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Topological Properties of 2-Dimensional Silicon-Carbons

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ABSTRACT There are immense applications of graph theory in chemistry and in the study of molecular structures, and after that, it has been increasing exponentially. Molecular graphs have points (vertices) representing atoms and lines (edges) that represent bonds between atoms. In this paper, we study the molecular graph of 2-D silicon–carbon Si_2C_3-I and Si_2C_3-II and analyzed its topological properties. For this purpose, we have computed topological indices, namely forgotten topological index, augmented Zagreb index, and Balaban index, and redefined first, second, and third Zagreb indices of 2-D silicon–carbon Si_2C_3-I and Si_2C_3-II.

INDEX TERMS Balaban index, forgotten index, augmented index, redefined first, second and third Zagreb indices, silicon-carbon.

I. INTRODUCTION

The importance of graph theory for chemistry stands mainly from the existence of isomerism, which is rationalized by chemical graph theory. The essence of chemistry is the combinatorics of atoms according to definite rules. Thus, the most adequate mathematical tools for this purpose are graph theory and combinatorics, the branches of mathematics which are closely related. The chemical graph theory contributes the prominent role in the area of chemical theory. Chemical compounds have a variety of applications in chemical graph theory, drug design, etc. The manipulation and examination of chemical structural information is made conceivable by using molecular descriptors. A great variety of topological indices are studied and used in theoretical chemistry, pharmaceutical researchers [26], [27].

Silicon has superiority over other semiconductor objects: It is, of low cost, nontoxic, its resources are unlimited, decades of research carried out about its purification, expansion and device manufacturing. It is utilized for all most recent electronic gadgets. The most stable structures of two-dimensional $2D$ silicon-carbon monolayer molecules with various stoichiometric pieces were anticipated in [18] which in view of the molecule swarm advancement meant as (PSO) method joined with thickness practical hypothesis improvement.

The graphene sheets were effectively disengaged in [20] and [21] and from that point to onward this honeycomb structured $2D$ material has roused and motivated serious research interests to a great extent in view of its exceptional electronic, mechanical, and optical properties, including its unusual quantum Hall impact, unrivaled electronic conductivity, and high mechanical quality. Specifically, the one of a kind electronic properties of graphene attract consideration regarding this $2D$ material is a potential possibility for applications in speedier and littler electronic devices. The carbon and silicon has a $2D$ allotrope with a honeycomb structure, in particular silicene. To date, heaps of exertion has been dedicated to open a bandgap in silicene sheets. A $2D$ silicon carbon (Si-C) monolayers can be seen as piece tunable materials between the immaculate $2D$ carbon monolayer graphene and the unadulterated $2D$ silicon vmonolayer-silicene. Bunches of endeavors have been directed towards anticipating the most stable structures of the SiC sheet read this [16], [17], and [30] for more data.

In the fields of chemical graph theory, molecular topology, and mathematical chemistry, a topological index also known as a connectivity index is a type of a molecular descriptor that is calculated based on the molecular graph of a chemical compound. More Preciously a topological index is a numeric amount related with a graph which describes the topology of the graph and is invariant under graph automorphism. There are some significant classes of topological indices such as degree based topological indices, degree based topological lists and tallying related polynomials and indices of graphs. The idea of topological record originated from work done by Wiener [29] while he was dealing with breaking point of paraffin. He named this index as *path number*. Later on, the path number was renamed as *Wiener index*. The Wiener index is the first and most concentrated topological index, both from hypothetical perspective, applications and characterized as the entirety of separations between all sets of vertices in G, for more points of interest see [11] and [12].

Let $G = (V, E)$ be a graph with vertex set V and edge set E. The degree $d(t)$ of a vertex t is the number of edges of G connecting with t. One of the oldest topological index is the first Zagreb index presented by I. Gutman and N. Trinajstic based on degree of vertices of G in 1972. Taken after by the first and second Zagreb indices, Furtula and Gutman [8] introduced Forgotten topological index (also called F-index) which was defined as:

$$F(G) = \sum_{st\in E(G)} \left(d(s)^2 + d(t)^2\right) \tag{1}$$

Propelled by the accomplishment of the ABC index, Furtula *et al.* [9] set forward its adjusted variant, that they fairly deficiently named Augmented Zagreb index and is characterized as:

$$AZI(G) = \sum_{st\in E(G)} \left(\frac{d(s)\cdot d(t)}{d(s)+d(t)-2}\right)^3 \tag{2}$$

Balaban *et al.* [4], [5] introduced a topological index based on the degree of the vertex and is called Balaban index. This Balaban index for a graph G of order n, size m is defined as:

$$J(G) = \frac{m}{m-n+2} \sum_{s,t\in E(G)} \frac{1}{\sqrt{d(s)\cdot d(t)}} \tag{3}$$

Ranjini *et al.* [22] re-defined the Zagreb indices namely the redefined first, second and third Zagreb indices for a graph G as:

$$ReZG_1(G) = \sum_{st\in E(G)} \frac{d(s)+d(t)}{d(s)\cdot d(t)} \tag{4}$$

$$ReZG_2(G) = \sum_{st\in E(G)} \frac{d(s)\cdot d(t))}{d(s)+d(t)} \tag{5}$$

$$ReZG_3(G) = \sum_{st\in E(G)} (d(s)\cdot d(t))(d(s)+d(t)) \tag{6}$$

II. APPLICATIONS OF TOPOLOGICAL INDICES

Furtula and Gutman [8] raised that the prescient capacity of Forgotten topological index is practically like that of first Zagreb index and for the acentric factor and entropy, and then to acquire correlation coefficients bigger than 0.95. This reality suggests the motivation behind why Forgotten topological index is helpful for testing the chemical and pharmacological properties of medication atomic structures. Recently, Gao *et al.* [10] showed the Forgotten topological index of some noteworthy medication atomic structures.

Mekenyan *et al.* [19] found that Balaban index correlate well with a range of physicochemical properties or with acute toxicity of ethers. However, Thakur *et al.* [28] found that the inhibition of carbonic anhydrase by sulphonamides was modeled well by Balaban index. Also the Balaban index increase with the molecular size and branching of molecules. This property of Balaban index is very useful for chemical and biological structures in Quantitative structure-activity relationship(QSPR). Balaban index is also useful for modification of heteroatoms. The Augmented Zagreb index provides a very good correlation for the stability of linear alkanes as well as the branched alkanes and for computing the strain energy of cyclo alkanes [9]. Bajaj *et al.* [6], who used redefined Zagreb indices to model the anti-inflammatory activity of N-arylanthranilic acids, and that of Dureja *et al.* [7], who found that redefined Zagreb indices are valuable in modeling the fraction bound and clearance of cephalosporins in humans. Moreover Zagreb type indices were found to occur for computation of the total π-electron energy of the molecules of Silicon Carbide Si_2C_3-$I[p,q]$ $2D$ structure within specific approximate expressions [13]. For further study of topological indices and their applications of chemical structures, see [1]–[3], [12], [14], [15], [24], and [25].

