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On Topological Properties of Symmetric Chemical Structures

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Abstract: The utilizations of graph theory in chemistry and in the study of molecule structures are more than someone's expectations, and, lately, it has increased exponentially. In molecular graphs, atoms are denoted by vertices and bonds by edges. In this paper, we focus on the molecular graph of (2D) silicon-carbon Si_2C_3-I and Si_2C_3-II. Moreover, we have computed topological indices, namely general Randić Zagreb types indices, geometric arithmetic index, atom–bond connectivity index, fourth atom–bond connectivity and fifth geometric arithmetic index of Si_2C_3-I and Si_2C_3-II.

Keywords: (2D) silicon-carbon Si_2C_3-I and Si_2C_3-II; atom–bond connectivity index; Zagreb types indices; geometric arithmetic index; general randić index

MSC: 05C12; 05C90

1. Introduction

Every structural formula that includes covalent bonded compounds or molecules are graphs. Along these lines, they are called molecular graphs. Recently, chemical graph theory tools are used for numeration, systematization of the problem in hand, it provides the process of arranging laws or rules according to a system or planning, nomenclature, it provides the connection between the compounds or atoms, and computer programming. The significance of graph theory tools for science stands for the most part from the presence of isomerism, which is excused by substance diagram hypothesis. The pith of chemistry is the combinatorics of molecules as per clear principles. Along these lines, the most satisfactory numerical apparatuses for this design are graph hypothesis and combinatorics, the branches of arithmetic that are nearly related.

Silicon has numerous preferences over other semiconductor materials: It is, of minimal effort, it is nontoxic, essentially its accessibility is boundless, and behind it many years of involvement in purging, development and gadget creation. It is utilized for all cutting edge electronic gadgets.

The most reliable structures of two-dimensional (2D) silicon-carbon monolayer mixes with different stoichiometric blends were expected in [1] which in light of the molecule swarm streamlining signified as (PSO) method joined with thickness utilitarian hypothesis optimization.

The graphene sheets were effectively confined in [2,3] and from that point forward this honeycomb organized 2D material has roused and enlivened concentrated research interests to a great extent as a result of its surprising mechanical, electronic and optical properties, including its anomalous quantum Lobby influence, overwhelming electronic conductivity, and high mechanical quality. In particular, the intriguing electronic properties of graphene pull in see for this 2D material as a potential probability for applications in speedier and smaller electronic gadgets.

Like carbon, silicon additionally has a 2D allotrope with a honeycomb structure, in particular silicene. To date, bunches of exertion have been given to open a bandgap in silicene sheets. In addition, 2D silicon–carbon $(Si - C)$ monolayers can be seen as creation tunable materials between the unadulterated 2D carbon monolayer-graphene and the unadulterated 2D silicon monolayer-silicene. Loads of endeavors have been directed towards anticipating the most stable structures of the SiC sheet read this [4,5] for more data.

Given a graph $G = (V, E)$ where V is the vertex set and E is the edge set of G, the degree $deg(s)$ of s is the quantity of spokes in G episode with s and is indicated as $d(s)$. A graph can be spoken to by a polynomial, a numerical esteem or by lattice frame. All the concepts of graph theory and combinatorics are used from the book of Harris et al. [6]. There are sure kinds of topological records for the most part capricious based, degree based and remove based files and so forth.

In 1975, *Milan Randić* [7] introduced the randic index as below:

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

In 1988, Bollobás et al. [8] and Amic et al. [9] introduced the general Randić index independently. For more details about Randić index, its properties and important results, see [10–13]. The general Randić index is defined as:

$$R_\alpha(G) = \sum_{st \in E(G)} (d(s)d(t))^\alpha.$$

Estrada et al. [14] defined atom–bond connectivity index as:

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

The geometric arithmetic index GA is introduced by Vukičević et al. [15] as:

$$GA(G) = \sum_{st \in E(G)} \frac{2\sqrt{d(s)d(t)}}{d(s) + d(t)}.$$

The Zagreb indices were introduced by Gutman and Trinajestic in [16,17]. For more details about Zagreb indices, its properties and important results, see [18–20]:

$$M_1(G) = \sum_{st \in E(G)} (d(s) + d(t)),$$

$$M_2(G) = \sum_{st \in E(G)} (d(s)d(t)).$$

Ghorbhani et al. [21] introduced the fourth version of atom–bond connectivity index ABC_4 as:

$$ABC_4(G) = \sum_{st \in E(G)} \sqrt{\frac{S(s) + S(t) - 2}{S(s)S(t)}},$$

where $S(s) = \sum_{st \in E(G)} d(t)$ and $S(t) = \sum_{st \in E(G)} d(s)$. For more details about the fourth version of atom–bond connectivity index, its properties and important results, see [9,22–25].

Graovoc et al. [26] introduced the fifth version of geometric arithmetic index GA_5 as:

$$GA_5(G) = \sum_{st \in E(G)} \frac{2\sqrt{S(s)S(t)}}{S(s) + S(t)}.$$

2. Applications of Topological Indices

The Randic index is a topological descriptor that has correlated with a lot of chemical characteristics of the molecules and has been found to the parallel to computing the boiling point and Kovats constants of the molecules. The atom–bond connectivity (ABC) 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 [14]. To correlate with certain physico-chemical properties, GA index has much better predictive power than the predictive power of the Randic connectivity index [27]. The first and second Zagreb index were found to occur for computation of the total π-electron energy of the molecules within specific approximate expressions [28]. These are among the graph invariants, who were proposed for measurement of skeleton of branching of the carbon-atom [17].

3. 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 neighbours method. Moreover, we use the Matlab for mathematical calculations and verifications. We also use the maple for plotting these mathematical results.

4. 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 represents 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 $15pq - 2p - 3q$.

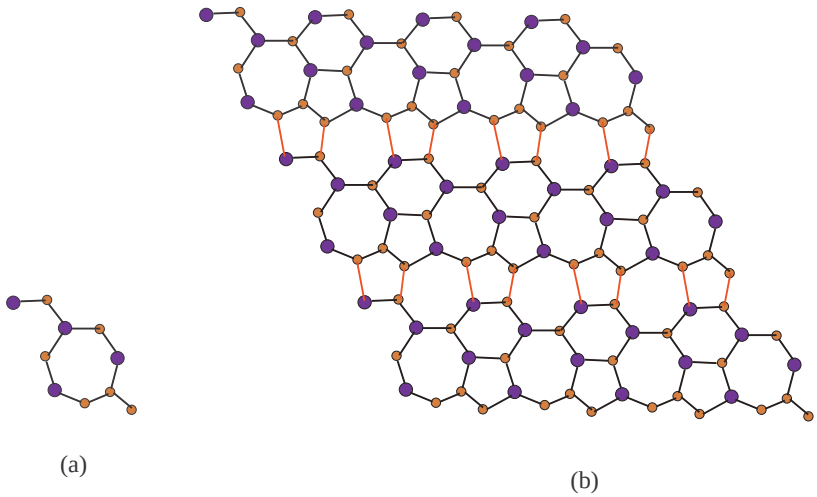

Figure 1. 2D structure of Si_2C_3-$I[p,q]$, (**a**) chemical unit cell of Si_2C_3-$I[p,q]$; (**b**) Si_2C_3-$I[4,3]$. Carbon atom C are brown and Silicon atom Si are blue.

