Computation of Several Banhatti and Reven Invariants of Silicon Carbides

Abid Mahboob, Muhammad Waheed Rasheed, Jalal Hatem Hussein Bayati and Iqra Hanif

1Department of Mathematics, Division of Science and Technology, University of Education Lahore, Pakistan
2Department 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 k-hyper 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 SiC4-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 1.

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 2. 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 3,4.

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 bond 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 elastic modulus, high thermal conductivity, hardness, and corrosion, and most significantly, the maintenance of elastic resistance at temperatures up to 1650°C. 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. 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$_3$-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. It was a distance-related 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 degree-based. The Zagreb indices are the oldest degree-related indices introduced for the analysis of the pi-electron 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-B-indices 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 δ(s, t). The number of edges attached to a vertex “s” is formed by its degree which is denoted by ϕ(s). A new concept of the edge degree is proposed recently as: ϕ(e) = ϕ(s) + ϕ(t) − 2. The maximum and minimum degree in a graph is represented by Δ(G) and δ(G).

- Kulli introduced the K-banhatti indices by inspiring the work of Zagreb indices. 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 $B_2(G)$ 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-indices is applicable to describe the properties of the path graphs and is used to compare the different graph operations. A specific structure of the SiC namely SiC$_3$–I [s, t] is analyzed by using the B-indices and Reyan indices. 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.

- 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. The modified first k-Banhatti index $mB_1(G)$ and second k-Banhatti index $mB_2(G)$ are determined as:

$$mB_1(G) = \sum_{se \in E(G)} \frac{1}{\phi(s) + \phi(e)}$$

$$mB_2(G) = \sum_{se \in E(G)} \frac{1}{\phi(s) \times \phi(e)}$$

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$_2$C$_3$-III [s, t] and several classes of the Jahangir graph.

- Kulli suggested the hyper B-indices for the simple and connected graphs such as cycle, complete, and bipartite graph. 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.
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:

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

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

Kulli et al. proposed the revan indices in 2017 for understanding the oxide and honeycomb networks. The numerical definition of the first Revan vertex index and third Revan index of a graph $G$ are stated below:

$$R_{01} = \sum_{s \in V(G)} r_G(s)^2$$

$$R_3(G) = \sum_{s \in V(G)} |r_G(s) - r_G(t)|$$

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. For more information related to graph theory see.

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$_4$-II[p, q].

Structural Representation of SiC$_4$-II[p, q]

The two-dimensional molecular structures of SiC$_4$-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$_4$-II[p, q] is as follows:

$$|V(\text{SiC}_4-II[p,q])| = 10pq$$

$$|E(\text{SiC}_4-II[p,q])| = 15pq - 4p - 2q$$

Vertex Partition

The whole vertex set of the graph SiC$_4$ - II[p, q] is partitioned into three classes according to the degree.
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 corresponding cardinality

<table>
<thead>
<tr>
<th>Φ(s)</th>
<th>Cardinality</th>
</tr>
</thead>
<tbody>
<tr>
<td>V₁</td>
<td>2</td>
</tr>
<tr>
<td>V₂</td>
<td>8p + 4q + 4</td>
</tr>
<tr>
<td>V₃</td>
<td>10pq – 8p – 4q + 2</td>
</tr>
</tbody>
</table>

Fundamental Outcomes for Silicon Carbide (SiC₄ – II[p, q])

In this section, there will be calculation for B₁(G), B₂(G), nB₁(G), nB₂(G), HB₁(G), HB₂(G), HR₁(G), HR₂(G), R₀(G), R₁(G) of the nanostructure silicon carbide SiC₄-II[p,q].

**Theorem 1:** The results of the first and second k-B-indices for the particular isomer of silicon carbide SiC₄-II[p,q] are determined as follows:

- B₁(G) = 210pq – 104p – 52q + 12
- B₂(G) = 360pq – 236p – 120q + 52

**Proof:** Let G \cong SiC₄-II[p,q] be the connected graph of SiC. The B₁-index for this graph is calculated by using Table 3 and the definition of the index given above.

\[ B₁(G) = \sum_{e \in E(G)} [\Phi(s) + \Phi(e)] = \sum_{e \in E(G)} [\Phi(s) + \Phi(e) + \Phi(t) + \Phi(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)] + (15pq – 10q – 18p + 10)(14) = 10 + 16p + 16 + 32p + 88q – 154 + 210pq – 140q – 252p + 140 = 210pq – 104p – 52q + 12

The B₂-index is determined as follows:

\[ B₂(G) = \sum_{e \in E(G)} [\Phi(s) \times \Phi(e)] = \sum_{e \in E(G)} [\Phi(s) \times \Phi(e) + \Phi(t) \times \Phi(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:

\[ nB₁(G) = \frac{30}{7}pq + \frac{9}{35}p + \frac{8}{105}q – \frac{559}{105} \]