III. METHODS

To compute our results we use the method of combinatorial computing, vertex partition method, edge partition method, graph theoretical tools, analytic techniques, degree counting method and sum of degrees of neighbors method. Moreover we use the Matlab for mathematical calculations and Maple for plotting these mathematical results.

IV. SILICON CARBIDE Si_2C_3-$I[p,q]$ 2D STRUCTURE

The $2D$ molecular graph of Silicon Carbide Si_2C_3-I is given in Figure 1. To describe its molecular graph we have used the settings in this way: we define p as the number of connected unit cells in a row(chain) and by q we represent the number of connected rows each with p number of cell. In Figure 2 we gave a demonstration how the cells connect in a row(chain) and how one row connects to another row. We will denote this molecular graph by Si_2C_3-$I[p,q]$. Thus the quantity of vertices in this graph is $10pq$ and the number of edges are $15pq - 2p - 3q$.

V. METHODOLOGY OF SILICON CARBIDE Si_2C_3-$I[p,q]$ FORMULAS

For the computation of these formulas for Silicon Carbide Si_2C_3-$I[p,q]$, we use first a unit cell then combine with another unit cell in horizontal direction and so on up to p unit cells. After this we use first a unit cell then combine

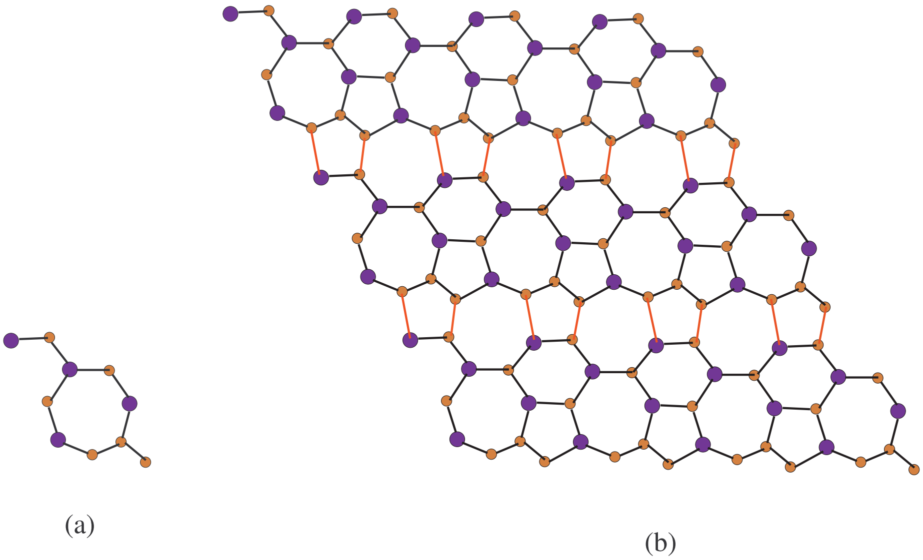


FIGURE 1. (a) Chemical unit cell of Si_2C_3-$I[p,q]$, (b) Si_2C_3-$I[4,3]$. Carbon atom C are brown and Silicon atom Si are blue.

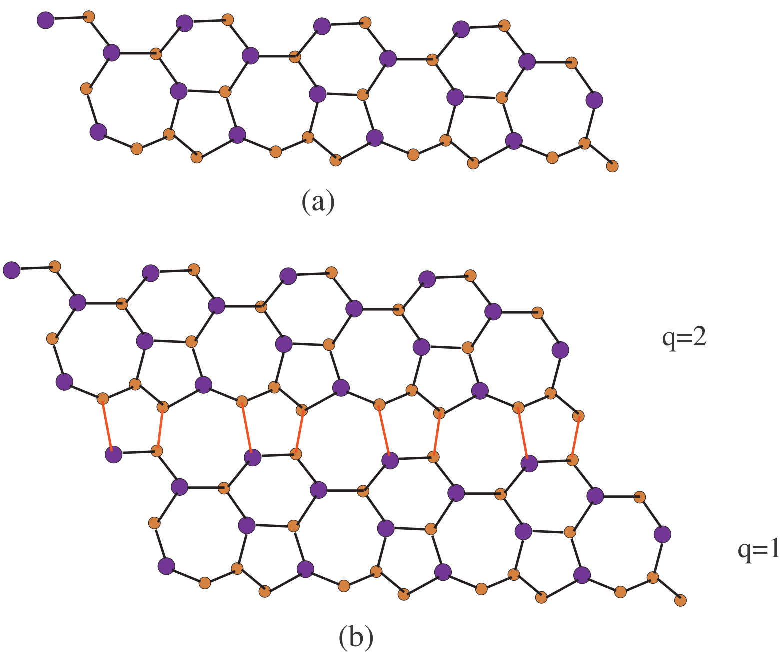


FIGURE 2. (a) Si_2C_3-$I[4,1]$, One row with $p = 4$ and $q = 1$ (b) Si_2C_3-$I[4,2]$, two rows are being connecting. Red lines(edges) connects the upper and lower rows.

with another unit cell in vertical direction and so on up to q unit cells, so we obtained Silicon Carbide $[p,q]$ structure see Figure 1. Now for the computation of vertices we use the Table 1, Table 2 and Matlab software for generalizing these formulas of vertices. In the following table, V_1 represents the quantity of vertices of degree 1, V_2 represents the quantity of vertices of degree 2 and V_3 represents the quantity of vertices of degree 3.

So finally we calculate the number of vertices of degree 1 are 2, the quantity of vertices of degree 2 are $4p+2+6(q-1)$ and the number of vertices of degree 3 are $10pq-4p-6q+2$.

TABLE 1. Vertex partition of Si_2C_3-$I[p,q]$.

$[p,q]$	$[1,1]$	$[1,2]$	$[1,3]$	$[2,1]$	$[2,2]$	$[2,3]$
V_1	2	2	2	2	2	2
V_2	6	12	18	10	16	2
V_3	2	6	10	8	22	36

To find topological indices of Si_2C_3-$I[p,q]$ we will take its edge partition as follows: The Table 3 shows the edge partition of Si_2C_3-$I[p,q]$ with $p,q \geq 1$. The edge set is partitioned into five sets, say, E_1, E_2, E_3, E_4, E_5 based on the degree of end vertices of each edge. The set E_1 contains one

TABLE 2. Vertex partition of Si_2C_3-$I[p,q]$.