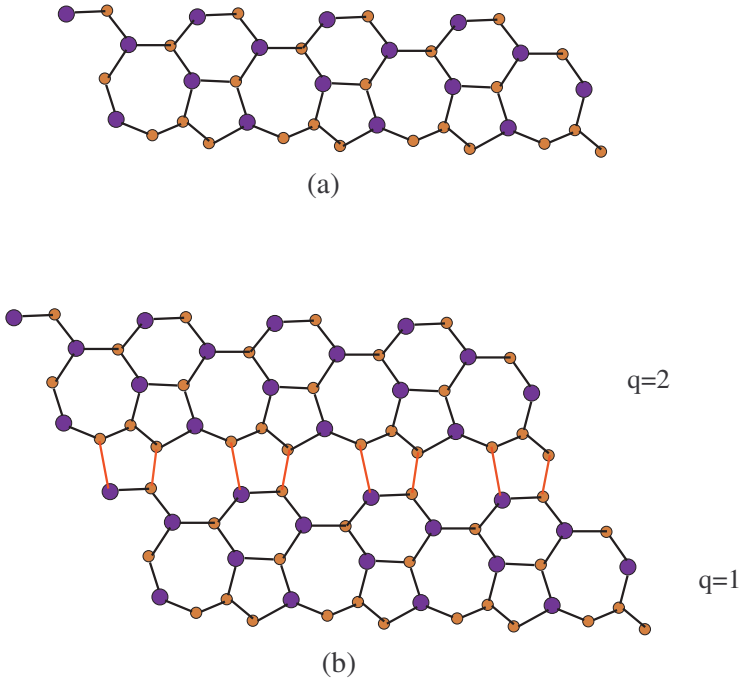

Figure 2. 2D structure of Si_2C_3-$I[p,q]$, (**a**) Si_2C_3-$I[4,1]$, one row with $p = 4$ and $q = 1$; (**b**) Si_2C_3-$I[4,2]$, two rows are being connecting. Red lines (edges) connects the upper and lower rows.

4.1. 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 and 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 and then combine with another unit cell in the vertical direction and so on up to q unit cells. Thus, we obtained Silicon Carbide $[p,q]$ structure (see Figure 1). Now, for the computation of vertices, we use the Table 1 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.

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

$[p,q]$	$[1,1]$	$[1,2]$	$[1,3]$	$[2,1]$	$[2,2]$	$[2,3]$	$[3,1]$	$[3,2]$	$[3,3]$	$[4,1]$	$[4,2]$	$[4,3]$
V_1	2	2	2	2	2	2	2	2	2	2	2	2
V_2	6	12	18	10	16	2	14	20	26	18	28	30
V_3	2	6	10	8	22	36	14	38	62	20	54	88

Thus, finally, we calculate he 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 $10pq - 4p - 6q + 2$.

To find the abstracted indices, we will partition the edges of Si_2C_3-$I[p,q]$ using the above methodology. Moreover, we use the combinatorial counting and standard edge partition. The first edge parcel contains one edge st, where $d(t) = 1$ and $\deg(u) = 2$. The second edge parcel contains again only one edge st, where $d(t) = 1$ and $\deg(u) = 3$. The third edge parcel contains $(p + 2q)$ edges st, where $d(t) = 2$ and $\deg(u) = 2$. The fourth edge parcel contains $6p - 1 + 8(q - 1)$ number of edges st, where $d(t) = 2$ and $\deg(u) = 3$. The fifth edge parcel contains $15pq - 9p - 13q + 7$ number of edges st, where $\deg(u) = d(t) = 3$. Table 2 shows the edge partition of Si_2C_3-$I[p,q]$ with $p, q \geq 1$. Finally, for comparison of these indices, we plot its diagram in maple software (see Figures 3,4,7 and 8).

Table 2. Edge partition of Si_2C_3-$I[p,q]$, $p,q \geq 1$.

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

4.2. Main Results for Silicon Carbide $Si_2C_3 - I[p,q]$

In this section, we compute the general result of topological indices for $Si_2C_3 - I[p,q]$. In addition, we construct the tables for these indices for small values of p,q. Moreover, we give graphical comparison and application of these indices.

- **Atom–bond connectivity index** $ABC\Big(Si_2C_3\text{-}I[p,q]\Big)$

Let G be the graph of Si_2C_3-$I[p,q]$. Then, from the edge partition of Si_2C_3-$I[p,q]$, which is given in Table 2, the atom–bond connectivity index is computed as (see Table 3):

$$\begin{aligned} ABC(G) &= \sum_{st\in E(G)} \sqrt{\frac{d(s)+d(t)-2}{d(s)d(t)}}, \\ ABC(G) &= (1)\sqrt{\frac{2+1-2}{2\times 1}} + (1)\sqrt{\frac{3+1-2}{3\times 1}} + (p+2q)\sqrt{\frac{2+2-2}{2\times 2}} \\ &+ (6p+8q-9)\sqrt{\frac{3+2-2}{3\times 2}} + (15pq-9p-13q+7)\sqrt{\frac{3+3-2}{3\times 3}}. \end{aligned}$$

After some easy calculations, we get:

$$ABC(G) = 10pq + p\left[6\frac{1}{\sqrt{2}} + \frac{\sqrt{2}}{2} - 6\right] + q\left[8\frac{1}{\sqrt{2}} + \frac{\sqrt{2}}{2} - \frac{26}{3}\right] - 8\frac{1}{\sqrt{2}} + \sqrt{\frac{2}{3}} + \frac{14}{3}.$$

Table 3. The atom–bond connectivity index.

$[p,q]$	$[1,1]$	$[2,2]$	$[3,3]$	$[4,4]$	$[5,5]$	$[6,6]$	$[7,7]$
$ABC(G)$	16.2	48.3	98.7	169.3	260.6	370.14	460.25

- **The General Randić index** $R_\alpha\Big(Si_2C_3\text{-}I[p,q]\Big)$

Let G be the graph of Si_2C_3-$I[p,q]$. Now, by using Table 2, the general Randić index for $\alpha = 1$ (see Table 4).

$$\begin{aligned} R_1(G) &= \sum_{st\in E(G)} (d(s)\times d(t)), \\ R_1(G) &= (1)(2\times 1) + (1)(3\times 1) + (p+2q)(2\times 2) \\ &+ (6p+8q-9)(3\times 2) + (15pq-9p-13q+7)(3\times 3), \\ R_1(G) &= 135pq - 41p - 61q + 14. \end{aligned}$$

Table 4. The Randić index for $\alpha = 1$.

$[p,q]$	$[1,1]$	$[2,2]$	$[3,3]$	$[4,4]$	$[5,5]$	$[6,6]$	$[7,7]$
$R_1(G)$	77	350	923	1776	2869	4262	5915

For $\alpha = -1$ (see Table 5),

$$\begin{aligned} R_{-1}(G) &= \sum_{st\in E(G)} \frac{1}{(d(s)\times d(t))}, \\ R_{-1}(G) &= (1)(\frac{1}{2\times 1}) + (1)(\frac{1}{3\times 1}) + (p+2q)(\frac{1}{2\times 2}) \\ &+ (6p+8q-9)(\frac{1}{3\times 2}) + (15pq-9p-13q+7)(\frac{1}{3\times 3}), \\ R_{-1}(G) &= \frac{5}{3}pq + \frac{1}{4}p + \frac{7}{18}q + \frac{1}{9}. \end{aligned}$$

Table 5. The Randić index for $\alpha = -1$.

$[p,q]$	$[1,1]$	$[2,2]$	$[3,3]$	$[4,4]$	$[5,5]$	$[6,6]$	$[7,7]$
$R_{-1}(G)$	2.41	11.32	18.11	29.12	41.23	53.42	65.32

For $\alpha = \frac{1}{2}$ (see Table 6),

$$\begin{aligned} R_{\frac{1}{2}}(G) &= \sum_{st\in E(G)} \sqrt{(d(s)\times d(t))}, \\ R_{\frac{1}{2}}(G) &= (1)(\sqrt{2\times 1}) + (1)(\sqrt{3\times 1}) + (p+2q)(\sqrt{2\times 2}) \\ &+ (6p+8q-9)(\sqrt{3\times 2}) + (15pq-9p-13q+7)(\sqrt{3\times 3}), \\ R_{\frac{1}{2}}(G) &= 45pq + p\left[\sqrt{66}-25\right] + q\left[\sqrt{68}-35\right] + \sqrt{2} + \sqrt{3} - 9\sqrt{6} + 21. \end{aligned}$$

Table 6. The Randić index for $\alpha = \frac{1}{2}$.

