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Computing Adriatic Indices of (2D) Silicon Carbons

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Abstract— Chemical graph theory is the combination of chemistry and graph theory, it is used for mathematical representation of mollecules for the sake of structural and physical properties of moleculer graph. Topological index is a numeric number which is calculated from a chemical network. Topological indices are used to associate structural properties such as topology and graph invariants of chemical graphs. In this paper we study the chemical graphs of (2D) silicon carbon $SiC_3 - I, SiC_3 - II, SiC_4 - I$ and $SiC_4 - II$. Moreover, we compute adriatic indices and their related polynomials, namely inverse sum indeg index and symmetric division degree index of $SiC_3 - I, SiC_3 - II, SiC_4 - I$ and $SiC_4 - II$.

Index Terms— Topological indices, silicon carbon $SiC_3 - I, SiC_3 - II, SiC_4 - I$ and $SiC_4 - II$, ISI index, SDD index

1 Introduction

CHEMICAL graph is the representation of a convenient model for any real or abstracted chemical system or a structure of a chemical system which is used to identify the interactions among atoms and bonds or groups of atoms and molecules. The pictorial representation of chemical graphs is used to study structural properties of a chemical graph, where its vertices being atoms and edges corresponds to covalent bonds. The study of chemical structures and the usage of graph theory is more than someone's expectations. Chemical graph theory is a topological branch of mathematical chemistry which applies graph theory to chemical modeling of chemical structures. It is used for mathematical representation of molecules for the sake of physical properties of molecular graphs. Danial and Rouvary [1] described introduction and fundamentals of chemical graph theory.

Topological index of a graph is a numerical value which can be associated to a graph. Topological indices can be calculated from molecular graphs in which vertices and edges are represented by atoms and bonds respectively. Our research is based on mathematical chemistry which deals with mathematical representation of graphs and studies structural properties of chemical graphs and it comprises an extensive research. Molecular graphs are the basic models of chemical graph theory. In this sense, a topological index is a type of molecular descriptor which is calculated for a molecular graph of chemical phenomena. In 2004, after the productive separation of graphene sheets, the 2-dimensional structure of honeycomb urged researchers due to its remarkable properties like electronic, mechanical and optical. In [2], Pengfi Li et al. explored 2-dimensional silicon carbon monolayers compounds, with compositions of different ratios. Silicon is also a group-IV element and it has also 2-dimensional allotrope with the structure of honey comb, namely silicene. The silicene sheet show a weakely buckled local geometry, it's not like graphene sheet which is flat. The 2-dimensional silicon carbon monolayers can be seen as the composition of tunable materials between the pure 2-dimensional silicon monolayer.

Some of the most important degree based topological indices are bond additive, i.e. they are calculated as the sum of bond partion contributions, e.g. Randic type indices and Balaban type indices. D. Vukicicevic and M. Gasperov [3] analyzed the computation methods of bond partition contributions of these bond additive descriptors. They extracted the general conccepts, based on those concepts, they introducesd a large class of molecular descriptors. This class of descriptors is named as adriatic indices. A special subclass of these descriptors consists of 148 discrete adriatic indices. They are analyzed through testing sets provided by the IYMAC (International Academy of Mathematical Chemistry), they have good predictive properties in many cases. It is possible that they could improve various QSAR and QSPR properties [4] [5].

A graph G is an ordered pair $G = \big(V(G), E(G)\big)$ of two sets, where $V(G)$ is a nonempty set of discrete points or atoms called vertices and $E(G)$ is a set of arcs or bonds connecting two vertices called edges. The number of vertices in $V(G)$ is called order and number of edges in $E(G)$ is called size of the graph G.

The number of edges incident with a vertex i in a graph G is called the degree of that vertex i in G, is denoted as d_i. In this paper we compute exact formulas for inverse sum indeg polynomial, symmetric division degree polynomial, inverse sum indeg index and symmetric division degree index. Inverse sum indeg (ISI) index is a discrete adriatic index, which is the best total surface area predicter for octane isomers. The ISI index was introduced by D. Vukicevic and M. Gasperov [3] as:

$$ISI(G) = \sum_{ij \in E(G)} \frac{d_i d_j}{d_i + d_j}$$

And the ISI polynomial is defined as:

$$ISI(G, x) = \sum_{ij \in E(G)} x^{\frac{d_{i+d\_j}}{d_i d_j} - 1}$$

Where $ISI(G) = \int_0^1 ISI(G, x)dx$.

The symmetric division degree (SDD) index is also an adriatic index. (See [6], [7] and [8]). The SDD index is defined as:

$$SDD(G) = \sum_{ij \in E(G)} \frac{d_i^2 + d_j^2}{d_i d_j}$$

And SDD polynomial is defined as

$$SDD(G,x) = \sum_{ij \in E(G)} x^{\frac{d_{i}d_{j}}{d_i^2+d_j^2}-1}$$

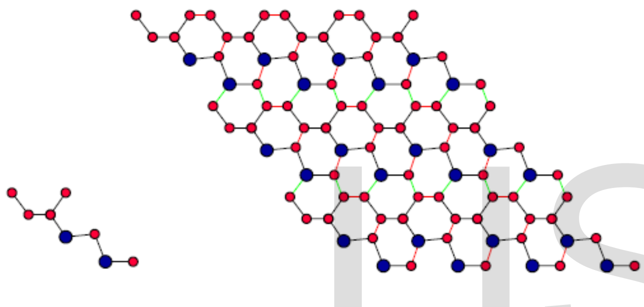
where $SDD(G) = \int_0^1 SDD(G,x)dx$.

We consider (2D) structures of $Si-C$ compounds with four different types namely $SiC_3-I, SiC_3-II, SiC_4-I$ and SiC_4-II.

2 Silicon Carbide $SiC_3 - I[a,b]$ 2D Structure

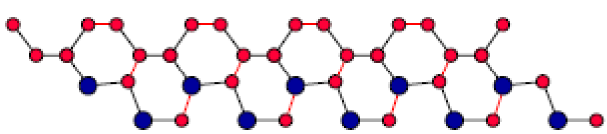
In this section ISI index, ISI polynomial, SDD index and SDD polynomials are computed for $SiC_3 - I$.

The 2D structure of silicon carbide graph $SiC_3 - I$ is shown in Figure 2.1 To describe its molecular graph we have used the setting in this way: we represented a as the number of connected cells in a row (or chain) and by b we defined the number of connected rows each with a number of cells. We denoted this molecular structure by $SiC_3 - I[a,b]$, whre a and b are natural numbers i.e. $a,b \geq 1$. Thus the order of this graph is $8ab$ where its size is $12ab-2a-3b$ for $a,b \geq 1$.

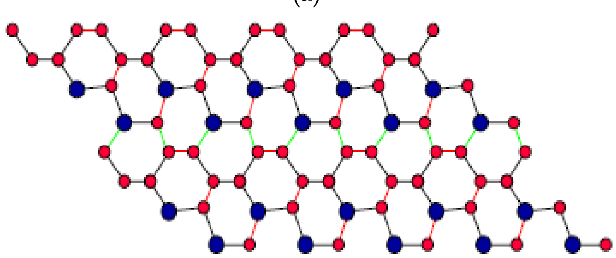


(a) (b)

Figure 2.1: The 2-dimensional structure of $SiC_3 - I[a,b]$, (a) One unit cell of $SiC_3 - I[a,b]$, (b) $SiC_3 - I[4,3]$. Silicon atoms Si are colored blue and carbon atoms C are colored red.



(a)



(b)

Figure 2.2: The 2D structure of $SiC_3 - I[a,b]$, (a) $SiC_3 - I[5,1]$, One row with $a=5$, $b=1$, red lines (edges\bonds) show how two cells are connected in a row (chain). (b) $SiC_3 - I[5,2]$ i.e. $a=5$, b=2, two rows are being connected by green lines (edges\bonds).

