



ANALYSIS OF CERTAIN SILICON CARBIDE GRAPHS BY USING IRREGULARITY INDICES

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Abstract

In the theoretical investigation of molecule structure, topological descriptors provide an effective approach to complicated quantum chemical calculations. They are extremely useful in studying the physical, chemical, and structural properties of chemical graphs, such as molecular weight, boiling temperature, and density. The study of chemical graphs through topological descriptors or indices are very important to understand their fundamental topologies. Silicon, the second most prevalent material on the planet, it has a wide range of industrial uses due to their thermal and chemical stability, non-oxidizing behavior and high melting point. In this research work, several degree-based irregularity topological indices were investigated for certain silicon carbide graphs i.e., $Si_2C_3-I(a,s)$, $Si_2C_3-II(a,s)$ and $Si_2C_3-III(a,s)$. The results for the computed topological indices for different types of silicon carbides are also presented graphically.

Keywords: Topological indices; Silicon carbides; Irregularity Indices.

Mathematics Subject Classification: 05C07, 05C35, 05C90, 05C92...

1. Introduction and Preliminaries

Molecular descriptors are important in mathematical chemistry, particularly in QSAR/QSPR research. A descriptors or indices represents molecular characteristics in term of a number that describes the molecule. The wiener index

was one of the first of its kind presented by Wiener. The π -electron energy of molecule was originated with the help of first and second zegreb indices [15]. First and second zegreb indices of a molecular graph is defined as

$$M_1(G) = \sum_{pq \in E(G)} (d_p + d_q). \quad (1)$$

$$M_2(G) = \sum_{pq \in E(G)} (d_p * d_q). \quad (2)$$

The well-known index is forgotten topological index (F), which is very helpful for medical scientists to grasp chemical characteristics of the new drugs and is defined [16] as:

$$F(G) = \sum_{pq \in E(G)} (d_r^2 + d_s^2). \quad (3)$$

Numerous topological indices present [1-3], but here we work on the irregularity indices. In the chemical graph theory, we apply the methods of graph theory to characterize chemical activities mathematically.

Konsalraj, et al., [4] computed the analytical expressions of irregularity indices for three significant classes of polycyclic aromatic hydrocarbons. The intriguing structures of these kinds of compounds have various potential applications in a wide range of domains, allowing for a structural study of their properties. Ahmed [5] worked on the irregularity measures of categorical product of graphs. The upper limits of irregularity indices of categorical product of connected graphs were demonstrated in the form of its graph elements. Kang, et al., [6] calculated the degree-based irregularity indices of probabilistic neural network. The probabilistic neural network results are applicable in material science and other practical disciplines. Irregularity

indices [14] computed in this article depicted in Table 1.

For additional comprehensive study on indices, we mention the following articles [7-12, 18-28] for readers.

Silicon carbides has unusual physical and chemical characteristics due to its semi conductance and nontoxicity. It is outperforming their semiconductors due to their properties and low-cost manufacturing procedures [13]. Because silicon carbides save electricity, they are utilized to replace many metal components found in digital devices.

Let G be an undirected, without loop simple molecular graph with $V(G)$ and $E(G)$ as the vertex and edge sets. The degree of a vertex $p \in V(G)$ is symbolized by d_p , and the edge connecting vertices p and q is symbolized by $j = pq$, where $j \in E(G)$. If the degree of all the vertices of graph (G) is same then it is regular, otherwise it is said to be irregular. For undefined terms and notations, we mention the readers to Robin J. Wilson book [14].

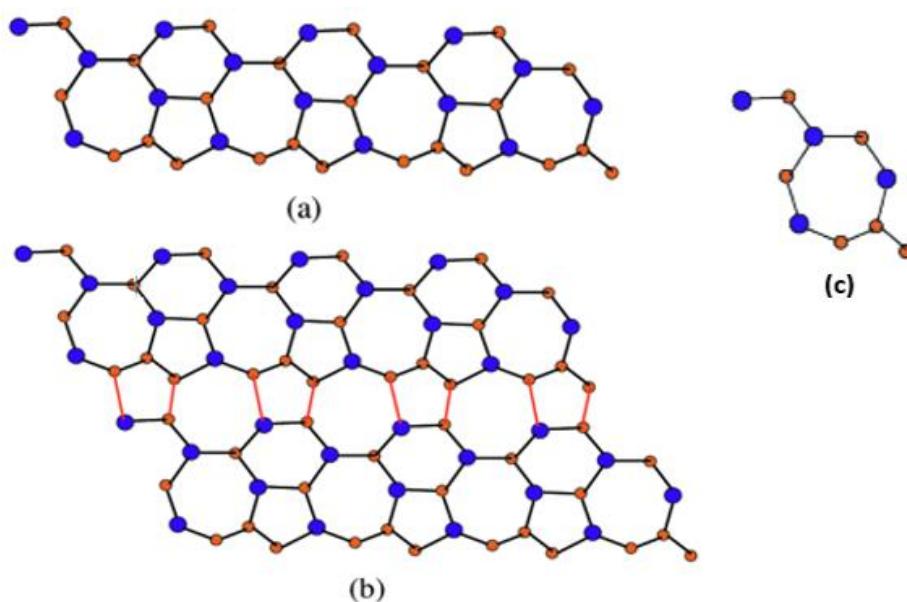
Table 1:Irregularity indices.

1).	$VAR(G) = \frac{M_1(G)}{i} - \left(\frac{2j}{i}\right)^2$	2).	$AL(G) = \sum_{pq \in E(G)} d_p - d_q $
3).	$IR1(G) = F(G) - \frac{2j}{i} M_1(G)$	4).	$IR2(G) = \sqrt{\frac{M_2(G)}{j}} - \frac{2j}{i}$
5).	$IRF(G) = F(G) - 2M_2(G)$	6).	$IRFW(G) = \frac{IRF(G)}{M_2(G)}$
7).	$IRA(G) = \sum_{pq \in E(G)} (d_p^{-1/2} - d_q^{-1/2})^2$	8).	$IRB(G) = \sum_{pq \in E(G)} (d_p^{1/2} - d_q^{1/2})^2$
9).	$IRC(G) = \sum_{pq \in E(G)} \frac{\sqrt{d_p d_q}}{j} - \frac{2j}{i}$	10).	$IRDIF(G) = \sum_{pq \in E(G)} \left \frac{d_p}{d_q} - \frac{d_q}{d_p} \right $
11).	$IRL(G) = \sum_{pq \in E(G)} \ln d_p - \ln d_q $	12).	$IRLU(G) = \sum_{pq \in E(G)} \frac{ d_p - d_q }{\min(d_p, d_q)}$
13).	$IRLF(G) = \sum_{pq \in E(G)} \frac{ d_p - d_q }{\sqrt{d_p d_q}}$	14).	$IRLA(G) = \sum_{pq \in E(G)} \frac{ d_p - d_q }{d_p + d_q}$
15).	$IRDI(G) = \sum_{pq \in E(G)} \ln\{1 + d_p - d_q \}$	16).	$IRGA(G) = \sum_{pq \in E(G)} \ln \frac{d_p + d_q}{(2)\sqrt{d_p d_q}}$

2. Main Results

Consider the 2D molecular structure of silicon carbide ($Si_2C_3-I(a,s)$) as depicted in Figure 1 having a shown the number of unit cell in each row and s shows the number of rows (see Figure

1(a)). Silicon Carbide ($Si_2C_3-I(a,s)$) has $10as$ vertices and $15as - 2a - 3s$ edges. According to Table 2, the edge set of ($Si_2C_3-I(a,s)$) can be divided into five sets by the degree of the vertices based on the structure analysis.