$[p,q]$	$[1,1]$	$[2,2]$	$[3,3]$	$[4,4]$	$[5,5]$	$[6,6]$	$[7,7]$
$R_{\frac{1}{2}}(G)$	49.31	60.34	80.41	97.11	117.32	140.56	162.87

For $\alpha = -\frac{1}{2}$ (see Table 7),

$$\begin{aligned} R_{-\frac{1}{2}}(G) &= \sum_{st\in E(G)} \frac{1}{\sqrt{(d(s)\times d(t))}}, \\ R_{-\frac{1}{2}}(G) &= (1)(\frac{1}{\sqrt{2\times 1}}) + (1)(\frac{1}{\sqrt{3\times 1}}) + (p+2q)(\frac{1}{\sqrt{2\times 2}}) \\ &+ (6p+8q-9)(\frac{1}{\sqrt{3\times 2}}) + (15pq-9p-13q+7)(\frac{1}{\sqrt{3\times 3}}), \\ R_{-\frac{1}{2}}(G) &= 5pq + p\left[\frac{1}{\sqrt{6}}6 - \frac{5}{2}\right] + q\left[\frac{1}{\sqrt{6}}8 - \frac{10}{3}\right] + \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{3}} - \frac{9}{\sqrt{6}} + \frac{7}{3}. \end{aligned}$$

Table 7. The Randić index for $\alpha = \frac{-1}{2}$.

$[p,q]$	$[1,1]$	$[2,2]$	$[3,3]$	$[4,4]$	$[5,5]$	$[6,6]$	$[7,7]$
$R_{\frac{-1}{2}}(G)$	7.42	25.18	51.23	87.04	110.41	143.32	170.44

- **The geometric arithmetic index** $GA\left(Si_2C_3\text{-}I[p,q]\right)$

Let G be the graph of Silicon Carbide $Si_2C_3\text{-}I[p,q]$. Now, by using Table 2, the geometric arithmetic index is computed as below (see Table 8):

$$\begin{aligned} GA(G) &= \sum_{st\in E(G)} \frac{2\sqrt{d(s)d(t)}}{d(s)+d(t)}, \\ GA(G) &= (1)\frac{2\sqrt{2}}{2+1} + (1)\frac{2\sqrt{3}}{3+1} + (p+2q)\frac{2\sqrt{4}}{2+2} + (6p+8q-9)\frac{2\sqrt{6}}{3+2} \\ &+ (15pq-9p-13q+7)\frac{2\sqrt{9}}{3+3}, \\ GA(G) &= 15pq + p\left[\frac{12\sqrt{6}}{5}-8\right] + q\left[\frac{16\sqrt{6}}{5}-11\right] + \frac{2\sqrt{2}}{3} + \frac{\sqrt{3}}{2} - \frac{18\sqrt{6}}{5} + 7. \end{aligned}$$

Table 8. The geometric arithmetic index.

$[p,q]$	$[1,1]$	$[2,2]$	$[3,3]$	$[4,4]$	$[5,5]$	$[6,6]$	$[7,7]$
$GA(G)$	19.251	68.29	141.12	248.41	358.32	470.15	590.32

- **First and second Zagreb index**

Let G be the graph of Si_2C_3-$I[p,q]$. Now, by using Table 2, the first and second Zagreb indices are computed as below (see Table 9 and 10):

$$\begin{aligned} M_1(G) &= \sum_{st\in E(G)} (d(s)+d(t)), \\ M_1(G) &= (1)(2+1) + (1)(3+1) + (p+2q)(2+2) + (6p+8q-9)(3+2) \\ &+ (15pq-9p-13q+7)(3+3), \\ M_1(G) &= 90pq - 20p - 30q + 4, \\ M_2(G) &= \sum_{st\in E(G)} (d(s)d(t)), \\ M_2(G) &= (1)(2\times 1) + (1)(3\times 1) + (p+2q)(2\times 2) + (6p+8q-9)(3\times 2) \\ &+ (15pq-9p-13q+7)(3\times 3), \\ M_2(G) &= 135pq - 41p - 61q + 14. \end{aligned}$$

Table 9. The first Zagreb index.

$[p,q]$	$[1,1]$	$[2,2]$	$[3,3]$	$[4,4]$	$[5,5]$	$[6,6]$	$[7,7]$
$M_1(G)$	44	264	664	1244	2046	3456	4874

Table 10. The second Zagreb index.

$[p,q]$	$[1,1]$	$[2,2]$	$[3,3]$	$[4,4]$	$[5,5]$	$[6,6]$	$[7,7]$
$M_2(G)$	47	350	923	1766	2879	4268	6425

- **Comparison of topological indices for** Si_2C_3-$I[p,q]$

In this section, we presented the comparison of above calculated topological indices for Si_2C_3-$I[p,q]$ with $p = 1,2,3,...,1500$ and $q = 1,2,3,...,1500$ graphically in Figure 3.

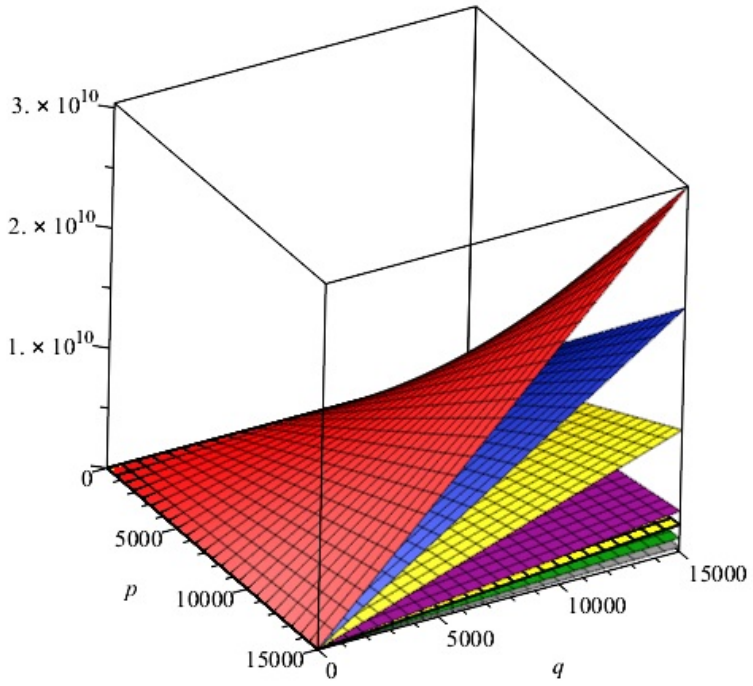

Figure 3. Comparison of indices, first and second Zagreb indexes, ABC index, GA index, ABC_4 index, GA_5 index, and general Randić index for$\alpha \in \{1, -1, 1/2, -1/2\}$ of 2D structure of Si_2C_3-$I[p, q]$. R_1, Red; $R_{\frac{1}{2}}$, orange; $R_{-\frac{1}{2}}$, Green; R_{-1},Gray; ABC, Cayn; GA,Niagara purple; M_1, Niagara Navy; M_2, off white.

Table 11 demonstrates the edge parcel in light of the degree total of end vertices of each edge of the chemical graph Si_2C_3-$I[p, q]$ for $p, q \geq 2$.

Table 11. Edge partition of Si_2C_3-$I[p, q]$.

