

## **Computation of Several Banhatti and Reven Invariants of Silicon Carbides**

Abid Mahboob<sup>1\*</sup> 🔎 🛇, Muhammad Waheed Rasheed<sup>1</sup> 🔍 🖉, Jalal Hatem Hussein Bayati<sup>2</sup>

and Iqra Hanif<sup>1</sup>

<sup>1</sup>Department of Mathematics, Division of Science and Technology, University of Education Lahore, Pakistan <sup>2</sup>Department of Mathematics, College, and Science for Women, University of Baghdad, Baghdad, Iraq \*Corresponding Author.

Received 11/12/2022, Revised 03/02/2023, Accepted 05/02/2023, Published 20/06/2023

This work is licensed under a Creative Commons Attribution 4.0 International License.

#### Abstract

Expressions for the molecular topological features of silicon carbide compounds are essential for quantitative structure-property and structure-activity interactions. Chemical Graph Theory is a subfield of computational chemistry that investigates topological indices of molecular networks that correlate well with the chemical characteristics of chemical compounds. In the modern age, topological indices are extremely important in the study of graph theory. Topological indices are critical tools for understanding the core topology of chemical structures while examining chemical substances. In this article, compute the first and second k-Banhatti index, modified first and second k-Banhatti index, first and second hyper Revan indices, first Revan vertex index, and third Revan index for Silicon Carbide SiC4-II [p, q] for all values of p and q.

**Keywords:** Banhatti Indices, Hyper Banhatti Indices, Hyper Revan indices, Silicon carbide SiC<sub>4</sub>-II [p, q], Topological Indices.

#### Introduction

Mathematical chemistry is a field of theoretical chemistry that uses mathematical approaches to discuss molecule structure without necessarily using quantum mechanics. Graph theory can be used to represent a chemical structure, with vertices representing atoms and edges representing chemical bonds. Chemical graph theory is a field of mathematical chemistry that bridges the gap between mathematics, chemistry, and graph theory to solve chemical issues mathematically. If there is a connection between any two vertices in a network, it is said to be connected <sup>1</sup>.

A molecular descriptor, also known as a topological graph index, is a mathematical formula that may be applied to any graph that describes a molecule structure. The topological index is used extensively in this field of research to investigate the topological features of various chemical structures.

The topological index is a numerical parameter associated with a chemical compound's molecular network. Topological indices are numerical values that describe the entire structure of a graph <sup>2</sup>. The topological indices are effective in predicting the physicochemical characteristics and bioactivity of the chemical compound. In mathematical chemistry, molecular descriptors serve an important role, particularly in the quantitative structure-property relationship (QSPR) and quantitative structure-activity relationship (QSAR) studies <sup>3-6</sup>.

Silicon Carbide (SiC) was the first substance to exhibit covalent bonds between C and Si atoms, which were commonly found in diatomic layers. These layers combine to produce tetrahedral orientated C and Si atom molecules with a short bound length and high binding strength. Silicon carbide is the most extensively applicable material in

structural ceramics. Numerous applications have been facilitated by properties such as resistance to abrasion, Low density, low thermal expansion, high modulus, high thermal elastic conductivity. hardness, and corrosion, and most significantly, the maintenance of elastic resistance at temperatures up to 1650° C<sup>7</sup>. SiC finds numerous applications in a variety of industries due to its special properties, including abrasive and cutting tools, structural materials, automobile parts, foundry crucibles, electric systems, electronic circuit elements, power electronic devices, LEDs, astronomy, heating elements, nuclear fuel particles, jewelry, steel production, and quantum physics <sup>8</sup>. This is the backbone of the superior mechanical and chemical stability of SiC. Moissanite is an extremely rare mineral that contains SiC. In this paper, the particular isomer of the silicon carbides  $SiC_4$ -II[p, q] is examined by using some of the vertex and edges degree-related topological indices.

The first T-index was the Wiener index, given by a famous chemist, H. Wiener<sup>9</sup>. It was a distancerelated index used to calculate the boiling point of the paraffin and named "path number" by Wiener. All the indices used in this article are vertex degreebased. The Zagreb indices are the oldest degreerelated indices introduced for the analysis of the pielectron energy of chemical compounds. Kulli proposed the first and second k-Banhatti indices by drawing inspiration from the work of the Zagreb indices. The modified form of B-indices is just the inverse of the classical B-indices. The hyper-Bindices are squares of B-indices, just like the hyper-Zagreb indices.

#### **Fundamental Definitions**

Suppose G is the graph that stands for all the chemical structures of the isomers of silicon carbide. All the chemical graphs used in this manuscript are simple, 2 dimensional, and planar. The nodes of the chemical networks are represented by "s" and "t" connected by the edges "e" to make the complex graphs. The distance between any two vertices "s" and "t" is the shortest path between them and is represented by  $\partial(s, t)$ . The number of edges attached to a vertex "s" is formed by its degree which is denoted by  $\Phi(s)$ . A new concept of the edge degree is proposed recently as;  $\Phi(e) = \Phi(s) + \Phi(t) - 2$ . The maximum and minimum degree in a graph is represented by  $\Delta(G)$  and  $\delta(G)$ .