Figure 1: Molecular graphs of ($Si_2C_3-I(4,1)$), ($Si_2C_3-I(4,2)$) and ($Si_2C_3-I(1,1)$).

For the silicon carbide ($Si_2C_3-I(a,s)$) first-Zagreb index (M_1), second-Zagreb index (M_2) and forgotten index (F) are

$$\begin{aligned} M_1[(Si_2C_3-I(a,s))] &= 90as - 20a - 30s + 4. \\ M_2[(Si_2C_3-I(a,s))] &= 135as - 41a - 61s + 14. \\ F[(Si_2C_3-I(a,s))] &= 270as - 76a - 114s + 24. \end{aligned}$$

computed by using Equation (1), (2) and (3) and Table 2 as follows:

Table 2: Edge separation of ($Si_2C_3-I(a,s)$)

$E(d_p, d_q)$	Number of edges
(1, 2)	1
(1, 3)	1
(2, 2)	$a + 2s$
(2, 3)	$6a + 8s - 9$
(3, 3)	$15as - 9a - 13s + 7$

Theorem 2.1.

Let G be the Silicon Carbide ($Si_2C_3-I(a,s)$), then

$$I.VAR(G) = \frac{10a^2s - 4a^2 - 12a + 15as^2 - 9s^2 + 10as}{25as^2}.$$

$$II.AL(G) = 6a + 8s - 6.$$

$$III.IR1(G) = \frac{2(-20a^2 + 50a^2s - 60as + 75as^2 - 45s^2 + 4a + 30as + 6s)}{5as}.$$

$$IV.IR2(G) = \frac{5as \sqrt{\frac{135as - 41a - 61s + 14}{15as - 2a - 3s}} + 2a - 15as + 3s}{5as}.$$

$$V.IRF(G) = 6a + 8s - 4.$$

$$VI.IRFW(G) = \frac{6a + 8s - 4}{135as - 41a - 61s + 14}.$$

$$VII.IRA(G) = -\frac{14}{3} - \sqrt{2} - \frac{2}{3}\sqrt{3} + 5a - 2a\sqrt{6} + \frac{20s}{3} - \frac{8s}{3}\sqrt{6} + 3\sqrt{6}.$$

$$VIII.IRB(G) = -38 - 2\sqrt{2} - 2\sqrt{3} - 12a\sqrt{6} + 30a - 16s\sqrt{6} + 40s + 18\sqrt{6}.$$

$$IX.IRC(G) = \frac{\sqrt{2} + \sqrt{3} - 25a - 35s + (6a + 8s - 9)\sqrt{6} + 45as + 21}{15as - 2a - 3s} - \frac{15as - 2a - 3s}{5as}.$$

$$X.IRDIF(G) = \frac{25}{6} + \frac{5}{6}(6a + 8s - 9).$$

$$XI.IRL(G) = 2.4327a + 3.2436s - 1.8572.$$

$$XII.IRLU(G) = 3a + 4s - \frac{3}{2}.$$

$$XIII.IRLF(G) = \frac{1}{\sqrt{2}} + \frac{2}{\sqrt{3}} + (6a + 8s - 9)\frac{1}{\sqrt{6}}.$$

$$XIV.IRLA(G) = \frac{6}{5}a + \frac{8}{5}s - \frac{29}{30}.$$

$$XV.IRDI(G) = 4.1589a + 5.5452s - 4.4466.$$

$$XVI.IRGA(G) = 0.1223a + 0.1631s + 0.01916.$$

Proof: Table 2 shows the edges of the type $E(d_p, d_q)$ where pq is an edge. By using Table 2, we acquire the following results:

$$\begin{aligned} VAR(G) &= \frac{M_1(G)}{i} - \left(\frac{2j}{i}\right)^2. \\ VAR(G) &= \frac{4 - 20a - 30s + 90as}{10as} - \left(\frac{2(15as - 2a - 3s)}{10as}\right)^2. \\ VAR(G) &= \frac{10a^2s - 4a^2 - 12a + 15as^2 - 9s^2 + 10as}{25as^2}. \end{aligned}$$

$$\mathbf{AL}(\mathbf{G}) = \sum_{pq \in E(G)} |\mathbf{d}_p - \mathbf{d}_q|.$$

$$AL(G) = |1 - 2| + |1 - 3| + (a + 2s)|2 - 2| + (6a + 8s - 9)|2 - 3| \\ + (15as - 9a - 13s + 7)|3 - 3|.$$

$$AL(G) = 6a + 8s - 6.$$

$$\mathbf{IR1}(\mathbf{G}) = \mathbf{F}(\mathbf{G}) - \frac{2j}{i} \mathbf{M}_1(\mathbf{G}).$$

$$= (24 - 76a - 114s + 270as) - \frac{(15as - 2a - 3s)}{5as} (4 - 20a - 30s + 90as).$$

$$IR1(G) = \frac{2(-20a^2 + 50a^2s - 60as + 75as^2 - 45s^2 + 4a + 30as + 6s)}{5as}.$$

$$\mathbf{IR2}(\mathbf{G}) = \sqrt{\frac{\mathbf{M}_2(\mathbf{G})}{j}} - \frac{2j}{i}.$$

$$IR2(G) = \sqrt{\frac{135as - 41a - 61s + 14}{15as - 2a - 3s}} - \frac{2(15as - 2a - 3s)}{10as}.$$

$$IR2(G) = \frac{5as \sqrt{\frac{135as - 41a - 61s + 14}{15as - 2a - 3s}} + 2a - 15as + 3s}{5as}.$$

$$\mathbf{IRF}(\mathbf{G}) = \mathbf{F}(\mathbf{G}) - 2\mathbf{M}_2(\mathbf{G}).$$

$$IRF(G) = (24 - 76a - 114s + 270as) - 2(135as - 41a - 61s + 14).$$

$$IRF(G) = 6a + 8s - 4.$$

$$\mathbf{IRFW}(\mathbf{G}) = \frac{\mathbf{IRF}(\mathbf{G})}{\mathbf{M}_2(\mathbf{G})}.$$

$$IRFW(G) = \frac{6a + 8s - 4}{135as - 41a - 61s + 14}.$$

$$\mathbf{IRA}(\mathbf{G}) = \sum_{pq \in E(G)} (\mathbf{d}_p^{-1/2} - \mathbf{d}_q^{-1/2})^2.$$

$$IRA(G) = \left(1 - \frac{1}{\sqrt{2}}\right)^2 + \left(1 - \frac{1}{\sqrt{3}}\right)^2 + (a + 2s)\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{2}}\right)^2 + (6a + 8s - 9)\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}}\right)^2 \\ + (15as - 9a - 13s + 7)\left(\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{3}}\right)^2.$$

$$IRA(G) = -\frac{14}{3} - \sqrt{2} - \frac{2}{3}\sqrt{3} + 5a - 2a\sqrt{6} + \frac{20s}{3} - \frac{8s}{3}\sqrt{6} + 3\sqrt{6}.$$