$(d(s), d(t))$	(S_u, S_v)	**Frequency**
(2, 1)	(4, 2)	1
(3, 1)	(5, 3)	1
(2, 2)	(5, 5)	$p + 2q$
(3, 2)	(5, 5)	1
(3, 2)	(7, 4)	1
(3, 2)	(7, 5)	$2(q + 1)$
(3, 2)	(5, 6)	1
(3, 2)	(7, 6)	$4p + 2q - 7$
(3, 2)	(8, 6)	$2(q - 1)$
(3, 2)	(8, 5)	$2p + 2q - 5$
(3, 3)	(8, 7)	1
(3, 3)	(8, 8)	$p + 2q - 4$
(3, 3)	(9, 7)	$2p + 2q - 3$
(3, 3)	(9, 8)	$2p + 4q - 7$
(3, 3)	(9, 9)	$15pq - 14p - 21q + 20$

- **The fourth atom–bond connectivity index** $ABC_4\Big(Si_2C_3 - I[p, q]\Big)$.

Let G be the graph of Silicon Carbide of type Si_2C_3-$I[p,q]$. Now, by using Table 11, the fourth atom–bond connectivity index is computed as below (see Table 12):

$$\begin{aligned}
ABC_4(G) &= \sum_{st\in E(G)} \sqrt{\frac{S(s)+S(t)-2}{S(s)S(t)}},\\
ABC_4(G) &= (1)\sqrt{\frac{4+2-2}{4\times 2}} + (1)\sqrt{\frac{5+3-2}{5\times 3}} + (p+2q+1)\sqrt{\frac{5+5-2}{5\times 5}}\\
&+ 2(q-1)\sqrt{\frac{7+5-2}{7\times 5}} + (1)\sqrt{\frac{5+6-2}{5\times 6}} + (4p+2q-7)\sqrt{\frac{7+6-2}{7\times 6}}\\
&+ 2(q-1)\sqrt{\frac{8+6-2}{8\times 6}} + (2p+2q-5)\sqrt{\frac{8+5-2}{8\times 5}} + (1)\sqrt{\frac{7+4-2}{7\times 4}}\\
&+ (1)\sqrt{\frac{8+7-2}{8\times 7}} + (p+2q-4)\sqrt{\frac{8+8-2}{8\times 8}} + (2p+2q-3)\sqrt{\frac{9+7-2}{9\times 7}}\\
&+ (2p+4q-7)\sqrt{\frac{9+8-2}{9\times 8}} + (15pq-14p-21q+20)\sqrt{\frac{9+9-2}{9\times 9}}.
\end{aligned}$$

After an easy calculation, we get:

$$\begin{aligned}
ABC_4(G) &= 20/3pq - \frac{56}{9}p - \frac{25}{3}q\\
&+ p\left[\frac{2\sqrt{2}}{5} + 4\sqrt{\frac{11}{42}} + \sqrt{\frac{11}{10}} + \frac{\sqrt{14}}{8} + \frac{2\sqrt{2}}{3} + \frac{1}{3}\sqrt{\frac{15}{2}}\right]\\
&+ q\left[\frac{4\sqrt{2}}{5} + 2\sqrt{\frac{2}{7}} + 2\sqrt{\frac{11}{42}} + \sqrt{\frac{11}{10}} + \frac{\sqrt{14}}{4} + \frac{2\sqrt{2}}{3} + \frac{2}{3}\sqrt{\frac{15}{2}}\right]\\
&+ \frac{1}{\sqrt{2}} + \sqrt{\frac{2}{5}} + \frac{2\sqrt{2}}{5} - 2\sqrt{\frac{2}{7}} + \frac{3}{\sqrt{30}} - 7\sqrt{\frac{11}{42}} - \frac{5}{2}\sqrt{\frac{11}{10}} + \frac{3}{2}\frac{1}{\sqrt{7}}\\
&+ \frac{1}{2}\sqrt{\frac{13}{14}} - \frac{\sqrt{14}}{2} - \sqrt{2} - \frac{7}{6}\sqrt{\frac{15}{2}} + \frac{71}{9}.
\end{aligned}$$

Table 12. The fourth atom–bond connectivity index.

$[p,q]$	$[1,1]$	$[2,2]$	$[3,3]$	$[4,4]$	$[5,5]$	$[6,6]$	$[7,7]$
$ABC_4(G)$	9.42	32.21	68.26	106.18	156.24	214.52	287.32

- **The fifth geometric arithmetic index** $GA_5\left(Si_2C_3 - I[p,q]\right)$

Let G be the graph of Si_2C_3-$I[p,q]$. Now, by using Table 11, the fifth geometric arithmetic index is computed as below (see Table 13):

$$GA_5(G) = \sum_{st\in E(G)} \frac{2\sqrt{S(s)S(t)}}{S(s)+S(t),}$$

$$\begin{aligned}
GA_5(G) &= (1)\frac{2\sqrt{4\times 2}}{4+2} + (1)\frac{2\sqrt{5\times 3}}{5+3} + (p+2q+1)\frac{2\sqrt{5\times 5}}{5+5} \\
&+ 2(q-1)\frac{2\sqrt{7\times 5}}{7+5} + (1)\frac{2\sqrt{5\times 6}}{5+6} + (4p+2q-7)\frac{2\sqrt{7\times 6}}{7+6} \\
&+ 2(q-1)\frac{2\sqrt{8\times 6}}{8+6} + (2p+2q-5)\frac{2\sqrt{8\times 5}}{8+5} + (1)\frac{2\sqrt{7\times 4}}{7+4} \\
&+ (1)\frac{2\sqrt{8\times 7}}{8+7} + (p+2q-4)\frac{2\sqrt{8\times 8}}{8+8} + (2p+2q-3)\frac{2\sqrt{9\times 7}}{9+7} \\
&+ (2p+4q-7)\frac{2\sqrt{9\times 8}}{9+8} + (15pq-14p-21q+20)\frac{2\sqrt{9\times 9}}{9+9},
\end{aligned}$$

$$\begin{aligned}
GA_5(G) &= 15pq + p\left[\frac{8}{13}\sqrt{42} + \frac{8}{13}\sqrt{10} + \frac{3}{4}\sqrt{7} + \frac{24}{17}\sqrt{2} - 12\right] \\
&+ q\left[\frac{1}{3}\sqrt{35} + \frac{4}{13}\sqrt{42} + \frac{4\sqrt{12}}{7} + \frac{8}{13}\sqrt{10} + \frac{3}{4}\sqrt{7} + \frac{48}{17}\sqrt{2} - 17\right] \\
&+ \frac{2\sqrt{2}}{3} + \frac{\sqrt{15}}{4} - \frac{\sqrt{35}}{3} + \frac{2\sqrt{30}}{11} - \frac{14\sqrt{42}}{13} - \frac{4\sqrt{12}}{7} - \frac{20\sqrt{10}}{13} \\
&+ \frac{4\sqrt{7}}{11} + \frac{4\sqrt{14}}{15} - \frac{9\sqrt{7}}{8} - \frac{84\sqrt{2}}{17} + 17.
\end{aligned}$$

Table 13. The fifth geometric arithmetic index.

$[p,q]$	$[1,1]$	$[2,2]$	$[3,3]$	$[4,4]$	$[5,5]$	$[6,6]$	$[7,7]$
$GA_5(G)$	19.26	69.31	143.28	251.21	304.25	360.56	412.32

- **Comparison of topological indices for** Si_2C_3-$I[p,q]$

In this section, we presented the comparison of above calculated topological indices for Si_2C_3-$I[p,q]$ graphically in Figure 4.