- Baghdad Science Journal
- Kulli introduced the K-banhatti indices by inspiring the work of Zagreb indices<sup>10</sup>. He analyzed various graphs such as cycle graphs, complete graphs, complete bipartite graphs, and regular graphs by using B-indices. The first k-Banhatti index  $B_1(G)$  and second k-Banhatti index  $B_1(G)$  are computed as:

$$B_1(G) = \sum_{se \in E(G)} [\Phi(s) + \Phi(e)]$$
$$B_2(G) = \sum_{se \in E(G)} [\Phi(s) \times \Phi(e)]$$

The B-induces is applicable to describe the properties of the path graphs and is used to compare the different graph operations<sup>11</sup>. A specific structure of the SiC namely SiC<sub>3</sub>–I [s, t] is analyzed by using the B-indices and Revan indices <sup>12</sup>. Nanomaterials are complex substances or materials that are synthesized and used on a tiny scale. The B-indices are used to explore the structure of different nanomaterials and famous Jahangir graphs<sup>13,14</sup>.

• Kulli suggested the first and second forms of modified B-indices. He applied these indices to study the behavior of connected graphs such as path, cycle, complete and bipartite graphs <sup>15</sup>. The modified first k-Banhatti index <sup>m</sup>B<sub>2</sub>(G) and second k-Banhatti index <sup>m</sup>B<sub>2</sub>(G) are determined as:

<sup>m</sup>
$$B_1$$
 (G) =  $\sum_{se \in E(G)} \frac{1}{\Phi(s) + \Phi(e)}$   
<sup>m</sup> $B_2$  (G) =  $\sum_{se \in E(G)} \frac{1}{\Phi(s) \times \Phi(e)}$ 

Many topological indices are used to explore the different isomers of the silicon carbides, due to the requirement of silicon in the modern world. The modified indices are used to discuss the structure of  $Si_2C_3$ -III [s, t] and several classes of the Jahangir graph <sup>16, 17</sup>.

• Kulli suggested the hyper B-indices for the simple and connected graphs such as cycle, complete, and bipartite graph<sup>18</sup>. The formulas of the first k-hyper Banhatti index  $HB_1(G)$  and second k-hyper Banhatti index  $HB_2(G)$  are given below:

$$HB_1(G) = \sum_{se \in E(G)} [\Phi(s) + \Phi(e)]^2$$
$$HB_2(G) = \sum_{se \in E(G)} [\Phi(s) \times \Phi(e)]^2$$

All the forms of the B-indices are introduced by inspiring the different forms of Zagreb indices.

For the recent use and applications of B-indice see <sup>19-21</sup>.

• The mathematical form of the first hyper Revan indices  $HR_1(G)$  and second hyper Revan indices  $HR_2(G)$  are written in the following way:

 $HR_1(G) = \sum_{st \in E(G)} [r_G(s) + r_G(t)]^2$ 

 $HR_2(G) = \sum_{\text{st} \in E(G)} [r_G(s) \times r_G(t)]^2$ 

• Kulli et al. proposed the revan indices in 2017 for understanding the oxide and honeycomb networks<sup>22</sup>. The numerical definition of the first

#### **Materials and Methods**

#### **Method and Strategies**

Numerous methods, including vertex and edge partitioning, graph analytic tools, and combinatorial algorithms, are utilized to calculate the results. All of the degree-related indices are calculated by hand using a basic calculator, and the calculations are rechecked using MATLAB. Because two major variables are employed at the same time, their graphs are three-dimensional. Mathematica is used to create the 3D graphs, while Chem-Draw is used to construct the chemical structures of SiC<sub>4</sub>-II[p, q].



Revan vertex index and third Revan index of a graph G are stated below:  $R_{01} = \sum_{c \in V(C)} r_c (s)^2$ 

$$R_{3}(G) = \sum_{st \in (G)} |r_{G}(s) - r_{G}(t)|$$

where  $r_G(t) = \Delta(G) + \delta(G) - \Phi(t)$  and *st* means that the vertex *s* and vertex *t* are adjacent in G. Revan indices have good correlation with not only the general mathematical graphs but also with the chemical graphs <sup>23-26</sup>. For more information related to graph theory see<sup>27,28</sup>.