$$\mathbf{IRB}(\mathbf{G}) = \sum_{pq \in E(G)} (\mathbf{d}_p^{1/2} - \mathbf{d}_q^{1/2})^2.$$

$$IRB(G) = (1 - \sqrt{2})^2 + (1 - \sqrt{3})^2 + (a + 2s)(\sqrt{2} - \sqrt{2})^2 + (6a + 8s - 9)(\sqrt{2} - \sqrt{3})^2 \\ + (15as - 9a - 13s + 7)(\sqrt{3} - \sqrt{3})^2.$$

$$IRB(G) = -38 - 2\sqrt{2} - 2\sqrt{3} - 12a\sqrt{6} + 30a - 16s\sqrt{6} + 40s + 18\sqrt{6}.$$

$$\mathbf{IRC}(\mathbf{G}) = \sum_{pq \in E(G)} \frac{\sqrt{\mathbf{d}_p \mathbf{d}_q}}{j} - \frac{2j}{i}.$$

$$IRC(G) = \frac{\sqrt{2} + \sqrt{3} + (a + 2s)\sqrt{4} + (6a + 8s - 9)\sqrt{6} + (15as - 9a - 13s + 7)\sqrt{9}}{15as - 2a - 3s} - \frac{2(15as - 2a - 3s)}{10as}.$$

$$IRC(G) = \frac{\sqrt{2} + \sqrt{3} - 25a - 35s + (6a + 8s - 9)\sqrt{6} + 45as + 21}{15as - 2a - 3s} - \frac{15as - 2a - 3s}{5as}.$$

$$IRDIF(G) = \sum_{pq \in E(G)} \left| \frac{d_p}{d_q} - \frac{d_q}{d_p} \right|.$$

$$IRDIF(G) = \left| \frac{1}{2} - 2 \right| + \left| \frac{1}{3} - 3 \right| + (6a + 8s - 9) \left| \frac{2}{3} - \frac{3}{2} \right|$$

$$IRDIF(G) = \frac{25}{6} + \frac{5}{6}(6a + 8s - 9).$$

$$IRL(G) = \sum_{pq \in E(G)} |\ln d_p - \ln d_q|.$$

$$IRL(G) = |\ln 1 - \ln 2| + |\ln 1 - \ln 3| + (a + 2s)|\ln 2 - \ln 2| + (6a + 8s - 9)|\ln 2 - \ln 3| + (15as - 9a - 13s + 7)|\ln 3 - \ln 3|.$$

$$IRL(G) = 2.4327a + 3.2436s - 1.8572.$$

$$IRLU(G) = \sum_{pq \in E(G)} \frac{|d_p - d_q|}{\min(d_p, d_q)}.$$

$$IRLU(G) = \frac{|1 - 2|}{1} + \frac{|1 - 3|}{1} + (a + 2s) \frac{|2 - 2|}{2} + (6a + 8s - 9) \frac{|2 - 3|}{2} + (15as - 9a - 13s + 7) \frac{|3 - 3|}{3}.$$

$$IRLU(G) = 3a + 4s - \frac{3}{2}.$$

$$IRLF(G) = \sum_{pq \in E(G)} \frac{|d_p - d_q|}{\sqrt{d_p d_q}}.$$

$$IRLF(G) = \frac{|1 - 2|}{\sqrt{2}} + \frac{|1 - 3|}{\sqrt{3}} + (a + 2s) \frac{|2 - 2|}{\sqrt{4}} + (6a + 8s - 9) \frac{|2 - 3|}{\sqrt{6}} + (15as - 9a - 13s + 7) \frac{|3 - 3|}{\sqrt{9}}.$$

$$IRLF(G) = \frac{1}{\sqrt{2}} + \frac{2}{\sqrt{3}} + (6a + 8s - 9) \frac{1}{\sqrt{6}}.$$

$$IRLA(G) = \sum_{pq \in E(G)} \frac{|d_p - d_q|}{d_p + d_q}.$$

$$IRLA(G) = \frac{|1 - 2|}{3} + \frac{|1 - 3|}{4} + (a + 2s) \frac{|2 - 2|}{4} + (6a + 8s - 9) \frac{|2 - 3|}{5} + (15as - 9a - 13s + 7) \frac{|3 - 3|}{6}.$$

$$IRLA(G) = \frac{6}{5}a + \frac{8}{5}s - \frac{29}{30}.$$

$$IRDI(G) = \sum_{pq \in E(G)} \ln\{1 + |d_p - d_q|\}.$$

$$IRDI(G) = \ln\{1 + |1 - 2|\} + \ln\{1 + |1 - 3|\} + (a + 2s)\ln\{1 + |2 - 2|\} + (6a + 8s - 9)\ln\{1 + |2 - 3|\} + (15as - 9a - 13s + 7)\ln\{1 + |3 - 3|\}.$$

$$IRDI(G) = \ln\{2\} + \ln\{3\} + (6a + 8s - 9) \ln\{2\}.$$

$$IRDI(G) = 4.1589a + 5.5452s - 4.4466.$$

$$IRGA(G) = \sum_{pq \in E(G)} \ln \frac{d_p + d_q}{(2)\sqrt{d_p d_q}}.$$

$$IRGA(G) = \ln \frac{1+2}{(2)\sqrt{2}} + \ln \frac{1+3}{(2)\sqrt{3}} + (a+2s) \left(\ln \frac{2+2}{(2)\sqrt{4}} \right) + (6a+8s-9) \left(\ln \frac{2+3}{(2)\sqrt{6}} \right) \\ + (15as - 9a - 13s + 7) \left(\ln \frac{3+3}{(2)\sqrt{9}} \right).$$

$$IRGA(G) = \ln \frac{3}{2\sqrt{2}} + \ln \frac{4}{(2)\sqrt{3}} + (6a+8s-9) \left(\ln \frac{5}{(2)\sqrt{6}} \right).$$

$$IRGA(G) = 0.1223a + 0.1631s + 0.01916.$$

Consider the 2D molecular structure of silicon carbide ($Si_2C_3-II(a,s)$) as depicted in

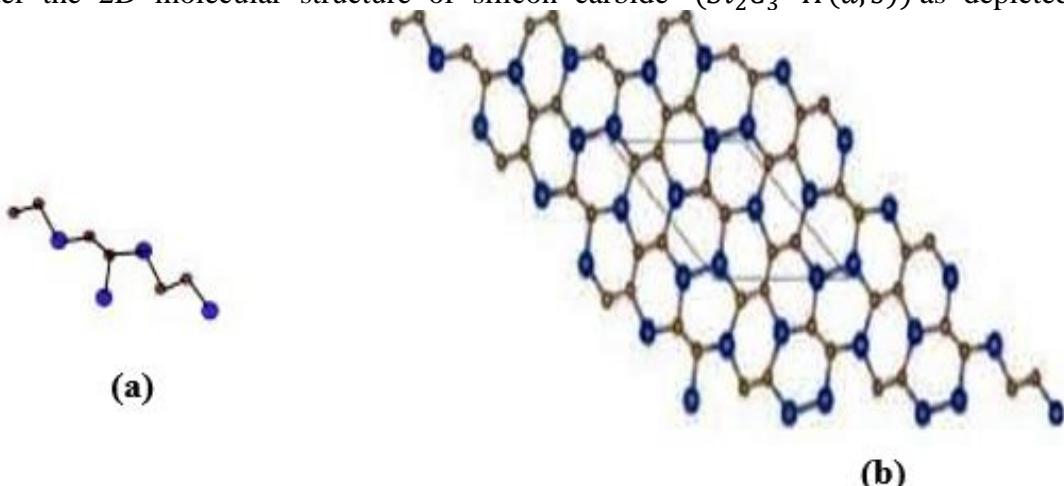


Figure 2 having a shown the number of unit cell in each row and s shows the number of rows. Silicon Carbide ($Si_2C_3-II(a,s)$) has $10as$ vertices and $15as - 3a - 3s$ edges. According to Table 3 the edge set of ($Si_2C_3-II(a,s)$) can be divided into five sets by the degree of the vertices based on the structure analysis.

