Research Article

On Generalized Topological Indices of Silicon-Carbon

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Let $G$ be a graph with $n$ vertices and $\Gamma(u)$ be the degree of its $u$-th vertex ($\Gamma(x)$ is the degree of $u$). In this article, we compute the generalization of Zagreb index, the generalized Zagreb index, the first and second hyper $F$-indices, the sum connectivity $F$-index, and the product connectivity $F$-index graphs of $\text{Si}_2C_3^{-I}[p, q]$, $\text{Si}_2C_3^{-II}[p, q]$, $\text{Si}_2C_3^{-III}[p, q]$, and $\text{SiC}_3^{-III}[p, q]$.

1. Introduction

Mathematical chemistry is a branch of theoretical chemistry that discusses about the molecular structure by mathematical methods without necessarily referring to quantum mechanics. Molecular descriptors play a significant role in mathematical chemistry especially in QSPR/QSAR investigations [1]. A chemical structure can be represented by using graph theory, where vertices denote atoms and edges denote chemical bonds. Chemical graph theory is a branch of mathematical chemistry that it is a subject that connects mathematics, chemistry, and graph theory and solves problems arising in chemistry mathematically (for more details you can see [2–8]).

In chemical graph theory, a graph of molecule is a simple connected graph, in which atoms and chemical bonds are represented by vertices and edges, respectively. A graph is connected if there is a connection between any pair of vertices. Among them, special place is reserved for so-called topological descriptors or topological indices. Actually, topological indices are numeric quantities that tell us about the whole structure of graph. The topological indices are useful in the prediction of physicochemical properties and the bioactivity of the chemical compounds [9–11].

The topological indices of 2-dimensional silicon-carbons are computed in [12], in [13], Kwun et al. On the Multiplicative Degree-Based Topological Indices of Silicon-Carbon $\text{Si}_2C_3^{-I}[p, q]$ and $\text{Si}_2C_3^{-II}[p, q]$, in [14], Imran et al. On Topological Properties of Symmetric Chemical Structures in [15], Idrees et al. Molecular Descriptors of Benzenoid System, in [16], Kulli. $F$-indices of Chemical Networks, in [6], in [17], Gao et al. the Redefined first, second and third Zagreb Indices of Titania Nanotubes $TiO_2[m, n]$ and in [18], Kang et al. computed the topological indices of 2-dimensional silicon-carbon. For more details, see [19–23].

Bearing this in mind, it seems to be purposeful to compute the generalization of Zagreb index, the generalized Zagreb index, the first and second hyper $F$-indices, the sum connectivity $F$-index, and the product connectivity $F$-index of $\text{Si}_2C_3^{-I}[p, q], \text{Si}_2C_3^{-II}[p, q], \text{Si}_2C_3^{-III}[p, q]$, and $\text{SiC}_3^{-III}[p, q]$. 
Throughout this paper, all graphs will be assumed simple that is without loops, multiple, or directed edges. Let $G = (n, m)$ be a simple graph with vertex set $V(G) = \{v_1, v_2, v_3, \ldots, v_n\}$ and edge set $E(G), |E(G)| = m$. Also, let $d_i$ be the degree of vertex $v_i$ in graph $G$, for $i = 1, 2, \ldots, n$. The concept of valence in chemistry and the concept of degree in a graph are somehow closely related. For details on bases of graph theory, we refer to the book [24]. If two vertices $u$ and $v$ of the graph $G$ are adjacent, then the edge connecting them will be denoted by $uv$. The number of first neighbors of the vertex $u \in V(G)$ is its degree and will be denoted by $\Gamma(u)$.

In [25], the authors defined a new index, named generalization of Zagreb index:

$$M_{a,\beta} = M_{a,\beta}(G) = \sum_{uv \in E(G)} \frac{(\Gamma(u) \times \Gamma(v))^a}{(\Gamma(u) + \Gamma(v))^\beta},$$

(1)

where $a$ and $\beta$ are arbitrary real numbers. Few years later, the same index was proposed in [26] under the name second Gourava index, obtained as a special case of the generalized Zagreb index $M_{r,s}$ introduced in [27]:

$$M_{r,s} = M_{r,s}(G) = \sum_{uv \in E(G)} [(\Gamma(u)^r \times \Gamma(v)^s) + (\Gamma(u)^s \times \Gamma(v)^r)].$$

(2)

In [28], Gobadi et al. defined the hyper $F$-index or the first hyper $F$-index of a graph $G$ as

$$HF_1(G) = \sum_{uv \in E(G)} (\Gamma(u)^2 + \Gamma(v)^2)^2.$$  

(3)

In [16], the second hyper $F$-index of a graph is defined as

$$HF_2(G) = \sum_{uv \in E(G)} (\Gamma(u)^2 \times \Gamma(v)^2)^2.$$  

(4)

In [16], the author introduced the sum connectivity $F$-index and the product connectivity $F$-index of a graph $G$, defined as

$$SF(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{\Gamma(u)^2 + \Gamma(v)^2}},$$

$$PF(G) = \sum_{uv \in E(G)} \frac{1}{\Gamma(u)^2 \times \Gamma(v)^2}.$$  

(5)

The concept of silicon carbide was introduced by an American scientist in 1891. But nowadays, we can produce silicon carbide artificially by silica and carbon. Till 1929, silicon carbide was known as the hardest material on Earth. Here, we will find out the generalization of Zagreb index, the generalized Zagreb index, the first and second hyper $F$-indices, the sum connectivity $F$-index, and the product connectivity $F$-index.

This paper is organized as follows. In Section 2, we compute the generalization of Zagreb index, the generalized Zagreb index, the first and second hyper $F$-indices, the sum connectivity $F$-index, and the product connectivity $F$-index graphs of $Si_2C_3 - I[p, q]$. In Section 3, we compute the generalization of Zagreb index, the generalized Zagreb index, the first and second hyper $F$-indices, the sum connectivity $F$-index, and the product connectivity $F$-index graphs of $Si_2C_3 - II[p, q]$. In Section 4, we compute the generalization of Zagreb index, the generalized Zagreb index, the first and second hyper $F$-indices, the sum connectivity $F$-index, and the product connectivity $F$-index graphs of $Si_2C_3 - III[p, q]$. In Section 5, we compute the generalization of Zagreb index, the generalized Zagreb index, the first and second hyper $F$-indices, the sum connectivity $F$-index, and the product connectivity $F$-index graphs of $Si_2C_3 - IV[p, q]$.

For more details about these indices, see [12, 13, 29–39].

2. Results for Silicon-Carbon $Si_2C_3 - I[p, q]$

In this section, we compute the generalization of Zagreb index, the generalized Zagreb index, the first and second hyper $F$-indices, the sum connectivity $F$-index, and the product connectivity $F$-index graphs of $Si_2C_3 - I[p, q]$. In Figure 1, one unit of $Si_2C_3 - I$ is shown. Molecular graph of $S_2C_3 - I$ is shown in Figure 2, in which $p$ denotes the number of cells attached in a single row and $q$ denotes the number of total rows where each row contains $p$ cells. In Figures 3 and 4, we demonstrate how cells are connected in one row (chain) and how one row is connected to another row. In Figures 1–4, carbon atoms are shown as brown, and silicon atoms Si are shown as blue.

**Remark 1** (see [12]). The graph $Si_2C_3 - I[p, q]$ contains $10pq$ vertices and $15pq - 2p - 3q$ edges.

We start by proving the carbon nanocones for the redefined Zagreb indices.