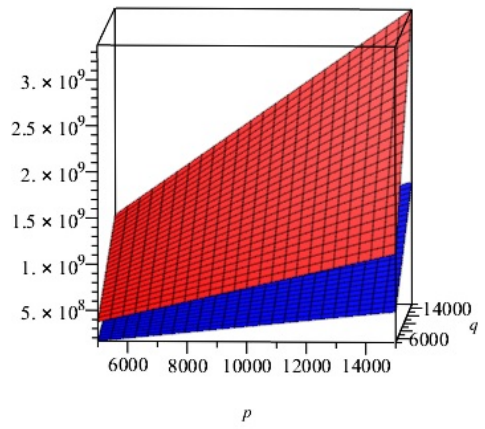

Figure 4. Comparison of ABC_4 and GA_5 indices of 2D structure of Si_2C_3-$I[p,q]$. Blue and red colors represents ABC_4 and GA_5, respectively.

5. 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 represent the number of connected rows, each with p number of cells.

In Figure 6, we gave a demonstration of 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 $15pq - 3p - 3q$.

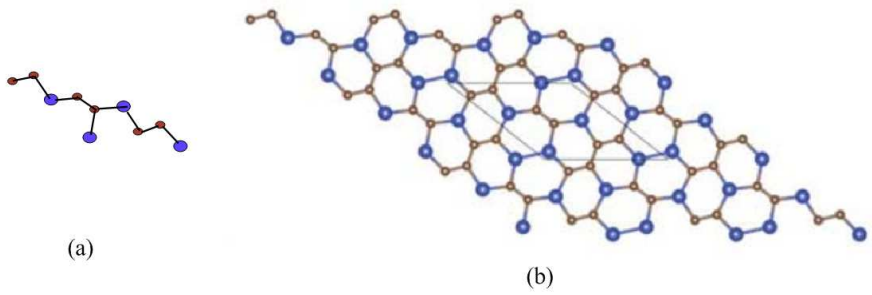

Figure 5. 2D structure of Si_2C_3-$II[p,q]$, (**a**) chemical unit cell of Si_2C_3-$II[p,q]$; (**b**) Si_2C_3-$II[3,3]$. Carbon atom C are brown and Silicon atom Si are blue

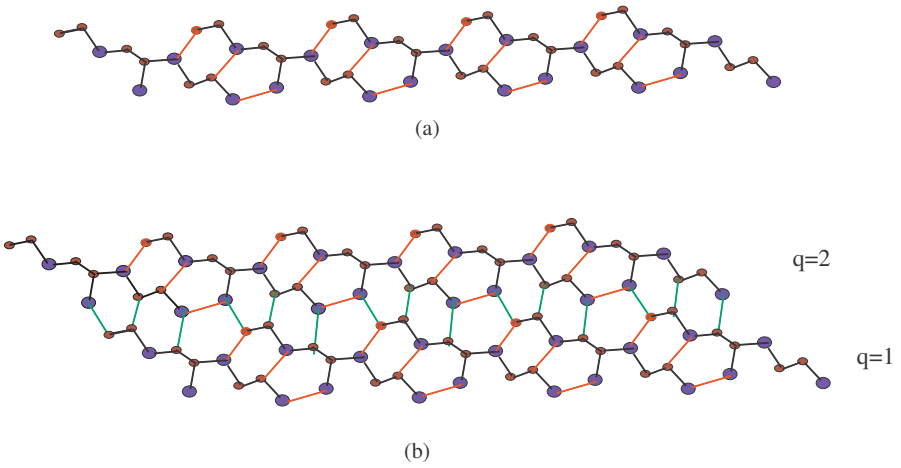

Figure 6. 2D structure of Si_2C_3-$II[p,q]$, (**a**) Si_2C_3-$II[5,1]$, one row with $p = 5$ and $q = 1$. Red lines show the connection between the unit cells; (**b**) Si_2C_3-$II[5,2]$, and two rows are connecting. Green lines (edges) connect the upper and lower rows.

5.1. 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 first use a unit cell and then combine it with another unit cell in the horizontal direction and so on up to p unit cells. After this, we use first a unit cell and then combine it with another unit cell in the vertical direction and so on up to q unit cells. Thus, we obtained Silicon Carbide Si_2C_3-$II[p,q]$ structure (see Figure 5). Now, for the computation of vertices, we use Table 14 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.

Table 14. Vertex partition of Si_2C_3-$II[p,q]$.

$[p,q]$	$[1,1]$	$[1,2]$	$[1,3]$	$[2,1]$	$[2,2]$	$[2,3]$	$[3,1]$	$[3,2]$	$[3,3]$	$[4,1]$	$[4,2]$	$[4,3]$
V_1	3	3	3	3	3	3	3	3	3	3	3	3
V_2	6	12	18	12	18	24	18	24	30	24	30	36
V_3	1	5	9	5	19	33	9	33	57	13	47	81

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 the abstracted indices, we will partition the edges of Si_2C_3-$II[p,q]$ using the above methodology. Moreover, we use the combinatorial counting and standard edge partition. The first edge parcel contains 2 edge st, where $\deg(u)=2$ and $d(t)=1$. The second edge parcel contains only one edge st, where $\deg(u)=3$ and $d(t)=1$. The third edge parcel contains $2(p+q)$ edges st, where $\deg(u)=2$ and $d(t)=2$. The fourth edge parcel contains $8p+8q-14$ number of edges st, where $\deg(u)=3$ and $d(t)=2$. The fifth edge parcel contains $15pq-13p-13q+11$ number of edges st, where $\deg(u)=d(t)=3$. Table 15 shows the edge partition of Si_2C_3-$II[p,q]$ with $p,q\geq 1$.

Table 15. 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)	$15pq-13p-13q+11$

5.2. Main Results for Silicon Carbide $Si_2C_3-II[p,q]$

In this section, we compute the general result of topological indices for $Si_2C_3-II[p,q]$. In addition, we construct the tables for these indices for small values of p,q. Moreover, we give graphical comparison and application of these indices.

- **Atom–bond connectivity index** $ABC\Big(Si_2C_3\text{-}IO[p,q]\Big)$

Let G be the graph of Silicon Carbide of type Si_2C_3-$II[p,q]$. Then, from the edge partition of Si_2C_3-$II[p,q]$ which is given in Table 15, the atom–bond connectivity index can be calculated as (see Table 16):

$$\begin{aligned}
ABC(G) &= \sum_{st\in E(G)}\sqrt{\frac{d(s)+d(t)-2}{d(s)d(t)}},\\
ABC(G) &= (2)\sqrt{\frac{2+1-2}{2\times 1}}+(1)\sqrt{\frac{3+1-2}{3\times 1}}+(2p+2q)\sqrt{\frac{2+2-2}{2\times 2}}\\
&+ (8p+8q-14)\sqrt{\frac{3+2-2}{3\times 2}}+(15pq-13p-13q+11)\sqrt{\frac{3+3-2}{3\times 3}},\\
ABC(G) &= 10pq+(p+q)\left[\frac{10}{\sqrt{2}}-\frac{26}{3}\right]-12\frac{1}{\sqrt{2}}+\sqrt{\frac{2}{3}}+\frac{22}{3}.
\end{aligned}$$

Table 16. The atom–bond connectivity index.

$[p,q]$	$[1,1]$	$[2,2]$	$[3,3]$	$[4,4]$	$[5,5]$	$[6,6]$	$[7,7]$
$ABC(G)$	13.25	45.26	95.17	165.26	240.32	330.15	440.14

- **The general Randić index** $R_\alpha\Big(Si_2C_3\text{-}II[p,q]\Big)$

Let G be the graph of Si_2C_3-$II[p,q]$. Now, by using Table 15, the general Randić index for $\alpha = 1$ (see Table 17),

$$\begin{aligned} R_1(G) &= \sum_{st\in E(G)} (d(s)\times d(t)), \\ R_1(G) &= (2)(2\times 1)+(1)(3\times 1)+(2p+2q)(2\times 2) \\ &+ (8p+8q-14)(3\times 2)+(15pq-13p-13q+11)(3\times 3), \\ R_1(G) &= 135pq-61p-61q+22. \end{aligned}$$

Table 17. The Randić index for $\alpha = 1$.