For the silicon carbide ($Si_2C_3-II(a,s)$) first-Zagreb index (M_1), second-Zagreb index (M_2) and forgotten index (F) is computed by using Equation (1), (2) and (3) and Table 3.

$$M_1[(Si_2C_3-II(a,s))] = 90as - 30a - 30s + 6.$$

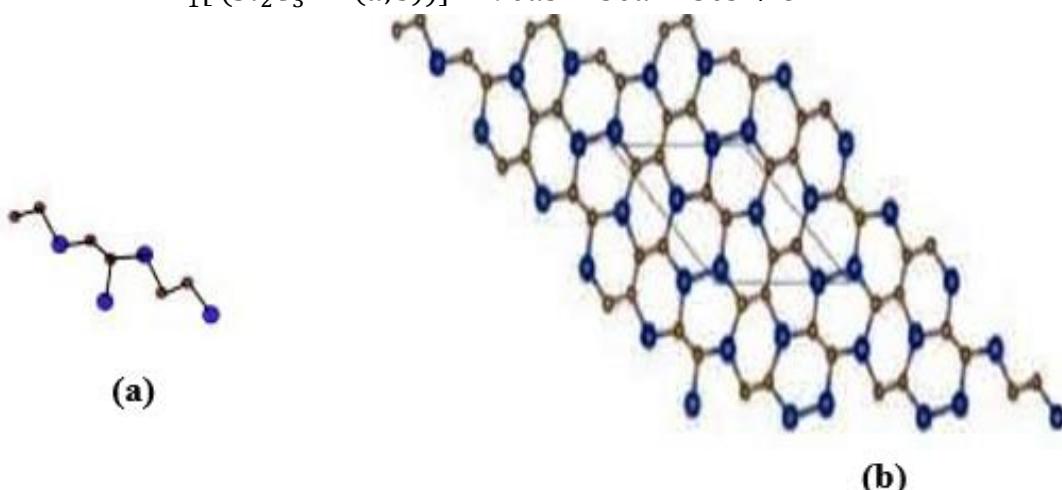


Figure 2: Molecular graphs of ($Si_2C_3-II(1,1)$) and ($Si_2C_3-II(3,3)$).

$$M_2[(Si_2C_3-II(a,s))] = 135as - 61a - 61s + 22.$$

$$F[(Si_2C_3-II(a,s))] = 270as - 114a - 114s + 36.$$

Table 3: Edge separation of $(Si_2C_3-II(a,s))$.

$E(d_p, d_q)$	Number of edges
(1, 2)	2
(1, 3)	1
(2, 2)	$2a + 2s$
(2, 3)	$2(4a + 4s - 7)$
(3, 3)	$15as - 13(a + s) + 11$

Theorem 2.2.

Let G be the Silicon Carbide $(Si_2C_3-II(a,s))$, then

$$\text{i.} VAR(G) = \frac{3(5a^2s - 3a^2 - 6as + 5as^2 - 3s^2 + 5as)}{25as^2}.$$

$$\text{ii.} AL(G) = 8a + 8s - 10.$$

$$\text{iii.} IRI(G) = \frac{6(-15a^2 + 25a^2s - 30as + 25as^2 - 15s^2 + 3a + 15as + 3s)}{5as}.$$

$$\text{iv.} IR2(G) = \frac{5as\sqrt{\frac{135as - 61a - 61s + 22}{15as - 3a - 3s}} + 3a - 15as + 3s}{5as}.$$

$$\text{v.} IRF(G) = 8a + 8s - 8.$$

$$\text{vi.} IRFW(G) = \frac{8(a+s-1)}{135as - 61a - 61s + 22}.$$

$$\text{vii.} IRA(G) = -\frac{2}{3}(2\sqrt{6} - 5)(13\sqrt{6} - 17\sqrt{3} - 21\sqrt{2} + 2a + 2s + 29).$$

$$\text{viii.} IRB(G) = -2(2\sqrt{6} - 5)(10\sqrt{6} - 13\sqrt{3} - 16\sqrt{2} + 4a + 4s + 18).$$

$$\text{ix.} IRC(G) = \frac{2\sqrt{2} + \sqrt{3} - 35a - 35s + 2(4a + 4s - 7)\sqrt{6} + 45as + 33}{15as - 3a - 3s} - \frac{15as - 3a - 3s}{5as}.$$

$$\text{x.} IRDIF(G) = \frac{20}{3}(a + s) - 6.$$

$$\text{xi.} IRL(G) = 3.2436a + 3.2436s - 3.1915.$$

$$\text{xii.} IRLU(G) = 4a + 4s - 3.$$

$$\text{xiii.} IRLF(G) = \frac{1}{3}(\sqrt{3} + \sqrt{2} + 4a + 4s - 7)\sqrt{6}.$$

$$\text{xiv.} IRLA(G) = \frac{8}{5}(a + s) - \frac{49}{30}.$$

$$\text{xv.} IRDI(G) = 5.5452a + 5.5452s - 7.2191.$$

$$\text{xvi.} IRGA(G) = 0.1631a + 0.1631s - 0.08280.$$

Proof: Table 3 shows the edges of the type $E(d_p, d_q)$ where pq is an edge. By using Table 3, we acquire the following results:

$$VAR(G) = \frac{M_1(G)}{i} - \left(\frac{2j}{i}\right)^2.$$

$$VAR(G) = \frac{90as - 30a - 30s + 6}{10as} - \left(\frac{2(15as - 3a - 3s)}{10as}\right)^2.$$

$$VAR(G) = \frac{3(5a^2s - 3a^2 - 6as + 5as^2 - 3s^2 + 5as)}{25as^2}.$$

$$AL(G) = \sum_{pq \in E(G)} |d_p - d_q|.$$

$$AL(G) = 2|1 - 2| + |1 - 3| + (2a + 2s)|2 - 2| + 2(4a + 4s - 7)|2 - 3| + (15as - 13(a + s) + 11)|3 - 3|.$$

$$AL(G) = 8a + 8s - 10.$$

$$\begin{aligned} \mathbf{IR1}(G) &= F(G) - \frac{2j}{i} M_1(G) \\ &= (270as - 114a - 114s + 36) - \frac{(15as - 3a - 3s)}{5as} (90as - 30a - 30s + 6). \\ IRI(G) &= \frac{6(-15a^2 + 25a^2s - 30as + 25as^2 - 15s^2 + 3a + 15as + 3s)}{5as}. \end{aligned}$$

