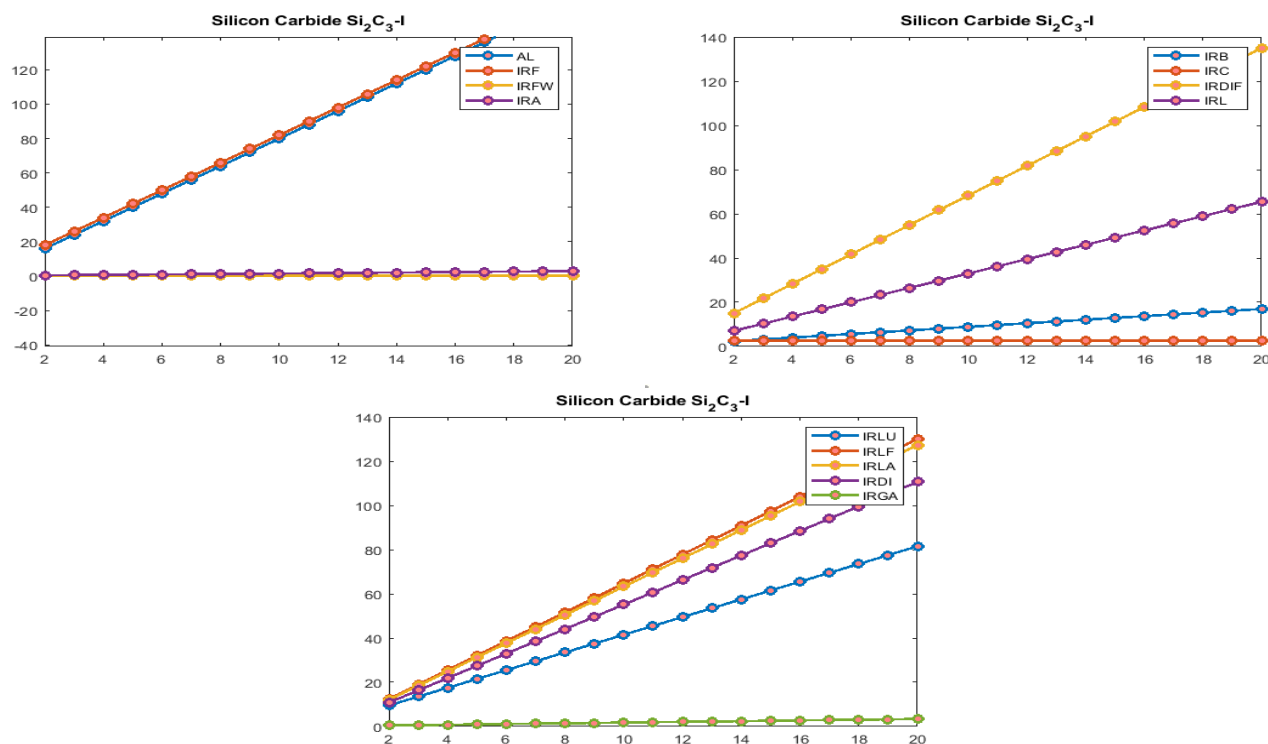


Figure 4: Comparison of topological indices of *SiliconCarbide* $Si_2C_3 - I$ Network

5.1 Discussion

Figure 4 illustrates the variation of different graph-theoretic indices for the silicon carbide graph $Si_2C_3 - I$ for $n = 2, \dots, 20$. Overall, most indices exhibit a clear and approximately linear increasing trend as the graph parameter increases. In the first subplot, AI , IRF , and $IRFW$ show very similar growth and attain values close to 135, whereas IRA remains near zero. In the second subplot, IRC and $IRID$ display the highest growth rates, reaching approximately 135, while $IRIL$ increases to about 65 and IRB remains comparatively small. These results demonstrate that the investigated indices respond differently to the structural growth of the graph. The third subplot further shows a nearly linear increase in $IRLI$, $IRLF$, $IRLA$, and $IRDL$, with $IRLF$ and $IRLA$ attaining the largest values, followed by $IRDL$ and $IRLI$. In contrast, $IRGA$ remains close to zero throughout the considered range. The overall behavior indicates that the majority of the indices are strongly dependent on the structural size of $Si_2C_3 - I$, while the nearly constant indices show comparatively low sensitivity. Thus, the graphical analysis provides a clear comparison of the growth patterns of the considered indices and highlights their usefulness for characterizing the structural properties of the silicon carbide graph.

