COMPUTING TOPOLOGICAL INDICES OF 2-DIMENSIONAL SILICON-CARBONS

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The applications of graph theory in chemistry and in the study of molecule structures are important, and lately, it has increased exponentially. Molecular graphs have points (vertices) representing atoms (regardless of type) and lines (edges) that represents chemical bonds (regardless of type) between atoms. In this article, we study the molecular graph of $(2D)$ *silicon-carbon* Si_2C_3*-III and* SiC_3*-III. Moreover, we have computed and gave close formulas of degree based additive topological indices mainly first and second Zagreb index, general Randić, atom bond connectivity index(ABC), geometric arithmetic index(GA), fourth atom bond connectivity and fifth* GA*index of* Si_2C_3*-III and* SiC_3*-III.*

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1. Introduction

A chemical structure can be represented by using graph theory, where vertices denotes atoms and edges denotes chemical bonds. Molecular descriptors play a significant role in mathematical chemistry especially in QSPR/QSAR investigations. Among them, special place is reserved for so-called topological descriptors or topological indices. A topological index is the value of a specific mathematical function which indicates some useful information about molecular structure. A benchmark data sets, [5], can be found at *www.moleculardescriptors.eu.* This data set contains 16 physicochemical properties of octanes: boiling point (BP), melting point (MP), heat capacity at

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V constant (CV), heat capacity at P constant (CP), Entropy (S), density ($DENS$), enthalpy of vaporization ($HVAP$), standard enthalpy of vaporization ($DHVAP$), enthalpy of formation ($HFORM$), standard enthalpy of formation ($DHFORM$), motor octane number (MON), molar refraction (MR), acentric factor ($AcenFac$), total surface area (TSA), octanolwater partition coefficient ($LogP$), and molar volume (MV). This data contains and compare ABC, GA index, General Randić index, ABC_4, GA_5. Researchers have found topological index to be powerful and useful tool in the description of molecular structure. Some applications related to topological indices of molecular graphs are given in [2, 7, 8, 9, 10, 11, 13, 17, 18, 20, 26, 27, 28, 29].

Each structural formulas that incorporate covalent bonded compounds or atoms are diagrams. Thusly they are called molecular graphs or, basic diagrams or its better to state constitutional graphs. In chemistry, graph theory gives the premise to definition, numeration, systematization of the issue close by, it gives the way toward organizing laws or standards as per a framework or arranging, terminology, it gives the association between the compounds or atoms, and PC programming. The significance graph theory for science stands fundamentally from the presence of isomerism, which is supported by chemical graph theory. Silicon is a semiconductor material that has many extra edges over other same type of materials: like, It's cost is very low, it is nontoxic, in reality its availability is unlimited, many years of experience in its purification, production and device manufacturing. Its being utilized almost in all the latest electronic based devices. One of the most stable structures of two-dimensional ($2D$) silicon-carbon single layer compounds having different stoichiometric compositions were concluded in [22] that was based on the particle-swarm optimization represented by (PSO) technique combined with density functional theory optimization. Sheets of graphene were successfully isolated in 2004,[23, 24] and since then this hexagon(honeycomb) structured $2D$ material has motivated and energized research interests chiefly because of the extraordinary electronic, optical properties, and mechanical. Also particularly, the uniquely existing electronic properties of graphene attract consideration to this $2D$ material as a probable candidate for utilization in better and minor electronic devices. To date, lots of devotion and endeavors has given to open a bandgap in silicene sheets. The $2D$ siliconcarbon ($Si{-}C$) single layers can be scene as configurable (or tunable) materials between the pure $2D$ carbon singlelayer-graphene and the pure $2D$ silicon singlelayer-silicene. Lots of attempts have been conducted trying anticipating the most stable structures of the SiC sheet for more details read this [31, 32].

We consider $2D$ $Si - C$ compounds with two different types of SiC structure based on low-energy metastable structures for each Si. The types are Si_2C_3-I and Si_2C_3-II that denotes the lowest-energy and the second lowest energy structure respectively. More details about the edge and vertex sets about these molecules graphs are in the next section. We have computed the

ABC, GAindex, General Randić index, ABC_4, GA_5 of Si_2C_3-I and Si_2C_3-II molecule graphs.

Consider a chemical graph $G = (V, E)$ with V the vertex set and E the edge set of G. The degree (or valency) of vertex p is the number of edges incident with p and is represented by d_p. There are some types of topological indices namely eccentric based, degree based and distance based indices etc. In this article, we dealt with degree based topological indices.
One of the earliest degree dependent index was deduced by *Milan Randić* [25] in 1975, characterized as:

$$R_{-\frac{1}{2}}(G) = \sum_{pq\in E(G)} \frac{1}{\sqrt{d_p d_q}}.$$

In 1988, Bollobás *et al.* [3] and Amic *et al.* [1] proposed the general Randić index independently. For more details about Randić index, its properties and important results [4, 19, 21]. The general Randić index, characterized as:

$$R_\alpha(G) = \sum_{pq\in E(G)} (d_p d_q)^\alpha \tag{1}$$

Among degree dependent topological indices, ABC index of vital importance and introduced by Estrada *et al.* [6] and characterized as:

$$ABC(G) = \sum_{pq\in E(G)} \sqrt{\frac{d_p + d_q - 2}{d_p d_q}}. \tag{2}$$

The GAindex GA of a graph G is introduced by Vukičević *et al.* [30] and is defined as

$$GA(G) = \sum_{pq\in E(G)} \frac{2\sqrt{d_p d_q}}{d_p + d_q}. \tag{3}$$

One of the important degree dependent topological index is the first Zagreb index. It was introduced in 1972 by [16]. Later on, second Zagreb index is introduced by [15]. Both first and second Zagreb index is formulated as

$$M_1(G) = \sum_{pq\in E(G)} (d_p + d_q). \tag{4}$$

$$M_2(G) = \sum_{pq\in E(G)} (d_p d_q). \tag{5}$$

A well known topological index fourth version of ABC ABC_4 of a graph G is introduced by Ghorbhani *et al.* [12] and is defined as

$$ABC_4(G) = \sum_{pq\in E(G)} \sqrt{\frac{S_p + S_q - 2}{S_p S_q}}, \tag{6}$$

here $S_p = \sum_{pq\in E(G)} d_q$, $S_q = \sum_{pq\in E(G)} d_p$.
Another very famous topological descriptor fifth version of GAindex GA_5 of a graph G is introduced by Graovoc *et al* [14] and characterized as:

$$GA_5(G) = \sum_{pq\in E(G)} \frac{2\sqrt{S_pS_q}}{S_p+S_q}. \quad (7)$$

2. Silicon Carbide Si_2C_3-$III[n,m]$ $2D$ structure

In this section, additive topological indices mainly ABC, GA index, fourth ABC ABC_4, fifth GAindex GA_5, general Randić index, first and second Zagreb index of Si_2C_3-$III[n,m]$ are computed. Moreover, close formulas are derived which are helpful for the study analysis of properties of molecular structures of Si_2C_3-$III[n,m]$.