**Theorem 1.** Let $Si_2C_3 - I[p, q]$ be the silicon carbide. Then,

$$M_{a,\beta}(Si_2C_3 - I[p, q]) = 9^a \times \frac{(15pq - 9p - 13q + 7)}{6^b} + 6^a \times \frac{(6p + 8q - 9)}{5^b} + (p + 2q) \times \frac{2^a}{3^b} + \frac{3^a}{4^b} \times \frac{4^{a-}\beta}{3^b} + \frac{3^a}{4^b}.$$  

$$M_{r,s}(Si_2C_3 - I[p, q]) = (6p + 8q - 9) \times (2^r \times 3^s + 2^s \times 3^r) + (30pq - 18p - 26q + 14) \times 3^{r+\tau}$$  

$$+ (2p + 4q) \times 2^{r+\tau} + 2^s \times 3^r + 3^s \times 3^\tau.$$  

(6)

**Proof.** Consider the graph silicon carbide $Si_2C_3 - I[p, q]$. By Remark 1, the graph $Si_2C_3 - I[p, q]$ contains $10pq$ vertices and $15pq - 2p - 3q$ edges. From the graph of $Si_2C_3 - I[p, q]$ silicon carbide, we can see that there are three partitions, $V_{(1)} = \{v \in V(Si_2C_3 - I[p, q]) \mid \Gamma(v) = 1\}$, $V_{(2)} = \{v \in V(Si_2C_3 - I[p, q]) \mid \Gamma(v) = 2\}$, and $V_{(3)} = \{v \in V(Si_2C_3 - I[p, q]) \mid \Gamma(v) \geq 3\}$. In $V_{(2)}$, the number of vertices is equal to $10pq$ and the number of cells attached in a single row is $p$. The number of rows is $q$. Therefore, the number of total rows is $q$. In each row, there are $p$ cells. In $V_{(3)}$, the number of vertices is equal to the number of total rows, which is $q$. The number of cells attached in a single row is $p$. Therefore, the number of total rows is $q$. In each row, there are $p$ cells. In $V_{(4)}$, the number of vertices is equal to the number of total rows, which is $q$. The number of cells attached in a single row is $p$. Therefore, the number of total rows is $q$. In each row, there are $p$ cells. In $V_{(5)}$, the number of vertices is equal to the number of total rows, which is $q$. The number of cells attached in a single row is $p$. Therefore, the number of total rows is $q$. In each row, there are $p$ cells.
\[ C_3 - I[p, q] \mid \Gamma(v) = 2 \], and \[ V_{(3)} = \{ v \in V(Si_2C_3 - I[p, q]) \mid \Gamma(v) = 3 \}. \] The edge set of the \( Si_2C_3 - I[p, q] \) can be partitioned as follows:

\[ E_1 = \{ e = uv \in E(Si_2C_3 - I[p, q]) \mid \Gamma(u) = 1 \text{ and } \Gamma(v) = 2 \}, \]
\[ E_2 = \{ e = uv \in E(Si_2C_3 - I[p, q]) \mid \Gamma(u) = 1 \text{ and } \Gamma(v) = 3 \}, \]
\[ E_3 = \{ e = uv \in E(Si_2C_3 - I[p, q]) \mid \Gamma(u) = 2 \text{ and } \Gamma(v) = 2 \}, \]
\[ E_4 = \{ e = uv \in E(Si_2C_3 - I[p, q]) \mid \Gamma(u) = 2 \text{ and } \Gamma(v) = 3 \}, \]
\[ E_5 = \{ e = uv \in E(Si_2C_3 - I[p, q]) \mid \Gamma(u) = 3 \text{ and } \Gamma(v) = 3 \}. \]

(7)

From the molecular graph of \( Si_2C_3 - I[p, q] \), we can observe that \[ |E_1| = 1, |E_2| = 1, |E_3| = p + 2q, |E_4| = 6p - 1 + 8(q - 1), \text{ and } |E_5| = 15pq - 9p - 13q + 7. \]

Thus, by definition generalization Zagreb index of \( Si_2C_3 - I[p, q] \), we have

\[ (7) \]
\[ M_{n,p}(S_i C_3 - I[p, q]) = \sum_{u \in E(S_i C_3 - I[p, q])} \frac{(\Gamma(u) \times \Gamma(v))^\alpha}{(\Gamma(u) + \Gamma(v))^\beta} \]
\[ = \sum_{u \in E_i(S_i C_3 - I[p, q])} \frac{(\Gamma(u) \times \Gamma(v))^\alpha}{(\Gamma(u) + \Gamma(v))^\beta} + \sum_{u \in E_i(S_i C_3 - I[p, q])} \frac{(\Gamma(u) \times \Gamma(v))^\alpha}{(\Gamma(u) + \Gamma(v))^\beta} \]
\[ + \sum_{u \in E_i(S_i C_3 - I[p, q])} \frac{(\Gamma(u) \times \Gamma(v))^\alpha}{(\Gamma(u) + \Gamma(v))^\beta} \]
\[ = \frac{(1 \times 2)^\alpha}{(1 + 2)^\beta} + \frac{(1 \times 3)^\alpha}{(1 + 3)^\beta} + (p + 2q) \times \frac{(2 \times 2)^\alpha}{(2 + 2)^\beta} \]
\[ + (6p - 1 + 8q - 13q + 7) \times \frac{(3 \times 3)^\alpha}{(3 + 3)^\beta} = g^\alpha \times \frac{(15pq - 9p - 13q + 7)}{6^\beta} + 6^\alpha \times \frac{(6p + 8q - 9)}{5^\beta} + (p + 2q) \times 4^{\alpha-\beta} + \frac{2^\alpha}{3^\alpha} + \frac{3^\alpha}{4^\beta}. \]

which is the required (18) result.

By definition of the generalized Zagreb index of \( S_i C_3 - I[p, q] \), we have

\[ M_{r,2}(S_i C_3 - I[p, q]) = \sum_{u \in E(S_i C_3 - I[p, q])} (\Gamma(u)^r \times \Gamma(v)^r + \Gamma(u)^r \times \Gamma(v)^r) \]
\[ = \sum_{u \in E_i(S_i C_3 - I[p, q])} (\Gamma(u)^r \times \Gamma(v)^r + \Gamma(u)^r \times \Gamma(v)^r) \]
\[ + \sum_{u \in E_i(S_i C_3 - I[p, q])} (\Gamma(u)^r \times \Gamma(v)^r + \Gamma(u)^r \times \Gamma(v)^r) \]
\[ + \sum_{u \in E_i(S_i C_3 - I[p, q])} (\Gamma(u)^r \times \Gamma(v)^r + \Gamma(u)^r \times \Gamma(v)^r) \]
\[ + \sum_{u \in E_i(S_i C_3 - I[p, q])} (\Gamma(u)^r \times \Gamma(v)^r + \Gamma(u)^r \times \Gamma(v)^r) \]
\[ = (1^r \times 2^r + 1^r \times 2^r) + (1^r \times 3^r + 1^r \times 3^r) \]
\[ + (p + 2q) \times (2^r \times 2^r + 2^r \times 2^r) + (6p - 1 + 8q - 13q + 7) \]
\[ \times (3^r \times 3^r + 3^r \times 3^r) = (2^r \times 3^r + 2^r \times 3^r) \]
\[ + (30pq - 18p - 26q + 14) \times 3^{r+r} + (2p + 4q) \times 2^{3r + 4} + 2^r + 2^r + 3^r + 3^r. \]
which is the required (19) result.

Proof. Consider the graph silicon carbide $\text{Si}_2\text{C}_3 - I[p,q]$. By Remark 1, the graph $\text{Si}_2\text{C}_3 - I[p,q]$ contains $10pq$ vertices and $15pq - 2p - 3q$ edges. By definition of the first hyper $F$-index of $\text{Si}_2\text{C}_3 - I[p,q]$, we have

$$HF_1(\text{Si}_2\text{C}_3 - I[p,q]) = \sum_{u \in E(\text{Si}_2\text{C}_3 - I[p,q])} (\Gamma(u)^2 + \Gamma(v)^2)^2$$

$$= \sum_{u \in E_1(\text{Si}_2\text{C}_3 - I[p,q])} (\Gamma(u)^2 + \Gamma(v)^2)^2 + \sum_{u \in E_2(\text{Si}_2\text{C}_3 - I[p,q])} (\Gamma(u)^2 + \Gamma(v)^2)^2$$

$$+ \sum_{u \in E_3(\text{Si}_2\text{C}_3 - I[p,q])} (\Gamma(u)^2 + \Gamma(v)^2)^2$$

$$= (1^2 + 2^2)^2 + (1^2 + 3^2)^2 + (p + 2q) \times (2^2 + 2^3)^2 + (6p - 1 + 8(q - 1))$$

$$\times (2^2 + 3^2)^2 + (15pq - 9p - 13q + 7) \times (3^2 + 3^2)^2$$

$$= 4860pq - 1838p - 2732q + 872.$$ 

which is the required (10) result.