In the graph of silicon carbide $SiC_3 - I[a,b]$ for $a,b \geq 1$, there are three types of vertex sets based on the degree of vertices (or atoms) the vertex sets and their cardinalities are:

$$V_1 = \{i \in V(SiC_3 - I[a,b]) | d_i = 1\}, |V_1| = 3$$
$$V_2 = \{i \in V(SiC_3 - I[a,b]) | d_i = 2\}, |V_2| = 4a+6b-6$$
$$V_3 = \{i \in V(SiC_3 - I[a,b]) | d_i = 3\}, |V_3| = 8ab-4a-6b+3$$

Similarly with respect to an edge $e = ij$ of type (d_i, d_j), $E(SiC_3 - I[a,b])$ is partioned into five sets, their set descriptions and cardinalities are given as:

$$E_{1,2} = \{ij \in E(SiC_3 - I[a,b]) \,|\, d_i = 1, d_j = 2\}, |E_{1,2}| = 2$$
$$E_{1,3} = \{ij \in E(SiC_3 - I[a,b]) \,|\, d_i = 1, d_j = 3\}, |E_{1,3}| = 1$$
$$E_{2,2} = \{ij \in E(SiC_3 - I[a,b]) \,|\, d_i = 2, d_j = 2\},$$
$$|E_{2,2}| = \begin{cases} 3b-1 & \text{for } a=1, b\geq 1 \\ 2a+2b-3 & \text{for } a>1, b \geq 1 \end{cases}$$
$$E_{2,3} = \{ij \in E(SiC_3 - I[a,b]) \,|\, d_i = 2, d_j = 3\},$$
$$|E_{2,3}| = \begin{cases} 6b-4 & \text{for } a=1, b\geq 1 \\ 4a+8b-8 & \text{for } a>1, b \geq 1 \end{cases}$$
$$E_{3,3} = \{ij \in E(SiC_3 - I[a,b]) \,|\, d_i = 3, d_j = 3\},$$
$$|E_{3,3}| = \begin{cases} 12ab-2a-12b+2 & \text{for } a=1, b\geq 1 \\ 12ab-8a-13b+8 & \text{for } a>1, b \geq 1 \end{cases}$$

Table 1. Shows this edge partition of $SiC_3 - I[a,b]$ for $a,b \geq 1$.

E_{d_i,d_j}	Frequency
$E_{1,2}$	2
$E_{1,3}$	1
$E_{2,2}$	$\begin{cases} 3b-1 & \text{for } a=1, b\geq 1 \\ 2a+2b-3 & \text{for } a>1, b \geq 1 \end{cases}$
$E_{2,3}$	$\begin{cases} 6b-4 & \text{for } a=1, b\geq 1 \\ 4a+8b-8 & \text{for } a>1, b \geq 1 \end{cases}$
$E_{3,3}$	$\begin{cases} 12ab-2a-12b+2 & \text{for } a=1, b\geq 1 \\ 12ab-8a-13b+8 & \text{for } a>1, b \geq 1 \end{cases}$

Our first theorem is about computation ISI polynomial of silicon carbide graph $SiC_3 - I[a,b]$ for $a,b \geq 1$.

Theorem 2.1: ISI polynomial of the silicon carbide graph $G \cong SiC_3 - I[a,b]$ for $a,b \geq 1$, is given as:

1. For $a=1, b \geq 1$
$$ISI(G,x) = 3b-1+2x^{\frac{1}{2}}+x^{\frac{1}{3}}+(6b-4)x^{-\frac{1}{6}}+(12ab-2a-12b+2)x^{-\frac{1}{3}}.$$
2. For $a>1, b\geq 1$
$$ISI(G,x) = 2a+2b-3+2x^{\frac{1}{2}}+x^{\frac{1}{3}}+(4a+8b-14)x^{-\frac{1}{6}}+(12ab-8a-13b+8)x^{-\frac{1}{3}}.$$

Proof: For given graph, by using edge partition from Table 1,

1. For $a=1, b\geq 1$

$$ISI(G,x) = \sum_{ij\in E(G)} x^{\frac{d_i+d_j}{d_id_j}-1}$$
$$= \sum_{ij\in E_{1,2}} x^{\frac{d_{i}+d\_j}{d_id_j}-1} + \sum_{ij\in E_{1,3}} x^{\frac{d_{i}+d\_j}{d_id_j}-1} + \sum_{ij\in E_{2,2}} x^{\frac{d_{i}+d\_j}{d_id_j}-1} + \sum_{ij\in E_{2,3}} x^{\frac{d_{i}+d\_j}{d_id_j}-1} + \sum_{ij\in E_{3,3}} x^{\frac{d_{i}+d\_j}{d_id_j}-1}$$
$$= (2)x^{\frac{1+2}{1\times 2}-1}+(1)x^{\frac{1+3}{1\times 3}-1}+(3b-1)x^{\frac{2+2}{2\times 2}-1}+(6b-4)x^{\frac{2+3}{2\times 3}-1}+(12ab-2a-12b+2)x^{\frac{3+3}{3\times 3}-1}$$

$= 3b - 1 + 2x^{\frac{1}{2}} + x^{\frac{1}{3}} + (6b-4)x^{-\frac{1}{6}} + (12ab - 2a - 12b + 2)x^{-\frac{1}{3}}.$

2. For $a > 1, b \geq 1$

$ISI(G,x) = \sum_{ij\in E(G)} x^{\frac{d_{i+d\_j}}{d_i d_j}-1}$

$= \sum_{ij\in E_{1,2}} x^{\frac{d_{i+d\_j}}{d_i d_j}-1} + \sum_{ij\in E_{1,3}} x^{\frac{d_{i+d\_j}}{d_i d_j}-1} + \sum_{ij\in E_{2,2}} x^{\frac{d_{i+d\_j}}{d_i d_j}-1} + \sum_{ij\in E_{2,3}} x^{\frac{d_{i+d\_j}}{d_i d_j}-1} + \sum_{ij\in E_{3,3}} x^{\frac{d_{i+d\_j}}{d_i d_j}-1}$

$= (2)x^{\frac{1+2}{1\times 2}-1} + (1)x^{\frac{1+3}{1\times 3}-1} + (2a+2b-3)x^{\frac{2+2}{2\times 2}-1} + (4a+8b-8)x^{\frac{2+3}{2\times 3}-1} + (12ab-8a-13b+8)x^{\frac{3+3}{3\times 3}-1}$

$= 2a + 2b - 3 + 2x^{\frac{1}{2}} + x^{\frac{1}{3}} + (4a+8b-14)x^{-\frac{1}{6}} + (12ab - 8a - 13b + 8)x^{-\frac{1}{3}}.$

As a particular result, we computed ISI index of $SiC_3 - I[a,b]$ in the following corollary.

Corollary: 2.1 ISI index of $G \cong SiC_3 - I[a,b]$ silicon carbide graph for $a, b \geq 1$, is given as:

1. $ISI(G) = 18ab - 3a - \frac{39}{5}b - \frac{43}{60}$ for $a = 1, b \geq 1$
2. $ISI(G) = 18ab - \frac{26}{5}a - \frac{79}{10}b + \frac{89}{60}$ for $a > 1, b \geq 1$

Proof:

1. $ISI(G) = \int_0^1 ISI(G,x)dx = \int_0^1 \left[3b - 1 + 2x^{\frac{1}{2}} + x^{\frac{1}{3}} + (6b-4)x^{-\frac{1}{6}} + (12ab - 2a - 12b + 2)x^{-\frac{1}{3}}\right]dx$

$= \left|(3b-1)x + \frac{4}{3}x^{\frac{3}{2}} + \frac{3}{4}x^{\frac{4}{3}} + \frac{6(6b-4)}{5}x^{\frac{5}{6}} + \frac{3(12ab-2a-12b+2)}{2}x^{\frac{2}{3}}\right|_0^1 = 18ab - 3a - \frac{39}{5}b - \frac{43}{60}$

2. $ISI(G) = \int_0^1 ISI(G,x)dx = \int_0^1 [= 2a + 2b - 3 + 2x^{\frac{1}{2}} + x^{\frac{1}{3}} + (4a+8b-14)x^{-\frac{1}{6}} + (12ab - 8a - 13b + 8)x^{-\frac{1}{3}}]dx$

$= \left|(2a+2b-3)x + \frac{4}{3}x^{\frac{3}{2}} + \frac{3}{4}x^{\frac{4}{3}} + \frac{6(4a+8b-14)}{5}x^{\frac{5}{6}} + 3(12ab - 8a - 13b + 8)x^{\frac{2}{3}}\right|_0^1$

$= 18ab - \frac{26}{5}a - \frac{79}{10}b + \frac{89}{60}$

Next we compute SDD polynomial of silicon carbide graph of $SiC_3 - I[a,b]$ for $a, b \geq 1$.