$[p,q]$	$[3,1]$	$[3,2]$	$[3,3]$	$[4,1]$	$[4,2]$	$[4,3]$
V_1	2	2	2	2	2	2
V_2	14	20	26	18	28	30
V_3	14	38	62	20	54	88

TABLE 3. Edge partition of Si_2C_3-$I[p,q]$.

$(d(s),\ d(t))$	Frequency
$(2,\ 1)$	1
$(3,\ 1)$	1
$(2,\ 2)$	$p+2q$
$(3,\ 2)$	$6p-1+8(q-1)$
$(3,\ 3)$	$15pq-9p-13q+7$

edges of type uv such that $d(s)=2$, $d(t)=1$, E_2 contains one edge of type uv such that $d(s)=3$, $d(t)=1$, E_3 contains $p+2q$ edge of type uv such that $d(s)=2$, $d(t)=2$, E_4 contains $6p-1+8(q-1)$ edges of type uv such that $d(s)=3$, $d(t)=2$, E_5 contains $15pq-9p-13q+7$ edges of type uv such that $d(s)=3$, $d(t)=3$.

Theorem 1: Consider the graph of silicon carbide Si_2C_3-$I[p,q]$, then its Forgotten index is

$$F(Si_2C_3\text{-}I[p,q]) = 24-76p-114q+270pq$$

Proof: Let G be the graph of silicon carbide Si_2C_3-$I[p,q]$. Then by using Table 3 and equation (1) the Forgotten index is computed below:

$$F(G) = \sum_{s,t\in E(G)} \left(d(s)^2+d(t)^2\right)$$

$$\begin{aligned} F(G) &= \sum_{st\in E_1}[d(s)^2+d(t)^2] + \sum_{st\in E_2}[d(s)^2+d(t)^2] \\ &\quad + \sum_{st\in E_3}[d(s)^2+d(t)^2] + \sum_{st\in E_4}[d(s)^2+d(t)^2] \\ &\quad + \sum_{st\in E_5}[d(s)^2+d(t)^2] \end{aligned}$$

$$\begin{aligned} F(G) &= 5\mid E_1(Si_2C_3\text{-}I[p,q])\mid +10\mid E_2(Si_2C_3\text{-}I[p,q])\mid \\ &\quad +8\mid E_3(Si_2C_3\text{-}I[p,q])\mid +13\mid E_4(Si_2C_3\text{-}I[p,q])\mid \\ &\quad +18\mid E_5(Si_2C_3\text{-}I[p,q])\mid \\ &= 5(1)+10(1)+8(p+2q) \\ &\quad +13(6p-1+8(q-1)) \\ &\quad +18(15pq-9p-13q+7) \\ &= 24-76p-114q+270pq \end{aligned}$$

□

Theorem 2: Consider the graph of silicon carbide Si_2C_3-$I[p,q]$, then its Augmented Zagreb index is

$$AZI(Si_2C_3\text{-}I[p,q]) = \frac{1223}{64}-\frac{2977}{64}p - \frac{4357}{64}q+\frac{10935}{64}pq$$

Proof: Let G be the graph of silicon carbide Si_2C_3-$I[p,q]$. Then by using Table 3 and equation (2) the Augmented Zagreb index is computed below:

$$AZI(G) = \sum_{st\in E(G)}\left(\frac{d(s)\cdot d(t)}{d(s)+d(t)-2}\right)^3$$

$$\begin{aligned} AZI(G) &= \sum_{st\in E_1}\left(\frac{d(s)\cdot d(t)}{d(s)+d(t)-2}\right)^3 \\ &\quad + \sum_{st\in E_2}\left(\frac{d(s)\cdot d(t)}{d(s)+d(t)-2}\right)^3 \\ &\quad + \sum_{st\in E_3}\left(\frac{d(s)\cdot d(t)}{d(s)+d(t)-2}\right)^3 \\ &\quad + \sum_{st\in E_4}\left(\frac{d(s)\cdot d(t)}{d(s)+d(t)-2}\right)^3 \\ &\quad + \sum_{st\in E_5}\left(\frac{d(s)\cdot d(t)}{d(s)+d(t)-2}\right)^3 \\ &= 8\mid E_1(Si_2C_3\text{-}I[p,q])\mid \\ &\quad +\frac{27}{8}\mid E_2(Si_2C_3\text{-}I[p,q])\mid \\ &\quad +8\mid E_3(Si_2C_3\text{-}I[p,q])\mid \\ &\quad +8\mid E_4(Si_2C_3\text{-}I[p,q])\mid \\ &\quad +\frac{729}{64}\mid E_5(Si_2C_3\text{-}I[p,q])\mid \end{aligned}$$

$$\begin{aligned} AZI(G) &= 8(1)+\frac{27}{8}(1)+8(p+2q)+8(6p-1+8(q-1)) \\ &\quad +\frac{729}{64}(15pq-9p-13q+7) \\ &= \frac{1223}{64}-\frac{2977}{64}p-\frac{4357}{64}q+\frac{10935}{64}pq \end{aligned}$$

□

Theorem 3: Consider the graph of silicon carbide $G\cong Si_2C_3$-$I[p,q]$, then its Balaban index is

$$\begin{aligned} J(G) &= \frac{15pq-2p-3q}{5pq-2p-3q+2}\left[\frac{7}{3}+\frac{\sqrt{2}}{2}\right] \\ &\quad +\frac{15pq-2p-3q}{5pq-2p-3q+2}\left[\frac{\sqrt{3}}{3}-\frac{5}{2}p\right] \\ &\quad +\frac{15pq-2p-3q}{5pq-2p-3q+2}\left[\frac{-10}{3}q+5pq\right] \\ &\quad +\frac{15pq-2p-3q}{5pq-2p-3q+2}\left[\frac{6p+8q-9}{\sqrt{6}}\right] \end{aligned}$$

Proof: Let G be the graph of silicon carbide Si_2C_3-$I[p,q]$. Then by using Table 3 and equation (3) the