By definition of the second hyper $F$-index of $\text{Si}_2\text{C}_3 - I[p,q]$, we have

$$HF_2(\text{Si}_2\text{C}_3 - I[p,q]) = \sum_{u \in E(\text{Si}_2\text{C}_3 - I[p,q])} (\Gamma(u)^2 + \Gamma(v)^2)^2$$

$$= \sum_{u \in E_1(\text{Si}_2\text{C}_3 - I[p,q])} (\Gamma(u)^2 + \Gamma(v)^2)^2 + \sum_{u \in E_2(\text{Si}_2\text{C}_3 - I[p,q])} (\Gamma(u)^2 + \Gamma(v)^2)^2$$

$$+ \sum_{u \in E_3(\text{Si}_2\text{C}_3 - I[p,q])} (\Gamma(u)^2 + \Gamma(v)^2)^2$$

$$= (1^2 \times 2^2)^2 + (1^2 \times 3^2)^2 + (p + 2q) \times (2^2 \times 2^3)^2 + (6p - 1 + 8(q - 1))$$

$$\times (2^2 \times 3^2)^2 + (15pq - 9p - 13q + 7) \times (3^2 \times 3^2)^2$$

$$= 98415pq - 51017p - 74413q + 34360.$$
which is the required (11) result.

Theorem 3. Let $\text{Si}_2\text{C}_3 - I[p, q]$ be the silicon carbide. Then,

$$SF(\text{Si}_2\text{C}_3 - I[p, q]) = \sqrt{2} \times \left(\frac{5pq}{2} - \frac{3p}{2} - \frac{13q}{6} + \frac{7}{6}\right) + \sqrt{2}$$

$$\times \left(\frac{pq}{4} + \frac{q}{2}\right) + \sqrt{13} \times \left(\frac{6p + 8q - 9}{13} + \frac{q}{2}\right)$$

$$+ \frac{\sqrt{5}}{5} + \frac{\sqrt{10}}{10}.$$  

(14)

$$PF(\text{Si}_2\text{C}_3 - I[p, q]) = \frac{9kn^2}{4} - \frac{27kn}{20} + \frac{k}{10}.$$  

(15)

Proof. Consider the graph silicon carbide $\text{Si}_2\text{C}_3 - I[p, q]$. By Remark 1, the graph $\text{Si}_2\text{C}_3 - I[p, q]$ contains $10pq$ vertices and $15pq - 2p - 3q$ edges. By definition of the sum connectivity F-index of $\text{Si}_2\text{C}_3 - I[p, q]$, we have

$$SF(\text{Si}_2\text{C}_3 - I[p, q]) = \sum_{uv \in E(\text{Si}_2\text{C}_3 - I[p, q])} \frac{1}{\Gamma(u)^2 + \Gamma(v)^2} + \sum_{uv \in E_1(\text{Si}_2\text{C}_3 - I[p, q])} \frac{1}{\Gamma(u)^2 + \Gamma(v)^2}$$

$$+ \sum_{uv \in E_2(\text{Si}_2\text{C}_3 - I[p, q])} \frac{1}{\Gamma(u)^2 + \Gamma(v)^2} + \sum_{uv \in E_3(\text{Si}_2\text{C}_3 - I[p, q])} \frac{1}{\Gamma(u)^2 + \Gamma(v)^2} + \sum_{uv \in E_4(\text{Si}_2\text{C}_3 - I[p, q])} \frac{1}{\Gamma(u)^2 + \Gamma(v)^2}.$$  

(16)

$$= \frac{1}{\sqrt{1^2 + 2^2}} + \frac{1}{\sqrt{1^2 + 3^2}} + (p + 2q) \times \left(\frac{1}{\sqrt{2^2 + 2^2}}\right) + (6p - 1 + 8(q - 1)) \times \left(\frac{1}{\sqrt{2^2 + 3^2}}\right)$$

$$\times \left(\frac{1}{\sqrt{3^2 + 3^2}}\right) + (15pq - 9p - 13q + 7) \times \left(\frac{1}{\sqrt{3^2 + 3^2}}\right)$$

$$= \sqrt{2} \times \left(\frac{5pq}{2} - \frac{3p}{2} - \frac{13q}{6} + \frac{7}{6}\right) + \sqrt{2} \times \left(\frac{pq}{4} + \frac{q}{2}\right)$$

$$+ \sqrt{13} \times \left(\frac{6p + 8q - 9}{13} + \frac{q}{2}\right) + \frac{\sqrt{5}}{5} + \frac{\sqrt{10}}{10}.$$

which is the required (14) result.

By definition of product connectivity F-index of $\text{Si}_2\text{C}_3 - I[p, q]$, we have
\[ PF(Si_2C_3 - I[p,q]) = \sum_{uv \in E(Si_2C_3 - I[p,q])} \frac{1}{\Gamma(u)^2 + \Gamma(v)^2} \]

\[ = \sum_{uv \in E_i(Si_2C_3 - I[p,q])} \frac{1}{\Gamma(u)^2 + \Gamma(v)^2} + \sum_{uv \in E_i(Si_2C_3 - I[p,q])} \frac{1}{\Gamma(u)^2 + \Gamma(v)^2} \]

\[ + \sum_{uv \in E_i(Si_2C_3 - I[p,q])} \frac{1}{\Gamma(u)^2 + \Gamma(v)^2} \]

\[ = \frac{1}{\sqrt{1^2 \times 2^2}} + \frac{1}{\sqrt{1^2 \times 3^2}} + (p + 2q) \times \left( \frac{1}{\sqrt{2^2 \times 2^2}} \right) + (6p - 1 + 8(q - 1)) \]

\[ \times \left( \frac{1}{\sqrt{2^2 \times 3^2}} \right) + (15pq - 9p - 13q + 7) \times \left( \frac{1}{\sqrt{3^2 \times 3^2}} \right) \]

\[ = \frac{5pq}{3} + \frac{p + 7q + 1}{4} \]

which is the required (15) result.

\[ M_{a,b}(Si_2C_3 - II[p,q]) = 9^a \times \frac{(15pq - 9p - 13q + 7)}{6^b} \]

\[ + 6^a \times \frac{(6p + 8q - 9)}{5^b} + (p + 2q) \]

\[ \times 4^{a+b} \times 2^a \times 3^a \times 4^b \]

\[ M_{r,s}(Si_2C_3 - II[p,q]) = (6p + 8q - 9) \times (2' \times 3' \times 2' \times 3') \]

\[ + (30pq - 18p - 26q + 14) \times 3^{*+r} \]

\[ + (2p + 4q) \times 2^{*+r} + 2' + 2' + 3' + 3'. \]

3. Results for Silicon-Carbon \( Si_2C_3 - II[p,q] \)

In this section, we compute the generalization of Zagreb index, the generalized Zagreb index, the first and second hyper F-indices, the sum connectivity F-index, and the product connectivity F-index graphs of \( Si_2C_3 - II[p,q] \). In Figure 5, one unit of \( Si_2C_3 - II \) is given. By connecting \( p \) cells in a row and then connecting \( q \) rows where each row contains \( p \) cells, we get molecular graph of \( Si_2C_3 - II \). The molecular graph of \( Si_2C_3 - II \) is shown in Figure 6 for \( p = 3 \) and \( q = 4 \). Figures 7 and 8 demonstrate how cells are connected in a row (chain) and how a row is connected to another row. We will use \( Si_2C_3 - II[p,q] \) to represent this molecular graph.

Remark 2 (see [12]). The graph \( Si_2C_3 - II[p,q] \) contains \( 10pq \) vertices and \( 15pq - 3p - 3q \) edges.

We start by proving the silicon carbide for the generalization of Zagreb index.

Theorem 4. Let \( Si_2C_3 - II[p,q] \) be the silicon carbide. Then,

**Proof.** Consider the graph silicon carbide \( Si_2C_3 - II[p,q] \). By Remark 2, the graph \( Si_2C_3 - II[p,q] \) contains \( 10pq \) vertices and \( 15pq - 2p - 3q \) edges. From the graph of \( Si_2C_3 - II[p,q] \) silicon carbide, we can see that there are three partitions, \( V_{(1)} = \{ v \in V(Si_2C_3 - II[p,q]) \mid \Gamma(v) = 1 \}, \)

\( V_{(2)} = \{ v \in V(Si_2C_3 - II[p,q]) \mid \Gamma(v) = 2 \}, \) and \( V_{(3)} = \{ v \in V(Si_2C_3 - II[p,q]) \mid \Gamma(v) = 3 \} \). The edge set of the \( Si_2C_3 - II[p,q] \) can be partitioned as follows:
which is the required (18) result.

From the molecular graph of $S_iC_3 - II[p, q]$, we can observe that $|E_1| = 2, |E_2| = 1, |E_3| = 2p + 2q, |E_4| = 8p + 8q - 14$, and $|E_5| = 14pq - 13p - 13q + 11$.