$$\begin{aligned} IR2(G) &= \sqrt{\frac{M_2(G)}{j}} - \frac{2j}{i} \\ &= \sqrt{\frac{135as - 61a - 61s + 22}{15as - 3a - 3s}} - \frac{2(15as - 3a - 3s)}{10as}. \\ IR2(G) &= \frac{5as \sqrt{\frac{135as - 61a - 61s + 22}{15as - 3a - 3s}} + 3a - 15as + 3s}{5as}. \\ IRF(G) &= F(G) - 2M_2(G). \end{aligned}$$

$$IRF(G) = (270as - 114a - 114s + 36) - 2(135as - 61a - 61s + 22).$$

$$IRF(G) = 8a + 8s - 8.$$

$$\begin{aligned} IRFW(G) &= \frac{IRF(G)}{M_2(G)}. \\ IRFW(G) &= \frac{8(a + s - 1)}{135as - 61a - 61s + 22}. \end{aligned}$$

$$\begin{aligned} IRA(G) &= \sum_{pq \in E(G)} (d_p^{-1/2} - d_q^{-1/2})^2. \\ IRA(G) &= 2\left(1 - \frac{1}{\sqrt{2}}\right)^2 + \left(1 - \frac{1}{\sqrt{3}}\right)^2 + (2a + 2s)\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{2}}\right)^2 \\ &\quad + 2(4a + 4s - 7)\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}}\right)^2 \\ &\quad + (15as - 13(a + s) + 11)\left(\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{3}}\right)^2. \end{aligned}$$

$$IRA(G) = -\frac{2}{3}(2\sqrt{6} - 5)(13\sqrt{6} - 17\sqrt{3} - 21\sqrt{2} + 2a + 2s + 29).$$

$$IRB(G) = \sum_{pq \in E(G)} (d_p^{1/2} - d_q^{1/2})^2.$$

$$\begin{aligned} IRB(G) &= 2(1 - \sqrt{2})^2 + (1 - \sqrt{3})^2 + (2a + 2s)(\sqrt{2} - \sqrt{2})^2 \\ &\quad + 2(4a + 4s - 7)(\sqrt{2} - \sqrt{3})^2 \\ &\quad + (15as - 13(a + s) + 11)(\sqrt{3} - \sqrt{3})^2. \end{aligned}$$

$$IRB(G) = -2(2\sqrt{6} - 5)(10\sqrt{6} - 13\sqrt{3} - 16\sqrt{2} + 4a + 4s + 18).$$

$$IRC(G) = \sum_{pq \in E(G)} \frac{\sqrt{d_p d_q}}{j} - \frac{2j}{i}.$$

$$\begin{aligned} IRC(G) &= \frac{2\sqrt{2} + \sqrt{3} + (2a + 2s)\sqrt{4} + 2(4a + 4s - 7)\sqrt{6} + (15as - 13(a + s) + 11)\sqrt{9}}{15as - 3a - 3s} \\ &\quad - \frac{2(15as - 3a - 3s)}{10as}. \end{aligned}$$

$$IRC(G) = \frac{2\sqrt{2} + \sqrt{3} - 35a - 35s + 2(4a + 4s - 7)\sqrt{6} + 45as + 33}{15as - 3a - 3s} - \frac{15as - 3a - 3s}{5as}.$$

$$IRDIF(G) = \sum_{pq \in E(G)} \left| \frac{d_p}{d_q} - \frac{d_q}{d_p} \right|.$$

$$IRDIF(G) = 2 \left| \frac{1}{2} - 2 \right| + \left| \frac{1}{3} - 3 \right| + 2(4a + 4s - 7) \left| \frac{2}{3} - \frac{3}{2} \right|$$

$$IRDIF(G) = \frac{20}{3}(a + s) - 6.$$

$$IRL(G) = \sum_{pq \in E(G)} |\ln d_p - \ln d_q|.$$

$$IRL(G) = 2|\ln 1 - \ln 2| + |\ln 1 - \ln 3| + (2a + 2s)|\ln 2 - \ln 2| \\ + 2(4a + 4s - 7)|\ln 2 - \ln 3| + (15as - 13(a + s) + 11)|\ln 3 - \ln 3|.$$

$$IRL(G) = 3.2436a + 3.2436s - 3.1915.$$

$$IRLU(G) = \sum_{pq \in E(G)} \frac{|d_p - d_q|}{\min(d_p, d_q)}.$$

$$IRLU(G) = 2 \left(\frac{|1 - 2|}{1} \right) + \frac{|1 - 3|}{1} + (2a + 2s) \frac{|2 - 2|}{2} + 2(4a + 4s - 7) \frac{|2 - 3|}{2} + (15as - 13(a + s) + 11) \frac{|3 - 3|}{3}.$$

$$IRLU(G) = 4a + 4s - 3.$$

$$IRLF(G) = \sum_{pq \in E(G)} \frac{|d_p - d_q|}{\sqrt{d_p d_q}}.$$

$$IRLF(G) = 2 \left(\frac{|1 - 2|}{\sqrt{2}} \right) + \frac{|1 - 3|}{\sqrt{3}} + (2a + 2s) \frac{|2 - 2|}{\sqrt{4}} + 2(4a + 4s - 7) \frac{|2 - 3|}{\sqrt{6}} + (15as - 13(a + s) + 11) \frac{|3 - 3|}{\sqrt{9}}.$$

$$IRLF(G) = \frac{1}{3}(\sqrt{3} + \sqrt{2} + 4a + 4s - 7)\sqrt{6}.$$

$$IRLA(G) = \sum_{pq \in E(G)} \frac{|d_p - d_q|}{d_p + d_q}.$$

$$IRLA(G) = 2 \left(\frac{|1 - 2|}{3} \right) + \frac{|1 - 3|}{4} + (2a + 2s) \frac{|2 - 2|}{4} + 2(4a + 4s - 7) \frac{|2 - 3|}{5} + (15as - 13(a + s) + 11) \frac{|3 - 3|}{6}.$$

$$IRLA(G) = \frac{8}{5}(a + s) - \frac{49}{30}.$$

$$IRDI(G) = \sum_{pq \in E(G)} \ln \{1 + |d_p - d_q|\}.$$

$$IRDI(G) = 2(\ln \{1 + |1 - 2|\}) + \ln \{1 + |1 - 3|\} + (2a + 2s) \ln \{1 + |2 - 2|\} \\ + 2(4a + 4s - 7) \ln \{1 + |2 - 3|\} + (15as - 13(a + s) + 11) \ln \{1 + |3 - 3|\}.$$

$$IRDI(G) = 2(\ln \{2\}) + \ln \{3\} + 2(4a + 4s - 7) \ln \{2\}.$$

$$IRDI(G) = 5.5452a + 5.5452s - 7.2191.$$

$$IRGA(G) = \sum_{pq \in E(G)} \ln \frac{d_p + d_q}{(2)\sqrt{d_p d_q}}$$

$$IRGA(G) = 2\ln \frac{1+2}{(2)\sqrt{2}} + \ln \frac{1+3}{(2)\sqrt{3}} + (2a+2s)\left(\ln \frac{2+2}{(2)\sqrt{4}}\right) + 2(4a+4s-7)\left(\ln \frac{2+3}{(2)\sqrt{6}}\right)$$

$$+ (15as - 13(a+s) + 11)\left(\ln \frac{3+3}{(2)\sqrt{9}}\right).$$

$$IRGA(G) = 2\left(\ln \frac{3}{2\sqrt{2}}\right) + \ln \frac{4}{(2)\sqrt{3}} + 2(4a+4s-7)\left(\ln \frac{5}{(2)\sqrt{6}}\right).$$

$$IRGA(G) = 0.1631a + 0.1631s - 0.08280.$$

Consider the 2D molecular structure of silicon carbide ($Si_2C_3-III(a,s)$) as depicted in