Balaban index is computed below:

$$J(G)=\frac{m}{m-n+2}\sum_{st\in E(G)}\frac{1}{\sqrt{d(s).d(t)}}$$

$$J(G)=\frac{m}{m-n+2}\left[\sum_{st\in E_1}\frac{1}{\sqrt{d(s).d(t)}}+\sum_{st\in E_2}\frac{1}{\sqrt{d(s).d(t)}}\right]+\frac{m}{m-n+2}\left[\sum_{st\in E_3}\frac{1}{\sqrt{d(s).d(t)}}+\sum_{st\in E_4}\frac{1}{\sqrt{d(s).d(t)}}\right]+\frac{m}{m-n+2}\left[\sum_{st\in E_5}\frac{1}{\sqrt{d(s).d(t)}}\right]$$

$$=\frac{15pq-2p-3q}{5pq-2p-3q+2}\left[\frac{1}{\sqrt{2}}\mid E_1(Si_2C_3\text{-}I[p,q])\mid\right]+\frac{15pq-2p-3q}{5pq-2p-3q+2}\left[\frac{1}{\sqrt{3}}\mid E_2(Si_2C_3\text{-}I[p,q])\mid\right]+\frac{15pq-2p-3q}{5pq-2p-3q+2}\left[\frac{1}{2}\mid E_3(Si_2C_3\text{-}I[p,q])\mid\right]+\frac{15pq-2p-3q}{5pq-2p-3q+2}\left[\frac{1}{\sqrt{6}}\mid E_4(Si_2C_3\text{-}I[p,q])\mid\right]+\frac{15pq-2p-3q}{5pq-2p-3q+2}\left[\frac{1}{3}\mid E_5(Si_2C_3\text{-}I[p,q])\mid\right]$$

$$J(G)=\frac{15pq-2p-3q}{5pq-2p-3q+2}\left[\frac{1}{\sqrt{2}}(1)+\frac{1}{\sqrt{3}}(1)+\frac{1}{2}(p+2q)\right]+\frac{15pq-2p-3q}{5pq-2p-3q+2}\left[\frac{1}{\sqrt{6}}(6p-1+8(q-1))\right]+\frac{15pq-2p-3q}{5pq-2p-3q+2}\left[\frac{1}{3}(15pq-9p-13q+7)\right]$$

$$J(G)=\frac{15pq-2p-3q}{5pq-2p-3q+2}\left[\frac{7}{3}+\frac{\sqrt{2}}{2}\right]+\frac{15pq-2p-3q}{5pq-2p-3q+2}\left[\frac{\sqrt{3}}{3}-\frac{5}{2}p\right]+\frac{15pq-2p-3q}{5pq-2p-3q+2}\left[\frac{-10}{3}q+5pq\right]+\frac{15pq-2p-3q}{5pq-2p-3q+2}\left[\frac{6p+8q-9}{\sqrt{6}}\right]$$

□

Theorem 4: Consider the silicon carbide $Si_2C_3\text{-}I[p,q]$, then its redefine first, second and third Zagreb indices are:

$$ReG_1(Si_2C_3\text{-}I[p,q])=10pq$$

$$ReG_2(Si_2C_3\text{-}I[p,q])=\frac{67}{60}-\frac{53}{10}p-\frac{79}{10}q+\frac{45}{2}pq$$

$$ReG_3(Si_2C_3\text{-}I[p,q])=126-290p-430q+810pq$$

Proof: Let G be the graph of silicon carbide $Si_2C_3\text{-}I[p,q]$. Then by using Table 3 and equations (4)-(6), we have

$$ReG_1(G)=\sum_{st\in E(G)}\frac{d(s)+d(t)}{d(s)\cdot d(t)}=\sum_{st\in E_1}\frac{d(s)+d(t)}{d(s)\cdot d(t)}+\sum_{st\in E_2}\frac{d(s)+d(t)}{d(s)\cdot d(t)}+\sum_{st\in E_3}\frac{d(s)+d(t)}{d(s)\cdot d(t)}+\sum_{st\in E_4}\frac{d(s)+d(t)}{d(s)\cdot d(t)}+\sum_{st\in E_5}\frac{d(s)+d(t)}{d(s)\cdot d(t)}$$

$$ReG_1(G)=\frac{3}{2}\mid E_1(Si_2C_3\text{-}I[p,q])\mid+\frac{4}{3}\mid E_2(Si_2C_3\text{-}I[p,q])\mid+1\mid E_3(Si_2C_3\text{-}I[p,q])\mid+\frac{5}{6}\mid E_4(Si_2C_3\text{-}I[p,q])\mid+\frac{2}{3}\mid E_5(Si_2C_3\text{-}I[p,q])\mid$$

$$=\frac{3}{2}(1)+\frac{4}{3}(1)+1(p+2q)+\frac{5}{6}(6p-1+8(q-1))+\frac{2}{3}(15pq-9p-13q+7)=10pq$$

$$ReG_2(G)=\sum_{st\in E(G)}\frac{d(s)\cdot d(t)}{d(s)+d(t)}=\sum_{st\in E_1}\frac{d(s)\cdot d(t)}{d(s)+d(t)}+\sum_{st\in E_2}\frac{d(s)\cdot d(t)}{d(s)+d(t)}+\sum_{st\in E_3}\frac{d(s)\cdot d(t)}{d(s)+d(t)}+\sum_{st\in E_4}\frac{d(s)\cdot d(t)}{d(s)+d(t)}+\sum_{st\in E_5}\frac{d(s)\cdot d(t)}{d(s)+d(t)}$$

$$=\frac{2}{3}\mid E_1(Si_2C_3\text{-}I[p,q])\mid+\frac{3}{4}\mid E_2(Si_2C_3\text{-}I[p,q])\mid+1\mid E_3(Si_2C_3\text{-}I[p,q])\mid+\frac{6}{5}\mid E_4(Si_2C_3\text{-}I[p,q])\mid+\frac{3}{2}\mid E_5(Si_2C_3\text{-}I[p,q])$$

$$ReG_2(G)=\frac{2}{3}(1)+\frac{3}{4}(1)+1(p+2q)$$

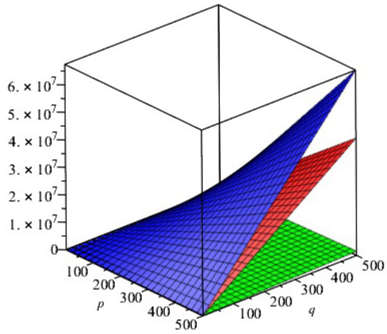


FIGURE 3. **Comparison of Forgotten index $F(G)$, Augmented Zagreb index $AZI(G)$ and Balaban index $J(G)$ of Si_2C_3-$I[p,\ q]$.**