Theorem:2.2 SDD polynomial of silicon carbide graph $G \cong SiC_3 - I[a,b]$ for $a, b \geq 1$, is given as:

1. For $a = 1, b \geq 1$

$SDD(G,x) = 2x^{-\frac{3}{5}} + x^{-\frac{7}{10}} + (6b-4)x^{-\frac{7}{13}} + (12ab - 2a - 9b + 1)x^{-\frac{1}{2}}.$

2. For $a > 1, b \geq 1$

$SDD(G,x) = 2x^{-\frac{3}{5}} + x^{-\frac{7}{10}} + (4a+8b-8)x^{-\frac{7}{13}} + (12ab - 6a - 11b + 5)x^{-\frac{1}{2}}.$

Proof: For given graph, by using edge partition from Table 1,

1. For $a = 1, b \geq 1$

$SDD(G,x) = \sum_{ij\in E(G)} x^{\frac{d_{id\_j}}{d_i^2+d_j^2}-1} = \sum_{ij\in E_{1,2}} x^{\frac{d_{id\_j}}{d_i^2+d_j^2}-1} + \sum_{ij\in E_{1,3}} x^{\frac{d_{id\_j}}{d_i^2+d_j^2}-1} + \sum_{ij\in E_{2,2}} x^{\frac{d_{id\_j}}{d_i^2+d_j^2}-1} + \sum_{ij\in E_{2,3}} x^{\frac{d_{id\_j}}{d_i^2+d_j^2}-1} + \sum_{ij\in E_{3,3}} x^{\frac{d_{id\_j}}{d_i^2+d_j^2}-1} = (2)x^{\frac{1\times 2}{1^2+2^2}-1} + (1)x^{\frac{1\times 3}{1^2\times 3^2}-1} + (3b-1)x^{\frac{2\times 2}{2^2+2^2}-1} + (6b-4)x^{\frac{2\times 3}{2^2+3^2}-1} + (12ab-2a-12b+2)x^{\frac{3\times 3}{3^2+3^2}-1}$

$= 2x^{-\frac{3}{5}} + x^{-\frac{7}{10}} + (6b-4)x^{-\frac{7}{13}} + (12ab - 2a - 9b + 1)x^{-\frac{1}{2}}$

2. For $a > 1, b \geq 1$

$SDD(G,x) = \sum_{ij\in E(G)} x^{\frac{d_{id\_j}}{d_i^2+d_j^2}-1}$

$= \sum_{ij\in E_{1,2}} x^{\frac{d_{id_j}}{d_i^2+d_j^2}-1} + \sum_{ij\in E_{1,3}} x^{\frac{d_{id_j}}{d_i^2+d_j^2}-1} + \sum_{ij\in E_{2,2}} x^{\frac{d_{id_j}}{d_i^2+d_j^2}-1} + \sum_{ij\in E_{2,3}} x^{\frac{d_{id_j}}{d_i^2+d_j^2}-1} + \sum_{ij\in E_{3,3}} x^{\frac{d_{id_j}}{d_i^2+d_j^2}-1}$

$= (2)x^{\frac{1\times 2}{1^2+2^2}-1} + (1)x^{\frac{1\times 3}{1^2\times 3^2}-1} + (2a+2b-3)x^{\frac{2\times 2}{2^2+2^2}-1} + (4a+8b-8)x^{\frac{2\times 3}{2^2+3^2}-1} + (12ab-8a-13b+7)x^{\frac{3\times 3}{3^2+3^2}-1}$

$= 2x^{-\frac{3}{5}} + x^{-\frac{7}{10}} + (4a+8b-8)x^{-\frac{7}{13}} + (12ab - 6a - 11b + 5)x^{-\frac{1}{2}}$

As a particular result, we computed SDD index of $SiC_3 - I[a,b]$ in the following corollary.

Corollary: 2.2 SDD index of $G \cong SiC_3 - I[a,b]$ silicon carbide graph for $a, b \geq 1$, is given as:

1. $SDD(G) = 24ab - 4a - 5b + \frac{11}{3}$ for $a = 1, b \geq 1$
2. $SDD(G) = 24ab - \frac{10}{3}a - \frac{14}{3}b + 1$ for $a > 1, b \geq 1$

Proof:

1. $SDD(G) = \int_0^1 SDD(G,x)dx = \int_0^1 [2x^{-\frac{3}{5}} + x^{-\frac{7}{10}} + (6b-4)x^{-\frac{7}{13}} + (12ab - 2a - 9b + 1)x^{-\frac{1}{2}}]dx$

$= \left|5x^{\frac{2}{5}} + \frac{10}{3}x^{\frac{3}{10}} + \frac{13(6b-4)}{6}x^{\frac{6}{13}} + 2(12ab - 2a - 9b + 1)\sqrt{x}\right|_0^1 = 24ab - 4a - 5b + \frac{11}{3}$

2. $SDD(G) = \int_0^1 SDD(G,x)dx = \int_0^1 [2x^{-\frac{3}{5}} + x^{-\frac{7}{10}} + (4a + 8b - 8)x^{-\frac{7}{13}} + (12ab - 6a - 11b + 5)x^{-\frac{1}{2}}]dx$

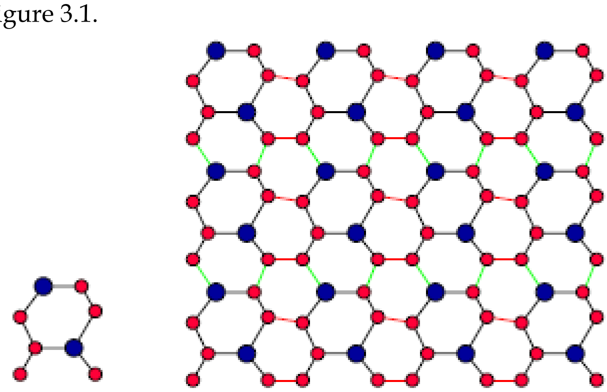
$= \left|5x^{\frac{2}{5}} + \frac{10}{3}x^{\frac{3}{10}} + \frac{13(4a+8b-8)}{6}x^{\frac{6}{13}} + 2(12ab - 6a - 11b + 5)\sqrt{x}\right|_0^1$

$= 24ab - \frac{10}{3}a - \frac{14}{3}b + 1$

3 SILICON CARBIDE $SiC_3 - II[a,b]$ 2D STRUCTURE

In this section ISI index, ISI polynomial, SDD index and SDD polynomials are computed for $SiC_3 - II$.

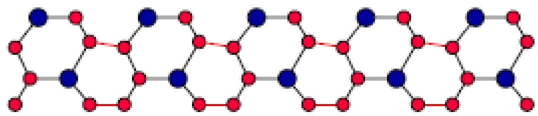
The 2D structure of silicon carbide graph $SiC_3 - II$ is shown in Figure 3.1.



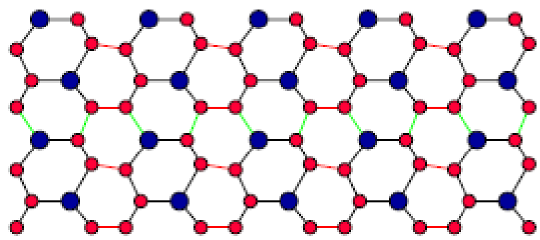
(a) (b)

Figure 3.1: The 2-dimensional structure of $SiC_3 - II[a,b]$, (a) One unit cell of $SiC_3 - II[a,b]$, (b) $SiC_3 - II[4,3]$. Silicon atoms Si are colored blue and carbon atoms C are colored red.