$[p,q]$	[1,1]	[2,2]	[3,3]	[4,4]	[5,5]	[6,6]	[7,7]
$R_1(G)$	35	318	871	1694	2459	4024	5714

For $\alpha = -1$ (see Table 18),

$$\begin{aligned} R_{-1}(G) &= \sum_{st\in E(G)} \frac{1}{(d(s)\times d(t))}, \\ R_{-1}(G) &= (2)(\frac{1}{2\times 1})+(1)(\frac{1}{3\times 1})+(2p+2q)(\frac{1}{2\times 2})+(8p+8q-14)(\frac{1}{3\times 2}) \\ &+ (15pq-13p-13q+11)(\frac{1}{3\times 3}), \\ R_{-1}(G) &= \frac{5}{3}pq+\frac{7}{18}p+\frac{7}{18}q+\frac{2}{9}. \end{aligned}$$

Table 18. The Randić index for $\alpha = -1$.

$[p,q]$	[1,1]	[2,2]	[3,3]	[4,4]	[5,5]	[6,6]	[7,7]
$R_{-1}(G)$	2.10	9.12	16.28	28.11	39.12	50.12	63.41

For $\alpha = \frac{1}{2}$ (see Table 19),

$$\begin{aligned} R_{\frac{1}{2}}(G) &= \sum_{st\in E(G)} \sqrt{(d(s)\times d(t))}, \\ R_{\frac{1}{2}}(G) &= (2)(\sqrt{2\times 1})+(1)(\sqrt{3\times 1})+(2p+2q)(\sqrt{2\times 2}) \\ &+ (8p+8q-14)(\sqrt{3\times 2})+(15pq-13p-13q+11)(\sqrt{3\times 3}), \\ R_{\frac{1}{2}}(G) &= 45pq+(p+q)\left[8\sqrt{6}-35\right]+2\sqrt{2}+\sqrt{3}-14\sqrt{6}+33. \end{aligned}$$

Table 19. The Randić index for $\alpha = \frac{1}{2}$.

$[p,q]$	[1,1]	[2,2]	[3,3]	[4,4]	[5,5]	[6,6]	[7,7]
$R_{\frac{1}{2}}(G)$	48.32	58.23	79.11	95.21	115.23	135.25	160.13

For $\alpha = \frac{-1}{2}$ (see Table 20),

$$\begin{aligned} R_{-\frac{1}{2}}(G) &= \sum_{st\in E(G)} \frac{1}{\sqrt{(d(s)\times d(t))}}, \\ R_{-\frac{1}{2}}(G) &= (2)(\frac{1}{\sqrt{2\times 1}}) + (1)(\frac{1}{\sqrt{3\times 1}}) + (2p+2q)(\frac{1}{\sqrt{2\times 2}}) \\ &+ (8p+8q-14)(\frac{1}{\sqrt{3\times 2}}) + (15pq-13p-13q+11)(\frac{1}{\sqrt{3\times 3}}), \\ R_{-\frac{1}{2}}(G) &= 5pq + (p+q)\left[\frac{8}{\sqrt{6}} - \frac{10}{3}\right] + \sqrt{2} + \frac{1}{\sqrt{3}} - \frac{14}{\sqrt{6}} + \frac{11}{3}. \end{aligned}$$

Table 20. The Randić index for $\alpha = \frac{-1}{2}$.

$[p,q]$	[1, 1]	[2, 2]	[3, 3]	[4, 4]	[5, 5]	[6, 6]	[7, 7]
$R_{\frac{-1}{2}}(G)$	6.21	23.51	48.25	84.36	108.32	133.42	168.24

- **The geometric arithmetic index** $GA\left(Si_2C_3\text{-}II[p,q]\right)$

Let G be the graph of Silicon Carbide $Si_2C_3\text{-}II[p,q]$. Now, by using Table 15, the geometric arithmetic index is computed as below (see Table 21):

$$\begin{aligned} GA(G) &= \sum_{st\in E(G)} \frac{2\sqrt{d(s)d(t)}}{d(s)+d(t)}, \\ GA(G) &= (2)\frac{2\sqrt{2}}{2+1} + (1)\frac{2\sqrt{3}}{3+1} + (2p+2q)\frac{2\sqrt{4}}{2+2} + (8p+8q-14)\frac{2\sqrt{6}}{3+2} \\ &+ (15pq-13p-13q+11)\frac{2\sqrt{9}}{3+3}, \\ GA(G) &= 15pq + (p+q)\left[\frac{16\sqrt{6}}{5} - 11\right] + \frac{4\sqrt{2}}{3} + \frac{\sqrt{3}}{2} - \frac{28\sqrt{6}}{5} + 11. \end{aligned}$$

Table 21. The geometric arithmetic index.

$[p,q]$	[1, 1]	[2, 2]	[3, 3]	[4, 4]	[5, 5]	[6, 6]	[7, 7]
$GA(G)$	18.35	64.21	135.11	236.42	346.12	460.25	580.12

- **The first and second Zagreb index**

Let G be the graph of $Si_2C_3\text{-}II[p,q]$. Now, by using Table 15, the first Zagreb index is computed as below (see Table 22):

$$\begin{aligned} M_1(G) &= \sum_{st\in E(G)} (d(s)+d(t)), \\ M_1(G) &= (2)(2+1) + (1)(3+1) + (2p+2q)(2+2) + (8p+8q-14)(3+2) \\ &+ (15pq-13p-13q+11)(3+3), \\ M_1(G) &= 90pq - 30p - 30q + 6. \end{aligned}$$

Table 22. The first Zagreb index.

$[p,q]$	[1, 1]	[2, 2]	[3, 3]	[4, 4]	[5, 5]	[6, 6]	[7, 7]
$M_1(G)$	36	246	636	1206	1836	3244	4634

The second Zagreb index is computed below (see Table 23):

$$\begin{aligned} M_2(G) &= \sum_{st\in E(G)} (d(s)d(t)) = R_1(G), \\ M_2(G) &= (2)(2\times 1)+(1)(3\times 1)+(2p+2q)(2\times 2)+(8p+8q-14)(3\times 2) \\ &+ (15pq-13p-13q+11)(3\times 3), \\ M_2(G) &= 135pq-61p-61q+22. \end{aligned}$$

Table 23. The second Zagreb index.

$[p,q]$	$[1,1]$	$[2,2]$	$[3,3]$	$[4,4]$	$[5,5]$	$[6,6]$	$[7,7]$
$M_2(G)$	35	318	871	1694	2654	4064	6248

- **Comparison of topological indices for** $Si_2C_3-II[p,q]$

In this section, we presented the comparison of above calculated topological indices for $Si_2C_3-II[p,q]$ graphically in Figure 7.

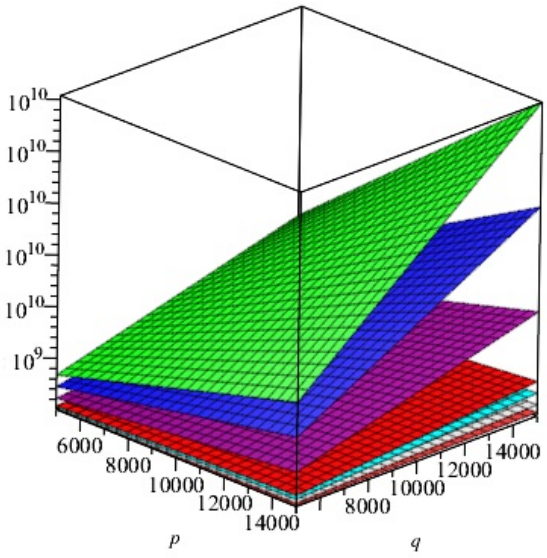

Figure 7. Comparison of indices, first and second Zagreb indexes, ABC index, GA index, ABC_4 index, GA_5 index, and general Randić index for$\alpha \in \{1,-1,1/2,-1/2\}$ of 2D structure of Si_2C_3-$II[p,q]$. R_1,Green; $R_{\frac{1}{2}}$, Purple; $R_{-\frac{1}{2}}$, Gray; R_{-1},Orange; ABC, Cayn; GA,Red; M_1, Blue; M_2, yellow.