The $2D$ molecular graph of Silicon Carbide Si_2C_3-$III[n,m]$ is given in Fig.1, for more details see [22]. To describe its molecular graph we have used the settings in this way: we define n as the number of connected unit cells in a row(chain) and by m we represents the number of connected rows each with n number of cell. In Fig.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-$III[n,m]$. Thus the number of vertices in this graph is $10mn$ and the number of edges are $15mn-2n-3m$.
In $Si_2C_3-III[m,n]$, for $n,m\geq 1$, we have divided the vertices in three

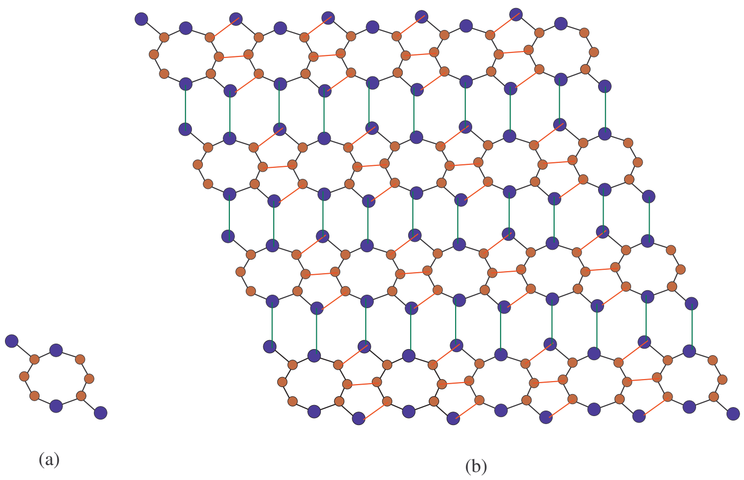

FIGURE 1. $2D$ structure of $Si_2C_3-III[n,m]$, (a) chemical unit cell of $Si_2C_3-III[n,m]$, (b) $Si_2C_3-III[5,4]$. Carbon atom C are brown and Silicon atom Si are blue.

sets based on the degree of vertices. The set of vertices degree 1 is denoted by V_1 and it has 2 elements. The set V_2 represents the vertices with degree

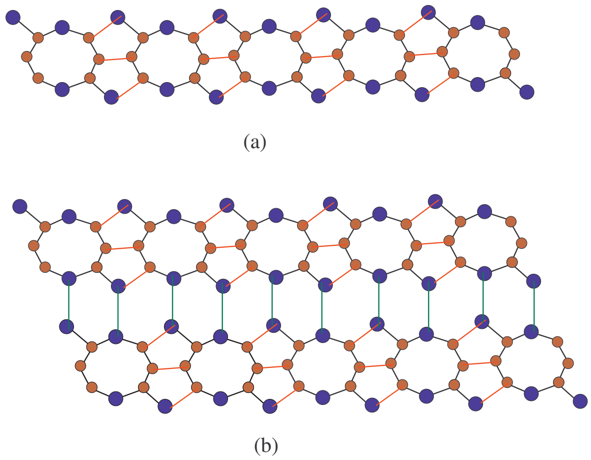

FIGURE 2. $2D$ structure of Si_2C_3-$III[n,m]$,(a) Si_2C_3-$I[5,1]$, One row with $n = 5$ and $m = 1$, red lines(edges) show the connection between the unit cell in a chain(b) Si_2C_3-$III[5,2]$, two rows are being connecting. Green lines(edges) connects the upper and lower rows(chains).

2 and it has $4n + 3m - 1$ elements. Similarly, the set of vertices degree 3 is denoted by V_3 and it has $10mn - 4n - 3m - 1$ elements. To find the topological indices we will partition the edges of Si_2C_3-$III[n,m]$. The edges of Si_2C_3-$III[n,m]$ are divided into four sets based on the degree of end vertices, say E_1, E_2, E_3 and E_4. The set E_1 contains 2 edges pq, where $d_p = 1$, $d_q = 3$. The set E_2 contains $2m + 2$ edges pq, where $d_p = 2$ and $d_q = 2$. The set E_3 contains $8n + 8m - 12$ edges pq, where $d_p = 2$ and $d_q = 3$. The set E_4 contains $15mn - 10n - 13m + 8$ edges pq, where $d_p = d_q = 3$. The Table 1 shows this edge partition of Si_2C_3-$III[n,m]$ for $m, n \geq 1$. The Randić index $R_\alpha(G)$ of

TABLE 1. Degree based partition of edges of Si_2C_3-$III[n,m]$, of end vertices of each edge

$(d_p,\ d_q)$	Frequency
$(1,\ 3)$	2
$(2,\ 2)$	$2m + 2$
$(2,\ 3)$	$8n + 8m - 12$
$(3,\ 3)$	$15mn - 10n - 13m + 8$

Si_2C_3-$III[n,m]$ are computed below.

Theorem 2.1. *Consider the graph $G \cong Si_2C_3\text{-}III[n,m]$ be the graph of Silicon Carbide, then its general Randić indices are;*

$$R_\alpha(G) = \begin{cases} 135mn - 61m - 42n + 14, & if\ \alpha = 1, \\ \frac{5mn}{3} + \frac{7m}{18} + \frac{2n}{9} + \frac{1}{18}, & if\ \alpha = -1, \\ 45mn - 35m + \sqrt{6}(8n + 8m - 12) - 30n + 2\sqrt{3} + 28. & if\ \alpha = \frac{1}{2}, \\ 5mn - \frac{10n}{3} - \frac{10m}{3} + \frac{11}{3} + \frac{\sqrt{6}(8n+8m-12)}{6} + \frac{2\sqrt{3}}{3} & if\ \alpha = -\frac{1}{2}. \end{cases}$$

Proof. Let G be the graph of $Si_2C_3\text{-}III[n,m]$. The above result can be proved by using Table 1 and equation (1), so the general Randić index for $\alpha = 1$.

$$\begin{aligned} R_1(G) &= \sum_{pq \in E(G)} (d_p \times d_q) \\ R_1(G) &= (2)(1 \times 3) + (2m + 2)(2 \times 2) + (8n + 8m - 12)(2 \times 3) \\ &+ (15mn - 10n - 13m + 8)(3 \times 3) \\ R_1(G) &= 135mn - 61m - 42n + 14 \end{aligned}$$