Overall, the graphical results demonstrate that most of the investigated indices exhibit linear or near-linear growth with respect to the graph parameter. This behavior indicates that the increasing structural complexity of the $Si_2C_3 - I$ graph has a systematic influence on the corresponding graph invariants. The indices with larger slopes are more sensitive to structural changes, whereas those remaining close to zero show comparatively weak sensitivity. Hence, the obtained results provide a useful comparative description of the structural properties of the silicon carbide $Si_2C_3 - I$ graph and demonstrate the applicability of the considered graph-theoretic indices for its structural characterization.

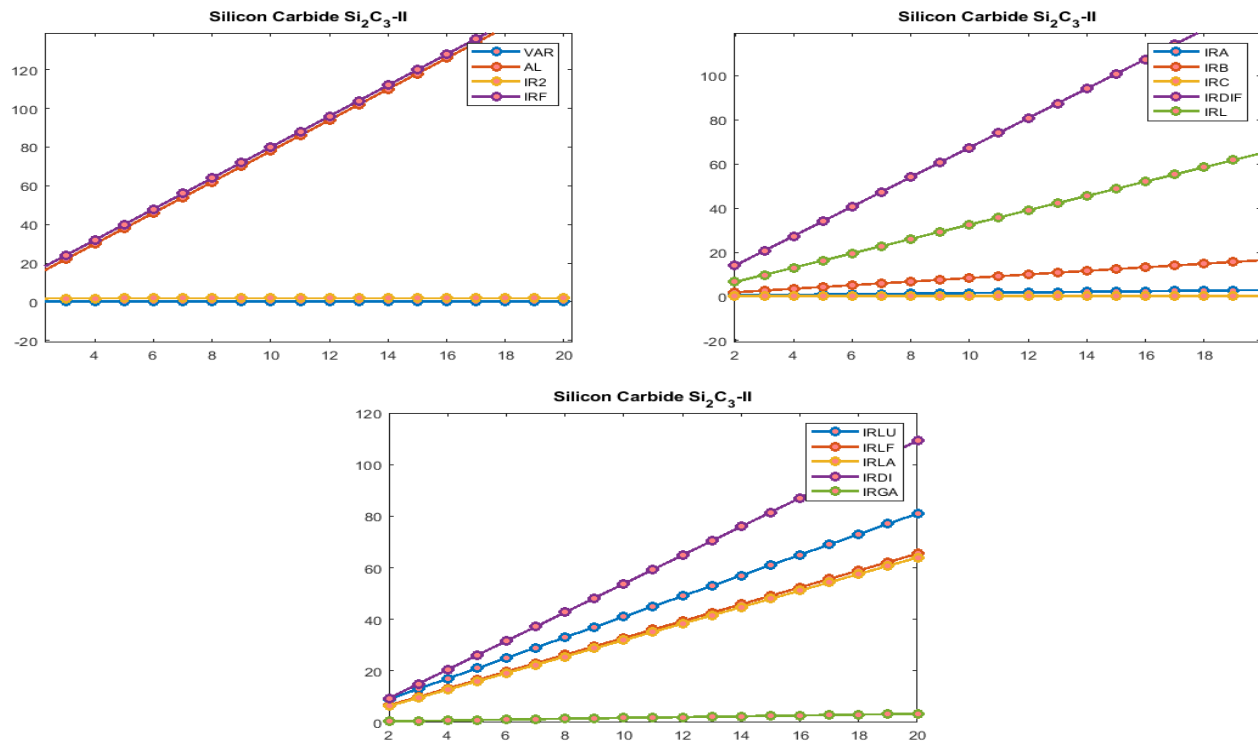


Figure 5: Comparison of topological indices of *SiliconCarbide* $Si_2C_3 - II$ Network

5.2 Discussion

Figure 5 presents a comparison of the topological indices of the silicon carbide $Si_2C_3 - II$ network for the considered range of the graph parameter. In the first subplot, VAR , AI , $R2$, and RFI exhibit a nearly linear increasing trend, with VAR showing the largest growth and attaining a value of approximately 135. In contrast, the remaining indices remain very close to zero. The second subplot shows that RA increases most rapidly and reaches a value of about 110, followed by RDF , which increases to approximately 65. The indices RAC and RDC show comparatively small growth, while RLF remains nearly constant. These results demonstrate that the considered topological indices have different sensitivities to the structural expansion of the $Si_2C_3 - II$ network.