For the description of its chemical graph we have used the setting in this way: we represented a as the number of connected cells in a row (or chain) and by b we defined the number of connected rows each with a number of cells. We denoted this molecular structure by $SiC_3 - II[a, b]$, whre a and b are natural numbers i.e. $a, b \geq 1$. Thus the order of this graph is $8ab$ where its size is $12ab - 2a - 2b$ for $a, b \geq 1$.



(a)



(b)

Figure 3.2: The 2D structure of $SiC_3 - II[a, b]$, (a) $SiC_3 - II[5,1]$, One row with $a = 5$ and $b = 1$, red lines (edges) show how two cells are connected in a row (chain). (b) $SiC_3 - II[5,2]$ i.e. $a = 5$, b=2, two rows are being connected by green lines (edges).

In the graph of silicon carbide $SiC_3 - II[a, b]$ for $a, b \geq 1$, there are three types of vertex sets based on the degree of vertices the vertex sets and their cardinalities are:

$$V_1 = \{i \in V(SiC_3 - II[a, b]) | d_i = 1\}, |V_1| = 2$$
$$V_2 = \{i \in V(SiC_3 - II[a, b]) | d_i = 2\}, |V_2| = 4a + 4b - 4$$
$$V_3 = \{i \in V(SiC_3 - II[a, b]) | d_i = 3\}, |V_3| = 8ab - 4a - 4b + 2$$

Similarly with respect to an edge $e = ij$ of type (d_i, d_j), $E(SiC_3 - II[a, b])$ is partioned into four sets, their set descriptions and cardinalities are given as:

$$E_{1,3} = \{ij \in E(SiC_3 - I[a, b]) | d_i = 1, d_j = 3\}, |E_{1,3}| = 1$$
$$E_{2,2} = \{ij \in E(SiC_3 - I[a, b]) | d_i = 2, d_j = 2\}, \ |E_{2,2}| = 2a + 1$$
$$E_{2,3} = \{ij \in E(SiC_3 - I[a, b]) | d_i = 2, d_j = 3\},$$
$$|E_{2,3}| = 4a + 8b - 10$$
$$E_{3,3} = \{ij \in E(SiC_3 - I[a, b]) | d_i = 3, d_j = 3\},$$
$$|E_{3,3}| = 12ab - 8a - 10b + 7$$

Table 2. Shows this edge partition of $SiC_3 - II[a, b]$ for $a, b \geq 1$.

E_{d_i,d_j}	Frequency
$E_{1,3}$	2
$E_{2,2}$	$2a + 1$
$E_{2,3}$	$4a + 8b - 10$
$E_{3,3}$	$12ab - 8a - 10b + 7$

In the following theorem we calculate ISI polynomial of silicon carbide graph $SiC_3 - II[a, b]$ for $a, b \geq 1$.

Theorem 3.1: ISI polynomial of the silicon carbide graph $G \cong SiC_3 - II[a, b]$ for $a, b \geq 1$, is given as:

$$ISI(G, x) = 3a + 1 + 2x^{\frac{1}{3}} + (4a + 8b - 10)x^{-\frac{1}{6}} + (12ab - 8a - 10b + 7)x^{-\frac{1}{3}}.$$

Proof: For given graph, by using edge partition from Table 2,

$$ISI(G, x) = \sum_{ij \in E(G)} x^{\frac{d_{i+}d\_j}{d_i d_j} - 1} = \sum_{ij \in E_{1,3}} x^{\frac{d_{i+}d\_j}{d_i d_j} - 1} + \sum_{ij \in E_{2,2}} x^{\frac{d_{i+}d\_j}{d_i d_j} - 1} + \sum_{ij \in E_{2,3}} x^{\frac{d_{i+}d\_j}{d_i d_j} - 1} + \sum_{ij \in E_{3,3}} x^{\frac{d_{i+}d\_j}{d_i d_j} - 1}$$
$$= (2)x^{\frac{1+3}{1\times 3} - 1} + (2a + 1)x^{\frac{2+2}{2\times 2} - 1} + (4a + 8b - 10)x^{\frac{2+3}{2\times 3} - 1} + (12ab - 8a - 10b + 7)x^{\frac{3+3}{3\times 3} - 1} = 3a + 1 + 2x^{\frac{1}{3}} + (4a + 8b - 10)x^{-\frac{1}{6}} + (12ab - 8a - 10b + 7)x^{-\frac{1}{3}}.$$

As a particular result, we computed ISI index of $SiC_3 - II[a, b]$ in the following corollary.

Corollary: 3.1 ISI index of $G \cong SiC_3 - II[a, b]$ silicon carbide graph for $a, b \geq 1$, is given as:

$$ISI(G) = 18ab - \frac{26}{5}a - \frac{27}{5}b + 1$$

Proof:

$$ISI(G) = \int_0^1 ISI(G, x)dx = \int_0^1 \left[3b - 1 + 2x^{\frac{1}{2}} + x^{\frac{1}{3}} + (6b - 4)x^{-\frac{1}{6}} + (12ab - 2a - 12b + 2)x^{-\frac{1}{3}}\right] dx$$
$$= \left|(2a + b)x + \frac{3}{2}x^{\frac{4}{3}} + \frac{6(4a+8b-10)}{5}x^{\frac{5}{6}} + \frac{3(12ab-8a-10b+7)}{2}x^{\frac{2}{3}}\right|_0^1$$
$$= 18ab - \frac{26}{5}a - \frac{27}{5}b + 1$$

Next theorem is about computation of SDD polynomial for the silicon carbide graph $SiC_3 - II[a, b]$, $a, b \geq 1$.

Theorem:3.2 SDD polynomial of the silicon carbide graph $G \cong SiC_3 - II[a, b]$ for $a, b \geq 1$, is given as:

$$SDD(G, x) = 2x^{-\frac{7}{10}} + (4a + 8b - 10)x^{-\frac{7}{13}} + (12ab - 6a - 10b + 8)x^{-\frac{1}{2}}.$$

Proof: For given graph, by using edge partition from Table 2,

$$SDD(G, x) = \sum_{ij \in E(G)} x^{\frac{d_i d\_j}{d_i^2 + d_j^2} - 1} = \sum_{ij \in E_{1,3}} x^{\frac{d_i d\_j}{d_i^2 + d_j^2} - 1} + \sum_{ij \in E_{2,2}} x^{\frac{d_i d\_j}{d_i^2 + d_j^2} - 1} + \sum_{ij \in E_{2,3}} x^{\frac{d_i d\_j}{d_i^2 + d_j^2} - 1} + \sum_{ij \in E_{3,3}} x^{\frac{d_i d\_j}{d_i^2 + d_j^2} - 1}$$
$$= (2)x^{\frac{1\times 3}{1^2\times 3^2} - 1} + (2a + 1)x^{\frac{2\times 2}{2^2+2^2} - 1} + (4a + 8m - 10)x^{\frac{2\times 3}{2^2+3^2} - 1} + (12ab - 8a - 10b + 7)x^{\frac{3\times 3}{3^2+3^2} - 1}$$
$$= 2x^{-\frac{7}{10}} + (4a + 8b - 10)x^{-\frac{7}{13}} + (12ab - 6a - 10b + 8)x^{-\frac{1}{2}}$$

As a particular result, we computed SDD index of $SiC_3 - II[a, b]$ in the following corollary.