For $\alpha = -1$, the formula of Randić index takes the following form.

$$\begin{aligned} R_{-1}(G) &= \sum_{pq \in E(G)} \frac{1}{(d_p \times d_q)} \\ R_{-1}(G) &= (2)\left(\frac{1}{1 \times 3}\right) + (2m + 2)\left(\frac{1}{2 \times 2}\right) + (8m + 8n - 12)\left(\frac{1}{2 \times 3}\right) \\ &+ (15mn - 10n - 13m + 8)\left(\frac{1}{3 \times 3}\right) \\ R_{-1}(G) &= \frac{5mn}{3} + \frac{7m}{18} + \frac{2n}{9} + \frac{1}{18} \end{aligned}$$

For $\alpha = \frac{1}{2}$, the formula of Randić index takes the following form.

$$\begin{aligned} R_{\frac{1}{2}}(G) &= \sum_{pq \in E(G)} \sqrt{(d_p \times d_q)} \\ R_{\frac{1}{2}}(G) &= (2)(\sqrt{1 \times 3}) + (2m + 2)(\sqrt{2 \times 2}) + (8n + 8m - 12)(\sqrt{2 \times 3}) \\ &+ (15mn - 10n - 13m + 8)(\sqrt{3 \times 3}) \\ R_{\frac{1}{2}}(G) &= 45mn - 35m + \sqrt{6}(8n + 8m - 12) - 30n + 2\sqrt{3} + 28. \end{aligned}$$

For $\alpha = -\frac{1}{2}$, the formula of Randić index takes the following form.

$$\begin{aligned}
R_{-\frac{1}{2}}(G) &= \sum_{pq\in E(G)} \frac{1}{\sqrt{(d_p \times d_q)}} \\
R_{-\frac{1}{2}}(G) &= (2)\left(\frac{1}{\sqrt{1\times 3}}\right) + (2m+2)\left(\frac{1}{\sqrt{2\times 2}}\right) + (8n+8m-12)\left(\frac{1}{\sqrt{2\times 3}}\right) \\
&+ (15mn-10n-13m+8)\left(\frac{1}{\sqrt{3\times 3}}\right) \\
R_{-\frac{1}{2}}(G) &= 5mn - \frac{10n}{3} - \frac{10m}{3} + \frac{11}{3} + \frac{\sqrt{6}(8n+8m-12)}{6} + \frac{2\sqrt{3}}{3}
\end{aligned}$$

□

The ABC of Si_2C_3-$III[n,m]$ is computed in the following Theorem.

Theorem 2.2. *Consider the graph $G \cong Si_2C_3$-$III[n,m]$ of Silicon Carbide with $m,n \geq 1$, then its ABC index is equal to*

$$ABC(G) = 10mn - \frac{26m}{3} - \frac{20n}{3} + \frac{(15m+15n+2\sqrt{3}-18)\sqrt{2}}{3} + \frac{16}{3}.$$

Proof. Let G be the graph of Si_2C_3-$III[n,m]$ with $m,n \geq 1$. Then by using from Table 1 and the equation (2), the ABC index is computed as.

$$\begin{aligned}
ABC(G) &= \sum_{pq\in E(G)} \sqrt{\frac{d_p+d_q-2}{d_p d_q}} \\
ABC(G) &= (2)\sqrt{\frac{1+3-2}{1\times 3}} + (2m+2)\sqrt{\frac{2+2-2}{2\times 2}} + (8n+8m-12)\sqrt{\frac{2+3-2}{2\times 3}} \\
&+ (15mn-10n-13m+8)\sqrt{\frac{3+3-2}{3\times 3}}.
\end{aligned}$$

After some easy calculations, we get:

$$ABC(G) = 10mn - \frac{26m}{3} - \frac{20n}{3} + \frac{(15m+15n+2\sqrt{3}-18)\sqrt{2}}{3} + \frac{16}{3}$$

□

A close formula of GA index GA of Si_2C_3-$III[n,m]$ is computed in the following Theorem.

Theorem 2.3. *Consider the graph $G \cong Si_2C_3$-$III[n,m]$, for $m,n \geq 1$, then its* GA *index is equal to*

$$GA(G) = 15mn - 10n - 11m + \frac{2\sqrt{6}(8n+8m-12)}{15} + \sqrt{3} + 10.$$

Proof. Let G be the graph of Silicon Carbide Si_2C_3-$III[n,m]$. The by using Table 1 and the equation (3) the GA index is computed as below:

$$\begin{aligned} GA(G) &= \sum_{pq\in E(G)} \frac{2\sqrt{d_pd_q}}{d_p+d_q} \\ GA(G) &= (2)\left(\frac{2\sqrt{3}}{3+1}\right) + (2m+2)\left(\frac{2\sqrt{4}}{2+2}\right) + (8n+8m-12)\left(\frac{2\sqrt{6}}{2+3}\right) \\ &+ (15mn-10n-13m+8)\left(\frac{2\sqrt{9}}{3+3}\right) \\ GA(G) &= 15mn-10n-11m+\frac{2\sqrt{6}(8n+8m-12)}{15}+\sqrt{3}+10 \end{aligned}$$

□

In the next Theorem, we compute first and second Zagreb index of Si_2C_3-$III[n,m]$.

Theorem 2.4. *Consider the graph $G \cong Si_2C_3$-$III[n,m]$, for $m,n \geq 1$, then its first and second Zagreb indices are equal to*

$$\begin{aligned} M_1(G) &= 90mn-30m-20n+4 \\ M_2(G) &= 135mn-61m-42n+14. \end{aligned}$$

Proof. Let G be the graph of Si_2C_3-$III[n,m]$. Then by using Table 1 and the equations (4), (5) the first Zagreb indices are computed as below:

$$\begin{aligned} M_1(G) &= \sum_{pq\in E(G)} (d_p+d_q). \\ M_1(G) &= (2)(1+3)+(2m+2)(2+2)+(8n+8m-12)(2+3) \\ &+ (15mn-10n-13m+8)(3+3) \\ M_1(G) &= 90mn-30m-20n+4 \end{aligned}$$

From Theorem 2.1 the second Zagreb index is computed below:

$$M_2(G) = \sum_{pq\in E(G)} (d_pd_q) = R_1(G) = 135mn-61m-42n+14$$

□

The Table 2 shows the edge partition based on the degree sum of end vertices of each edge of the chemical graph Si_2C_3-$III[n,m]$ for $n,m \geq 2$. We have computed ABC_4, GA_5 index by using Table 2. A close formula of ABC_4 index of Si_2C_3-$III[n,m]$ is computed in the following Theorem.