#### Structural Representation of SiC<sub>4</sub>-II[p, q]

The two-dimensional molecular structures of SiC<sub>4</sub>-II[p, q] are demonstrated in Fig.1 and Fig.2. Unit cells form the basis for all chemical structures and are used to construct chemical building blocks. The length of the row increases if the unit cells are attached in the "p" direction, but the number of rows increases if the unit cells are attached in the "q" direction. The representation of the number of nodes and links in SiC<sub>4</sub>-II [p, q] is as follows:

$$|V(SiC_4 - II[p, q])| = 10pq$$

$$E(SiC_4 - II[p, q])| = 15pq - 4p - 2q$$

- M

(a) A unit cell of SiC<sub>4</sub> – II[p, q]
 (b) SiC<sub>4</sub> – II[p, q] for p=3, q=3.
 Figure 1.Two dimensional structure of SiC<sub>4</sub> – II[p, q]



(a) SiC<sub>4</sub>–II[p, q], one row with p=4 and q=1 (b) SiC<sub>4</sub> – II[p, q] for Figure 2. Two dimensional structure of SiC<sub>4</sub> – II[p, q]

# =1 (b) SiC<sub>4</sub> – II[p, q] for p=4, q=2

#### **Vertex Partition**

The whole vertex set of the graph  $SiC_4 - II[p, q]$  is partitioned into three classes according to the degree.

The vertex sets with one, two, and three degrees are represented by  $V_1$ ,  $V_2$ , and  $V_3$ , respectively. Table. 1, shows the general form of all the vertex degrees with

their frequencies and the general form of total vertices and edges is shown in Table. 2. These generalizations of the three parcels of vertices are done with the help of Matlab.

Table 1. Vertex degree with the correspondingcardinality

$\Phi(s)$	Cardinality		
$V_1$	2		
$V_2$	8p + 4q - 4		
$V_3$	10pq - 8p - 4q + 2		

# Table 2. Cardinality of nodes and edges for SiC<sub>4</sub>-II [p, q]

**Baghdad Science Journal** 

 Total vertices	Total edges		
10pq	15pq - 4p - 2q		

#### **Edge Partition:**

The edge set of SiC<sub>4</sub>-II[p, q] is partitioned by using the methods described above. There are four different edge divisions of SiC<sub>4</sub>-II[p, q] that are described in Table 3. The first edge pack has 2 edges, where  $\Phi(s) = 1$  and  $\Phi(t) = 2$ . The second edge pack consists of 2h + 2 edges, where  $\Phi(s)=2$  and  $\Phi(t) =$ 2. The third edge bundle is composed of 12p + 8q -14 edges, where  $\Phi(s)=2$  and  $\Phi(t) = 3$ . The fourth edge packet is composed of 15pq - 10q - 18p +10 edges, where  $\Phi(s) = 3$  and  $\Phi(t) = 3$ .

Table 3. Degree-based	nartition of edges	of SiC4-IIIn.	ոլ
Table 5. Degree-based	par unon or cuges	or 51C4-11[p,	ЧJ

I uble of Degree bused purtition of euges of blet H[p, q]					
Edges	$ig( \Phi(s), \Phi(t) ig)$	Frequency	<b>Φ</b> ( <b>e</b> )	$r_{G}(s)$	$r_{G}(t)$
E <sub>1</sub>	(1,2)	2	1	3	2
$E_2$	(2,2)	(2p + 2)	2	2	2
$E_3$	(2,3)	(12p + 8q - 14)	3	2	1
$E_4$	(3,3)	(15pq - 10q - 18p + 10)	4	1	1

#### Fundamental Outcomes for Silicon Carbide $(SiC_4 - II[p,q])$

In this section, there will be calculation for  $B_1(G)$ ,  $B_2(G)$ ,  ${}^{n_j}B_1(G)$ ,  ${}^{n_j}B_2(G)$ ,  $HB_1(G)$ ,  $HB_2(G)$ ,  $HR_1(G)$ ,  $HR_2(G)$ ,  $R_{01}(G)$ ,  $R_3(G)$  of the nanostructure silicon carbide SiC<sub>4</sub>-II[p,q].

**Theorem 1:** The results of the first and second k-Bindices for the particular isomer of silicon carbide  $SiC_4$ -II[p, q] are determined as follows:

52

$$B_1(G) = 210pq - 104p - 52q +$$

$$B_2$$
 (G)=360 $pq$  – 236 $p$  – 120 $q$  +

**Proof:** Let  $G \cong SiC_4$ -II[p, q] be the connected graph of SiC. The B<sub>1</sub>-index for this graph is calculated by using Table 3 and the definition of the index given above.

$$B_{1}(G) = \sum_{se \in E(G)} [\Phi(s) + \Phi(e)]$$
  
= 
$$\sum_{se \in E(G)} [\Phi(s) + \Phi(e) + \Phi(t) + \Phi(e)]$$

2[(1 + 1) + (2 + 1)] + (2k + 1)

Φ(e)]

$$= 2[(1 + 1) + (2 + 1)] + (2h + 2)[(2 + 2) + (2 + 2)] + (12h + 8u - 14) \times [(2 + 3) + (3 + 3)] + (15hu - 10u - 18h + 10)[(3 + 4) + (3 + 4)] = 2(5) + (2p + 2)(8) + (12p + 2)(8) + (12p$$

= 10 + 16p + 16 + 32p + 88q -154 + 210pq - 140q - 252p + 140 = 210pq - 104p - 52q + 12