Corollary: 3.2 SDD index of $G \cong SiC_3 - II[a, b]$ silicon carbide graph for $a, b \geq 1$, is given as:

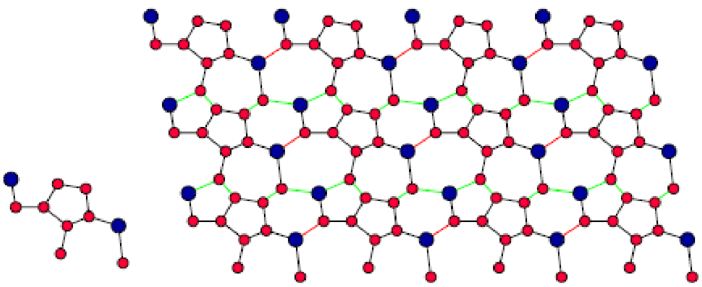
$$SDD(G) = 24ab - \frac{10}{3}a - \frac{8}{3}b + 1$$

Proof:

$$SDD(G) = \int_0^1 SDD(G, x)dx = \int_0^1 [2x^{-\frac{7}{10}} + (4a + 8b - 10)x^{-\frac{7}{13}} + (12ab - 6a - 10b + 8)x^{-\frac{1}{2}}]dx$$
$$= \left|\frac{20}{3}x^{\frac{3}{10}} + \frac{13(4a+8b-10)}{6}x^{\frac{6}{13}} + 2(12ab - 6a - 10b + 8)\sqrt{x}\right|_0^1 = 24ab - \frac{10}{3}a - \frac{8}{3}b + 1$$

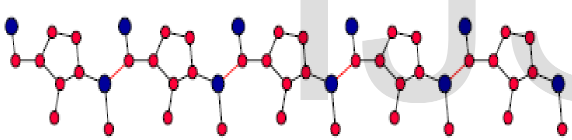
4 Silicon Carbide $SiC_4 - I[a, b]$ 2D Structure

In this section ISI index, ISI polynomial, SDD index and SDD polynomials are computed for $SiC_4 - I$.
The 2D structure of silicon carbide graph $SiC_4 - I$is shown in Figure 4.1, To describe its chemical graph we have used the setting in this way: we represented a as the number of connected cells in a row (or chain) and by b we defined the number of connected rows each with a number of cells. We denoted this molecular structure by $SiC_4 - I[a, b]$, whre a and b are natural numbers i.e. $a, b \geq 1$. Thus the order of this graph is $10ab$ where its size is $15ab - 4a - 2b + 1$ for $a, b \geq 1$.

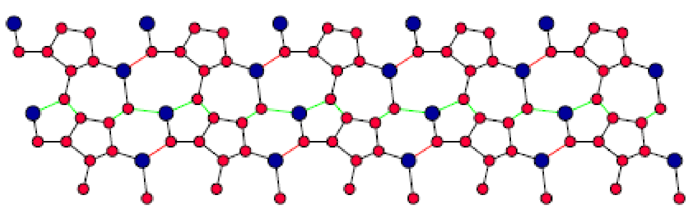


(a) (b)

Figure 4.1: The 2-dimensional structure of $SiC_4 - I[a, b]$,
(a) One unit cell of $SiC_4 - I[a, b]$, (b) $SiC_4 - I[4,3]$. Silicon atoms Si are colored blue and carbon atoms C are colored red.



(a)



(b)

Figure 4.2: The 2D structure of $SiC_4 - I[a, b]$, (a) $SiC_4 - I[5,1]$, One row with $a = 5$ and $b = 1$, red lines (edges) show how two cells are connected in a row (chain). (b) $SiC_4 - I[5,2]$ i.e. $a = 5$, b=2, two rows are being connected by green lines (edges).

In graph of silicon carbide $SiC_4 - I[a, b]$ for $a, b \geq 1$, there are three types of vertex sets based on the degree of vertices (or atoms) the vertex sets and their cardinalities are:

$$V_1 = \{i \in V(SiC_4 - I[a, b]) | d_i = 1\}, |V_1| = 3a$$
$$V_2 = \{i \in V(SiC_4 - I[a, b]) | d_i = 2\}, |V_2| = 2a + 4b - 2$$
$$V_3 = \{i \in V(SiC_4 - I[a, b]) | d_i = 3\}, |V_3| = 10ab - 5a - 4b + 2$$

Similarly with respect to an edge $e = ij$ of type (d_i, d_j), $E(SiC_4 - I[a, b])$ is partioned into five sets, their set descriptions and cardinalities are given as:

$$E_{1,2} = \{ij \in E(SiC_4 - I[a, b]) | d_i = 1, d_j = 2\}, |E_{1,2}| = 2$$
$$E_{1,3} = \{ij \in E(SiC_4 - I[a, b]) | d_i = 1, d_j = 3\}, |E_{1,3}| = 3a - 2$$
$$E_{2,2} = \{ij \in E(SiC_4 - I[a, b]) | d_i = 2, d_j = 2\},$$
$$|E_{2,2}| = a + 2b - 2$$
$$E_{2,3} = \{ij \in E(SiC_4 - I[a, b]) | d_i = 2, d_j = 3\},$$
$$|E_{2,3}| = 2a + 4b - 2$$
$$E_{3,3} = \{ij \in E(SiC_4 - I[a, b]) | d_i = 3, d_j = 3\},$$
$$|E_{3,3}| = 15ab - 10a - 8b + 5$$

Table 3. Shows this edge partition of $SiC_4 - I[a, b]$ for $a, b \geq 1$.

E_{d_i,d_j}	Frequency
$E_{1,2}$	2
$E_{1,3}$	$3a - 2$
$E_{2,2}$	$a + 2b - 2$
$E_{2,3}$	$2a + 4b - 2$
$E_{3,3}$	$15ab - 10a - 8b + 5$

Next we compute exact formula of ISI polynomial for the silicon carbide graph $SiC_4 - I[a, b], a, b \geq 1$.

Theorem 4.1: ISI polynomial of the silicon carbide graph $G \cong SiC_4 - I[a, b]$ for $a, b \geq 1$, is given as:

$$ISI(G, x) = a + 2b - 2 + 2x^{\frac{1}{2}} + (3a - 2)x^{\frac{1}{3}} + (2a + 4b - 2)x^{-\frac{1}{6}} + (15ab - 10a - 8b + 5)x^{-\frac{1}{3}}.$$

Proof: For given graph, by using edge partition from Table 3,

$$ISI(G, x) = \sum_{ij \in E(G)} x^{\frac{d_i + d_j}{d_i d_j} - 1}$$
$$= \sum_{ij \in E_{1,2}} x^{\frac{d_i + d\_j}{d_i d_j} - 1} + \sum_{ij \in E_{1,3}} x^{\frac{d_i + d\_j}{d_i d_j} - 1} + \sum_{ij \in E_{2,2}} x^{\frac{d_i + d\_j}{d_i d_j} - 1} + \sum_{ij \in E_{2,3}} x^{\frac{d_i + d\_j}{d_i d_j} - 1} + \sum_{ij \in E_{3,3}} x^{\frac{d_i + d\_j}{d_i d_j} - 1}$$
$$= (2)x^{\frac{1+2}{1\times2} - 1} + (3a - 2)x^{\frac{1+3}{1\times3} - 1} + (a + 2b - 2)x^{\frac{2+2}{2\times2} - 1} + (2a + 4b - 2)x^{\frac{2+3}{2\times3} - 1} + (15ab - 10a - 8b + 5)x^{\frac{3+3}{3\times3} - 1}$$
$$= a + 2b - 2 + 2x^{\frac{1}{2}} + (3a - 2)x^{\frac{1}{3}} + (2a + 4b - 2)x^{-\frac{1}{6}} + (15ab - 10a - 8b + 5)x^{-\frac{1}{3}}.$$

As a particular result, we computed ISI index of $SiC_4 - I[a, b]$ in the following corollary.

Corollary: 4.1 ISI index of $G \cong SiC_4 - I[a, b]$ silicon carbide graph for $a, b \geq 1$, is given as:

$$ISI(G) = \frac{45}{2}ab - \frac{187}{20}a - \frac{26}{5}b + \frac{44}{15}$$

Proof:

$$ISI(G) = \int_0^1 ISI(G, x)dx = \int_0^1 \Big[a + 2b - 2 + 2x^{\frac{1}{2}} + (3a - 2)x^{\frac{1}{3}} + (2a + 4b - 2)x^{-\frac{1}{6}} + (15ab - 10a - 8b + 5)x^{-\frac{1}{3}}\Big] dx$$
$$= \Big|(a + 2b - 2)x + \frac{4}{3}x^{\frac{3}{2}} + \frac{3(3a-2)}{4}x^{\frac{4}{3}} + \frac{6(2a+4b-2)}{5}x^{\frac{5}{6}} + \frac{3(15ab-10a-8b+5)}{2}x^{\frac{2}{3}}\Big|_0^1 = \frac{45}{2}ab - \frac{187}{20}a - \frac{26}{5}b + \frac{44}{15}.$$

In next theorem, we compute SDD polynomial of silicon carbide graph $SiC_4 - I[a,b]$ for $a, b \geq 1$.