Thus, by definition generalization of $S_iC_3 - II[p, q]$, we have

\[
M_{a,b}(S_iC_3 - II[p, q]) = \sum_{u \in E(S_iC_3 - II[p, q])} \frac{(\Gamma (u) \times \Gamma (v))^a}{(\Gamma (u) + \Gamma (v))^b}
\]

\[
= \sum_{u \in E_1(S_iC_3 - II[p, q])} \frac{(\Gamma (u) \times \Gamma (v))^a}{(\Gamma (u) + \Gamma (v))^b} + \sum_{u \in E_2(S_iC_3 - II[p, q])} \frac{(\Gamma (u) \times \Gamma (v))^a}{(\Gamma (u) + \Gamma (v))^b}
\]

\[
+ \sum_{u \in E_3(S_iC_3 - II[p, q])} \frac{(\Gamma (u) \times \Gamma (v))^a}{(\Gamma (u) + \Gamma (v))^b} + \sum_{u \in E_4(S_iC_3 - II[p, q])} \frac{(\Gamma (u) \times \Gamma (v))^a}{(\Gamma (u) + \Gamma (v))^b}
\]

\[
= 2 \times \frac{(1 \times 2)^a}{(1 + 2)^b} + \frac{(1 \times 3)^a}{(1 + 3)^b} + (2p + 2q) \times \frac{(2 \times 2)^a}{(2 + 2)^b}
\]

\[
+ (8p + 8q - 14) \times \frac{(2 \times 3)^a}{(2 + 3)^b} + (15pq - 13p - 13q + 11)
\]

\[
\times \frac{(3 \times 3)^a}{(3 + 3)^b} = 9^a \times \frac{(15pq - 13p - 13q + 11)}{6^b} + 6^a \times \frac{(8p + 8q - 14)}{5^b}
\]

\[
+ (2p + 2q) \times 4^{a-b} + 2 \times \frac{2^a}{3^b} + \frac{3^a}{4^b}
\]

which is the required (18) result.
By definition of the generalized Zagreb index of $Si_2C_3 - II[p, q]$, we have

\[ M_{r,s}(Si_2C_3 - I[p, q]) = \sum_{uv \in E(Si_2C_3 - I[p, q])} (\Gamma(u)^r \times \Gamma(v)^s + \Gamma(u)^s \times \Gamma(v)^r) \]

\[ = \sum_{uv \in E_i(Si_2C_3 - I[p, q])} (\Gamma(u)^r \times \Gamma(v)^s + \Gamma(u)^s \times \Gamma(v)^r) \]

\[ + \sum_{uv \in E_i(Si_2C_3 - I[p, q])} (\Gamma(u)^s \times \Gamma(v)^r + \Gamma(u)^r \times \Gamma(v)^s) \]

\[ + \sum_{uv \in E_i(Si_2C_3 - I[p, q])} (\Gamma(u)^s \times \Gamma(v)^r + \Gamma(u)^r \times \Gamma(v)^s) \]

\[ + \sum_{uv \in E_i(Si_2C_3 - I[p, q])} (\Gamma(u)^r \times \Gamma(v)^s + \Gamma(u)^s \times \Gamma(v)^r) \]

\[ = 2 \times (1^r \times 2^s + 1^s \times 2^r) + (1^r \times 3^s + 1^s \times 3^r) \]

\[ + (2p + 2q) \times (2^r \times 2^s + 2^s \times 2^r) + (8p + 8q - 14) \]

\[ \times (2^r \times 3^s + 2^s \times 3^r) + (15pq - 13p - 13q + 11) \times (3^r \times 3^s + 3^r \times 3^s) \]

\[ = (8p - 6) \times (2^r \times 3^s + 2^r \times 3^s) + (30pq - 26p - 26q + 22) \times 3^{rr} \]

\[ + (4p + 4q) \times 2^{rr} + 2 \times 2^r + 2 \times 2^s + 3^r + 3^s. \]

which is the required (19) result. \[ \square \]

**Proof.** Consider the graph silicon carbide $Si_2C_3 - II[p, q]$. By Remark 2, the graph $Si_2C_3 - II[p, q]$ contains 10pq vertices and 15pq - 2p - 3q edges. By definition of the first hyper F-index of $Si_2C_3 - II[p, q]$, we have

\[ HF_1(Si_2C_3 - II[p, q]) = 4860pq - 2732p - 2732q + 1348, \]

\[ HF_2(Si_2C_3 - II[p, q]) = 98415pq - 74413p - 74413q + 54140. \]

---

\[
HF_1(Si_2C_3 - II[p, q]) = \sum_{uv \in E(Si_2C_3 - II[p, q])} \left( \Gamma(u)^2 + \Gamma(v)^2 \right)^2
\]

\[ = \sum_{uv \in E_i(Si_2C_3 - II[p, q])} \left( \Gamma(u)^2 + \Gamma(v)^2 \right)^2 + \sum_{uv \in E_i(Si_2C_3 - II[p, q])} \left( \Gamma(u)^2 + \Gamma(v)^2 \right)^2 \]

\[ + \sum_{uv \in E_i(Si_2C_3 - II[p, q])} \left( \Gamma(u)^2 + \Gamma(v)^2 \right)^2 + \sum_{uv \in E_i(Si_2C_3 - II[p, q])} \left( \Gamma(u)^2 + \Gamma(v)^2 \right)^2 \]

\[ = 2 \times (1^2 + 2^2)^2 + (1^2 + 3^2)^2 + (2p + 2q) \times (2^2 + 2^2)^2 + (8p + 8q - 14) \]

\[ \times (2^2 + 3^2)^2 + (15pq - 13p - 13q + 11) \times (3^2 + 3^2)^2 \]

\[ = 4860pq - 2732p - 2732q + 1348. \]
which is the required (23) result. By definition of the second hyper F-index of $Si_2C_3 - II[p,q]$, we have

\[
HF_2(Si_2C_3 - II[p,q]) = \frac{1}{\sqrt{\Gamma(u)^2 + \Gamma(v)^2}} \left( \Gamma(u)^2 \times \Gamma(v)^2 \right)^2 
\]

\[
= \sum_{uv\in E(Si_2C_3 - II[p,q])} \left( \Gamma(u)^2 \times \Gamma(v)^2 \right)^2 + \sum_{uv\in E_1(Si_2C_3 - II[p,q])} \left( \Gamma(u)^2 \times \Gamma(v)^2 \right)^2 
\]

\[
+ \sum_{uv\in E_1(Si_2C_3 - II[p,q])} \left( \Gamma(u)^2 \times \Gamma(v)^2 \right)^2 + \sum_{uv\in E_2(Si_2C_3 - II[p,q])} \left( \Gamma(u)^2 \times \Gamma(v)^2 \right)^2 
\]

\[
= 2 \times \left( 1^2 \times 2^2 \right)^2 + \left( 1^2 \times 3^2 \right)^2 + \left( 2^2 \times 2^2 \right)^2 + (8p + 8q - 14) \times \left( 2^2 \times 3^2 \right)^2 + (15pq - 13p - 13q + 11) \times \left( 3^2 \times 3^2 \right)^2 
\]

\[
= 98415pq - 74413p - 74413q + 54140. 
\]

which is the required (24) result. □

**Theorem 6.** Let $Si_2C_3 - II[p,q]$ be the silicon carbide. Then,

\[
SF(Si_2C_3 - II[p,q]) = \sqrt{2} \times \left( \frac{5pq}{2} - \frac{13p}{6} - \frac{13q}{6} + \frac{11}{6} \right) + \sqrt{2} \times \left( \frac{p + q}{2} \right) + \sqrt{13} \times \left( \frac{8p + 8q - 14}{13} \right) + \frac{2 \times \sqrt{5}}{5} + \frac{\sqrt{10}}{10} 
\]

(27)

\[
PF(Si_2C_3 - II[p,q]) = \frac{5pq}{3} + \frac{7p}{18} + \frac{7q}{18} + \frac{2}{9} 
\]

(28)