The B<sub>2</sub>(G)-index is determined as follows:  

$$B_2(G) = \sum_{se \in E(G)} [\Phi(s) \times \Phi(e)]$$

$$= \sum_{se \in E} [\Phi(s) \times \Phi(e) + \Phi(t) \times \Phi(e)]$$

Φ(e)]

$$= 2[(1 \times 1) + (2 \times 1)] + (2p + 2)[(2 \times 2) + (2 \times 2)] + (12p + 8q - 14) \times [(2 \times 3) + (3 \times 3)] + (15pq - 10q - 18p + 10)[(3 \times 4) + (3 \times 4)] = 2(3) + (2p + 2)(8) + (12p + 8q - 14)(15) + (15pq - 10q - 18p + 10)(24) = 6 + 16p + 16 + 180p + 120q - 210 + 360pq - 240q - 432p + 240 = 360pq - 236p - 120q + 52$$

**Theorem 2:** The outcomes of the first and second modified k-B-indices for the special isomer of SiC are determined as:

$${}^{\mathrm{m}}B_{1}(\mathrm{G}) = \frac{30}{7}\mathrm{pq} + \frac{9}{35}p + \frac{8}{105}q - \frac{559}{105}$$
$${}^{\mathrm{m}}B_{2}(\mathrm{G}) = \frac{5}{3}\mathrm{pq} + \frac{4}{3}p + 5q - \frac{16}{9}$$

**Proof:** Let  $G \cong \text{SiC}_4\text{-II}[p, q]$  be the planar graph of SiC. By using the values of the edge partition and vertex division given in Table 3, The  ${}^{n_j}B_1(G)$ -index can be easily computed.

$${}^{m}B_{1}(G) = \sum_{se \in E(G)} \frac{1}{\Phi(s) + \Phi(e)}$$

$${}^{m}B_{1}(G) = \sum_{se \in E} \frac{1}{\Phi(s) + \Phi(e)} + \frac{1}{\Phi(t) + \Phi(e)}$$

$$= 2 \left[\frac{1}{2} + \frac{1}{3}\right] + ((2p + 2)) \left[\frac{1}{4} + \frac{1}{4}\right] + (12p + 8q - 14) \left[\frac{1}{5} + \frac{1}{6}\right] + (15pq - 10q - 18p + 10) \left[\frac{1}{7} + \frac{1}{7}\right]$$

$$= 2 \left[\frac{5}{6}\right] + (2p + 2) \left[\frac{2}{4}\right] + (12p + 8q - 14) \left[\frac{11}{30}\right] + (15pq - 10q - 18p + 10) \left[\frac{2}{7}\right]$$

$$= \frac{10}{6} + \frac{4}{4}p + \frac{4}{4} + \frac{132}{30}p + \frac{88}{30}q - \frac{154}{30} + \frac{30}{7}pq - \frac{20}{7}q - \frac{36}{7}p + \frac{20}{7}$$

$$= \frac{30}{7}pq + \frac{9}{35}p + \frac{8}{105}q - \frac{559}{105}$$
From Table. 3 and the formula of  ${}^{m}B_{2}(G)$ -index:

$${}^{n_{j}}B_{2}(G) = \sum_{se \in E(G)} \frac{1}{\Phi(s) \times \Phi(e)}$$

$$= \sum_{se \in E} \frac{1}{\Phi(s) \times \Phi(e)} + \frac{1}{\Phi(t) \times \Phi(e)}$$

$$= 2[1 + \frac{1}{2}] + (2p + 2) \left[\frac{1}{4} + \frac{1}{4}\right] + (12p + 2)\left[\frac{1}{4} + \frac{1}{4}\right] + (12p + 2)\left[\frac{1}{12} + \frac{1}{12}\right]$$

$$= 2 \left[\frac{3}{2}\right] + (2p + 2) \left[\frac{1}{2}\right] + (12p + 8q - 2)\left[\frac{1}{2}\right] + (15pq - 10q - 18p + 10)\left[\frac{1}{6}\right]$$

$$= \frac{6}{2} + \frac{2}{2}p + \frac{2}{2} + \frac{60}{18}p + \frac{120}{18}q - \frac{70}{18} + \frac{15}{6}pq - \frac{10}{6}q - \frac{18}{6}p + \frac{10}{6}$$

$$= \frac{5}{3}pq + \frac{4}{3}p + 5q - \frac{16}{9}$$

Theorem 3: The final values of the hyper k-Bindices for the particular isomer of the SiC are given as follows:

$$HB_1(G) = 1470pq -$$

$$492q + 216$$

968p -

$$HB_2(G) = 4320pq - 3716p -$$

1944q + 1316

**Proof:** Suppose G is representing the simple structure of SiC<sub>4</sub>-II[p, q]. The general structure of SiC<sub>4</sub>-II[p, q] is divided into the four groups of the edges given in Table 3. By utilizing Table 3,  $HB_1$ index is computed as follows:

$$HB_{1}(G) = \sum_{st} [\Phi(s) + \Phi(e)]^{2}$$
  
=  $\sum_{st \in E(G)} [(\Phi(s) + \Phi(e))^{2} + (\Phi(t) + \Phi(e))^{2}]$   
=  $2[(1+1)^{2} + (2+1)^{2}] + (2p + 2)[(2+2)^{2} + (2+2)^{2}] + (12p + 8q - 14)$   
×  $[(2+3)^{2} + (3+3)^{2}] + (15pq - 10q - 18p + 10)[(3+4)^{2} + (3+4)^{2}]$ 