Theorem:4.2 SDD polynomial of the silicon carbide graph $G \cong SiC_4 - I[a,b]$ for $a, b \geq 1$, is given as:

$$SDD(G,x) = 2x^{-\frac{3}{5}} + (3a-2)x^{-\frac{7}{10}} + (2a+4b-2)x^{-\frac{7}{13}} + (15ab - 9a - 6b + 3)x^{-\frac{1}{2}}.$$

Proof: For given graph, by using edge partition from Table 3,

$$SDD(G,x) = \sum_{ij \in E(G)} x^{\frac{d_i d_j}{d_i^2 + d_j^2} - 1} = \sum_{ij \in E_{1,2}} x^{\frac{d_i d_j}{d_i^2 + d_j^2} - 1} + \sum_{ij \in E_{1,3}} x^{\frac{d_i d_j}{d_i^2 + d_j^2} - 1} + \sum_{ij \in E_{2,2}} x^{\frac{d_i d_j}{d_i^2 + d_j^2} - 1} + \sum_{ij \in E_{2,3}} x^{\frac{d_i d_j}{d_i^2 + d_j^2} - 1} + \sum_{ij \in E_{3,3}} x^{\frac{d_i d_j}{d_i^2 + d_j^2} - 1}$$

$$= (2)x^{\frac{1\times2}{1^2\times2^2} - 1} + (3a-2)x^{\frac{1\times3}{1^2\times3^2} - 1} + (a + 2b - 2)x^{\frac{2\times2}{2^2+2^2} - 1} + (2a + 4b - 2)x^{\frac{2\times3}{2^2+3^2} - 1} + (15ab - 10a - 8b + 5)x^{\frac{3\times3}{3^2+3^2} - 1}$$

$$= 2x^{-\frac{3}{5}} + (3a-2)x^{-\frac{7}{10}} + (2a+4b-2)x^{-\frac{7}{13}} + (15ab - 9a - 6b + 3)x^{-\frac{1}{2}}$$

As a particular result, we computed SDD index of $SiC_4 - I[a,b]$ in the following corollary.

Corollary: 4.2 SDD index of $G \cong SiC_4 - I[a,b]$ silicon carbide graph for $a, b \geq 1$, is given as:

$$SDD(G) = 30ab - \frac{11}{3}a - \frac{10}{3}b$$

Proof:

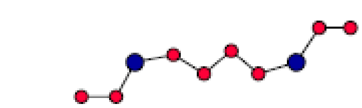
$$SDD(G) = \int_0^1 SDD(G,x)dx = \int_0^1 [2x^{-\frac{3}{5}} + (3a-2)x^{-\frac{7}{10}} + (2a+4b-2)x^{-\frac{7}{13}} + (15ab - 9a - 6b + 3)x^{-\frac{1}{2}}]dx$$

$$= \left| 5x^{\frac{2}{5}} + \frac{10(3a-2)}{3}x^{\frac{3}{10}} + \frac{13(2a+4b-2)}{6}x^{\frac{6}{13}} + 2(15ab - 9a - 6b + 3)\sqrt{x} \right|_0^1 = 30ab - \frac{11}{3}a - \frac{10}{3}b$$

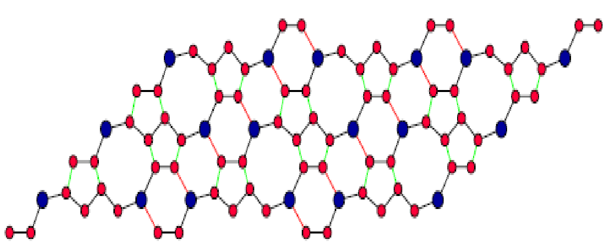
5 Silicon Carbide $SiC_4 - II[a,b]$ 2D Structure

In this section ISI index, ISI polynomial, SDD index and SDD polynomials are computed for $SiC_4 - II$.

The 2D structure of silicon carbide graph $SiC_4 - II$is shown in Figure 5.1. To describe its chemical graph we have used the setting in this way: we represented a as the number of connected cells in a row (or chain) and by b we defined the number of connected rows each with a number of cells. We denoted this molecular structure by $SiC_4 - II[a,b]$, whre a and b are natural numbers i.e. $a, b \geq 1$. Thus the order of this graph is $10ab$ where its size is $15ab - 4a - 2b$ for $a, b \geq 1$.

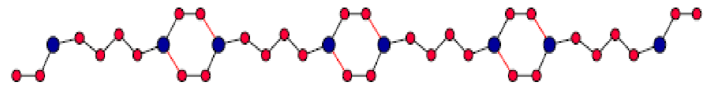


(a)

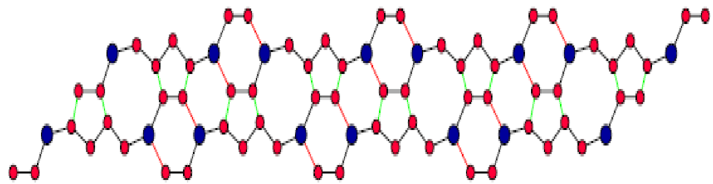


(b)

Figure 4.1: The 2-dimensional structure of $SiC_4 - II[a,b]$, (a) One unit cell of $SiC_4 - II[a,b]$, (b) $SiC_4 - II[3,3]$. Silicon atoms Si are colored blue and carbon atoms C are colored red.



(a)



(b)

Figure 4.2: The 2D structure of $SiC_4 - II[a,b]$, (a) $SiC_4 - II[4,1]$, One row with $a = 4$ and $b = 1$, red lines (edges) show how two cells are connected in a row (chain). (b) $SiC_4 - II[4,2]$ i.e. $a = 3$, b=2, two rows are being connected by green lines (edges).

In graph of silicon carbide $SiC_4 - II[a,b]$ for $a, b \geq 1$, there are three types of vertex sets based on the degree of vertices the vertex sets and their cardinalities are:

$$V_1 = \{i \in V(SiC_4 - II[a,b]) | d_i = 1\}, |V_1| = 2$$

$$V_2 = \{i \in V(SiC_4 - II[a,b]) | d_i = 2\}, |V_2| = 8a + 4b - 4$$

$$V_3 = \{i \in V(SiC_4 - II[a,b]) | d_i = 3\}, |V_3| = 10ab - 8a - 4b + 2$$

Similarly with respect to an edge $e = ij$ of type (d_i, d_j), $E(SiC_4 - I[a,b])$ is partioned into four sets, their set descriptions and cardinalities are given as:

$$E_{1,2} = \{ij \in E(SiC_4 - II[a,b]) | d_i = 1, d_j = 2\}, |E_{1,2}| = 2$$

$$E_{2,2} = \{ij \in E(SiC_4 - II[a,b]) | d_i = 2, d_j = 2\},$$

$$|E_{2,2}| = \begin{cases} 5a + 2 & \text{for } b = 1, a \geq 1 \\ 2a + 2 & \text{for } b > 1, a \geq 1 \end{cases}$$

$$E_{2,3} = \{ij \in E(SiC_4 - II[a,b]) | d_i = 2, d_j = 3\},$$

$$|E_{2,3}| = \begin{cases} 6a - 6 & \text{for } b = 1, a \geq 1 \\ 12a + 8b - 14 & \text{for } b > 1, a \geq 1 \end{cases}$$

$$E_{3,3} = \{ij \in E(SiC_4 - II[a,b]) | d_i = 3, d_j = 3\},$$

$$|E_{3,3}| = \begin{cases} 15ab - 15a - 2b + 2 & \text{for } b = 1, a \geq 1 \\ 15ab - 18a - 10b + 10 & \text{for } b > 1, a \geq 1 \end{cases}$$

Table 5. Shows this edge partition of $SiC_4 - II[a,b]$ for $a, b \geq 1$.