Table 24 demonstrates the edge parcel in light of the degree total of end vertices of each edge of the chemical graph Si_2C_3-$II[p,q]$ for $p,q \geq 2$.

Table 24. Edge partition of Si_2C_3-$II[p,q]$.

$(d(s),\ d(t))$	$(S_u,\ S_v)$	Frequency
(2, 1)	(3, 2)	2
(3, 1)	(7, 3)	1
(2, 2)	(4, 3)	2
(2, 2)	(5, 4)	2
(2, 2)	(5, 5)	$2p+2q-4$
(3, 2)	(7, 5)	$2p+2q$
(3, 2)	(7, 6)	$2p+2q-2$
(3, 2)	(8, 6)	$2p+2q-6$
(3, 2)	(8, 5)	$2p+2q-6$
(3, 3)	(8, 7)	2
(3, 3)	(8, 8)	$2(p+q-4)$
(3, 3)	(7, 7)	2
(3, 3)	(9, 7)	$2p+2q-3$
(3, 3)	(9, 8)	$2p+2q-5$
(3, 3)	(9, 9)	$15pq-19p-19q+23$

- **The fourth atom–bond connectivity index** $ABC_4\Big(Si_2C_3-II[p,q]\Big)$

Let G be the graph of Silicon Carbide of type Si_2C_3-$II[p,q]$. Now, by using Table 24, the fourth atom–bond connectivity index is computed as (see Table 25):

$$\begin{aligned}
ABC_4(G) &= \sum_{st\in E(G)}\sqrt{\frac{S(s)+S(t)-2}{S(s)S(t)}},\\
ABC_4(G) &= (2)\sqrt{\frac{3+2-2}{3\times 2}}+(1)\sqrt{\frac{7+3-2}{7\times 3}}+(2)\sqrt{\frac{4+3-2}{4\times 3}}+(2)\sqrt{\frac{5+4-2}{5\times 4}}\\
&+ (2p+2q-4)\sqrt{\frac{5+5-2}{5\times 5}}+(2p+2q)\sqrt{\frac{7+5-2}{7\times 5}}+2(p+q-1)\sqrt{\frac{7+6-2}{7\times 6}}\\
&+ (2p+2q-6)\sqrt{\frac{8+6-2}{8\times 6}}+(2p+2q-6)\sqrt{\frac{8+5-2}{8\times 5}}+(2)\sqrt{\frac{8+7-2}{8\times 7}}\\
&+ 2(p+q-4)\sqrt{\frac{8+8-2}{8\times 8}}+(2)\sqrt{\frac{7+7-2}{7\times 7}}+(2p+2q-3)\sqrt{\frac{9+7-2}{9\times 7}}\\
&+ (2p+2q-5)\sqrt{\frac{9+8-2}{9\times 8}}+(15pq-19p-19q+23)\sqrt{\frac{9+9-2}{9\times 9}}.
\end{aligned}$$

After an easy calculation, we get:

$$\begin{aligned}
ABC_4(G) &= \frac{20}{3}pq\\
&+ (p+q)\left[\frac{22\sqrt{2}}{15}+2\sqrt{\frac{2}{7}}+2\sqrt{\frac{11}{42}}+\sqrt{\frac{11}{10}}+\frac{\sqrt{14}}{4}+\frac{1}{3}\sqrt{\frac{15}{2}}-67/9\right]\\
&+ \sqrt{2}+2\sqrt{\frac{2}{21}}+\frac{2}{5}\sqrt{\frac{5}{3}}+\sqrt{\frac{7}{5}}-\frac{13\sqrt{2}}{5}-2\sqrt{\frac{11}{42}}-3\sqrt{\frac{11}{10}}\\
&+ \sqrt{\frac{13}{14}}-\sqrt{14}+\frac{4\sqrt{3}}{7}-\frac{5}{6}\sqrt{\frac{15}{2}}+\frac{65}{9}.
\end{aligned}$$

Table 25. The fourth atom–bond connectivity index.

$[p,q]$	$[1,1]$	$[2,2]$	$[3,3]$	$[4,4]$	$[5,5]$	$[6,6]$	$[7,7]$
$ABC_4(G)$	7.21	28.23	64.11	101.21	142.28	208.44	266.64

- **The fifth geometric arithmetic index** $GA_5\left(Si_2C_3 - II[p,q]\right)$

Let G be the graph of Si_2C_3-$II[p,q]$. Now, by using Table 24, the fifth geometric arithmetic index is computed as (see Table 26):

$$\begin{aligned}
GA_5(G) &= \sum_{st\in E(G)} \frac{2\sqrt{S(s)S(t)}}{S(s)+S(t)},\\
GA_5(G) &= (2)\frac{2\sqrt{3\times 2}}{3+2} + (1)\frac{2\sqrt{7\times 3}}{7+3} + (2)\frac{2\sqrt{4\times 3}}{4+3} + (2)\frac{2\sqrt{5\times 4}}{5+4}\\
&+ (2p+2q-4)\frac{2\sqrt{5\times 5}}{5+5} + (2p+2q)\frac{2\sqrt{7\times 5}}{7+5} + 2(p+q-1)\frac{2\sqrt{7\times 6}}{7+6}\\
&+ (2p+2q-6)\frac{2\sqrt{8\times 6}}{8+6} + (2p+2q-6)\frac{2\sqrt{8\times 5}}{8+5} + (2)\frac{2\sqrt{8\times 7}}{8+7}\\
&+ 2(p+q-4)\frac{2\sqrt{8\times 8}}{8+8} + (2)\frac{2\sqrt{7\times 7}}{7+7} + (2p+2q-3)\frac{2\sqrt{9\times 7}}{9+7}\\
&+ (2p+2q-5)\frac{2\sqrt{9\times 8}}{9+8} + (15pq-19p-19q+23)\frac{2\sqrt{9\times 9}}{9+9},\\
GA_5(G) &= 15pq + (p+q)\left[\frac{\sqrt{35}}{3} + \frac{4\sqrt{42}}{13} + \frac{8\sqrt{3}}{7} + \frac{8\sqrt{10}}{13} + \frac{3\sqrt{7}}{4} + \frac{24\sqrt{2}}{17} - 15\right]\\
&+ \frac{4\sqrt{6}}{5} + \frac{\sqrt{21}}{5} + \frac{8\sqrt{3}}{7} + \frac{8\sqrt{5}}{9} - \frac{4\sqrt{42}}{13} - \frac{24\sqrt{3}}{7} - \frac{24\sqrt{10}}{13} + \frac{8\sqrt{14}}{15}\\
&- \frac{9\sqrt{7}}{8} - \frac{60\sqrt{2}}{17} + 13.
\end{aligned}$$

Table 26. The fifth geometric arithmetic index.

$[p,q]$	$[1,1]$	$[2,2]$	$[3,3]$	$[4,4]$	$[5,5]$	$[6,6]$	$[7,7]$
$GA_5(G)$	17.12	64.34	139.18	246.42	298.24	354.54	408.44

- **Comparison of topological indices for** Si_2C_3-$II[p,q]$

We presented the comparison of topological indices for Si_2C_3-$II[p,q]$ graphically in Figure 8.