**Baghdad Science Journal** = 2[13] + (2p + 2) [32] + (12p + 2)8q - 14) [61] + (2p + 4q - 2) [61] +(15pq - 10q - 18p + 10) [98] = 26 + 64p + 64 + 732p + 488q -854 + 1470pq - 980q - 1764p + 980= 1470pq - 968p - 492q + 216The HB<sub>2</sub>-index of graph G is determined as:  $HB_2(G) = \sum_{se} [\Phi(s) \times \Phi(e)]^2$  $= \sum_{st \in E(G)} \left[ (\Phi(s) \times \Phi(e))^2 + (\Phi(t) \times \Phi(e))^2 \right]$ 

 $= 2[(1 \times 1)^{2} + (2 \times 1)^{2}] + (2p + 2)[(2 \times 1)^{2}] + (2p + 2)](2 \times 1)^{2}$  $(2)^{2} + (2 \times 2)^{2} + (12p + 8q - 14)[(2 \times 3)^{2} +$  $(3 \times 3)^2$ ]  $+(15pq - 10q - 18p + 10)[(3 \times 4)^{2} +$ 

$$(3 \times 4)^2$$
]  
= 2[5] + (2p + 2) [32] + (12p + 8q -

14) [117] + (15pq - 10p - 8q + 5) [188]10 + 64p + 64 + 1404p + 936q -= 1638 + 4320pq - 2880q - 5184p + 2880

$$= 4320pq - 3716p - 1944q + 1316$$

Theorem 4: The final results of the first and second Revan indices for the SiC<sub>4</sub>-II[p, q] are computed as:  $HR_1(G) =$ 60pq + 68p +

$$32q - 4$$

$$HR_2(G) = 15pq + 62p +$$

22q + 58

 $\Phi(e))^{2}$ 

**Proof:** Consider  $G \cong SiC_4$ -II[p, q] as a simple graph of SiC. The  $HR_1(G)$  is calculated as follows.

$$HR_{1}(G) = \sum_{st \in E} [r_{G}(s) + r_{G}(t)]^{2}$$
  
= 2[(3 + 2)<sup>2</sup>] + (2h + 2)[(2 + 2)<sup>2</sup>] +  
(12h + 8u - 14)[(2 + 1)<sup>2</sup>]  
+(15hu - 10u - 18h + 10)[(1 +

1)4

$$= 50 + 32p + 32 + 108p + 72q - 126 + 60pq - 40q - 72p + 40$$

$$= 60pq + 68p + 32q - 4$$

The  $HR_2(G)$ -index can be calculated by using the data given in Table 3.

$$HR_{2}(G) = \sum_{\text{st} \in E(G)} [r_{G}(s) \times r_{G}(t)]^{2}$$
  
= 2[(3 × 2)<sup>2</sup>] + (2p + 2)[(2 × 2)<sup>2</sup>] +  
(12p + 8q - 14)[(2 × 1)<sup>2</sup>]  
+(15pq - 10p - 8q + 10)[(1 × 1)<sup>2</sup>]  
= 72 + 32p + 32 + 48p + 32q - 56 +  
15pq - 10q - 18p + 10

= 15pq + 62p + 22q + 58

Theorem 5: The final values of the first and third Revan indices for SiC<sub>4</sub>-II[p, q] are given below.

$$R_{01}(G) = 10pq + 24p + 12q + 4$$

$$R_3(G) = 12p + 8q - 12$$

**Proof:** Suppose  $G \cong SiC_4$ -II[p, q] is the connected graph of SiC. The  $R_{01}(G)$  is calculated as follows,

Page | 1103



 $R_{01}(G) = \sum_{s \in V(G)} r_G(s)^2$ =  $\sum_{vr_3} [r_G(s^2)] + \sum_{vr_2} [r_G(s^2)]$ +  $\sum_{vr_1} [r_G(s^2)]$ = 2 (3)<sup>2</sup> + (8p + 4q - 4) (2)<sup>2</sup> + (10pq - 8p - 4q + 2) (1)<sup>2</sup> = 2 (9) + 32p + 16q - 16 + 10pq - 8p - 4q + 2 = 10pq + 24p + 12q + 4

The  $R_3(G)$ -Index is determined by using its mathematical definition and the data given in Table 3.