In the third subplot, RLA exhibits the highest growth and reaches a value of approximately 110, while RLI increases to nearly 80. The indices RLF and RFL show similar moderate linear growth and attain values of about 65, whereas $IRGA$ remains close to zero. Overall, the majority of the investigated indices display a clear linear dependence on the graph parameter, indicating a systematic relationship between the network size and its topological characteristics. The differences in the slopes of the curves further provide a comparative measure of the sensitivity of the indices and demonstrate their effectiveness in characterizing the structural properties of the silicon carbide $Si_2C_3 - II$ network.

Overall, the graphical analysis of the topological indices for the silicon carbide $Si_2C_3 - II$ network reveals a consistent and predominantly linear growth pattern with increasing graph parameter. The results show that different indices exhibit different growth rates, reflecting their varying sensitivity to the structural changes of the network. Some indices attain relatively large values, while others remain close to zero, indicating distinct structural characteristics captured by the corresponding topological measures. Therefore, the obtained results provide a clear comparative understanding of the structural behavior of the $Si_2C_3 - II$ network and confirm that the investigated topological indices are useful mathematical tools for its structural characterization and analysis.

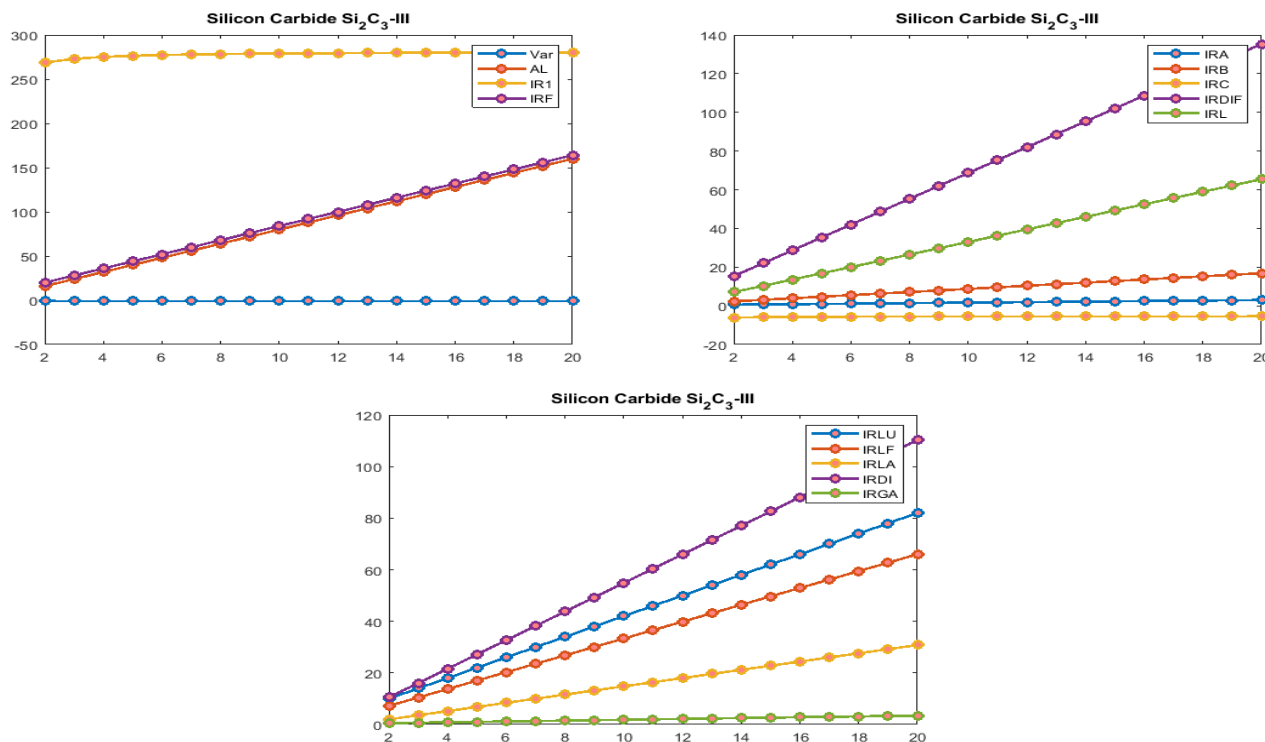


Figure 6: Comparison of topological indices of *SiliconCarbide* $Si_2C_3 - III$ Network

5.3 Discussion

Figure 6 illustrates the comparison of different topological indices for the silicon carbide $Si_2C_3 - III$ network. In the first subplot, AI remains nearly constant at a high value of approximately 270, whereas $IR1$ and IRF exhibit a clear and almost linear increase, reaching values of about 165 at $n = 20$. The index VAR remains close to zero throughout the considered range. In the second subplot, RA shows the most prominent linear growth and attains a value of approximately 135, followed by RDF , which increases to nearly 65. The indices RBC and RDC show relatively small increases, while RLF remains close to zero. These results indicate that the considered indices respond differently to the structural growth of the $Si_2C_3 - III$ network.

The third subplot further demonstrates approximately linear growth for the investigated indices. In particular, $IRDI$ exhibits the highest growth, reaching approximately 110, followed by $IRLU$, which attains nearly 80, and $IRLF$, which reaches about 65. The index $IRLA$ shows a comparatively lower increase, while $IRGA$ remains nearly constant at a very small value. Overall, the results demonstrate that most of the topological indices increase systematically with the graph parameter, although their growth rates differ considerably. This variation reflects the different structural features captured by the corresponding indices and provides a useful basis for comparing the topological characteristics of the $Si_2C_3 - III$ network.