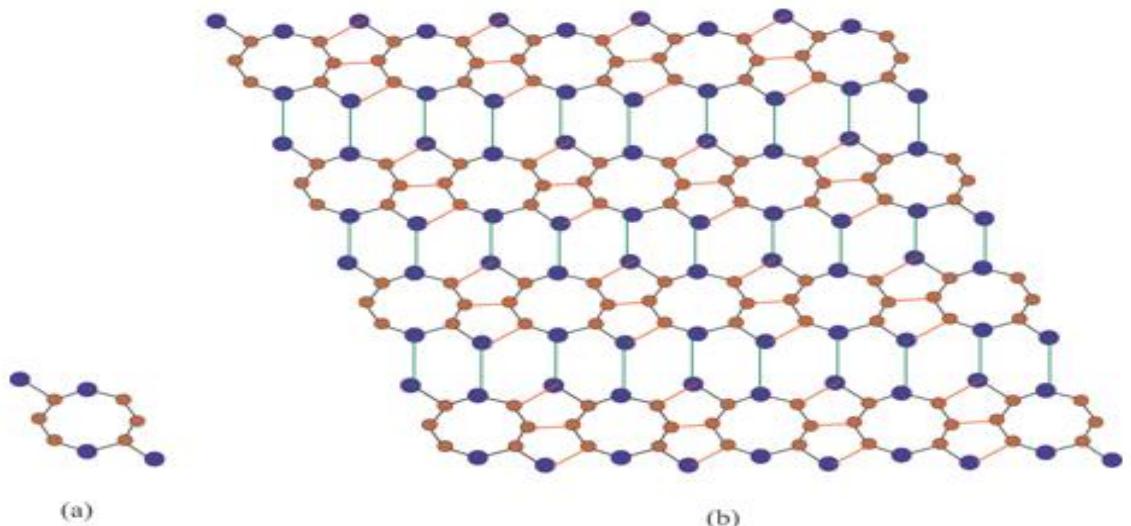


Figure 3 having a shown the number of unit cell in each row and s shows the number of rows. Silicon Carbide ($Si_2C_3-III(a,s)$) has $10as$ vertices and $15as - 2a - 3s$ edges. According to Table 4, the edge set of ($Si_2C_3-III(a,s)$) can be divided into four sets by the degree of the vertices based on the structure analysis.

For the silicon carbide ($Si_2C_3-III(a,s)$) first-Zagreb index (M_1), second-Zagreb index (M_2) and forgotten index (F) is computed by using Equation (1), (2) and (3) and Table 4.

$$M_1[(Si_2C_3-III(a,s))] = 90as - 20a - 30s + 4.$$

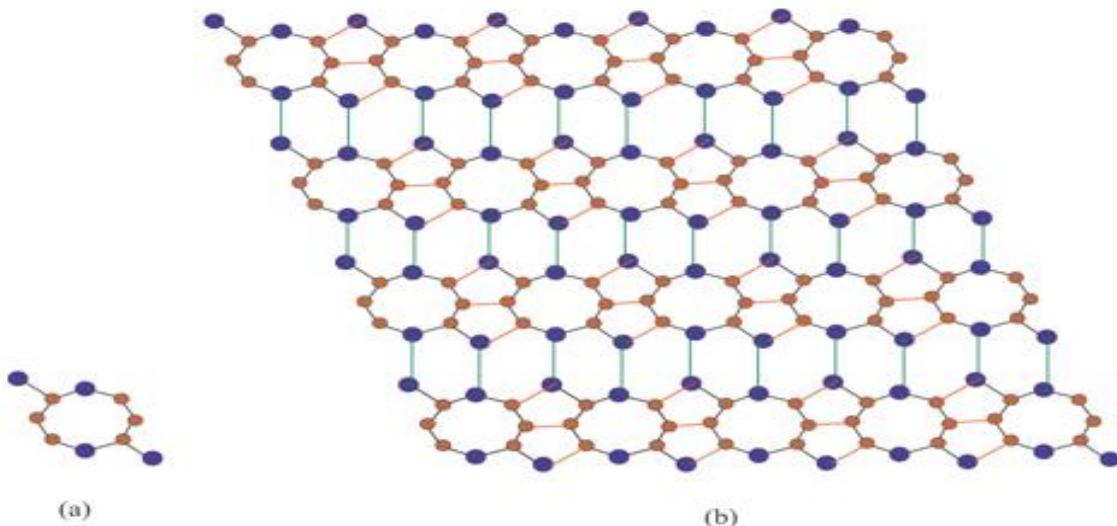


Figure 3: Molecular graphs of ($Si_2C_3-III(1,1)$) and ($Si_2C_3-III(5,4)$).

$$M_2[(Si_2C_3-III(a,s))] = 135as - 42a - 61s + 14.$$

$$F[(Si_2C_3-III(a,s))] = 270as - 76a - 114s + 24.$$

Table 4: Edge separation of $(Si_2C_3-III(a,s))$.

$E(d_p, d_q)$	Number of edges
(1, 3)	2
(2, 2)	$2 + 2s$
(2, 3)	$4(2a + 2s - 3)$
(3, 3)	$15as - 10a - 13s + 8$

Theorem 2.3.

Let G be the Silicon Carbide $(Si_2C_3-III(a,s))$, then

$$I.VAR(G) = \frac{10a^2s - 4a^2 - 12a + 15as^2 - 9s^2 + 10as}{25as^2}.$$

$$II.AL(G) = 8(a + s - 1).$$

$$III.IR1(G) = \frac{2(-20a^2 + 50a^2s - 60as + 75as^2 - 45s^2 + 4a + 30as + 6s)}{5as}.$$

$$IV.IR2(G) = \frac{5as \sqrt{\frac{135as - 42a - 61s + 14}{15as - 2a - 3s}} + 2a - 15as + 3s}{5as}.$$

$$V.IRF(G) = 4(2a + 2s - 1).$$

$$VI.IRFW(G) = \frac{4(2a + 2s - 1)}{135as - 42a - 61s + 14}.$$

$$VII.IRA(G) = -\frac{2}{3}(2\sqrt{6} - 5)(8\sqrt{6} - 10\sqrt{3} - 12\sqrt{2} + 2a + 2s + 17).$$

$$VIII.IRB(G) = -4(2\sqrt{6} - 5)(4\sqrt{6} - 5\sqrt{3} - 6\sqrt{2} + 2a + 2s + 7).$$

$$IX.IRC(G) = \frac{2\sqrt{3} - 28 - 35s + 4(2a + 2s - 3)\sqrt{6} + 45as + 30a}{15as - 2a - 3s} - \frac{15as - 2a - 3s}{5as}.$$