E_{d_i,d_j}	Frequency
$E_{1,2}$	2
$E_{2,2}$	$\begin{cases} 5a + 2 & \text{for } b = 1, a \geq 1 \\ 2a + 2 & \text{for } b > 1, a \geq 1 \end{cases}$
$E_{2,3}$	$\begin{cases} 6a - 6 & \text{for } b = 1, a \geq 1 \\ 12a + 8b - 14 & \text{for } b > 1, a \geq 1 \end{cases}$
$E_{3,3}$	$\begin{cases} 15ab - 15a - 2b + 2 & \text{for } b = 1, a \geq 1 \\ 15ab - 18a - 10b + 10 & \text{for } b > 1, a \geq 1 \end{cases}$

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Next we compute ISI polynomial for the silicon carbide graph $SiC_4-II[a,b]$ for $a,b\ge 1$.

Theorem 5.1: ISI polynomial of the silicon carbide graph $G\cong SiC_4-II[a,b]$ for $a,b\ge 1$, is given as:

1. For $b=1, a\ge 1$
$$ISI(G,x)=5a+2+2x^{\frac{1}{2}}+(6a-6)x^{-\frac{1}{6}}+(15ab-15a-2b+2)x^{-\frac{1}{3}}.$$
2. For $b>1, a\ge 1$
$$ISI(G,x)=2a+2+2x^{\frac{1}{2}}+(12a+8b-14)x^{-\frac{1}{6}}+(15ab-18a-10b+10)x^{-\frac{1}{3}}.$$

Proof: For given graph, by using edge partition from Table 4,

1. For $b=1, a\ge 1$
$$ISI(G,x)=\sum_{ij\in E(G)}x^{\frac{d_i+d_j}{d_id_j}-1}=\sum_{ij\in E_{1,2}}x^{\frac{d_i+d_j}{d_id_j}-1}+ +\sum_{ij\in E_{2,2}}x^{\frac{d_i+d_j}{d_id_j}-1}+\sum_{ij\in E_{2,3}}x^{\frac{d_i+d_j}{d_id_j}-1}+\sum_{ij\in E_{3,3}}x^{\frac{d_i+d_j}{d_id_j}-1}$$
$$=(2)x^{\frac{1+2}{1\times2}-1}+(5a+2)x^{\frac{2+2}{2\times2}-1}+(6a-6)x^{\frac{2+3}{2\times3}-1}+(15ab-15a-2b+2)x^{\frac{3+3}{3\times3}-1}$$
$$=5a+2+2x^{\frac{1}{2}}+(6a-6)x^{-\frac{1}{6}}+(15ab-15a-2b+2)x^{-\frac{1}{3}}$$
2. For $b>1, a\ge 1$
$$ISI(G,x)=\sum_{ij\in E(G)}x^{\frac{d_i+d_j}{d_id_j}-1}=\sum_{ij\in E_{1,2}}x^{\frac{d_i+d_j}{d_id_j}-1}+ +\sum_{ij\in E_{2,2}}x^{\frac{d_i+d_j}{d_id_j}-1}+\sum_{ij\in E_{2,3}}x^{\frac{d_i+d_j}{d_id_j}-1}+\sum_{ij\in E_{3,3}}x^{\frac{d_i+d_j}{d_id_j}-1}$$
$$=(2)x^{\frac{1+2}{1\times2}-1}+(2a+2)x^{\frac{2+2}{2\times2}-1}+(12a+8b-14)x^{\frac{2+3}{2\times3}-1}+(15ab-18a-10b+10)x^{\frac{3+3}{3\times3}-1}=2a+2+2x^{\frac{1}{2}}+(12a+8b-14)x^{-\frac{1}{6}}+(15ab-18a-10b+10)x^{-\frac{1}{3}}$$

As a particular result, we computed ISI index of $SiC_4-II[a,b]$ in the following corollary.

Corollary: 5.1 ISI index of $G\cong SiC_4-II[a,b]$ silicon carbide graph for $a,b\ge 1$, is given as:

1. $ISI(G)=\frac{45}{2}ab-\frac{103}{10}a-3b-\frac{13}{15}$ for $b=1, b\ge 1$
2. $ISI(G)=\frac{45}{2}ab-\frac{53}{5}a-\frac{27}{5}b+\frac{23}{15}$ for $b>1, b\ge 1$

Proof:

1. $$ISI(G)=\int_0^1 ISI(G,x)dx=\int_0^1\left[5a+2+2x^{\frac{1}{2}}+(6a-6)x^{-\frac{1}{6}}+(15ab-15a-2b+2)x^{-\frac{1}{3}}\right]dx$$
$$=\left|(5a+2)x+\frac{4}{3}x^{\frac{3}{2}}+\frac{6(6a-6)}{5}x^{\frac{5}{6}}+\frac{3(15ab-15a-2b+2)}{2}x^{\frac{2}{3}}\right|_0^1$$
$$=\frac{45}{2}ab-\frac{103}{10}a-3b-\frac{13}{15}$$
2. $$ISI(G)=\int_0^1 ISI(G,x)dx=\int_0^1[2a+2+2x^{\frac{1}{2}}+(12a+8b-14)x^{-\frac{1}{6}}+(15ab-18a-10b+10)x^{-\frac{1}{3}}]dx$$
$$=\left|(2a+2)x+\frac{4}{3}x^{\frac{3}{2}}+\frac{6(12a+8b-14)}{5}x^{\frac{5}{6}}+\frac{3(15ab-18a-10b+2)}{2}x^{\frac{2}{3}}\right|_0^1=\frac{45}{2}ab-\frac{53}{5}a-\frac{27}{5}b+\frac{23}{15}$$

In the last theorem of this section we compute SDD polynomial of the silicon carbide graph $SiC_4-II[a,b]$ for $a,b\ge 1$.

Theorem:5.2 SDD polynomial of the silicon carbide graph $G\cong SiC_4-II[a,b]$ for $a,b\ge 1$, is given as:

1. For $b=1, a\ge 1$
$$SDD(G,x)=2x^{-\frac{3}{5}}+(6b-6)x^{-\frac{7}{13}}+(15ab-10a-2b+4)x^{-\frac{1}{2}}.$$
2. For $b>1, a\ge 1$
$$SDD(G,x)=2x^{-\frac{3}{5}}+(12a+8b-14)x^{-\frac{7}{13}}+(15ab-16a-10b+12)x^{-\frac{1}{2}}.$$

Proof: For given graph, by using edge partition from Table 4,

1. For $b=1, a\ge 1$
$$SDD(G,x)=\sum_{ij\in E(G)}x^{\frac{d_id_j}{d_i^2+d_j^2}-1}$$
$$=\sum_{ij\in E_{1,2}}x^{\frac{d_id_j}{d_i^2+d_j^2}-1}+\sum_{ij\in E_{2,2}}x^{\frac{d_id_j}{d_i^2+d_j^2}-1}+\sum_{ij\in E_{2,3}}x^{\frac{d_id_j}{d_i^2+d_j^2}-1}+\sum_{ij\in E_{3,3}}x^{\frac{d_id_j}{d_i^2+d_j^2}-1}=(2)x^{\frac{1\times2}{1^2+2^2}-1}+(5a+2)x^{\frac{2\times2}{2^2+2^2}-1}+(6b-6)x^{\frac{2\times3}{2^2+3^2}-1}+(15ab-15a-2b+2)x^{\frac{3\times3}{3^2+3^2}-1}$$
$$=2x^{-\frac{3}{5}}+(6b-6)x^{-\frac{7}{13}}+(15ab-10a-2b+4)x^{-\frac{1}{2}}$$
2. For $b>1, a\ge 1$
$$SDD(G,x)=\sum_{ij\in E(G)}x^{\frac{d_id_j}{d_i^2+d_j^2}-1}$$
$$=\sum_{ij\in E_{1,2}}x^{\frac{d_id_j}{d_i^2+d_j^2}-1}+\sum_{ij\in E_{2,2}}x^{\frac{d_id_j}{d_i^2+d_j^2}-1}+\sum_{ij\in E_{2,3}}x^{\frac{d_id_j}{d_i^2+d_j^2}-1}+\sum_{ij\in E_{3,3}}x^{\frac{d_id_j}{d_i^2+d_j^2}-1}=(2)x^{\frac{1\times2}{1^2+2^2}-1}+(2a+2)x^{\frac{2\times2}{2^2+2^2}-1}+(12a+8b-14)x^{\frac{2\times3}{2^2+3^2}-1}+(15ab-18a-10b+10)x^{\frac{3\times3}{3^2+3^2}-1}$$
$$=2x^{-\frac{3}{5}}+(12a+8b-14)x^{-\frac{7}{13}}+(15ab-16a-10b+12)x^{-\frac{1}{2}}$$

As a particular result, we computed SDD index of $SiC_4-II[a,b]$ in the following corollary.