**Proof.** Consider the graph silicon carbide $Si_2C_3 - II[p,q]$. By Remark 2, the graph $Si_2C_3 - II[p,q]$ contains 10 vertices and 15 $pq - 2p - 3q$ edges. By definition of the sum connectivity F-index of $Si_2C_3 - II[p,q]$, we have

\[
SF(Si_2C_3 - II[p,q]) = \sum_{uv\in E(Si_2C_3 - II[p,q])} \frac{1}{\sqrt{\Gamma(u)^2 + \Gamma(v)^2}} 
\]

\[
= \sum_{uv\in E_1(Si_2C_3 - II[p,q])} \frac{1}{\sqrt{\Gamma(u)^2 + \Gamma(v)^2}} + \sum_{uv\in E_2(Si_2C_3 - II[p,q])} \frac{1}{\sqrt{\Gamma(u)^2 + \Gamma(v)^2}} 
\]

\[
+ \sum_{uv\in E_1(Si_2C_3 - II[p,q])} \frac{1}{\sqrt{\Gamma(u)^2 + \Gamma(v)^2}} + \sum_{uv\in E_2(Si_2C_3 - II[p,q])} \frac{1}{\sqrt{\Gamma(u)^2 + \Gamma(v)^2}} 
\]

\[
= 2 \times \frac{1}{\sqrt{1^2 + 2^2}} + \frac{1}{\sqrt{1^2 + 3^2}} + (2p + 2q) \times \left( \frac{1}{\sqrt{2^2 + 2^2}} \right) + (8p + 8q - 14) \times \left( \frac{1}{\sqrt{2^2 + 3^2}} \right) + (15pq - 13p - 13q + 11) \times \left( \frac{1}{\sqrt{3^2 + 3^2}} \right) 
\]

\[
= \sqrt{2} \times \left( \frac{5pq}{2} - \frac{13p}{6} - \frac{13q}{6} + \frac{11}{6} \right) + \sqrt{2} \times \left( \frac{p + q}{2} \right) + \sqrt{13} \times \left( \frac{8p + 8q - 14}{13} \right) + \frac{2 \times \sqrt{5}}{5} + \frac{\sqrt{10}}{10}. 
\]
which is the required (27) result. By definition of product connectivity F-index of $Si_2C_3 - \text{II}[p, q]$, we have

$$PF(Si_2C_3 - \text{II}[p, q]) = \sum_{u \in E(Si_2C_3 - \text{II}[p, q])} \frac{1}{\Gamma(u)^2 \times \Gamma(v)^2}$$

$$= \sum_{u \in E_1(Si_2C_3 - \text{II}[p, q])} \frac{1}{\Gamma(u)^2 \times \Gamma(v)^2} + \sum_{u \in E_2(Si_2C_3 - \text{II}[p, q])} \frac{1}{\Gamma(u)^2 \times \Gamma(v)^2}$$

$$+ \sum_{u \in E_3(Si_2C_3 - \text{II}[p, q])} \frac{1}{\Gamma(u)^2 \times \Gamma(v)^2}$$

$$= 2 \times \frac{1}{\sqrt{12} \times 2^2} + \frac{1}{\sqrt{12} \times 3^2} + (2p + 2q) \times \left( \frac{1}{\sqrt{2} \times 2^2} \right) + (8p + 8q - 14)$$

$$\times \left( \frac{1}{\sqrt{2} \times 3^2} \right) + (15pq - 13p - 13q + 11) \times \left( \frac{1}{\sqrt{3} \times 3^2} \right)$$

$$= \frac{5pq}{3} + \frac{7p}{18} + \frac{7q}{18} + \frac{2}{9}$$

which is the required (28) result.

4. Results for Silicon-Carbon $Si_2C_3 - \text{III}[p, q]$

In this section, we compute the generalization of Zagreb index, the generalized Zagreb index, the first and second hyper $F$-indices, the sum connectivity $F$-index, and the product connectivity $F$-index of $Si_2C_3 - \text{III}[p, q]$. The 2D silicon-carbon ($Si-C$) single layers can be seen as configurable (or tunable) materials between the pure 2D carbon single-layer graphene and the pure 2D silicon single-layer silicene. Lots of attempts have been conducted trying to anticipate the most stable structures of the SiC sheet (for more details, see [40, 41]).

The 2D molecular graph of silicon carbide $Si_2C_3 - \text{III}[p, q]$ is given in Figure 9, where carbon atom $C$ is shown in brown color and silicon atom $Si$ is shown in blue color (for more details, see [42]). In Figure 10, we gave a demonstration how the cells connect in a row (chain) and how one row connects to another row; red lines (edges) show the connection between the unit cell in a chain and green lines (edges) connect the upper and lower rows (chains). We will denote this molecular graph by $Si_2C_3 - \text{III}[p, q]$.

Remark 3 (see [13]). The graph $Si_2C_3 - \text{I}[p, q]$ contains 10pq vertices and 15pq - 2p - 3q edges.

We start by proving the carbon nanocones for the redefined Zagreb indices.

Theorem 7. Let $Si_2C_3 - \text{III}[p, q]$ be the silicon carbide. Then,

$$M_{a, \beta}(Si_2C_3 - \text{III}[p, q]) = 9^a \times \frac{(15pq - 10p - 13q + 8)}{6^\beta}$$

$$+ 6^a \times \frac{(8p + 8q - 12)}{5^\beta} + (4 + 4q)$$

$$\times 4^{a-\beta} + \frac{2 \times 3^a}{4^\beta}.$$  

$$M_{r,s}(Si_2C_3 - \text{III}[p, q]) = (8p + 8q - 12) \times (2^r \times 3^s + 2^s) \times 3^r \times (30pq - 20p - 26q + 16)$$

$$\times 3^{r+s} \times (2 + 2q) \times 4^{s+r} + 2 \times 3^r$$

$$+ 2 \times 3^s.$$
Proof. Consider the graph silicon carbide $\text{Si}_2\text{C}_3 - \text{III}[p, q]$. By Remark 3, the graph $\text{Si}_2\text{C}_3 - \text{III}[p, q]$ contains $10pq$ vertices and $15pq - 2p - 3q$ edges. From the graph of $\text{Si}_2\text{C}_3 - \text{III}[p, q]$ silicon carbide, we can see that there are three partitions, $V_{(1)} = \{v \in V(\text{Si}_2\text{C}_3 - \text{III}[p, q]) | \Gamma(v) = 1\}$, $V_{(2)} = \{v \in V(\text{Si}_2\text{C}_3 - \text{III}[p, q]) | \Gamma(v) = 2\}$, and $V_{(3)} = \{v \in V(\text{Si}_2\text{C}_3 - \text{III}[p, q]) | \Gamma(v) = 3\}$. The edge set of the $\text{Si}_2\text{C}_3 - \text{III}[p, q]$ can be partitioned as follows:

$E_1 = \{e = uv \in E(\text{Si}_2\text{C}_3 - \text{III}[p, q]) | \Gamma(u) = 1 \text{ and } \Gamma(v) = 3\},$

$E_2 = \{e = uv \in E(\text{Si}_2\text{C}_3 - \text{III}[p, q]) | \Gamma(u) = 2 \text{ and } \Gamma(v) = 2\},$

$E_3 = \{e = uv \in E(\text{Si}_2\text{C}_3 - \text{III}[p, q]) | \Gamma(u) = 2 \text{ and } \Gamma(v) = 3\},$

$E_4 = \{e = uv \in E(\text{Si}_2\text{C}_3 - \text{III}[p, q]) | \Gamma(u) = 3 \text{ and } \Gamma(v) = 3\}.$

(33)
From the molecular graph of $Si_2C_3 - III[p,q]$, we can observe that $|E_1| = 2, |E_2| = p + 2q, |E_3| = 8p + 8q - 12$, and $|E_4| = 15pq - 10p - 13q + 8$.

Thus, by definition generalization of $Si_2C_3 - III[p,q]$, we have

$$M_{n,p}(Si_2C_3 - III[p,q]) = \sum_{uv \in E(Si_2C_3 - III[p,q])} \frac{(\Gamma(u) \times \Gamma(v))^a}{(\Gamma(u) + \Gamma(v))^p}$$

$$= \sum_{uv \in E_1(Si_2C_3 - III[p,q])} \frac{(\Gamma(u) \times \Gamma(v))^a}{(\Gamma(u) + \Gamma(v))^p} + \sum_{uv \in E_2(Si_2C_3 - III[p,q])} \frac{(\Gamma(u) \times \Gamma(v))^a}{(\Gamma(u) + \Gamma(v))^p}$$

$$+ \sum_{uv \in E_3(Si_2C_3 - III[p,q])} \frac{(\Gamma(u) \times \Gamma(v))^a}{(\Gamma(u) + \Gamma(v))^p} + \sum_{uv \in E_4(Si_2C_3 - III[p,q])} \frac{(\Gamma(u) \times \Gamma(v))^a}{(\Gamma(u) + \Gamma(v))^p}$$

$$= 2 \times \frac{(1 \times 3)^a}{(1 + 3)^p} + (p + 2q) \times \frac{(2 \times 2)^a}{(2 + 2)^p}$$

$$+ (8p + 8q - 12) \times \frac{(2 \times 3)^a}{(2 + 3)^p} + (15pq - 10p - 13q + 8)$$

$$\times \frac{(3 \times 3)^a}{(3 + 3)^p} = 9a \times \frac{(15pq - 10p - 13q + 8)}{6^p} + 6a \times \frac{(8p + 8q - 12)}{5^p}$$

$$+ (2 + 2q) \times 4^{a-\beta} + \frac{2 \times 3a}{4^p}$$

which is the required (31) result.