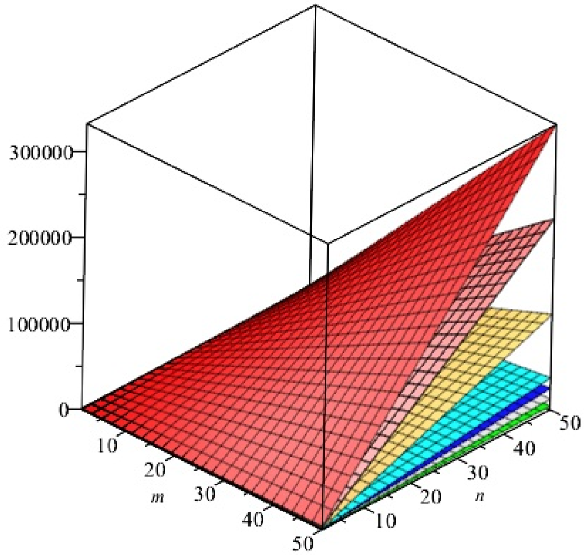

FIGURE 3. Comparison of indices, general Randić index for $\alpha \in \{1, -1, 1/2, -1/2\}$, ABC index, GA index and first Zagreb index of $2D$ structure of $G \cong SiC_3\text{-}III[n,m]$. The colors red, green, gold, blue , gray, cyan and orange represents $R_1(G)$, $R_{-1}(G)$ $R_{\frac{1}{2}}(G)$, $R_{-\frac{1}{2}}(G)$, $ABC(G)$, $GA(G)$, and $M_1(G)$, respectively. We can see that in the given domain $R_1(G)$ is more dominating and all the indices behave differently.

TABLE 2. Edge partition of $Si_2C_3\text{-}III[n,m]$, $m \geq 2$, $n \geq 2$ based on degree sum of end vertices of each edge.

$(S_p,\ S_q)$	Frequency
(3, 5)	2
(4, 5)	4
(5, 5)	$2m$
(5, 6)	2
(5, 7)	$4m-2$
(6, 7)	$8n+4m-14$
(7, 9)	$4n+4m-8$
(9, 9)	$15mn-14n-17m+16$

Theorem 2.5. *Consider the graph $G \cong Si_2C_3\text{-}III[n,m]$ with $n,m \geq 2$, then its ABC_4 index is equal to*

$$\begin{aligned} ABC_4(G) &= \frac{20mn}{3} - \frac{56n}{9} - \frac{68m}{9} + \frac{4\sqrt{2}m}{5} + \frac{\sqrt{30}}{5} + \frac{\sqrt{14}(4m-2)}{7} \\ &+ \frac{\sqrt{2}(4n+4m-8)}{3} + \frac{64}{9} + \frac{2\sqrt{10}}{5} + \frac{2\sqrt{35}}{5} + \frac{\sqrt{462}(8n+4m-14)}{42}. \end{aligned}$$

Proof. Let G be the graph of Silicon Carbide of type Si_2C_3-$III[n,m]$. The ABC_4 is computed by using Table 2 and equation (6) as below:

$$ABC_4(G) = \sum_{pq\in E(G)} \sqrt{\frac{S_p+S_q-2}{S_pS_q}}$$

$$\begin{aligned} ABC_4(G) &= (2)\sqrt{\frac{3+5-2}{3\times 5}}+(4)\sqrt{\frac{4+5-2}{4\times 5}}+(2m)\sqrt{\frac{5+5-2}{5\times 5}} \\ &+ (4m-2)\sqrt{\frac{5+7-2}{5\times 7}}+(8n+4m-14)\sqrt{\frac{6+7-2}{6\times 7}} \\ &+ (15mn-14n-17m+16)\sqrt{\frac{9+9-2}{9\times 9}}+(2)\sqrt{\frac{5+6-2}{5\times 6}} \\ &+ (4n+4m-8)\sqrt{\frac{7+9-2}{7\times 9}} \end{aligned}$$

After an easy calculation, we get:

$$\begin{aligned} ABC_4(G) &= \frac{20mn}{3}-\frac{56n}{9}-\frac{68m}{9}+\frac{4\sqrt{2}m}{5}+\frac{\sqrt{30}}{5}+\frac{\sqrt{14}(4m-2)}{7} \\ &+ \frac{\sqrt{2}(4n+4m-8)}{3}+\frac{64}{9}+\frac{2\sqrt{10}}{5}+\frac{2\sqrt{35}}{5}+\frac{\sqrt{462}(8n+4m-14)}{42} \end{aligned}$$

□

The GA_5 index of Si_2C_3-$III[n,m]$ is computed in the following Theorem.

Theorem 2.6. *Consider the graph $G \cong SiC_3$-$I[n,m]$ with $n,m \geq 2$, then its GA_5 index is equal to*

$$\begin{aligned} GA_5(G) &= 15mn-14n-15m+\frac{\sqrt{35}(4m-2)}{6}+\frac{2\sqrt{42}(8n+4m-14)}{13} \\ &+ \frac{3\sqrt{7}(4n+4m-8)}{8}+16+\frac{\sqrt{15}}{2}+\frac{16\sqrt{5}}{9}+\frac{4\sqrt{30}}{11}. \end{aligned}$$

Proof. Let G be the graph of Si_2C_3-$III[n,m]$. Then by using Table 2 and equation (7) the GA_5 index is computed as below:

$$GA_5(G) = \sum_{pq\in E(G)} \frac{2\sqrt{S_pS_q}}{S_p+S_q}$$

$$\begin{aligned} GA_5(G) &= (2)\frac{2\sqrt{3\times 5}}{3+5}+(4)\frac{2\sqrt{4\times 5}}{4+5}+(2m)\frac{2\sqrt{5\times 5}}{5+5}+(2)\frac{2\sqrt{5\times 6}}{6+5}\\ &+ (8n+4m-14)\frac{2\sqrt{6\times 7}}{6+7}+(4n+4m-8)\frac{2\sqrt{7\times 9}}{7+9}\\ &+ (15mn-14n-17m+16)\frac{2\sqrt{9\times 9}}{9+9}+(4m-2)\frac{2\sqrt{5\times 7}}{5+7} \end{aligned}$$