$$+\frac{6}{5}(6p-1+8(q-1))$$

$$+\frac{3}{2}(15pq-9p-13q+7)$$

$$=\frac{67}{60}-\frac{53}{10}p-\frac{79}{10}q+\frac{45}{2}pq$$

$$ReG_3(G)=\sum_{st\in E(G)}(d(s)\cdot d(t))(d(s)+d(t))$$

$$=\sum_{st\in E_1}(d(s)\cdot d(t))(d(s)+d(t))$$

$$+\sum_{st\in E_2}(d(s)\cdot d(t))(d(s)+d(t))$$

$$+\sum_{st\in E_3}(d(s)\cdot d(t))(d(s)+d(t))$$

$$+\sum_{st\in E_4}(d(s)\cdot d(t))(d(s)+d(t))$$

$$+\sum_{st\in E_5}(d(s)\cdot d(t))(d(s)+d(t))$$

$$ReG_3(G)=2(3)\mid E_1(Si_2C_3\text{-}I[p,q])\mid$$

$$+3(4)\mid E_2(Si_2C_3\text{-}I[p,q])\mid$$

$$+4(4)\mid E_3(Si_2C_3\text{-}I[p,q])\mid$$

$$+6(5)\mid E_4(Si_2C_3\text{-}I[p,q])\mid$$

$$+9(6)\mid E_5(Si_2C_3\text{-}I[p,q])\mid$$

$$=2(3)(1)+3(4)(1)+4(4)(p+2q)$$

$$+6(5)(6p-1+8(q-1))$$

$$+9(6)(15pq-9p-13q+7)$$

$$=126-290p-430q+810pq$$

□

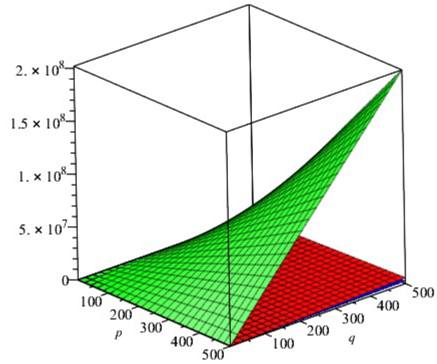


FIGURE 4. **Comparison of redefine first $ReG_1(G)$, second $ReG_2(G)$ and third Zagreb indices $ReG_3(G)$ of $Si_2C_3-I[p,\ q]$.**

TABLE 4. **Vertex partition of Si_2C_3-$II[p,q]$.**

$[p,q]$	$[1,1]$	$[1,2]$	$[1,3]$	$[2,1]$	$[2,2]$	$[2,3]$
V_1	3	3	3	3	3	3
V_2	6	12	18	12	18	24
V_3	1	5	9	5	19	33

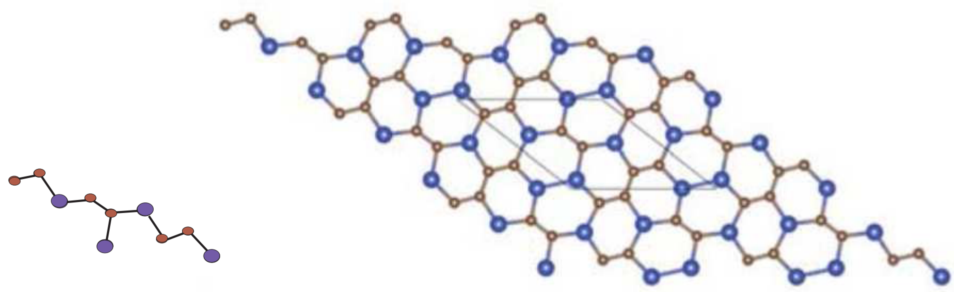
VI. SILICON CARBIDE Si_2C_3-$II[P,Q]$ 2D STRUCTURE

The $2D$ molecular graph of Silicon Carbide Si_2C_3-II is given in Figure 5. To describe its molecular graph we have used the settings in this way: we define p as the number of connected unit cells in a row(chain) and by q we represents the number of connected rows each with p number of cell. In Figure 6 we gave a demonstration how the cells connect in a row(chain) and how one row connects to another row. We will denote this molecular graph by Si_2C_3-$II[p,q]$. Thus the quantity of vertices in this graph is $10pq$ and the number of edges are $15pq-3p-3q$.

VII. METHODOLOGY OF SILICON CARBIDE Si_2C_3-$II[P,Q]$ FORMULAS

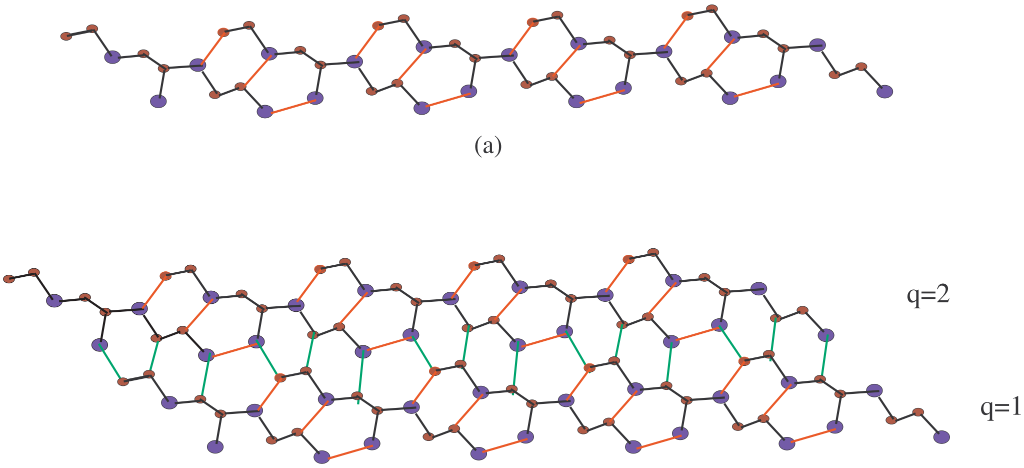
For the computation of these formulas for Silicon Carbide Si_2C_3-$II[p,q]$, we use first a unit cell then combine with another unit cell in horizontal direction and so on up to p unit cells. After this we use first a unit cell then combine with another unit cell in vertical direction and so on up to q unit cells, so we obtained Silicon Carbide Si_2C_3-$II[p,q]$ structure see Figure 5. Now for the computation of vertices we use the Table 4, Table 5 and Matlab software for generalizing these formulas of vertices. In the following table, V_1 represents the quantity of vertices of degree 1, V_2 represents the quantity of vertices of degree 2 and V_3 represents the quantity of vertices of degree 3. Now in general, the quantity of vertices of degree 1 are 3, the quantity of vertices of degree 2 are $6(p+q-1)$, the quantity of vertices of degree 3 are $10pq-6p-6q+3$.

To find topological indices of Si_2C_3-$II[p,q]$ we will take its edge partition as follows: The edge set is partitioned into five sets, say, E_1, E_2, E_3, E_4, E_5 based on the degree of end



(a) (b)

FIGURE 5. (a) Chemical unit cell of Si_2C_3-$II[p,q]$, (b) Si_2C_3-$II[3,3]$. Carbon atom C are brown and Silicon atom Si are blue.



(b)

FIGURE 6. (a) Si_2C_3-$II[5,1]$, One row with $p = 5$ and $q = 1$ (b) Si_2C_3-$II[5,2]$, two rows are connecting. Green lines(edges) connects the upper and lower rows.