Overall, the graphical analysis confirms that the topological indices of the $Si_2C_3 - III$ network exhibit distinct but systematic trends with increasing graph size. Several indices show strong linear growth, whereas others remain nearly constant or close to zero. The indices with larger slopes demonstrate greater sensitivity to structural changes in the network. Hence, the obtained results provide a clear comparative characterization of the $Si_2C_3 - III$ network and demonstrate the usefulness of the investigated topological indices in describing its structural properties.

6 Conclusion

In this study, the two-dimensional silicon carbide network Si_2C_3 was investigated from a graph-theoretical perspective. The molecular structure was represented as a mathematical graph, enabling the derivation and computation of sixteen irregularity-based topological indices, including the First Zagreb Index, Second Zagreb Index, Randić Index, Degree Variance, Albertson Irregularity Index, and several related irregularity measures. These indices provide quantitative descriptors of the structural complexity and irregularity of the silicon carbide network.

The obtained analytical results and graphical comparisons demonstrate that the considered topological indices effectively capture the structural characteristics of the Si_2C_3 network and exhibit distinct trends with respect to the network size. The findings further emphasize the applicability of graph-theoretical methods in the study of chemical and materials structures. The derived expressions provide a useful mathematical framework for the analysis of silicon carbide nanostructures and may

serve as a reference for future theoretical investigations. In particular, the present methodology can be extended to other silicon carbide configurations, higher-dimensional network structures, and additional classes of topological descriptors. Such extensions may provide further insight into the structural–property relationships of nanomaterials and support potential applications in materials science and nanotechnology.

Declarations

Consent to Publish declaration:

Not applicable

Consent to Participate declaration:

Not applicable

Author's contributions:

M.K: design the methodology, apply method, formal analysis, writing original draft, software, analysis. H.M: formal analysis, review original draft, software, supervision. M.S: formal analysis, review original draft, software, writing original draft.

Ethical Approval:

We hereby declare that this manuscript is the result of our independent creation. This manuscript does not contain any research achievements that have been published or written by other individuals or groups.

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Data Availability

The data used or analysed during the current study available from the corresponding author on reasonable request.

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