After an easy calculation, we get:

$$\begin{aligned} GA_5(G) &= 15mn-14n-15m+\frac{\sqrt{35}(4m-2)}{6}+\frac{2\sqrt{42}(8n+4m-14)}{13}\\ &+ \frac{3\sqrt{7}(4n+4m-8)}{8}+16+\frac{\sqrt{15}}{2}+\frac{16\sqrt{5}}{9}+\frac{4\sqrt{30}}{11}. \end{aligned}$$

□

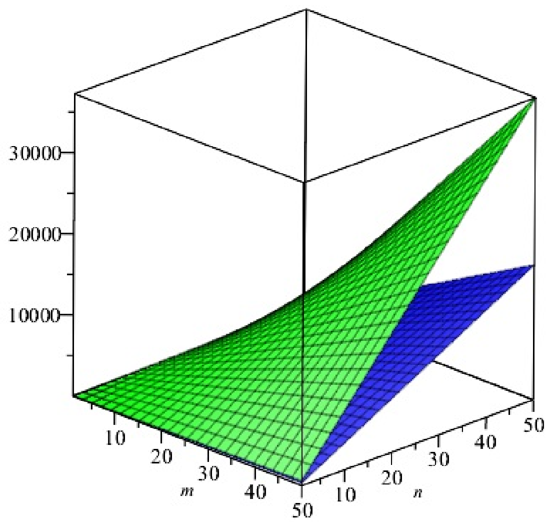

FIGURE 4. Comparison of $ABC_4(G)$ index and $GA_5(G)$ index of G equivalent to $2D$ structure of Si_2C_3-$III[n,m]$. The colors blue, green represents ABC_4 and GA_5 respectively. We can see that both are behaving differently.

3. Silicon Carbide SiC_3-$II[n,m]$ $2D$ structure

In this section, additive topological indices mainly ABC index, GA index, ABC_4 index, GA_5 index, general Randić index, first and second Zagreb indices of SiC_3-$III[n,m]$ are computed. Moreover, close formulas are derived which are helpful for the study analysis of properties of molecular structures of SiC_3-$III[n,m]$.

The $2D$ molecular graph of Silicon Carbide SiC_3-II is given in Fig.5, for more details see [22]. To describe its molecular graph we have used the settings in this way: we define n as the number of connected unit cells in a row(chain) and by m we represents the number of connected rows each with n number of cell. In Fig.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 SiC_3-$III[n,m]$. Thus the number of vertices in this graph is $8mn$ and the number of edges are $12mn-3n-2m$.

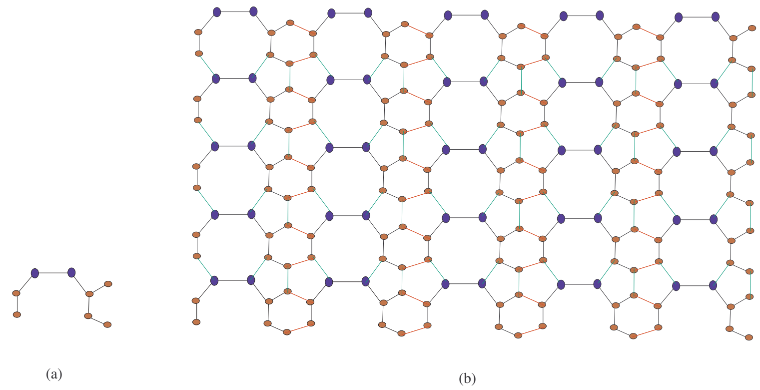

FIGURE 5. $2D$ structure of SiC_3-$III[n,m]$, (a) chemical unit cell of SiC_3-$III[n,m]$, (b) SiC_3-$III[5,5]$. Carbon atom C are brown and Silicon atom Si are blue

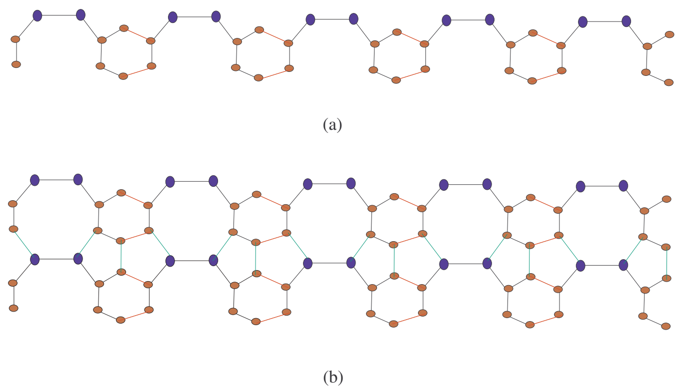

FIGURE 6. $2D$ structure of SiC_3-$III[n,m]$,(a) SiC_3-$III[5,1]$, One row with $n=5$ and $m=1$. Red lines show the connection between the unit cells(b) SiC_3-$III[5,2]$, two rows are connecting. Green lines(edges) connects the upper and lower rows.

In SiC_3-$III[n,m]$, for $n,m \geq 1$, we have divided the vertices in three sets based on the degree of vertices. The set of vertices having degree 1 is denoted by V_1 and it has 3 elements. The set V_2 represents the vertices with degree 2 and it has $4m + 6n - 6$ elements. Similarly, the set of vertices having degree 3 is denoted by V_3 and it has $8mn - 4m - 6n + 3$ elements. To find the topological indices we will partition the edges of SiC_3-$III[n, m]$. The edges of SiC_3-$III[n, m]$ are divided into five sets based on the degree of end vertices, say E_1, E_2, E_3, E_4 and E_5. The set E_1 contains 2 edges pq, where $d_p = 1$, $d_q = 2$. The set E_2 contains only one edge pq, where $d_p = 1$ and $d_q = 3$. The set E_3 contains $3n + 2m - 3$ edges pq, where $d_p = 2$ and $d_q = 2$. The set E_4 contains $6m + 4m - 8$ edges pq, where $d_p = 2$, $d_q = 3$. The set E_5 contains $12mn - 12n - 8m + 8$ edges pq, where $d_p = 3$, $d_q = 3$. The Table 3 shows the edge partition of SiC_3-$III[n, m]$ with $n, m \geq 1$.

Table 3. Degree based partition of edges of SiC_3-$III[n, m]$, of end vertices of each edge.

$(d_p,\ d_q)$	Frequency
(1, 2)	2
(1, 3)	1
(2, 2)	$3n + 2m - 3$
(2, 3)	$6n + 4m - 8$
(3, 3)	$12mn - 12n - 8m + 8$

The ABC index of SiC_3-$III[n, m]$ in the next Theorem is computed below.