$$X.IRDIF(G) = \frac{20}{3}(a + s) - \frac{14}{3}.$$

$$XI.IRL(G) = 3.2436a + 3.2436s - 2.66820.$$

$$XII.IRLU(G) = 4a + 4s - 2.$$

$$XIII.IRLF(G) = \frac{2}{3}(\sqrt{2} + 2a + 2s - 3)\sqrt{6}.$$

$$XIV.IRLA(G) = \frac{8}{5}(a + s) - \frac{7}{5}.$$

$$XV.IRDI(G) = 5.5452a + 5.5452s - 6.1206.$$

$$XVI.IRGA(G) = 0.1631a + 0.1631s + 0.04299.$$

Proof: Table 4 shows the edges of type $E(d_p, d_q)$ where pq is an edge. By using Table 4, we acquire the following results:

$$VAR(G) = \frac{M_1(G)}{i} - \left(\frac{2j}{i}\right)^2.$$

$$VAR(G) = \frac{90as - 20a - 30s + 4}{10as} - \left(\frac{2(15as - 2a - 3s)}{10as}\right)^2.$$

$$VAR(G) = \frac{10a^2s - 4a^2 - 12a + 15as^2 - 9s^2 + 10as}{25as^2}.$$

$$AL(G) = \sum_{pq \in E(G)} |d_p - d_q|.$$

$$AL(G) = 2|1 - 3| + (2 + 2s)|2 - 2| + 4(2a + 2s - 3)|2 - 3| + (15as - 10a - 13s + 8)|3 - 3|.$$

$$AL(G) = 8(a + s - 1).$$

$$IR1(G) = F(G) - \frac{2j}{i}M_1(G)$$

$$= (270as - 76a - 114s + 24) - \frac{(15as - 2a - 3s)}{5as} (90as - 20a - 30s + 4).$$

$$IR1(G) = \frac{2(-20a^2 + 50a^2s - 60as + 75as^2 - 45s^2 + 4a + 30as + 6s)}{5as}.$$

$$IR2(G) = \sqrt{\frac{M_2(G)}{j}} - \frac{2j}{i}.$$

$$IR2(G) = \sqrt{\frac{135as - 42a - 61s + 14}{15as - 2a - 3s}} - \frac{2(15as - 2a - 3s)}{10as}.$$

$$IR2(G) = \frac{5as\sqrt{\frac{135as - 42a - 61s + 14}{15as - 2a - 3s}} + 2a - 15as + 3s}{5as}.$$

$$IRF(G) = F(G) - 2M_2(G).$$

$$IRF(G) = (270as - 76a - 114s + 24) - 2(135as - 42a - 61s + 14).$$

$$IRF(G) = 4(2a + 2s - 1).$$

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

$$IRFW(G) = \frac{4(2a + 2s - 1)}{135as - 42a - 61s + 14}.$$

$$IRA(G) = \sum_{pq \in E(G)} (d_p^{-1/2} - d_q^{-1/2})^2.$$

$$IRA(G) = 2\left(1 - \frac{1}{\sqrt{3}}\right)^2 + (2 + 2s)\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{2}}\right)^2 + 4(2a + 2s - 3)\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}}\right)^2 \\ + (15as - 10a - 13s + 8)\left(\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{3}}\right)^2.$$

$$IRA(G) = -\frac{2}{3}(2\sqrt{6} - 5)(8\sqrt{6} - 10\sqrt{3} - 12\sqrt{2} + 2a + 2s + 17).$$

$$IRB(G) = \sum_{pq \in E(G)} (d_p^{1/2} - d_q^{1/2})^2.$$

$$IRB(G) = 2(1 - \sqrt{3})^2 + (2 + 2s)(\sqrt{2} - \sqrt{2})^2 + 4(2a + 2s - 3)(\sqrt{2} - \sqrt{3})^2 \\ + (15as - 10a - 13s + 8)(\sqrt{3} - \sqrt{3})^2.$$

$$IRB(G) = -4(2\sqrt{6} - 5)(4\sqrt{6} - 5\sqrt{3} - 6\sqrt{2} + 2a + 2s + 7).$$

$$IRC(G) = \sum_{pq \in E(G)} \frac{\sqrt{d_p d_q}}{j} - \frac{2j}{i}.$$

$$IRC(G) = \frac{2\sqrt{3} + (2 + 2s)\sqrt{4} + 4(2a + 2s - 3)\sqrt{6} + (15as - 10a - 13s + 8)\sqrt{9}}{15as - 2a - 3s} \\ - \frac{2(15as - 2a - 3s)}{10as}.$$

$$IRC(G) = \frac{2\sqrt{3} - 28 - 35s + 4(2a + 2s - 3)\sqrt{6} + 45as + 30a}{15as - 2a - 3s} - \frac{15as - 2a - 3s}{5as}.$$

$$IRDIF(G) = \sum_{pq \in E(G)} \left| \frac{d_p}{d_q} - \frac{d_q}{d_p} \right|.$$

$$IRDIF(G) = 2 \left| \frac{1}{3} - 3 \right| + 4(2a + 2s - 3) \left| \frac{2}{3} - \frac{3}{2} \right|$$

$$IRDIF(G) = \frac{20}{3}(a + s) - \frac{14}{3}.$$

$$IRL(G) = \sum_{pq \in E(G)} |\ln d_p - \ln d_q|.$$

$$IRL(G) = 2|\ln 1 - \ln 3| + (2 + 2s)|\ln 2 - \ln 2| + 4(2a + 2s - 3)|\ln 2 - \ln 3| + (15as - 10a - 13s + 8)|\ln 3 - \ln 3|.$$

$$IRL(G) = 3.2436a + 3.2436s - 2.66820.$$

$$IRLU(G) = \sum_{pq \in E(G)} \frac{|d_p - d_q|}{\min(d_p, d_q)}.$$

$$IRLU(G) = 2 \left(\frac{|1 - 3|}{1} \right) + (2 + 2s) \frac{|2 - 2|}{2} + 4(2a + 2s - 3) \frac{|2 - 3|}{2} + (15as - 10a - 13s + 8) \frac{|3 - 3|}{3}.$$

$$IRLU(G) = 4a + 4s - 2.$$

$$IRLF(G) = \sum_{pq \in E(G)} \frac{|d_p - d_q|}{\sqrt{d_p d_q}}.$$

$$IRLF(G) = 2 \left(\frac{|1 - 3|}{\sqrt{3}} \right) + (2 + 2s) \frac{|2 - 2|}{\sqrt{4}} + 4(2a + 2s - 3) \frac{|2 - 3|}{\sqrt{6}} + (15as - 10a - 13s + 8) \frac{|3 - 3|}{\sqrt{9}}.$$

$$IRLF(G) = \frac{2}{3}(\sqrt{2} + 2a + 2s - 3)\sqrt{6}.$$

$$IRLA(G) = \sum_{pq \in E(G)} \frac{|d_p - d_q|}{d_p + d_q}.$$

$$IRLA(G) = 2 \frac{|1 - 3|}{4} + (2 + 2s) \frac{|2 - 2|}{4} + 4(2a + 2s - 3) \frac{|2 - 3|}{5} + (15as - 10a - 13s + 8) \frac{|3 - 3|}{6}.$$