By definition of the generalized Zagreb index of $Si_2C_3 - III[p,q]$, we have

$$M_{r,s}(Si_2C_3 - III[p,q]) = \sum_{uv \in E(Si_2C_3 - III[p,q])} (\Gamma(u)^r \times \Gamma(v)^s + \Gamma(u)^s \times \Gamma(v)^r)$$

$$= \sum_{uv \in E_1(Si_2C_3 - III[p,q])} (\Gamma(u)^r \times \Gamma(v)^s + \Gamma(u)^s \times \Gamma(v)^r)$$

$$+ \sum_{uv \in E_2(Si_2C_3 - III[p,q])} (\Gamma(u)^r \times \Gamma(v)^s + \Gamma(u)^s \times \Gamma(v)^r)$$

$$+ \sum_{uv \in E_3(Si_2C_3 - III[p,q])} (\Gamma(u)^r \times \Gamma(v)^s + \Gamma(u)^s \times \Gamma(v)^r)$$

$$+ \sum_{uv \in E_4(Si_2C_3 - III[p,q])} (\Gamma(u)^r \times \Gamma(v)^s + \Gamma(u)^s \times \Gamma(v)^r)$$

$$= 2 \times (1^r \times 3^s + 1^s \times 3^r)$$

$$+ (p + 2q) \times (2^r \times 2^s + 2^s \times 2^r) + (8p + 8q - 12)$$

$$\times (2^r \times 3^s + 2^s \times 3^r) + (15pq - 10p - 13q + 8) \times (3^r \times 3^s + 3^s \times 3^r)$$

$$= (8p + 8q - 12) \times (2^r \times 3^s + 2^s \times 3^r) + (30pq - 20p - 26q + 16) \times 3^{s+r}$$

$$+ (4 + 4q) \times 2^{s+r} + 2 \times 3^r + 2 \times 3^s.$$
Theorem 8. Let $Si_2C_3 - III[p, q]$ be the silicon carbide. Then,
\[ HF_1(Si_2C_3 - III[p, q]) = 4860pq - 2732p - 2732q + 1348, \] (36)
\[ HF_2(Si_2C_3 - III[p, q]) = 98415pq - 74413p - 74413q + 54140. \] (37)

Proof. Consider the graph silicon carbide $Si_2C_3 - III[p, q]$. By Remark 3, the graph $Si_2C_3 - III[p, q]$ contains 10pq vertices and 15pq - 2p - 3q edges. By definition of the first hyper F-index of $Si_2C_3 - III[p, q]$, we have

\[
HF_1(Si_2C_3 - III[p, q]) = \sum_{uv \in E(Si_2C_3 - III[p, q])} (\Gamma(u)^2 + \Gamma(v)^2)^2
= \sum_{uv \in E_1(Si_2C_3 - III[p, q])} (\Gamma(u)^2 + \Gamma(v)^2)^2 + \sum_{uv \in E_2(Si_2C_3 - III[p, q])} (\Gamma(u)^2 + \Gamma(v)^2)^2
+ \sum_{uv \in E_3(Si_2C_3 - III[p, q])} (\Gamma(u)^2 + \Gamma(v)^2)^2 + \sum_{uv \in E_4(Si_2C_3 - III[p, q])} (\Gamma(u)^2 + \Gamma(v)^2)^2
= 2((1^2 + 3^2)^2 + (2p + 2)(2^2 + 2^2)^2 + (8p + 8q - 12)
\times(2^2 + 3^2)^2 + (15pq - 10p - 13q + 8)(3^2 + 3^2)^2
= 4860pq - 1888p - 2732q + 892.
\]

which is the required (36) result.

By definition of the second hyper F-index of $Si_2C_3 - III[p, q]$, we have

\[
HF_2(Si_2C_3 - III[p, q]) = \sum_{uv \in E(Si_2C_3 - III[p, q])} (\Gamma(u)^2 \times \Gamma(v)^2)^2
= \sum_{uv \in E_1(Si_2C_3 - III[p, q])} (\Gamma(u)^2 \times \Gamma(v)^2)^2 + \sum_{uv \in E_2(Si_2C_3 - III[p, q])} (\Gamma(u)^2 \times \Gamma(v)^2)^2
+ \sum_{uv \in E_3(Si_2C_3 - III[p, q])} (\Gamma(u)^2 \times \Gamma(v)^2)^2 + \sum_{uv \in E_4(Si_2C_3 - III[p, q])} (\Gamma(u)^2 \times \Gamma(v)^2)^2
= 2(1^2 \times 3^2)^2 + (2 + 2q)(2^2 \times 2^2)^2 + (8p + 8q - 12)
\times(2^2 \times 3^2)^2 + (15pq - 10p - 13q + 8)(3^2 \times 3^2)^2
= 98415pq - 54730p - 74413q + 37136.
\]

which is the required (37) result.

Theorem 9. Let $Si_2C_3 - III[p, q]$ be the silicon carbide. Then,
\[
SF(S_i_2 C_3 - III[p, q]) = \sqrt{2} \times \left( \frac{5pq}{2} - \frac{5p}{3} - \frac{13q}{6} + \frac{4}{3} \right) + \sqrt{13} \times \left( \frac{8p + 8q - 12}{13} \right) + \sqrt{2} \times \left( \frac{q + 1}{2} \right) + \sqrt{10} \times \frac{1}{5}, \tag{40}
\]

\[
PF(S_i_2 C_3 - III[p, q]) = \frac{5pq}{3} + \frac{2p}{9} + \frac{7q}{18} - \frac{5}{18}. \tag{41}
\]

**Proof.** Consider the graph silicon carbide \(S_i_2 C_3 - III[p, q]\). By Remark 3, the graph \(S_i_2 C_3 - III[p, q]\) contains 10pq vertices and 15pq - 2p - 3q edges. By definition of the sum connectivity F-index of \(S_i_2 C_3 - III[p, q]\), we have

\[
SF(S_i_2 C_3 - III[p, q]) = \sum_{uv \in E(S_i_2 C_3 - III[p, q])} \frac{1}{\sqrt{\Gamma(u)^2 + \Gamma(v)^2}}
\]

\[
= \sum_{uv \in E_1(S_i_2 C_3 - III[p, q])} \frac{1}{\sqrt{\Gamma(u)^2 + \Gamma(v)^2}} + \sum_{uv \in E_2(S_i_2 C_3 - III[p, q])} \frac{1}{\sqrt{\Gamma(u)^2 + \Gamma(v)^2}}
\]

\[
+ \sum_{uv \in E_3(S_i_2 C_3 - III[p, q])} \frac{1}{\sqrt{\Gamma(u)^2 + \Gamma(v)^2}}
\]

\[
= 2 \times \frac{1}{\sqrt{12 + 3^2}} + (2 + 2q) \times \left( \frac{1}{\sqrt{2^2 + 2^2}} \right) + (8p + 8q - 12) \times \left( \frac{1}{\sqrt{3^2 + 3^2}} \right)
\]

\[
\times \left( \frac{5pq}{2} - \frac{5p}{3} - \frac{13q}{6} + \frac{4}{3} \right) + \sqrt{13} \times \left( \frac{8p + 8q - 12}{13} \right)
\]

\[
+ \sqrt{2} \times \left( \frac{q + 1}{2} \right) + \sqrt{10} \times \frac{1}{5}, \tag{42}
\]

which is the required (40) result.