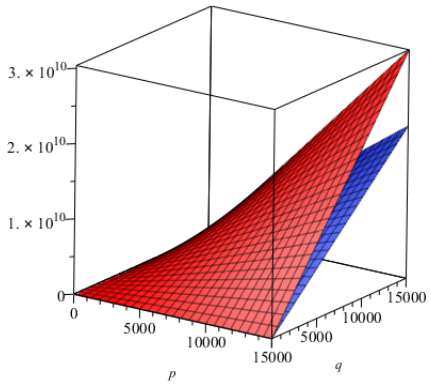

Figure 8. Comparison of ABC_4 and GA_5 indices of 2D structure of Si_2C_3-$II[p,q]$. Blue and red colors represents ABC_4 and GA_5, respectively.

6. Comparisons and Discussion

In this section, we have computed all indices for different values of p, q for both structures Si_2C_3-$I[p,q]$ and Si_2C_3-$II[p,q]$. In addition, we construct Tables 3–10, 12 and 13 for small values of p, q for these topological indices to the structure Si_2C_3-$I[p,q]$ and Tables 16–23, 25 and 26 to the structure Si_2C_3-$II[p,q]$. Now, from Tables 27 and 28, we can easily see that all indices are in increasing order as the values of p, q are increases. In addition, on the other hand, indices showed higher values for Si_2C_3-$I[p,q]$, as compared to those of Si_2C_3-$II[p,q]$.

The graphical representations of topological indices of Si_2C_3-$I[p,q]$ and Si_2C_3-$II[p,q]$ are depicted in Figures 3, 4, 7 and 8 for certain values of p, q.

Table 27. Comparison of all indices for Si_2C_3-$I[p,q]$.

$[p,q]$	ABC	R_1	R_{-1}	$R_{\frac{1}{2}}$	$R_{\frac{-1}{2}}$	GA	M_1	M_2	ABC_4	GA_5
$[1,1]$	16.2	77	2.41	49.31	7.42	19.25	44	47	9.42	19.26
$[2,2]$	48.3	350	11.32	60.34	25.18	68.29	264	350	32.21	69.31
$[3,3]$	98.7	923	18.11	80.41	51.23	141.12	664	923	68.26	143.28
$[4,4]$	169.3	1766	29.12	97.11	87.04	248.41	1244	1766	106.18	251.21

Table 28. Comparison of all indices for Si_2C_3-$II[p,q]$.

$[p,q]$	ABC	R_1	R_{-1}	$R_{\frac{1}{2}}$	$R_{\frac{-1}{2}}$	GA	M_1	M_2	ABC_4	GA_5
$[1,1]$	13.25	35	2.10	48.32	6.21	18.35	36	35	7.21	17.12
$[2,2]$	45.26	318	9.12	58.23	23.51	64.21	246	318	28.23	64.34
$[3,3]$	95.17	871	16.28	79.11	48.25	135.11	636	871	64.11	139.18
$[4,4]$	165.26	1694	28.11	95.21	84.39	236.42	1206	1694	101.21	246.42

Now, we presented the comparison of all topological indices using Table 27, for Si_2C_3-$I[p,q]$ in Figure 9 and using Table 28, for Si_2C_3-$II[p,q]$ in Figure 10.

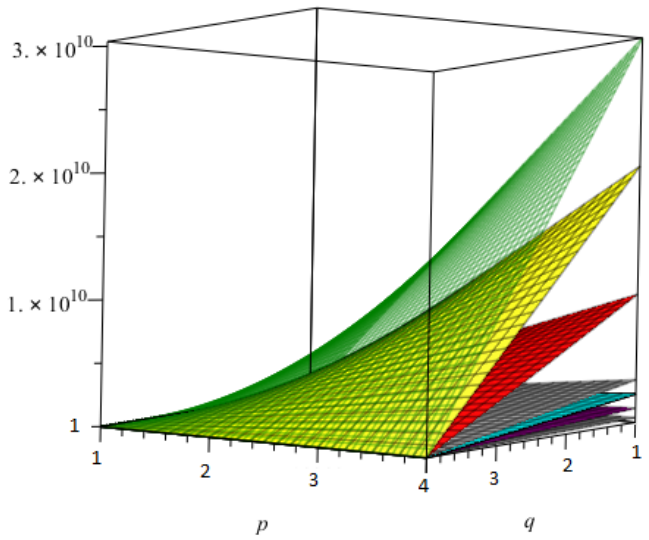

Figure 9. The comparison of all topological indices for Si_2C_3-$I[p,q]$.

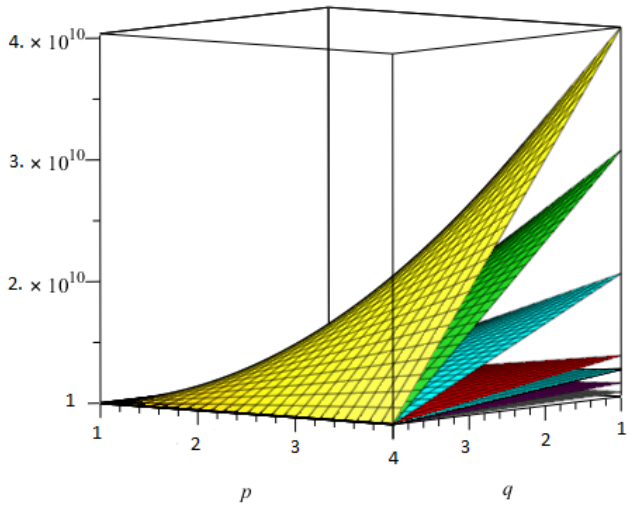

Figure 10. The comparison of all topological indices for Si_2C_3-$II[p,q]$.

7. Conclusions

We have studied and computed additive degree based topological indices, mainly atom–bond connectivity ABC index, general Randić index, first and second Zagreb index, geometric arithmetic GA index, fourth atom–bond connectivity ABC_4 index and fifth geometric arithmetic GA_5 index of two types of 2D Silicon Carbide, namely Si_2C_3-$I[p,q]$ and Si_2C_3-$II[p,q]$.

Since the Randic index is a topological descriptor that has correlated with a lot of chemical characteristics of the molecules. Thus, it has been found that the boiling point of Si_2C_3-$I[p,q]$ and Si_2C_3-$II[p,q]$-$I[p,q]$ is varying in increasing order for $\alpha \in \{1,-1,1/2,-1/2\}$.

Since the atom-bond connectivity (ABC) index provides a very good correlation for computing the strain energy of molecules, one can easily be seen that the strain energy of Si_2C_3-$I[p,q]$ and Si_2C_3-$II[p,q]$-$I[p,q]$ is high as the values of p,q increases.

In addition, GA index has much better predictive power than the predictive power of the Randic index, so the GA index is more useful than the Randic index for $\alpha \in \{-1,-1/2\}$ as compared to the Randic index for $\alpha \in \{1,1/2\}$ in the case of Si_2C_3-$I[p,q]$ and Si_2C_3-$II[p,q]$-$I[p,q]$.

Since the first and second Zagreb indexes were found to occur for computation of the total π-electron energy of the molecules, in the case of Si_2C_3-$I[p,q]$ and Si_2C_3-$II[p,q]$-$I[p,q]$, their values provide total π-electron energy in increasing order for higher values of p,q.

However, computing the distance based and counting related topological indices for these symmetrical chemical structures still remain open for investigation and as a challenge for researchers.

Author Contributions: M.I. and M.K.S. conceived, designed the experiments and analyzed the data. M.N. and M.A.I. performed experiments, some computations and wrote the initial draft of the paper which were validated and approved by M.I. and M.K.S. and wrote the final draft. All authors read and approved the final version of the paper.

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