TABLE 5. Vertex partition of Si_2C_3-$II[p,q]$.

$[p,q]$	$[3,1]$	$[3,2]$	$[3,3]$	$[4,1]$	$[4,2]$	$[4,3]$
V_1	3	3	3	3	3	3
V_2	18	24	30	24	30	36
V_3	9	33	57	13	47	81

vertices of each edge. The edge set E_1 contains 2 edges of type st such that $d(s) = 2$, $d(t) = 1$, E_2 contains one edge of type st such that $d(s) = 3$, $d(t) = 1$, E_3 contains $2p + 2q$ edges of type st such that $d(s) = 2$, $d(t) = 2$, E_4 contains $8p + 8q - 14$ edges of type st such that $d(s) = 3$, $d(t) = 2$, E_5 contains $15pq - 13p - 13q + 11$ edges of type st such that $d(s) = 3$, $d(t) = 3$. The Table 6 shows the edge partition of Si_2C_3-$II[p,q]$ with $p, q \geq 1$.

Theorem 5: Consider the silicon carbide Si_2C_3-$II[p,q]$, then its Forgotten index is equal to

$$F(Si_2C_3\text{-}II[p,q]) = 36 - 114p - 114q + 270pq$$

TABLE 6. Edge partition of Si_2C_3-$II[p,q]$.

$(d(s),\ d(t))$	$Frequency$
$(2,\ 1)$	2
$(3,\ 1)$	1
$(2,\ 2)$	$2p + 2q$
$(3,\ 2)$	$8p + 8q - 14$
$(3,\ 3)$	$15pq - 13p - 13q + 11$

Proof: Let G be the graph silicon carbide Si_2C_3-$II[p,q]$. Now by using Table 6 and equation (1) the Forgotten index is calculated as follows:

$$F(G) = \sum_{s,t \in E(G)} \left(d(s)^2 + d(t)^2\right)$$

$$F(G) = \sum_{st \in E_1} [d(s)^2 + d(t)^2] + \sum_{st \in E_2} [d(s)^2 + d(t)^2]$$
$$+ \sum_{st \in E_3} [d(s)^2 + d(t)^2] + \sum_{st \in E_4} [d(s)^2 + d(t)^2]$$

$$+\sum_{st\in E_5}[d(s)^2+d(t)^2]$$
$$= 5\mid E_1(Si_2C_3\text{-}II[p,q])\mid +10\mid E_2(Si_2C_3\text{-}II[p,q])\mid +8\mid E_3(Si_2C_3\text{-}II[p,q])\mid +13\mid E_4(Si_2C_3\text{-}II[p,q])\mid +18\mid E_5(Si_2C_3\text{-}II[p,q])\mid$$
$$= 5(2)+10(1)+8(2p+2q) +13(8p+8q-14)) +18(15pq-13p-13q+11)$$
$$= 36-114p-114q+270pq$$

□

Theorem 6: Consider the silicon carbide $Si_2C_3\text{-}II[p,q]$, then its Augmented Zagreb index is

$$AZI(Si_2C_3\text{-}II[p,q]) = \frac{2091}{64}-\frac{4357}{64}p -\frac{4357}{64}q+\frac{10935}{64}pq$$

Proof: Let G be the graph silicon carbide $Si_2C_3\text{-}II[p,q]$. Now by using Table 6 and equation (2) the Augmented Zagreb index is calculated as follows:

$$AZI(G) = \sum_{st\in E(G)}\left(\frac{d(s)\cdot d(t)}{d(s)+d(t)-2}\right)^3$$
$$AZI(G) = \sum_{st\in E_1}\left(\frac{d(s)\cdot d(t)}{d(s)+d(t)-2}\right)^3 + \sum_{st\in E_2}\left(\frac{d(s)\cdot d(t)}{d(s)+d(t)-2}\right)^3 + \sum_{st\in E_3}\left(\frac{d(s)\cdot d(t)}{d(s)+d(t)-2}\right)^3 + \sum_{st\in E_4}\left(\frac{d(s)\cdot d(t)}{d(s)+d(t)-2}\right)^3 + \sum_{st\in E_5}\left(\frac{d(s)\cdot d(t)}{d(s)+d(t)-2}\right)^3$$
$$AZI(G) = 8\mid E_1(Si_2C_3\text{-}II[p,q])\mid +\frac{27}{8}\mid E_2(Si_2C_3\text{-}II[p,q])\mid +8\mid E_3(Si_2C_3\text{-}II[p,q])\mid +8\mid E_4(Si_2C_3\text{-}II[p,q])\mid +\frac{729}{64}\mid E_5(Si_2C_3\text{-}II[p,q])\mid$$
$$= 8(2)+\frac{27}{8}(1)+8(2p+2q) +8(8p+8q-14) +\frac{729}{64}(15pq-13p-13q+11)$$
$$= \frac{2091}{64}-\frac{4357}{64}p-\frac{4357}{64}q+\frac{10935}{64}pq$$

□

Theorem 7: Consider the silicon carbide $G \cong Si_2C_3\text{-}II[p,q]$, then its Balaban index is given by:

$$J(G) = \frac{15pq-3p-3q}{5pq-3p-3q+2}\left[\frac{11}{3}+\sqrt{2}+\frac{\sqrt{3}}{3}\right] +\frac{15pq-3p-3q}{5pq-3p-3q+2}\left[-\frac{10}{3}p-\frac{10}{3}q+5pq\right] +\frac{15pq-3p-3q}{5pq-3p-3q+2}\left[\frac{\sqrt{6}}{6}(8p+8q-14)\right]$$

Proof: Let G be the graph silicon carbide $Si_2C_3\text{-}II[p,q]$. Now by using Table 6 and equation (3) the Balaban index is calculated as follows:

$$J(G) = \frac{m}{m-n+2}\sum_{st\in E(G)}\frac{1}{\sqrt{d(s).d(t)}}$$
$$J(G) = \frac{m}{m-n+2}\left[\sum_{st\in E_1}\frac{1}{\sqrt{d(s).d(t)}}+\sum_{st\in E_2}\frac{1}{\sqrt{d(s).d(t)}}\right] +\frac{m}{m-n+2}\left[\sum_{st\in E_3}\frac{1}{\sqrt{d(s).d(t)}}+\sum_{st\in E_4}\frac{1}{\sqrt{d(s).d(t)}}\right] +\frac{m}{m-n+2}\left[\sum_{st\in E_5}\frac{1}{\sqrt{d(s).d(t)}}\right]$$
$$J(G) = \frac{15pq-3p-3q}{5pq-3p-3q+2}\left[\frac{1}{\sqrt{2}}\mid E_1(Si_2C_3\text{-}II[p,q])\mid\right] +\frac{15pq-3p-3q}{5pq-3p-3q+2}\left[\frac{1}{\sqrt{3}}\mid E_2(Si_2C_3\text{-}II[p,q])\mid\right] +\frac{15pq-3p-3q}{5pq-3p-3q+2}\left[\frac{1}{2}\mid E_3(Si_2C_3\text{-}II[p,q])\mid\right] +\frac{15pq-3p-3q}{5pq-3p-3q+2}\left[\frac{1}{\sqrt{6}}\mid E_4(Si_2C_3\text{-}II[p,q])\mid\right] +\frac{15pq-3p-3q}{5pq-3p-3q+2}\left[\frac{1}{3}\mid E_5(Si_2C_3\text{-}II[p,q])\mid\right]$$
$$= \frac{15pq-3p-3q}{5pq-3p-3q+2}\left[\frac{1}{\sqrt{2}}(2)+\frac{1}{\sqrt{3}}(1)\right]$$