By definition of product connectivity F-index of \(S_i_2 C_3 - III[p, q]\), we have

\[
PF(S_i_2 C_3 - III[p, q]) = \sum_{uv \in E(S_i_2 C_3 - III[p, q])} \frac{1}{\Gamma(u)^2 \times \Gamma(v)^2}
\]

\[
= \sum_{uv \in E_1(S_i_2 C_3 - III[p, q])} \frac{1}{\Gamma(u)^2 \times \Gamma(v)^2} + \sum_{uv \in E_2(S_i_2 C_3 - III[p, q])} \frac{1}{\Gamma(u)^2 \times \Gamma(v)^2}
\]

\[
+ \sum_{uv \in E_3(S_i_2 C_3 - III[p, q])} \frac{1}{\Gamma(u)^2 \times \Gamma(v)^2}
\]

\[
= 2 \times \frac{1}{\sqrt{12 \times 3^2}} + (2 + 2q) \times \left( \frac{1}{\sqrt{2 \times 2^2}} \right) + (8p + 8q - 12) \times \left( \frac{1}{\sqrt{3 \times 3^2}} \right)
\]

\[
\times \left( \frac{5pq}{2} - \frac{5p}{3} - \frac{13q}{6} + \frac{4}{3} \right) + \sqrt{13} \times \left( \frac{8p + 8q - 12}{13} \right)
\]

\[
+ \sqrt{2} \times \left( \frac{q + 1}{2} \right) + \sqrt{10} \times \frac{1}{5}. \tag{43}
\]
which is the required (41) result. □

5. Results for Silicon-Carbon $Si_2C_3 - III[p, q]$ 

In this section, we compute the generalization of Zagreb index, the generalized Zagreb index, the first and second hyper $F$-indices, the sum connectivity $F$-index, and the product connectivity $F$-index graphs of $Si_2C_3 - III[p, q]$.

The 2D molecular graph of silicon carbide $SiC_3 - III$ is given in Figure 11, where carbon atom $C$ is shown in brown color and silicon atom $Si$ is shown in blue color (for more details, see [42]). In Figure 12, we gave a demonstration how the cells connect in a row (chain) and how one row connects to another row; red lines show the connection between the unit cells and green lines (edges) connect the upper and lower rows. We will denote this molecular graph by $SiC_3 - III[p, q]$.

Remark 4 (see [13]). The graph $SiC_3 - III[p, q]$ contains $8pq$ vertices and $12pq - 3p - 2q$ edges.

We start by proving the carbon nanocones for the redefined Zagreb indices.

**Theorem 10.** Let $Si_2C_3 - III[p, q]$ be the silicon carbide. Then,

\[
M_{\alpha, \beta}(SiC_3 - III[p, q]) = 9^n \times \frac{(12pq - 12p - 8q + 8)}{6^\beta} + 6^\alpha
\]

\[
\times \frac{(6p + 4q - 8)}{5^\beta} + (3p + 2q - 3)
\]

\[
\times 4\alpha + \beta + \frac{3^\alpha}{4^\beta} + \frac{2 \times 2^\alpha}{3^\beta}.
\]

\[
(44)
\]

\[
M_{r,s}(SiC_3 - III[p, q]) = (6p + 4q - 8) \times (2^r \times 3^s + 2^r
\]

\[
\times 3^s) + (24pq - 24p - 16q + 16)
\]

\[
\times 3^{r+s} + (6p + 4q - 6) \times 2^{r+s} + 3^r
\]

\[
+ 3^s + 2 \times 2^r + 2 \times 2^s.
\]

\[
(45)
\]

**Proof.** Consider the graph silicon carbide $Si_2C_3 - III[p, q]$. By Remark 4, the graph $SiC_3 - III[p, q]$ contains $8pq$ vertices and $12pq - 3p - 2q$ edges. From the graph of $SiC_3 - III[p, q]$ silicon carbide, we can see that there are three partitions, $V_{(1)} = \{v \in V(SiC_3 - III[p, q]) | \Gamma(v) = 1\}$, $V_{(2)} = \{v \in V(SiC_3 - III[p, q]) | \Gamma(v) = 2\}$, and $V_{(3)} = \{v \in V(SiC_3 - III[p, q]) | \Gamma(v) = 3\}$.

The edge set of the $Si_2C_3 - III[p, q]$ can be partitioned as follows:

\[
E_1 = \{e = uv \in E(SiC_3 - III[p, q]) | \Gamma(u) = 1 \text{ and } \Gamma(v) = 2\},
\]

\[
E_2 = \{e = uv \in E(SiC_3 - III[p, q]) | \Gamma(u) = 1 \text{ and } \Gamma(v) = 3\},
\]

\[
E_3 = \{e = uv \in E(SiC_3 - III[p, q]) | \Gamma(u) = 2 \text{ and } \Gamma(v) = 2\},
\]

\[
E_4 = \{e = uv \in E(SiC_3 - III[p, q]) | \Gamma(u) = 2 \text{ and } \Gamma(v) = 3\},
\]

\[
E_1 = \{e = uv \in E(SiC_3 - III[p, q]) | \Gamma(u) = 3 \text{ and } \Gamma(v) = 3\}.
\]

(46)

From the molecular graph of $Si_2C_3 - III[p, q]$, we can observe that $|E_1| = 2, |E_2| = 1, |E_3| = 3p + 2q - 3, |E_4| = 6p + 4q - 8$, and $|E_1| = (12pq - 12p - 8q + 8)$.

Thus, by definition generalization of $Si_2C_3 - III[p, q]$, we have
\[ M_{s,\beta}(\text{SiC}_3 - \text{III}[p, q]) = \sum_{uv \in E(\text{SiC}_3 - \text{III}[p, q])} \frac{(\Gamma(u) \times \Gamma(v))^a}{(\Gamma(u) + \Gamma(v))^\beta} \]

\[ = \sum_{uv \in E_1(\text{SiC}_3 - \text{III}[p, q])} \frac{(\Gamma(u) \times \Gamma(v))^a}{(\Gamma(u) + \Gamma(v))^\beta} + \sum_{uv \in E_2(\text{SiC}_3 - \text{III}[p, q])} \frac{(\Gamma(u) \times \Gamma(v))^a}{(\Gamma(u) + \Gamma(v))^\beta} + \sum_{uv \in E_3(\text{SiC}_3 - \text{III}[p, q])} \frac{(\Gamma(u) \times \Gamma(v))^a}{(\Gamma(u) + \Gamma(v))^\beta} + \sum_{uv \in E_4(\text{SiC}_3 - \text{III}[p, q])} \frac{(\Gamma(u) \times \Gamma(v))^a}{(\Gamma(u) + \Gamma(v))^\beta} \]

\[ = 2 \times \left( \frac{(1 \times 2)^a}{(1 + 2)^\beta} + \frac{(1 \times 3)^a}{(1 + 3)^\beta} + (3p + 2q - 3) \times \frac{(2 \times 2)^a}{(2 + 2)^\beta} + (6p + 4q - 8) \times \frac{(2 \times 3)^a}{(2 + 3)^\beta} + (12pq - 12p - 8q + 8) \times \frac{(3 \times 3)^a}{(3 + 3)^\beta} \right) \times \frac{9^a}{6^\beta} + 6^a \times \frac{(6p + 4q - 8)}{5^\beta} + (3p + 2q - 3) \times \frac{(4^a - \beta)}{3^\beta} + 2 \times \frac{2^a}{3^\beta} \]

which is the required (44) result.

By definition of the generalized Zagreb index of \( \text{SiC}_3 - \text{III}[p, q] \), we have

\[ M_{r,s}(\text{SiC}_3 - \text{III}[p, q]) = \sum_{uv \in E(\text{SiC}_3 - \text{III}[p, q])} (\Gamma(u)^r \times \Gamma(v)^s + \Gamma(u)^s \times \Gamma(v)^r) \]

\[ = \sum_{uv \in E_1(\text{SiC}_3 - \text{III}[p, q])} (\Gamma(u)^r \times \Gamma(v)^s + \Gamma(u)^s \times \Gamma(v)^r) + \sum_{uv \in E_2(\text{SiC}_3 - \text{III}[p, q])} (\Gamma(u)^r \times \Gamma(v)^s + \Gamma(u)^s \times \Gamma(v)^r) + \sum_{uv \in E_3(\text{SiC}_3 - \text{III}[p, q])} (\Gamma(u)^r \times \Gamma(v)^s + \Gamma(u)^s \times \Gamma(v)^r) + \sum_{uv \in E_4(\text{SiC}_3 - \text{III}[p, q])} (\Gamma(u)^r \times \Gamma(v)^s + \Gamma(u)^s \times \Gamma(v)^r) \]

\[ = 2 \times \left( \frac{(1 \times 2)^r \times (1 \times 3)^s + 1 \times 2 \times (3p + 2q - 3)}{1 \times 2 \times 3} + (3p + 2q - 3) \times \frac{(2 \times 2)^r \times (2 \times 3)^s + 2 \times 3}{2 \times 2 \times 3} + (3p + 2q - 3) \times \frac{(2 \times 3)^r \times (3 \times 3)^s + 3 \times 3}{3 \times 3 \times 3} + (3p + 2q - 3) \times \frac{(3 \times 3)^r \times (3 \times 3)^s + 4 \times 4}{3 \times 3 \times 3} \right) + (3p + 2q - 3) \times \frac{(2 \times 3)^r \times (3 \times 3)^s + 2 \times 2 \times 2}{3 \times 3 \times 3} \]