$$R_{3}(G) = \sum_{\text{st} \in G} |r_{G}(s) - r_{G}(t)|$$
  
= 2[1] + (2p + 2)[0] + (12p +  
8q - 14)[1] + (15pq - 10q - 18p + 10)[0]  
= 2 + 12p + 8q - 14  
= 12p + 8q - 12

#### **Numerical Analysis**

This section discusses the numerical results of silicon carbide, SiC4-[p, q]. Numerical data are quantities that may be measured and arranged properly. Different values of p and q are used to examine the variance at various points. When the values of the input parameters (p, q) change, the values of the output (topological indices) vary as well. Table 4 displays the numerical values of all topological indices. Table 4 shows that all of the outputs are positive for p = q = (2, 3, 4,...). The hyper-Banhatti indices have the greatest values, while the third Revan index has the lowest. The values of parameters (p, q) might be negative or positive, but positive and equal values are employed for the efficiency of computation and symmetry.

Baghdad Science Journal

Indices	(p, q)=[1, 1]	(p, q)=[2, 2]	(p, q)=[3, 3]	(p, q)=[4, 4]	(p, q)=[5, 5]
$B_1(G)$	66	540	1434	2748	4482
$B_2(G)$	56	780	2224	4388	7272
${}^{\mathrm{m}}B_{1}(G)$	-0.70	12.48	34.24	64.58	103.48
${}^{\mathrm{m}}B_{2}(G)$	6.22	17.56	32.22	50.22	71.56
$HB_1(G)$	226	3176	9066	17896	29666
$HB_2(G)$	-24	7276	23216	47796	81016
$HR_1(G)$	156	436	836	1356	1996
$HR_2(G)$	157	286	445	634	853
$R_{01}(G)$	50	116	202	308	434
$R_3(G)$	8	28	48	68	88

Table 4. Numerical Analysis for SiC<sub>4</sub>-II[n, a]

#### Graphical Expression of SiC<sub>4</sub>-II[p, q]

Fig. 3 demonstrates the variation in the outcomes of all topological indices. The variations of the parameters p and q are presented on the x- and yaxes, respectively, while the results of topological indices are given in three-dimensional space. All of the graphs in Fig. 3(a-e) were constructed using data from Table 4. Numerical analysis is an effective method for comparing data, and their graphs make the comparison extremely efficient. Graphs and charts reduce massive quantities of information into simple formats that express key ideas simply and efficiently. Graphs make information more accessible. This is particularly true when two or more groups of numbers are somehow connected. Graphs come in a variety of shapes and sizes, including bar charts, line graphs, area graphs, scatter plots, pie charts, pictographs, column charts, and bubble charts. For data analysis in this area, 3D space graphs are applied. The extreme values of the topological index are also depicted in these figures. These figures also show how the values of topological indices can change when p and q are changed. The relationship between topological indices and experimental measurements makes it simple to identify the characteristics of silicon structures SiC<sub>4</sub>-II[p, q].





(e) First and third Revan Indices Figure 3. The graphs of all the degree-related topological indices of SiC<sub>4</sub>-II[p, q]

#### Conclusion

Topological indices are useful in forecasting a chemical compound's physio-chemical properties. Silicon carbide SiC<sub>4</sub>-II[p, q] plays an important function in chemistry, particularly in assembly methods and host-guest reactions. The T-indices, namely the first and second k-Banhatti index ( $B_1(G)$ ,  $B_2(G)$ ), modified the first and second k-Banhatti index(<sup>m</sup>B<sub>1</sub> (G), <sup>m</sup>B<sub>2</sub>(G)), first and second k-hyper Banhatti index( $HB_1(G)$ ,  $HB_2(G)$ ), first and second

hyper Revan indices ( $HR_1(G)$ ,  $HR_2(G)$ ), first Revan vertex index and third Revan index( $R_{01}$  (G),  $R_3$  (G)) for Silicon Carbide SiC<sub>4</sub>-II[p, q] are calculated in this article. The correlation between the experimental values of SiC<sub>4</sub>-II[p, q] and T-indices describes the validity of T-indices. All the degree-based indices are suitable for the estimation of the physical and chemical features of SiC<sub>4</sub>-II[p, q].

#### **Data Availability**

In this article, no data were utilized.



#### **Author's Declaration**

- Conflicts of Interest: None.
- We hereby confirm that all the Figures and Tables in the manuscript are ours. Furthermore, any Figures and images that are not ours have been

#### **Author's Contribution Statement**

Conceptualization: A. M. and M. W. R. Methodology: M. W. R. and A. M. Investigation: M. W. R. Writing original draft preparation: I. H. Writing review and editing: I.H and M. W. R.