Theorem 3.1. *Consider the graph $G \cong SiC_3$-$III[n, m]$ of Silicon Carbide with $n, m \geq 1$, then its ABC index is equal to*

$$\begin{aligned} ABC(G) &= 8mn - 8n - \frac{16m}{3} + \frac{\sqrt{2}(3n + 2m - 3)}{2} \\ &+ \frac{\sqrt{2}(6n + 4m - 8)}{2} + \frac{16}{3} + \sqrt{2} + \frac{\sqrt{6}}{3}. \end{aligned}$$

Proof. Let G be the graph of Silicon Carbide of type SiC_3-$III[n, m]$. Then from the edge partition of SiC_3-$III[n, m]$ based on degrees of end vertices of each edge with their frequencies which is given in Table 3, and equation (2) the ABC index is computed as:

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

$$
\begin{aligned}
ABC(G) &= (2)\sqrt{\frac{1+2-2}{1\times 2}}+(1)\sqrt{\frac{1+3-2}{1\times 3}}+(3n+2m-3)\sqrt{\frac{2+2-2}{2\times 2}}\\
&+ (6n+4m-8)\sqrt{\frac{2+3-2}{2\times 3}}+(12mn-12n-8m+8)\sqrt{\frac{3+3-2}{3\times 3}}.\\
ABC(G) &= 8mn-8n-\frac{16m}{3}+\frac{\sqrt{2}(3n+2m-3)}{2}\\
&+ \frac{\sqrt{2}(6n+4m-8)}{2}+\frac{16}{3}+\sqrt{2}+\frac{\sqrt{6}}{3}.
\end{aligned}
$$

□

The Randić index $R_\alpha(G)$ of silicon carbide SiC_3-$III[n,m]$ is computed below.

Theorem 3.2. *Consider the graph $G \cong SiC_3$-$III[n,m]$ be the graph of Silicon Carbide, then its general Randić index is equal to*

$$
R_\alpha(G)=\begin{cases}
108mn-60n-40m+19, & if\ \alpha=1\\
\frac{4mn}{3}+\frac{5n}{12}+\frac{5m}{18}+\frac{11}{36}., & if\ \alpha=-1\\
36mn-30n-20m+18+\sqrt{6}(6n+4m-8)+2\sqrt{2}+\sqrt{3} & if\ \alpha=\frac{1}{2}\\
4mn-\frac{5n}{2}-\frac{5m}{3}+\frac{7}{6}+\frac{\sqrt{6}(6n+4m-8)}{6}+\sqrt{2}+\frac{\sqrt{3}}{3} & if\ \alpha=-\frac{1}{2}.
\end{cases}
$$

Proof. Let G be the graph of SiC_3-$III[n,m]$. The above result can be proved by using Table 3 and equation (1) the general Randić indices are computed as:
For $\alpha = 1$.

$$
\begin{aligned}
R_1(G) &= \sum_{pq\in E(G)}(d_p\times d_q)\\
R_1(G) &= (2)(1\times 2)+(1)(1\times 3)+(3n+2m-3)(2\times 2)+(6n+4m-8)(2\times 3)\\
&+ (12mn-12n-8m+8)(3\times 3)\\
R_1(G) &= 108mn-60n-40m+19
\end{aligned}
$$

For $\alpha = -1$, the formula of Randić index takes the following form.

$$
\begin{aligned}
R_{-1}(G) &= \sum_{pq\in E(G)}\frac{1}{(d_p\times d_q)}\\
R_{-1}(G) &= \left(\frac{2}{1\times 2}\right)+\left(\frac{1}{1\times 2}\right)+(3n+2m-3)\left(\frac{1}{2\times 2}\right)+(6n+4m-8)\left(\frac{1}{2\times 3}\right)\\
&+ (12mn-12n-8m+8)\left(\frac{1}{3\times 3}\right)\\
R_{-1}(G) &= \frac{4mn}{3}+\frac{5n}{12}+\frac{5m}{18}+\frac{11}{36}.
\end{aligned}
$$

For $\alpha = \frac{1}{2}$, the formula of Randić index takes the following form.

$$\begin{aligned}
R_{\frac{1}{2}}(G) &= \sum_{pq\in E(G)} \sqrt{(d_p \times d_q)} \\
R_{\frac{1}{2}}(G) &= (2)(\sqrt{1\times 2}) + (1)(\sqrt{1\times 3}) + (3n+2m-3)(\sqrt{2\times 2}) \\
&+ (12mn-8m-12n+8)(\sqrt{3\times 3}) + (6n+4m-8)(\sqrt{2\times 3}) \\
R_{\frac{1}{2}}(G) &= 36mn-30n-20m+18+\sqrt{6}(6n+4m-8)+2\sqrt{2}+\sqrt{3}.
\end{aligned}$$

For $\alpha = -\frac{1}{2}$, the formula of Randić index takes the following form.

$$\begin{aligned}
R_{-\frac{1}{2}}(G) &= \sum_{pq\in E(G)} \frac{1}{\sqrt{(d_p \times d_q)}} \\
R_{-\frac{1}{2}}(G) &= (2)\left(\frac{1}{\sqrt{1\times 2}}\right) + (1)\left(\frac{1}{\sqrt{1\times 3}}\right) + (3n+2m-3)\left(\frac{1}{\sqrt{2\times 2}}\right) \\
&+ (6n+4m-8)\left(\frac{1}{\sqrt{2\times 3}}\right) + (12mn-8m-12n+8)\left(\frac{1}{\sqrt{3\times 3}}\right) \\
R_{-\frac{1}{2}}(G) &= 4mn - \frac{5n}{2} - \frac{5m}{3} + \frac{7}{6} + \frac{\sqrt{6}(6n+4m-8)}{6} + \sqrt{2} + \frac{\sqrt{3}}{3}.
\end{aligned}$$

□

A close formula of GA index of SiC_3-$III[n,m]$ is computed in the following Theorem.

Theorem 3.3. *Consider the graph $G \cong SiC_3$-$III[n,m]$, for $n,m \geq 1$, then its GA index is equal to*

$$GA(G) = 12mn-9n-6m+5+\frac{2\sqrt{6}(6n+4m-8)}{5}+\frac{4\sqrt{2}}{3}+\frac{(\sqrt{3}}{2}$$

Proof. Let G be the graph of Silicon Carbide SiC_3-$III[n,m]$. Then by using Table 3 and equation (3) the GA index is computed as below:

$$\begin{aligned}
GA(G) &= \sum_{pq\in E(G)} \frac{2\sqrt{d_p d_q}}{d_p+d_q} \\
GA(G) &= (2)\left(\frac{2\sqrt{2}}{1+2}\right) + (1)\left(\frac{2\sqrt{3}}{3+1}\right) + (3n+2m-3)\left(\frac{2\sqrt{4}}{2+2}\right) \\
&+ (12mn-8m-12n+8)\left(\frac{2\sqrt{9}}{3+3}\right) + (6n+4m-8)\left(\frac{2\sqrt{6}}{2+3}\right) \\
GA(G) &= 12mn-9n-6m+5+\frac{2\sqrt{6}(6n+4m-8)}{5}+\frac{4\sqrt{2}}{3}+\frac{\sqrt{3}}{2}.
\end{aligned}$$

□

In the next Theorem, we have computed first and second Zagreb indices of SiC_3-$III[n,m]$.