$$+\frac{15pq-3p-3q}{5pq-3p-3q+2}\left[\frac{1}{2}(2p+2q)\right]$$
$$+\frac{15pq-3p-3q}{5pq-3p-3q+2}\left[\frac{1}{\sqrt{6}}(8p+8q-14)\right]$$
$$+\frac{15pq-3p-3q}{5pq-3p-3q+2}\left[\frac{1}{3}(15pq-13p-13q+11)\right]$$
$$J(G)=\frac{15pq-3p-3q}{5pq-3p-3q+2}\left[\frac{11}{3}+\sqrt{2}+\frac{\sqrt{3}}{3}\right]$$
$$+\frac{15pq-3p-3q}{5pq-3p-3q+2}\left[-\frac{10}{3}p-\frac{10}{3}q+5pq\right]$$
$$+\frac{15pq-3p-3q}{5pq-3p-3q+2}\left[\frac{\sqrt{6}}{6}(8p+8q-14)\right]$$

□

Theorem 8: Consider the silicon carbide $Si_2C_3\text{-}II[p,q]$, then its the redefine first, second and third Zagreb indices are

$$ReG_1(Si_2C_3\text{-}II[p,q])=10pq$$
$$ReG_2(Si_2C_3\text{-}II[p,q])=\frac{107}{60}-\frac{79}{10}p-\frac{79}{10}q+\frac{45}{2}pq$$
$$ReG_3(Si_2C_3\text{-}II[p,q])=198-430p-430q+810pq$$

Proof: Let G be the graph silicon carbide $Si_2C_3\text{-}II[p,q]$. Now by using Table 6 and equation (4)-(6) the redefine first, second and third Zagreb indices are calculated as follows:

$$ReG_1(G)=\sum_{st\in E(G)}\frac{d(s)+d(t)}{d(s)\cdot d(t)}$$
$$ReG_1(G)=\sum_{st\in E_1}\frac{d(s)+d(t)}{d(s)\cdot d(t)}+\sum_{st\in E_2}\frac{d(s)+d(t)}{d(s)\cdot d(t)}+\sum_{st\in E_3}\frac{d(s)+d(t)}{d(s)\cdot d(t)}+\sum_{st\in E_4}\frac{d(s)+d(t)}{d(s)\cdot d(t)}+\sum_{st\in E_5}\frac{d(s)+d(t)}{d(s)\cdot d(t)}$$
$$=\frac{3}{2}\mid E_1(Si_2C_3\text{-}I[p,q])\mid+\frac{4}{3}\mid E_2(Si_2C_3\text{-}I[p,q])\mid+(1)\mid E_3(Si_2C_3\text{-}I[p,q])\mid+\frac{5}{6}\mid E_4(Si_2C_3\text{-}I[p,q])\mid+\frac{2}{3}\mid E_5(Si_2C_3\text{-}I[p,q])\mid$$
$$=\frac{3}{2}(2)+\frac{4}{3}(1)+1(2p+2q)+\frac{5}{6}(8p+8q-14)+\frac{2}{3}(15pq-13p-13q+11)$$
$$=10pq$$
$$ReG_2(G)=\sum_{st\in E(G)}\frac{d(s)\cdot d(t)}{d(s)+d(t)}$$
$$ReG_2(G)=\sum_{st\in E_1}\frac{d(s)\cdot d(t)}{d(s)+d(t)}+\sum_{st\in E_2}\frac{d(s)\cdot d(t)}{d(s)+d(t)}+\sum_{st\in E_3}\frac{d(s)\cdot d(t)}{d(s)+d(t)}+\sum_{st\in E_4}\frac{d(s)\cdot d(t)}{d(s)+d(t)}+\sum_{st\in E_5}\frac{d(s)\cdot d(t)}{d(s)+d(t)}$$
$$=\frac{2}{3}\mid E_1(Si_2C_3\text{-}I[p,q])\mid+\frac{3}{4}\mid E_2(Si_2C_3\text{-}I[p,q])\mid+1\mid E_3(Si_2C_3\text{-}I[p,q])\mid+\frac{6}{5}\mid E_4(Si_2C_3\text{-}I[p,q])\mid+\frac{3}{2}\mid E_5(Si_2C_3\text{-}I[p,q])\mid$$
$$=\frac{2}{3}(2)+\frac{3}{4}(1)+1(2p+2q)+\frac{6}{5}(8p+8q-14)+\frac{3}{2}(15pq-13p-13q+11)$$
$$=\frac{107}{60}-\frac{79}{10}p-\frac{79}{10}q+\frac{45}{2}pq$$
$$ReG_3(G)=\sum_{st\in E(G)}(d(s)\cdot d(t))(d(s)+d(t))$$
$$ReG_3(G)=\sum_{st\in E_1}(d(s)\cdot d(t))(d(s)+d(t))+\sum_{st\in E_2}(d(s)\cdot d(t))(d(s)+d(t))+\sum_{st\in E_3}(d(s)\cdot d(t))(d(s)+d(t))+\sum_{st\in E_4}(d(s)\cdot d(t))(d(s)+d(t))+\sum_{st\in E_5}(d(s)\cdot d(t))(d(s)+d(t))$$
$$=2(3)\mid E_1(Si_2C_3\text{-}I[p,q])\mid+3(4)\mid E_2(Si_2C_3\text{-}I[p,q])\mid$$

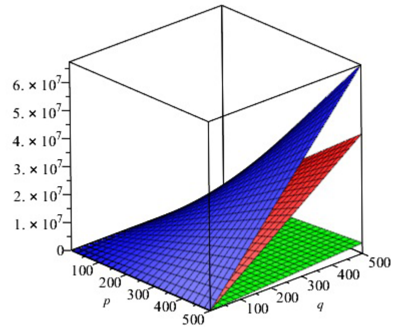


FIGURE 7. Comparison of Forgotten index $F(G)$, Augmented Zagreb index $AZI(G)$ and Balaban index $J(G)$ of G equivalent to $Si_2C_3\text{-}II[p,q]$.