$$IRLA(G) = \frac{8}{5}(a + s) - \frac{7}{5}.$$

$$IRDI(G) = \sum_{pq \in E(G)} \ln \{1 + |d_p - d_q|\}.$$

$$IRDI(G) = 2(\ln \{1 + |1 - 3|\}) + (2 + 2s)\ln \{1 + |2 - 2|\} + 4(2a + 2s - 3)\ln \{1 + |2 - 3|\} + (15as - 10a - 13s + 8)\ln \{1 + |3 - 3|\}.$$

$$IRDI(G) = 2(\ln \{3\}) + 4(2a + 2s - 3)\ln \{2\}.$$

$$IRDI(G) = 5.5452a + 5.5452s - 6.1206.$$

$$IRGA(G) = \sum_{pq \in E(G)} \ln \frac{d_p + d_q}{(2)\sqrt{d_p d_q}}.$$

$$IRGA(G) = 2 \left(\ln \frac{1 + 3}{(2)\sqrt{3}} \right) + (2 + 2s) \left(\ln \frac{2 + 2}{(2)\sqrt{4}} \right) + 4(2a + 2s - 3) \left(\ln \frac{2 + 3}{(2)\sqrt{6}} \right) + (15as - 10a - 13s + 8) \left(\ln \frac{3 + 3}{(2)\sqrt{9}} \right).$$

$$IRGA(G) = 2 \left(\ln \frac{4}{(2)\sqrt{3}} \right) + 4(2a + 2s - 3) \left(\ln \frac{5}{(2)\sqrt{6}} \right).$$

$$IRGA(G) = 0.1631a + 0.1631s + 0.04299.$$

Graphically Representation

Here we present graphically the results of above calculated irregular topological indices for different classes of Silicon Carbides, namely, $Si_2C_3-I(a,s)$, $Si_2C_3-II(a,s)$ and $Si_2C_3-III(a,s)$ (see Figures 4-6). In Table 5, we show the colors of the different irregular indices used in the graphical comparison.

Table 5. Colors used in graphically representations and their corresponding indices

$VAR(G)$		$AL(G)$	
$IR1(G)$		$IR2(G)$	
$IRF(G)$		$IRW(G)$	
$IRA(G)$		$IRB(G)$	
$IRC(G)$		$IRDIF(G)$	
$IRL(G)$		$IRLU(G)$	
$IRLF(G)$		$IRLA(G)$	
$IRDI(G)$		$IRGA(G)$	

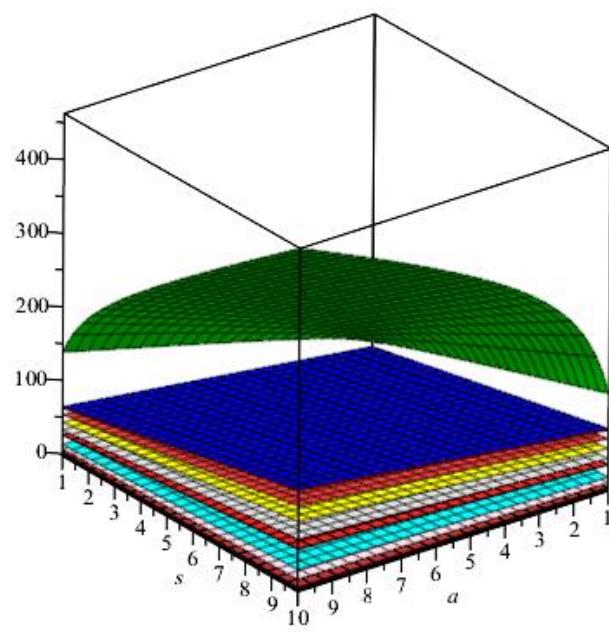


Figure 5: Graphically representation of irregularity indices for Silicon Carbide $Si_2C_3-I(a,s)$.

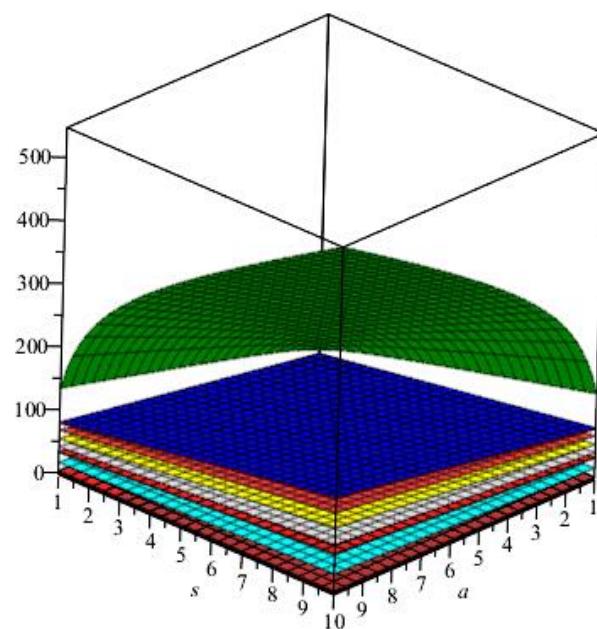


Figure 6: Graphically representation of irregularity indices for Silicon Carbide $Si_2C_3-II(a,s)$.

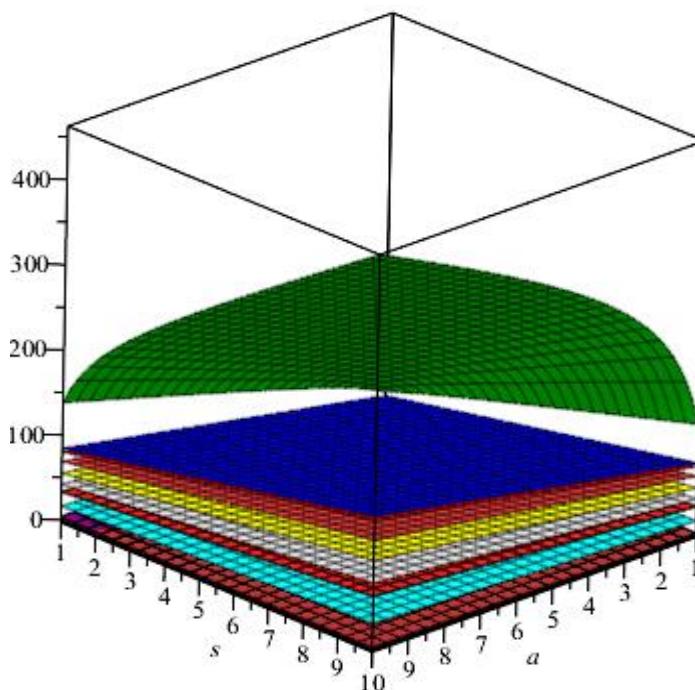


Figure 7: Graphically representation of irregularity indices for Silicon Carbide $Si_2C_3-III(a,s)$.

Conclusion

Indices are extremely essential in the subject of chemical graph theory. Topological indices are a practical way to convert chemical composition into numerical values. Many scholars have investigated topological indices for different graph families. Here, we calculate 16 different irregularity indices for the molecular graphs of Silicon carbides, after generalizing its molecular structure. Due to the wide range applications of silicon carbide in physics and chemistry, we examine $Si_2C_3-I(a,s)$, $Si_2C_3-II(a,s)$ and $Si_2C_3-III(a,s)$ graphically by using above calculated topological indices.

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