Theorem 3.4. *Consider the graph $G \cong SiC_3$-$III[n,m]$, for $n,m \geq 1$, then its first and second Zagreb indices are equal to*

$$\begin{aligned} M_1(G) &= 72mn - 30n - 20m + 6 \\ M_2(G) &= 108mn - 60n - 40m + 19. \end{aligned}$$

Proof. Let G be the graph of SiC_3-$III[n,m]$. Now, by using Table 3 and equation (4), (5) the first Zagreb index is computed as:

$$\begin{aligned} M_1(G) &= \sum_{pq \in E(G)} (d_p + d_q). \\ M_1(G) &= (2)(1+2) + (1)(1+3) + (3n+2m-3)(2+2) + (6n+4m-8)(2+3) \\ &+ (12mn - 8m - 12n + 8)(3+3) \\ M_1(G) &= 72mn - 30n - 20m + 6 \end{aligned}$$

By using Theorem 3.2 the second Zagreb index is computed below:

$$M_2(G) = \sum_{pq \in E(G)} (d_p d_q) = R_1(G) = 108mn - 60n - 40m + 19$$

□

The Table 4 shows the edge partition based on the degree sum of end vertices of each edge of the chemical graph SiC_3-$III[n,m]$ for $n,m \geq 2$. We have computed ABC_4 and GA_5 index by using Table 4.
A close formula of fourth bond connectivity index ABC_4 of SiC_3-$III[n,m]$ is computed in the following Theorem.

Theorem 3.5. *Consider the graph $G \cong SiC_3$-$III[n,m]$ with $n,m \geq 2$, then its fourth ABC index is equal to*

$$\begin{aligned} ABC_4(G) &= \frac{16mn}{3} - 8n - \frac{16m}{3} + \frac{\sqrt{35}(2n-1)}{10} + \frac{2\sqrt{2}(n+2m-3)}{5} \\ &+ \frac{\sqrt{110}(2m+2n-5)}{20} + \frac{\sqrt{462}(2n-2)}{42} + \frac{\sqrt{2}(2n+m-2)}{3} \\ &+ \frac{\sqrt{30}(4n+2m-7)}{12} + \sqrt{2} + \frac{\sqrt{6}}{2} + \frac{3\sqrt{7}}{7} + \frac{\sqrt{30}}{10} + \frac{17}{2} \\ &+ \frac{\sqrt{14}(2m+2n-4)}{7} + \frac{\sqrt{14}(m-2)}{8} \end{aligned}$$

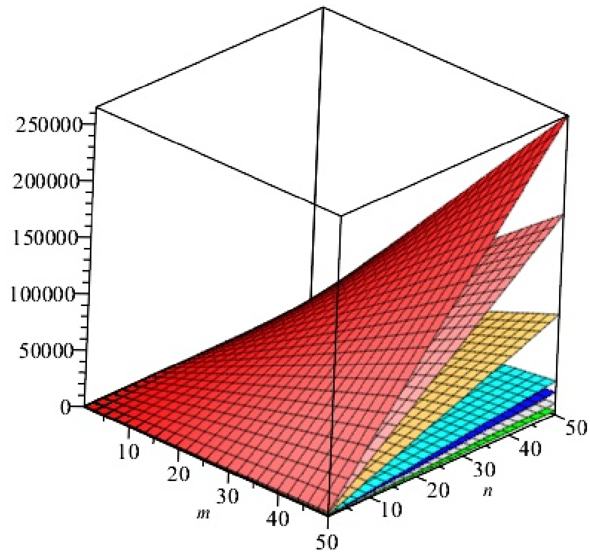

FIGURE 7. Comparison of indices, general Randić index for $\alpha \in \{1, -1, 1/2, -1/2\}$, ABC index, GA index and first Zagreb index of $2D$ structure of $G \cong SiC_3\text{-}III[n,m]$. The colors red, green, gold, blue , gray, cyan and orange represents $R_1(G)$, $R_{-1}(G)$ $R_{\frac{1}{2}}(G)$, $R_{-\frac{1}{2}}(G)$, $ABC(G)$, $GA(G)$, and $M_1(G)$, respectively. We can see that in the given domain $R_1(G)$ is more dominating and all the indices behave differently.

TABLE 4. Edge partition of $SiC_3\text{-}III[n,m]$, $m \geq 2$, $n \geq 2$, based on degree sum of end vertices of each edge.

$(S_p,\ S_q)$	Frequency
(2, 4)	2
(3, 8)	1
(4, 4)	1
(4, 5)	$2n-1$
(5, 5)	$n+2m-3$
(4, 7)	2
(5, 6)	1
(5, 7)	$2m+2n-4$
(5, 8)	$2m+2n-5$
(6, 7)	$2n-2$
(6, 8)	1
(7, 9)	$2n+m-2$
(8, 8)	$m-2$
(8, 9)	$4n+2m-7$
(9, 9)	$12mn-18n-12m+18$

Proof. Let G be the graph of Silicon Carbide of type SiC_3-$III[n,m]$, $n, m \geq 2$. The fourth ABC is computed by using Table 4 in the following calculations:

$$ABC_4(G) = \sum_{pq \in E(G)} \sqrt{\frac{S_p + S_q - 2}{S_p S_q}}$$

$$\begin{aligned}
ABC_4(G) &= (2)\sqrt{\frac{2+4-2}{2\times 4}} + (1)\sqrt{\frac{3+8-2}{3\times 8}} + (1)\sqrt{\frac{4+4-2}{4\times 4}} \\
&+ (n+2m-3)\sqrt{\frac{5+5-2}{5\times 5}} + (2)\sqrt{\frac{4+7-2}{4\times 7}} + (1)\sqrt{\frac{5+6-2}{5\times 6}} \\
&+ (2m+2n-4)\sqrt{\frac{5+7-2}{5\times 7}} + (2m+2n-5)\sqrt{\frac{5+8-2}{5\times 8}} \\
&+ (1)\sqrt{\frac{6+8-2}{6\times 8}} + (2n+m-2)\sqrt{\frac{7+9-2}{7\times 9}} + (m-2)\sqrt{\frac{8+8-2}{8\times 8}} \\
&+ (4n+2m-7)\sqrt{\frac{8+9-2}{8\times 9}} + (12mn-18n-12m+18)\sqrt{\frac{9+9-2}{9\times 9}} \\
&+ (2n-1)\sqrt{\frac{4+5-2}{4\times 5}} + (2n-2)\sqrt{\frac{6+7-2}{6\times 7}}
\end{aligned}$$