**Proof:** Let G \cong SiC₄-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 nB₁(G)-index can be easily computed.

Table 2. Cardinality of nodes and edges for SiC₄-II[p, q]

<table>
<thead>
<tr>
<th>Total vertices</th>
<th>Total edges</th>
</tr>
</thead>
<tbody>
<tr>
<td>10pq</td>
<td>15pq – 4p – 2q</td>
</tr>
</tbody>
</table>

Table 3. Degree-based partition of edges of SiC₄-II[p, q]

| Edges | (Φ(s), Φ(t)) | Frequency | Φ(e) | r⁶|s(Φ) | r⁶|t(Φ) |
|-------|---------------|-----------|------|---|------|------|
| E₁    | (1,2)         | 2         | 1    | 3 | 2    |      |
| E₂    | (2,2)         | (2p + 2)  | 2    | 2 | 2    |      |
| E₃    | (2,3)         | (12p + 8q – 14) | 3 | 2 | 1    |      |
| E₄    | (3,3)         | (15pq – 10q – 18p + 10) | 4 | 1 | 1    |      |
Theorem 3: The final values of the hyper k-B-indices for the particular isomer of SiC are given as follows:

\[ HB_1(G) = 1470pq - 968p - 492q + 216 \]
\[ HB_2(G) = 4320pq - 3716p - 1944q + 1316 \]

Proof: Suppose \( G \) is representing the simple structure of SiC-II[p, q]. The general structure of SiC-II[p, q] is divided into four groups of the edges given in Table 3. By utilizing Table 3, \( HB_1 \) - index is computed as follows:

\[ HB_1(G) = \sum_{s \in E(G)} \left[ \Phi(s) + \Phi(e) \right]^2 + (\Phi(t) + \Phi(e))^2 \]
\[ = \sum_{st \in E(G)} \left[ (\Phi(s) + \Phi(e))^2 + (\Phi(t) + \Phi(e))^2 \right] \]
\[ = 2(\{1 + 1\}^2 + (2 + 1)^2) + (2p + 2)(2 + 2)^2 + (2p + 8q - 14) \times (2 + 3)^2 + (3 + 4)^2 + (15pq - 10q - 18p + 10)(3 + 3)^2 \]
\[ \]
\[ \]

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

\[ R_{101}(G) = 10pq + 24p + 12q + 4 \]
\[ R_{20}(G) = 12p + 8q - 12 \]

Proof: Suppose \( G \) is the connected graph of SiC. The \( R_{101}(G) \) is calculated as follows,
\[ R_{01}(G) = \sum_{s \in V(G)} r_G(s)^2 \]
\[ = \sum_{v_r^3} r_G(s^2) + \sum_{v_r^2} [r_G(s^2)] \]
\[ = 2 (3)^2 + (8p + 4q - 4) (2)^2 + (10pq - 8p - 4q) \]
\[ + 2 \]
\[ = 10pq + 24p + 12q + 4 \]

The \( R_3(G) \)-Index is determined by using its mathematical definition and the data given in Table 3.
\[ R_3(G) = \sum_{s \in G} |r_G(s) - r_G(t)| \]
\[ = 2[1] + (2p + 2)[0] + (12p + 8q - 14)[1] + (15pq - 10q - 18p + 10)[0] \]
\[ = 2 + 12p + 8q - 14 \]
\[ = 12p + 8q - 12 \]

**Numerical Analysis**

This section discusses the numerical results of silicon carbide, SiC\( ^4 \). 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.