Corollary: 5.2 SDD index of $G\cong SiC_4-II[a,b]$ silicon carbide graph for $a,b\ge 1$, is given as:

1. $SDD(G)=30ab-7a-4b$ for $b=1, a\ge 1$
2. $SDD(G)=30ab-6a-\frac{8}{3}b-\frac{4}{3}$ for $b>1, a\ge 1$

Proof:

1. $$SDD(G)=\int_0^1 SDD(G,x)dx=\int_0^1[2x^{-\frac{3}{5}}+(6b-6)x^{-\frac{7}{13}}+(15ab-10a-2b+4)x^{-\frac{1}{2}}]dx$$
$$=\left|5x^{\frac{2}{5}}+\frac{13(6a-6)}{6}x^{\frac{6}{13}}+2(15ab-10a-2b+4)\sqrt{x}\right|_0^1=30ab-7a-4b$$
2. $$SDD(G)=\int_0^1 SDD(G,x)dx=\int_0^1[2x^{-\frac{3}{5}}+(12a+8b-14)x^{-\frac{7}{13}}+(15ab-16a-10b+12)x^{-\frac{1}{2}}]dx$$
$$=\left|5x^{\frac{2}{5}}+\frac{13(12a+8b-14)}{6}x^{\frac{6}{13}}+2(15ab-16a-10b+12)\sqrt{x}\right|_0^1=30ab-6a-\frac{8}{3}b-\frac{4}{3}$$

6 Analysis

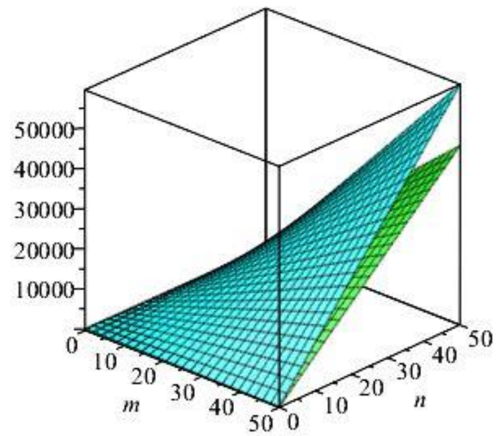
In this section we draw surface of topological indices computed in Scetion 2, Section 3, Section 4 and Section 5, and give comparision of these indices.

1. Using Corollary 2.1 and Corollary 2.2, we have the following details:

- ISI index of silicon carbide graph $SiC_3-I[a,b], a,b\ge 1$ is
  $ISI(G)=18ab-3a-\frac{39}{5}b-\frac{43}{60}$ for $a=1, b\ge 1$
  $ISI(G)=18ab-\frac{26}{5}a-\frac{79}{10}b+\frac{89}{60}$ for $a>1, b\ge 1$

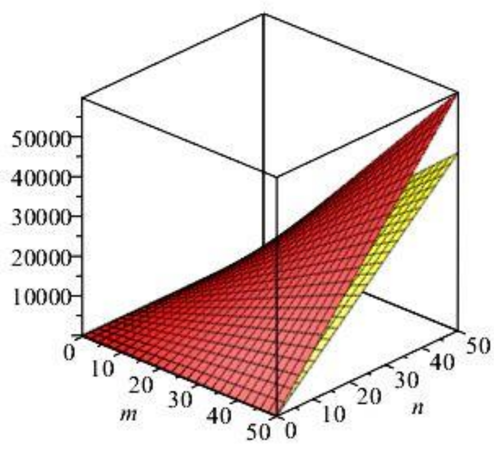
Its value at $a = b = 50$ is $2660789/60$ and green color sheet represents ISI index.

- SDD index of silicon carbide graph $SiC_3 - I[a,b], a,b \geq 1$ is
$SDD(G) = 24ab - 4a - 5b + \frac{11}{3}$ for $a = 1, b \geq 1$
$SDD(G) = 24ab - \frac{10}{3}a - \frac{14}{3}b + 1$ for $a > 1, b \geq 1$
Its value at $a = b = 50$ is 59601 and cyan color sheet represents SDD index.



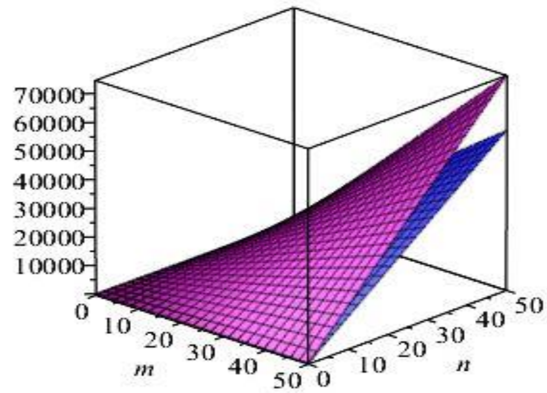
2. Using Corollary 3.1 and Corollary 3.2, we have the following details:

- ISI index of silicon carbide graph $SiC_3 - II[a,b], a,b \geq 1$ is
$$ISI(G) = 18ab - \frac{26}{5}a - \frac{27}{5}b + 1$$
Its value at $a = b = 50$ is 44471 and yellow color sheet represents ISI index.
- SDD index of silicon carbide graph $SiC_3 - II[a,b], a,b \geq 1$ is
$$SDD(G) = 24ab - \frac{10}{3}a - \frac{8}{3}b + 1$$
Its value at $a = b = 50$ is 59701 and red color sheet represents SDD index.



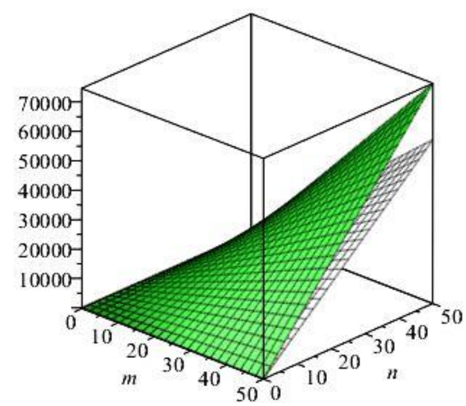
3. Using Corollary 4.1 and Corollary 4.2, we have the following details:

- ISI index of silicon carbide graph $SiC_4 - I[a,b], a,b \geq 1$ is
$ISI(G) = \frac{45}{2}ab - \frac{187}{20}a - \frac{26}{5}b + \frac{44}{15}$
Its value at $a = b = 50$ is $149872/15$ and blue color sheet represents ISI index.
- SDD index of silicon carbide graph $SiC_4 - I[a,b], a,b \geq 1$ is
$$SDD(G) = 30ab - \frac{11}{3}a - \frac{10}{3}b$$
Its value at $a = b = 50$ is 74650 and purple color sheet represents SDD index.



4. Using Corollary 5.1 and Corollary 5.2, we have the following details:

- ISI index of silicon carbide graph $SiC_4 - II[a,b], a,b \geq 1$ is
$ISI(G) = \frac{45}{2}ab - \frac{103}{10}a - 3b - \frac{13}{15}$ for $b = 1, a \geq 1$
. $ISI(G) = \frac{45}{2}ab - \frac{53}{5}a - \frac{27}{5}b + \frac{23}{15}$ for $b > 1, a \geq 1$
Its value at $a = b = 50$ is $831773/15$ and white color sheet represents ISI index.
- SDD index of silicon carbide graph $SiC_4 - II[a,b], a,b \geq 1$ is
$SDD(G) = 30ab - 7a - 4b$ for $b = 1, a \geq 1$
$SDD(G) = 30ab - 6a - \frac{8}{3}b - \frac{4}{3}$ for $b > 1, a \geq 1$
Its value at $a = b = 50$ is $223696/3$ and green color sheet represents SDD index.



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