After an easy calculation, we get:

$$\begin{aligned}
ABC_4(G) &= \frac{16mn}{3} - 8n - \frac{16m}{3} + \frac{\sqrt{35}(2n-1)}{10} + \frac{2\sqrt{2}(n+2m-3)}{5} \\
&+ \frac{\sqrt{110}(2m+2n-5)}{20} + \frac{\sqrt{462}(2n-2)}{42} + \frac{\sqrt{2}(2n+m-2)}{3} \\
&+ \frac{\sqrt{30}(4n+2m-7)}{12} + \sqrt{2} + \frac{\sqrt{6}}{2} + \frac{3\sqrt{7}}{7} + \frac{\sqrt{30}}{10} + \frac{17}{2} \\
&+ \frac{\sqrt{14}(2m+2n-4)}{7} + \frac{\sqrt{14}(m-2)}{8}
\end{aligned}$$

□

The GA_5 index of SiC_3-$III[n,m]$ is computed in the following Theorem.

Theorem 3.6. *Consider the graph $G \cong SiC_3\text{-}III[n,m]$ with $n,m \geq 2$, then its GA_5 index is equal to*

$$\begin{aligned} GA_5(G) &= 12mn + \frac{4\sqrt{5}(2n-1)}{9} - 17n - 9m + \frac{12\sqrt{2}(4n+2m-7)}{17} \\ &+ \frac{4\sqrt{10}(2m+2n-5)}{13} + \frac{2\sqrt{42}(2n-2)}{13} + \frac{3\sqrt{7}(2n+m-2)}{18} \\ &+ \frac{8\sqrt{7}}{11} + \frac{2\sqrt{30}}{11} + \frac{4\sqrt{3}}{17} + 14 + \frac{\sqrt{35}(2m+2n-4)}{6} \\ &+ \frac{4\sqrt{2}}{3} + \frac{4\sqrt{6}}{11} \end{aligned}$$

Proof. Let G be the graph of $SiC_3\text{-}III[n,m]$. The above result can be proved by using Table 4 and equation (7) as below:

$$GA_5(G) = \sum_{pq \in E(G)} \frac{2\sqrt{S_p S_q}}{S_p + S_q}$$

$$\begin{aligned} GA_5(G) &= (2)\frac{2\sqrt{2\times 4}}{2+4} + (1)\frac{2\sqrt{3\times 8}}{3+8} + (1)\frac{2\sqrt{4\times 4}}{4+4} \\ &+ (2)\frac{2\sqrt{4\times 7}}{4+7} + (1)\frac{2\sqrt{5\times 6}}{5+6} + (2m+2n-4)\frac{2\sqrt{5\times 7}}{5+7} \\ &+ (2n-2)\frac{2\sqrt{6\times 7}}{6+7} + (1)\frac{2\sqrt{6\times 8}}{6+8} + (2n+m-2)\frac{2\sqrt{7\times 9}}{7+9} \\ &+ (4n+2m-7)\frac{2\sqrt{8\times 9}}{8+9} + (12mn-18n-12m+18)\frac{2\sqrt{9\times 9}}{9+9} \\ &+ (n+2m-3)\frac{2\sqrt{5\times 5}}{5+5} + (2n-1)\frac{2\sqrt{4\times 5}}{4+5} \\ &+ (2m+2n-5)\frac{2\sqrt{5\times 8}}{5+8} + (m-2)\frac{2\sqrt{8\times 8}}{8+8} \end{aligned}$$

After an easy calculation, we get:

$$\begin{aligned} GA_5(G) &= 12mn + \frac{4\sqrt{5}(2n-1)}{9} - 17n - 9m + \frac{12\sqrt{2}(4n+2m-7)}{17} \\ &+ \frac{4\sqrt{10}(2m+2n-5)}{13} + \frac{2\sqrt{42}(2n-2)}{13} + \frac{3\sqrt{7}(2n+m-2)}{18} \\ &+ \frac{8\sqrt{7}}{11} + \frac{2\sqrt{30}}{11} + \frac{4\sqrt{3}}{17} + 14 + \frac{\sqrt{35}(2m+2n-4)}{6} \\ &+ \frac{4\sqrt{2}}{3} + \frac{4\sqrt{6}}{11} \end{aligned}$$

□

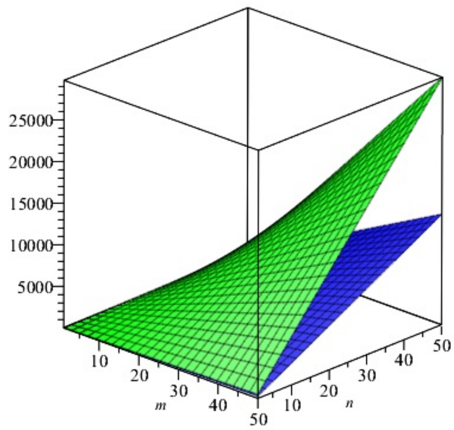

FIGURE 8. Comparison of $ABC_4(G)$ index and $GA_5(G)$ index of G equivalent to $2D$ structure of SiC_3-$III[n, m]$. The colors blue, green represents ABC_4 and GA_5 respectively. We can see that both are behaving differently.

4. Conclusion

We have studied and computed additive degree based topological indices mainly first and second Zagreb index, ABC index, GA GA index, fourth atom bond connectivity ABC_4 index, GA_5 index and general Randić index of two types of $2D$ Silicon Carbide, namely Si_2C_3-$III[n, m]$ and SiC_3-$III[n, m]$ chemical graphs for m-rows.

The graphical comparisons of topological indices of Si_2C_3-$III[n, m]$ and SiC_3-$III[n, m]$ are given in Fig.3, Fig.4, Fig.7 and Fig.8 for certain values of m, n. By varying the value of n, m the topological indices behaves differently. The comparison of indices as computed above mainly first Zagreb index, ABC index, GA index, ABC_4 index, GA_5 index, and general Randić index for$\alpha \in \{1, -1, 1/2, -1/2\}$ are depicted in Fig.3, Fig.4, Fig.7 and Fig.8.

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