#### References

- 1. Trinajstic, N. 2018. Chemical graph theory. CRC press; 2019. p. 352. https://doi.org/10.1201/9781315139111.
- Afzal F, Hussain S, Afzal D, Razaq S. Some New Degree Based Topological Indices via M-polynomial. *J Optim Theory Appl*. 2020 May 18; 41(4): 1061-1076. <u>https://doi.org/10.1080/02522667.2020.1744307</u>
- Alam SM, Jarad F, Mahboob A, Siddique I, Altunok T, Rasheed MW. A Survey on Generalized Topological Indices for Silicon Carbide Structure. J Chem. 2022 Jun 2; 2022: 1-11. https://doi.org/10.1155/2022/7311404
- Sardar MS, Ali MA, Ashraf F, Cancan M. On Topological Indices of Double and Strong Double Graph of Silicon Carbide Si<sub>2</sub> C<sub>3</sub> -I [p, q]. Eurasian Chem. Commun. 2023; 5: 37-49. DOI:10.22034/ecc.2023.356160.1519
- Pan YH, Khalid A, Ali P, Rehman AU, Siddiqui MK, Ishtiaq M, Liu JB. Topological Study of Polycyclic Silicon Carbide Structure. Polycycl Aromat Compd. 2022 Jan 8: 1-12. https://doi.org/10.1080/10406638.2021.2024861
- Ghods M, Rostami Z. Some Topological Indices for Silicon-Carbon Si<sub>2</sub>C<sub>3</sub>–I [p, q] and Some Inequalities Between Distance-Based and Degree-Based Indices in Silicon-Carbon Si<sub>2</sub>C<sub>3</sub>–I [p, q]. *Journal of Information and Optimization Sciences*. 2021 Jul 4; 42(5): 973-93. https://doi.org/10.1080/02522667.2020.1827506
- Sun K, Wang T, Gong W, Lu W, He X, Eddings EG, Fan M. Synthesis and Potential Applications of Silicon Carbide Nanomaterials/Nanocomposites. Ceram Int. 2022 Jul 30; 22(48): 32571-32587. https://doi.org/10.1016/j.ceramint.2022.07.204
- Saddow SE. Silicon Carbide Technology for Advanced Human Healthcare Applications. Micromachines. 2022 Feb 22; 13(3): 346-357. <u>https://doi.org/10.3390/mi13030346</u>
- Wiener H. Structural Determination of Paraffin Boiling Points. J Am Chem Soc.1947 Jan; 69(1): 17-20. https://doi.org/10.1021/ja01193a005

included with the necessary permission for republication, which is attached to the manuscript.

- Ethical Clearance: The project was approved by the local ethical committee in University of Education Lahore, Pakistan.

Supervision: A. M. and J. H. H. B. All authors read and agreed to the published version of the manuscript.

- Nazari ME, Chamua M, Bharali A, Sarma NK, Saikia R. M-Polynomial of Some Operations of Path and K-Banhatti Indices. Mathematical Statistician and Engineering Applications. 2022 Aug 2; 38-55. <u>http://philstat.org.ph</u>
- Mahboob A, Muhiuddin G, Siddique I, Alam SM. A View of Banhatti and Revan Indices in Chemical Graphs. J Math. 2022 Jul 31; 2022. <u>https://doi.org/10.1155/2022/5680712</u>
- Anjum MS, Safdar MU. K Banhatti and K Hyper-Banhatti Indices of Nanotubes. *J Eng Appl Sci*. 2019 Mar; 2(1):19-37. doi:10.30538/psrp-easl2019.0013
- 13. Siddique I, Muhiuddin G, Mahboob A, Rasheed MW. Research Article Various Uses of Topological Invariants in Jahangir Graph J[ $\beta$ ,  $\alpha$ ]. J Math. 2022 Sep. 13; 2022: 1-11. https://doi.org/10.1155/2022/4321206
- 14. Kulli VR. New K Banhatti Topological Indices. *Int j fuzzy math arch.* 2017; 12(1): 29-37. DOI: <u>http://dx.doi.org/10.22457/ijfma.v12n1a4</u>
- Afzal D, Ali S, Afzal F, Cancan M, Ediz S, Farahani MR. A Study of Newly Defined Degree-Based Topological Indices via M-Polynomial of Jahangir Graph. J Discrete Math Sci Cryptogr. 2021 Feb 17; 24(2): 427-38. https://doi.org/10.1080/09720529.2021.1882159
- 16. Zhao D, Zahid MA, Irfan R, Arshad M, Fahad A, Ahmad Z, Li L. Banhatti, Revan and Hyper-Indices of Silicon Carbide Si<sub>2</sub>C<sub>3</sub>-III [n, m]. Open Chem J. 2021 Jan 1; 19(1): 646-52. <u>https://doi.org/10.1515/chem-2020-0151</u>
- 17. Kulli VR. On K Hyper-Banhatti Indices and Coindices of Graphs. International Research Journal of Pure Algebra. 2016; 6(5): 300-304. <u>http://www.rjpa.info/index.php/rjpa/article/view/437</u>
- Kulli VR. K Banhatti Indices of Chloroquine and Hydroxychloroquine: Research Applied for the Treatment and Prevention of COVID-19. SSRG- Int J Appl Chem. 2020; 7(1): 63-68. <u>10.14445/23939133/IJAC-V7I1P113</u>