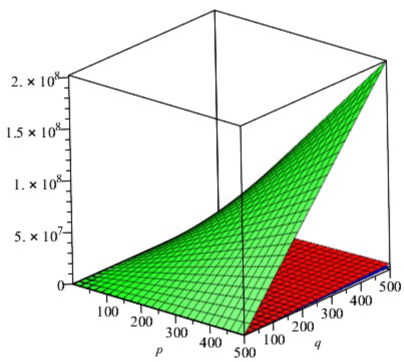


FIGURE 8. Comparison of redefine first $ReG_1(G)$, second $ReG_2(G)$ and third Zagreb indices $ReG_3(G)$ of $Si_2C_3\text{-}II[p,q]$. Blue, red and green represents $ReG_1(G)$, $ReG_2(G)$ and $ReG_3(G)$, respectively.

$$
\begin{aligned}
&+4(4)\mid E_3(Si_2C_3\text{-}I[p,q])\mid\\
&+6(5)\mid E_4(Si_2C_3\text{-}I[p,q])\mid\\
&+9(6)\mid E_5(Si_2C_3\text{-}I[p,q])\mid\\
=\;& 2(3)(2)+3(4)(1)+4(4)(2p+2q)\\
&+6(5)(8p+8q-14)\\
&+9(6)(15pq-13p-13q+11)\\
=\;& 198-430p-430q+810pq
\end{aligned}
$$

□

VIII. COMPARISONS AND DISCUSSIONS

- In this section we have computed all indices for different values of p, q for both structures $Si_2C_3\text{-}I[p,q]$ and $Si_2C_3\text{-}II[p,q]$. Now from Table 7 and Table 8, we can easily see that all indices are in increasing order as the values of p, q are increasing. But on the other hand indices showed higher values for $Si_2C_3\text{-}I[p,q]$ as compared to those of $Si_2C_3\text{-}II[p,q]$.
  The graphical representations of topological indices of $Si_2C_3\text{-}I[p,q]$ and $Si_2C_3\text{-}II[p,q]$ are depicted in Figure 3, Figure 4, Figure 7 and Figure 8 for certain values of p, q. Now we presented the comparison of all topological indices using Table 7, for $Si_2C_3\text{-}I[p,q]$ in Figure 9 and using Table 8, for $Si_2C_3\text{-}II[p,q]$ in Figure 10.
- The Zagreb types indices and polynomials were found to occur for the computation of the total π-electron energy of molecules. Thus, the total π-electron energy in increasing order in the case of $Si_2C_3\text{-}I[p,q]$ and $Si_2C_3\text{-}II[p,q]$ for higher values of p, q.
  The forgotten topological index is helpful for testing the substance and pharmacological properties of drug nuclear structures. So in the case of $Si_2C_3\text{-}I[p,q]$ and $Si_2C_3\text{-}II[p,q]$, its increasing value is useful for quick action during chemical reaction for drugs.
  The augmented Zagreb index displays a good correlation with the formation heat of heptanes and octane. So our computation for AZI index is play an important rule for formation heat of heptanes and octane as its values are in increasing order.

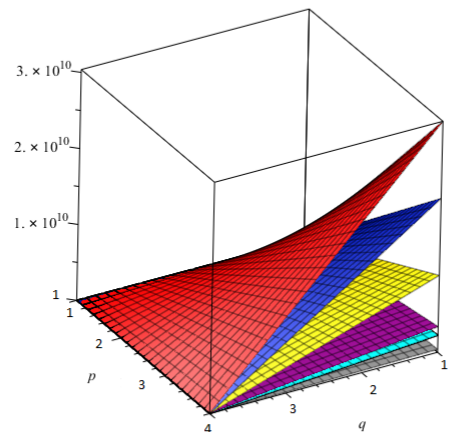


FIGURE 9. The comparison of all topological indices for $Si_2C_3\text{-}I[p,q]$.

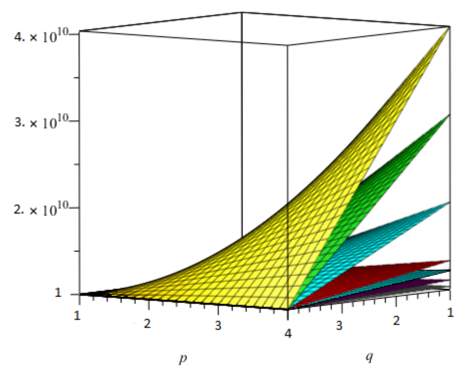


FIGURE 10. The comparison of all topological indices for $Si_2C_3\text{-}II[p,q]$.

TABLE 7. Comparison of all indices for $Si_2C_3\text{-}I[p,q]$.

$[p,q]$	F	AZI	J	ReG_1	ReG_2	ReG_3
[1, 1]	104	75.32	2.04	10	12.5	216
[2, 2]	724	473.35	5.18	40	63.18	1926
[3, 3]	1884	1213.06	15.25	90	153.11	5256
[4, 4]	3584	2294.48	32.18	160	221.32	10206

TABLE 8. Comparison of all indices for $Si_2C_3\text{-}II[p,q]$.

$[p,q]$	F	AZI	J	ReG_1	ReG_2	ReG_3
[1, 1]	78	64.32	1.8	10	8.9	148
[2, 2]	660	415.20	4.21	40	54.12	1718
[3, 3]	1782	1124.54	13.12	90	141.23	4908
[4, 4]	3444	2173.42	29.25	160	201.23	9718

Since the Balaban index correlate well with a range of physicochemical properties of molecule. So in the case of $Si_2C_3\text{-}I[p,q]$ and $Si_2C_3\text{-}II[p,q]$, the Balaban index correlate well with a range of physicochemical properties as well.

IX. CONCLUSION

In this paper we have studied and dealt with topological indices of $2D$ molecular graph of $Si_2C_3\text{-}I[p,q]$ and $Si_2C_3\text{-}II[p,q]$. We determined Forgotten index, Augmented Zagreb index and Balaban index and have computed the redefine Zagreb indices that is the redefine first, second and third Zagreb indices.

The graphical representations of Forgotten index, Augmented Zagreb index, Balaban index and redefine Zagreb indices of $Si_2C_3\text{-}I[p,q]$ and $Si_2C_3\text{-}II[p,q]$ are depicted in Figure 3, Figure 4, Figure 7, Figure 8 for some values of p, q. By varying the value of p, q in the given domain the Forgotten index, Augmented Zagreb index, Balaban index and redefine Zagreb indices behaves differently.

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