\[ = (6p + 4q - 8) \times (2 \times 3^r + 2 \times 3^s) + (24pq - 24p - 16q + 16) \times 3^{s+r} + (6p + 4q - 6) \times 2^{s+r} + 3^s + 3^r + 2 \times 2^r + 2 \times 2^s. \]
Theorem 11. Let $SiC_3 - III[p, q]$ be the silicon carbide. Then,

$$HF_1(SiC_3 - III[p, q]) = 3888pq - 2682p - 1788q + 1198,$$

(49)

$$HF_2(SiC_3 - III[p, q]) = 78732pq - 70188p - 46792q + 41465.$$  

(50)

which is the required (45) result. □

Proof. Consider the graph silicon carbide $SiC_3 - III[p, q]$. By Remark 4, the graph $SiC_3 - III[p, q]$ contains $8pq$ vertices and $12pq - 3p - 2q$ edges. By definition of the first hyper $F$-index of $SiC_3 - III[p, q]$, we have

$$HF_1(SiC_3 - III[p, q]) = \sum_{uv \in E(SiC_3 - III[p, q])} \left( (\Gamma(u)^2 + \Gamma(v)^2)^2 \right),$$

$$= \sum_{uv \in E_1(SiC_3 - III[p, q])} \left( (\Gamma(u)^2 + \Gamma(v)^2)^2 + \sum_{uv \in E_2(SiC_3 - III[p, q])} \left( (\Gamma(u)^2 + \Gamma(v)^2)^2 + \sum_{uv \in E_3(SiC_3 - III[p, q])} \left( (\Gamma(u)^2 + \Gamma(v)^2)^2 + \sum_{uv \in E_4(SiC_3 - III[p, q])} \left( (\Gamma(u)^2 + \Gamma(v)^2)^2 \right) \right) \right) \right),$$

(51)

which is the required (49) result.

By definition of the second hyper $F$-index of $Si_2C_3 - III[p, q]$, we have

$$HF_2(SiC_3 - III[p, q]) = \sum_{uv \in E(SiC_3 - III[p, q])} \left( (\Gamma(u)^3 \times (\Gamma(v))^3) \right)^2,$$

$$= \sum_{uv \in E_1(SiC_3 - III[p, q])} \left( (\Gamma(u)^3 \times (\Gamma(v))^3) \right)^2 + \sum_{uv \in E_2(SiC_3 - III[p, q])} \left( (\Gamma(u)^3 \times (\Gamma(v))^3) \right)^2 + \sum_{uv \in E_3(SiC_3 - III[p, q])} \left( (\Gamma(u)^3 \times (\Gamma(v))^3) \right)^2 + \sum_{uv \in E_4(SiC_3 - III[p, q])} \left( (\Gamma(u)^3 \times (\Gamma(v))^3) \right)^2,$$

(52)

$$= 2 \times (1^2 + 2^2)^2 + (1^2 + 3^2)^2 + (3p + 2q - 3) \times (2^2 + 2^2)^2 + (6p + 4q - 8) \times (2^2 + 3^2)^2 + (12pq - 12p - 8q + 8) \times (3^2 + 3^2)^2,$$

$$= 3888pq - 2682p - 1788q + 1198.$$
Theorem 12. Let SiC$_3$−III[p,q] be the silicon carbide. Then,

$$SF(SiC_3−III[p,q]) = \sqrt{2} \times \left( 2pq - \frac{4p}{3} - 2p + \frac{4}{3} \right) + \sqrt{13}$$

$$\times \left( \frac{6p + 4q - 8}{13} \right) + \sqrt{2}$$

$$\times \left( \frac{q}{2} + \frac{3q}{2} - \frac{3}{4} \right) + \frac{\sqrt{10}}{10} + \frac{2\sqrt{5}}{5}.$$  \hspace{1cm} (53)

$$PF(SiC_3−III[p,q]) = \frac{4pq}{3} + \frac{5p}{12} + \frac{5p}{18} + \frac{5}{36}.$$  \hspace{1cm} (54)

Proof. Consider the graph silicon carbide SiC$_3$−III[p,q]. By Remark 4, the graph SiC$_3$−III[p,q] contains 8pq vertices and 12pq − 3p − 2q edges. By definition of the sum connectivity F-index of SiC$_3$−III[p,q], we have

$$SF(SiC_3−III[p,q]) = \sum_{uv\in E(SiC_3−III[p,q])} \frac{1}{\Gamma(u)^2 + \Gamma(v)^2}$$

$$= \sum_{uv\in E_1(SiC_3−III[p,q])} \frac{1}{\Gamma(u)^2 + \Gamma(v)^2} + \sum_{uv\in E_2(SiC_3−III[p,q])} \frac{1}{\Gamma(u)^2 + \Gamma(v)^2}$$

$$+ \sum_{uv\in E_3(SiC_3−III[p,q])} \frac{1}{\Gamma(u)^2 + \Gamma(v)^2}$$

$$+ \sum_{uv\in E_4(SiC_3−III[p,q])} \frac{1}{\Gamma(u)^2 + \Gamma(v)^2}$$  \hspace{1cm} (55)

$$= 2 \times \frac{1}{\sqrt{1^2 + 2^2}} + \frac{1}{\sqrt{1^2 + 3^2}} + (3p + 2q - 3) \times \left( \frac{1}{\sqrt{2^2 + 2^2}} \right) + (6p + 4q - 8)$$

$$\times \left( \frac{1}{\sqrt{3^2 + 3^2}} \right) + (12pq - 12p - 8q + 8) \times \left( \frac{1}{\sqrt{3^2 + 3^2}} \right)$$

$$= \sqrt{2} \times \left( 2pq - \frac{4p}{3} - 2p + \frac{4}{3} \right) + \sqrt{13} \times \left( \frac{6p + 4q - 8}{13} \right)$$

$$+ \sqrt{2} \times \left( \frac{q}{2} + \frac{3q}{2} - \frac{3}{4} \right) + \frac{\sqrt{10}}{10} + \frac{2\sqrt{5}}{5}.$$
which is the required (53) result.

By definition of product connectivity F-index of $\text{Si}_2\text{C}_3 - \text{III}[p, q]$, we have

$$PF(\text{Si}_2\text{C}_3 - \text{III}[p, q]) = \sum_{uv \in E(\text{Si}_2\text{C}_3 - \text{III}[p, q])} \frac{1}{\sqrt{\Gamma(u)^2 \times \Gamma(v)^2}}$$

$$= \sum_{uv \in E_1(\text{Si}_2\text{C}_3 - \text{III}[p, q])} \frac{1}{\sqrt{\Gamma(u)^2 \times \Gamma(v)^2}} + \sum_{uv \in E_2(\text{Si}_2\text{C}_3 - \text{III}[p, q])} \frac{1}{\sqrt{\Gamma(u)^2 \times \Gamma(v)^2}}$$

$$+ \sum_{uv \in E_3(\text{Si}_2\text{C}_3 - \text{III}[p, q])} \frac{1}{\sqrt{\Gamma(u)^2 \times \Gamma(v)^2}}$$

$$= 2 \times \frac{1}{\sqrt{1^2 \times 2^2}} + \frac{1}{\sqrt{1^2 \times 3^2}} + (3p + 2q - 3) \times \left( \frac{1}{\sqrt{2^2 \times 2^2}} \right) + (6p + 4q - 8)$$

$$\times \left( \frac{1}{\sqrt{2^2 \times 3^2}} \right) + (12pq - 12p - 8q + 8) \times \left( \frac{1}{\sqrt{3^2 \times 3^2}} \right)$$

$$= \frac{4pq}{3} + \frac{5p}{12} + \frac{5p}{18} + \frac{5}{36}$$

which is the required (54) result.

6. Conclusion

In this paper, we computed the generalization of Zagreb index, the generalized Zagreb index, the first and second hyper F-indices, the sum connectivity F-index, and the product connectivity F-index graphs of $\text{Si}_2\text{C}_3 - \text{I}[p, q], \text{Si}_2\text{C}_3 - \text{II}[p, q], \text{Si}_2\text{C}_3 - \text{III}[p, q]$ and $\text{Si}_2\text{C}_3 - \text{III}[p, q]$.

Data Availability

The data used to support the findings of this study are cited at relevant places within the text as references.

Conflicts of Interest

The authors declare that there no conflicts of interest.

Authors’ Contributions

All authors contributed equally to this work.

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