- Kulli VR. Hyper Zagreb-K-Banhatti Indices of Graphs. International Journal of Mathematics Trends and Technology. 2020; 66(8): 123-30. (10.14445/22315373/IJMTT-V66I8P513)
- 20. Ranjini PS, Lokesha V, Kumar S. The K. Banhatti Indices of Certain Graphs. Southeast Asian Bull. Math. 2022 Jul 1; 46(4): 453-466. <u>http://www.seams-bull-</u> math.ynu.edu.cn/quick search result.jsp
- 21. Kulli VR. Revan Indices of Oxide and Honeycomb Networks. Int J Math. 2017 march 13; 4(5): 663-667. Available Online: http://ijmaa.in/
- 22. Aguilar-Sanchez R, Herrera-Gonzalez IF, Mendez-Bermudez JA, Sigarreta JM. Revan-Degree Indices on Random Graphs. *ArXiv.org*. 2022 Oct 10; 1-16.<u>https://doi.org/10.48550/arXiv.2210.04749</u>
- 23. Kamran M, Salamat N, Hussain Khan R, Abaid Ullah M, Hameed MS, Pandit MK. Computation of Revan Topological Indices for Phenol-Formaldehyde Resin. J Math. 2022 Apr 27; 1(2022): 1-10. <u>https://doi.org/10.1155/2022/8548771</u>

- 24. Kamran M, Delen S, Khan RH, Salamat N, Baig AQ, Cangul IN, Alam A. Physico-Chemical Characterization of Amylose and Amylopectin Using Revan Topological Indices. J Math. 2022 Jul 6; 2022: 1-12. https://doi.org/10.1155/2022/2840217
- 25. Narasimhan D, Vignesh R, Desikan K. Results on Revan and Hyper Revan Indices of Some HEX Derived Networks. *Adv Comput Math.* 2022 April 7; 419: 209-220. DOI: 10.1007/978-981-19-0471-4\_15
- 26. Omran AA, Oda HH. Hn-Domination in Graphs. Baghdad Sci. J. 2019; 16(1(Suppl.)): 242-247. DOI: <u>http://dx.doi.org/10.21123/bsj.2019.16.1(Suppl.).024</u> 2
- 27. Al-Harere MN, Bakhash PAK. Tadpole Domination in Graphs. Baghdad Sci J. 2018 Dec 9; 15(4): 466-471. DOI: <u>http://dx.doi.org/10.21123/bsj.2018.15.4.0466</u>
- Alsulami SH, Bayati JH. COVID-19 Infection Structure Analysis Based on Minimum Spanning Tree Visualization in the Kingdom of Saudi Arabia Regions. J Chem. 2022 Jul 26; 2022(Special Issue): 1-8. <u>https://doi.org/10.1155/2022/1726286</u>

### حساب العديد من ثوابت بنهاتي وريفين لكربيدات السيليكون

عابد محبوب<sup>1</sup> ، محمد وحيد رشيد<sup>1</sup> ، جلال حاتم حسين البياتى<sup>2</sup> و اقرا حنيف<sup>1</sup>

<sup>ل</sup>قسم الرياضيات، قسم العلوم والتكنولوجيا، جامعة التربية، لاهور ، باكستان <sup>2</sup>قسم الرياضيات، كلية العلوم للبنات، جامعة بغداد، بغداد، العراق

#### الخلاصة

تعد التعبيرات عن السمات الطوبولوجية الجزيئية لمركبات كربيد السيليكون ضرورية للتفاعلات الكمية للهيكل - الملكية والتفاعلات الهيكلية. نظرية الرسم البياني الكيميائية للمركبات الكيميائية. في العصر الحديث ، تعتبر المؤشرات الطوبولوجية مهمة للغاية في دراسة نظرية التي ترتبط جيدًا بالخصائص الكيميائية للمركبات الكيميائية. في العصر الحديث ، تعتبر المؤشرات الطوبولوجية مهمة للغاية في دراسة نظرية الرسم البياني. المؤشرات الطوبولوجية هي أدوات مهمة لفهم الهيكل الأساسي للهياكل الكيميائية أثناء فحص المواد الكيميائية. التشف مؤشر Banhatti الطوبولوجية هي أدوات مهمة لفهم الهيكل الأساسي للهياكل الكيميائية أثناء فحص المواد الكيميائية. في هذه المقالة ، اكتشف مؤشر Happer k-hyper k-hyper l الأول والثاني ، ومؤشر رأس Revan الأول ، ومؤشر Revan الثالث لـ كربيد السيليكون -SiC4 والتابي مؤلم و والثالث للميليكون -Revan الأول والثاني موقات المولي الكيميائية المولي المولي والي الكيميائية ال

الكلمات المفتاحية: مؤشرات بانهاتي، مؤشرات هايبر بانهاتي، مؤشرات هايبر ريفان، كربيد السيليكون [p, q] SiC<sub>4</sub>-II، المؤشرات الطوبولوجية.