**Table 4. Numerical Analysis for SiC\( ^4 \)-III\( [p, q] \)**

<table>
<thead>
<tr>
<th>Indices</th>
<th>( (p, q) = [1, 1] )</th>
<th>( (p, q) = [2, 2] )</th>
<th>( (p, q) = [3, 3] )</th>
<th>( (p, q) = [4, 4] )</th>
<th>( (p, q) = [5, 5] )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( B_1(G) )</td>
<td>66</td>
<td>540</td>
<td>1434</td>
<td>2748</td>
<td>4482</td>
</tr>
<tr>
<td>( B_2(G) )</td>
<td>56</td>
<td>780</td>
<td>2224</td>
<td>4388</td>
<td>7272</td>
</tr>
<tr>
<td>( m_B_1(G) )</td>
<td>-0.70</td>
<td>12.48</td>
<td>34.24</td>
<td>64.58</td>
<td>103.48</td>
</tr>
<tr>
<td>( m_B_2(G) )</td>
<td>6.22</td>
<td>17.56</td>
<td>32.22</td>
<td>50.22</td>
<td>71.56</td>
</tr>
<tr>
<td>( HB_1(G) )</td>
<td>226</td>
<td>3176</td>
<td>9066</td>
<td>17896</td>
<td>29666</td>
</tr>
<tr>
<td>( HB_2(G) )</td>
<td>-24</td>
<td>7276</td>
<td>23216</td>
<td>47796</td>
<td>81016</td>
</tr>
<tr>
<td>( HR_1(G) )</td>
<td>156</td>
<td>436</td>
<td>836</td>
<td>1356</td>
<td>1996</td>
</tr>
<tr>
<td>( HR_2(G) )</td>
<td>157</td>
<td>286</td>
<td>445</td>
<td>634</td>
<td>853</td>
</tr>
<tr>
<td>( R_{01}(G) )</td>
<td>50</td>
<td>116</td>
<td>202</td>
<td>308</td>
<td>434</td>
</tr>
<tr>
<td>( R_3(G) )</td>
<td>8</td>
<td>28</td>
<td>48</td>
<td>68</td>
<td>88</td>
</tr>
</tbody>
</table>

**Graphical Expression of SiC-\( ^4 \)-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 y-axes, 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\( ^4 \)-II\( [p, q] \).
**Conclusion**

Topological indices are useful in forecasting a chemical compound's physio-chemical properties. Silicon carbide $\text{SiC}_4\text{II}[p, q]$ 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($\text{m}B_1(G)$, $\text{m}B_2(G)$), 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($R_0(G)$, $R_3(G)$) for Silicon Carbide $\text{SiC}_4\text{II}[p, q]$ are calculated in this article. The correlation between the experimental values of $\text{SiC}_4\text{II}[p, q]$ 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 $\text{SiC}_4\text{II}[p, q]$.

**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 included with the necessary permission for re-publication, which is attached to the manuscript.
- Ethical Clearance: The project was approved by the local ethical committee in University of Education Lahore, Pakistan.

Author’s Contribution Statement


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

References


حساب العديد من ثوابت بنهائي ورفتين لكربيدات السيليكون

عابد محبوب1، محمد وحيد رشيد1، جلال حاتم حسين البطاني2، أفرا حنيف1

1قسم الرياضيات، قسم العلوم والتكنولوجيا، جامعة التربية، لاهاور، باكستان
2قسم الرياضيات، كلية العلوم للبنات، جامعة بغداد، بغداد، العراق

الخلاصة

تعتبر التعريفات عن السمات الطوبولوجية الجزيئية لمركبات كربيدي السيليكون ضرورية للتفاعلية الكيميائية، الملكية والتفاعلات الهيكلية. نظرية الرسم البياني الكيميائي هي حقل فرعى من الكيمياء الحسابية التي تبحث في المؤشرات الطوبولوجية للشبكات الكيميائية التي ترتبط جيدًا بالخصائص الكيميائية للكربون الكيميائي. في العصر الحديث، تعتبر المؤشرات الطوبولوجية مهمة للغاية في دراسة نظرية الرسم البياني. المؤشرات الطوبولوجية هي أدوات مهمة لفهم الهيكل الكيميائي للمركبات الكيميائية أثناء فحص المواد الكيميائية. في هذه المقالة، اكتشف مؤشر k-hyper k-hyper k-Banhatti، مؤشر k-Banhatti الأول والثاني، مؤشر SiC4 مanko، مؤشر Revan Hyper Revan، مؤشر Revan الأول والثاني، مؤشر Revan راس hyper 1، مؤشر Revan الأول والثاني، مؤشر Revan راس hyper 1، مؤشر Revan الأول والثاني، مؤشر Revan راس hyper 1، مؤشر Revan الأول والثاني، مؤشر Revan راس hyper 1، مؤشر Revan الأول والثاني، مؤشر Revan راس hyper 1، مؤشر Revan الأول والثاني، مؤشر Revan راس hyper 1، مؤشر Revan الأول والثاني، مؤشر Revan راس hyper 1، مؤشر Revan الأول والثاني، مؤشر Revan راس hyper 1، مؤشر Revan الأول والثاني، مؤشر Revan راس hyper 1، مؤشر Revan الأول والثاني، مؤشر Revan راس hyper 1، مؤشر Revan الأول والثاني، مؤشر Revan راس hyper 1، مؤشر Revan الأول والثاني، مؤشر Revan راس hyper 1، مؤشر Revan الأول والثاني، مؤشر Revan راس hyper 1، مؤشر Revan الأول والثاني، المؤشرات السيليكون، المؤشرات الطوبولوجية.