Research Article

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Banhatti, revan and hyper-indices of silicon carbide $\text{Si}_2\text{C}_3\text{-III}[n, m]$

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Abstract: In recent years, several structure-based properties of the molecular graphs are understood through the chemical graph theory. The molecular graph G of a molecule consists of vertices and edges, where vertices represent the atoms in a molecule and edges represent the chemical bonds between these atoms. A numerical quantity that gives information related to the topology of the molecular graphs is called a topological index. Several topological indices, contributing to chemical graph theory, have been defined and vastly studied. Recent inclusions in the class of the topological indices are the K-Banhatti indices. In this paper, we established the precise formulas for the first and second K-Banhatti, modified K-Banhatti, K-hyper Banhatti, and hyper Revan indices of silicon carbide $\text{Si}_2\text{C}_3\text{-III}[n, m]$. In addition, we present the graphical analysis along with the comparison of these indices for $\text{Si}_2\text{C}_3\text{-III}[n, m]$.

Keywords: Banhatti, hyper Banhatti, hyper Revan indices, silicon carbide $\text{Si}_2\text{C}_3\text{-III}[n, m]$

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1 Introduction

The chemical, physical, and physicochemical properties of a compound, which depends on its structure, can be effectively studied by means of the graph theory. A chemical structure of a compound can be described by a graph G , where the vertex set of G consists of the atoms of the compound and the edge set consists of the chemical bonds between the atoms. A graph can be recognized by connection table, polynomial, sequence of numbers, matrix or numeric number which is also called a topological index that represents the whole graph. A topological index got special attention as it predicts several information related to the molecular structure of the compounds. In the description of a chemical structure, a topological index is one of the most powerful tools with several intense applications in such as mathematical chemistry, the fields of control theory and quantitative structure–property relation (QSPR) and quantitative structure–activity relation (QSAR) investigations, see refs. [1,2]. For details regarding the recent contributions on the topological indices, see refs. [3–11].

Before proceeding further regarding the definitions of the topological indices studied in this paper, we recall the relevant notions and set the corresponding notations. For the notions and notations not described here we refer [12] to the readers. Throughout this paper, we denote a simple connected graph by G , distance between u and v by $d(u, v)$, the degree of a vertex u in G by $d(u)$, an edge e between the vertices u and v by $e = uv$, degree of an edge e by $d(e)$ (where $d(e) = d(u) + d(v) - 2$), and the maximum and minimum degree in a graph by $\Delta(G)$ and $\delta(G)$, respectively.

According to the settings described in the previous paragraph, the first K-Banhatti index $B_1(G)$ and second K-Banhatti index $B_2(G)$ are defined as follows:

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$$B_1(G) = \sum_{ue \in E(G)} [d(u) + d(e)],$$

$$B_2(G) = \sum_{ue \in E(G)} [d(u) \times d(e)].$$

The modified first K-Banhatti index ${}^m B_1(G)$ and second K-Banhatti index ${}^m B_2(G)$ are defined as follows:

$${}^m B_1(G) = \sum_{ue \in E(G)} \frac{1}{d(u) + d(e)},$$

$${}^m B_2(G) = \sum_{ue \in E(G)} \frac{1}{d(u) \times d(e)}.$$

The first K-hyper Bhanhatti index $HB_1(G)$ and second K-hyper Bhanhatti index $HB_2(G)$ are defined as follows:

$$HB_1(G) = \sum_{ue \in E(G)} [d(u) + d(e)]^2,$$

$$HB_2(G) = \sum_{ue \in E(G)} [d(u) \times d(e)]^2.$$

The first- and second-hyper Revan indices of G are defined as follows:

$$HR_1(G) = \sum_{uv \in E(G)} [r_G(u) + r_G(v)]^2,$$

$$HR_2(G) = \sum_{uv \in E(G)} [r_G(u)r_G(v)]^2,$$

where $r_G(v) = \Delta(G) + \delta(G) - d(v)$ and uv means that the vertex u and vertex v are adjacent in G . We refer [13–16] for details about these indices.

On the other hand, silicon is a nontoxic semiconductor material that has a very low cost when compared with other materials of the same type. Silicon is a vital

part of all electronic devices. The well-constructed structures of two-dimensional (2D) silicon–carbon single layer compounds having different stoichiometric compositions were concluded in ref. [17]. The 2D silicon–carbon single layer may be seen as configurable materials between the pure 2D carbon single layer, graphene, and the pure 2D silicon single layer, silicene. After many attempts, the structure of the SiC sheet (with remarkable stability) was predicted, and for further details about this structure, we refer [18–20] to the readers. We consider 2D SiC compounds with a different types of silicon carbide structure-based on low-energy metastable structures for each silicon, that is, $\text{Si}_2\text{C}_3\text{-III}$.

By keeping in view the importance of the topological indices in theoretical and computational nano-sciences, we compute $B_1(G)$, $B_2(G)$, ${}^m B_1(G)$, ${}^m B_2(G)$, $HB_1(G)$, $HB_2(G)$, $HR_1(G)$, $HR_2(G)$ of the nanostructure silicon carbide $\text{Si}_2\text{C}_3\text{-III}[n, m]$.

2 Materials and methods

In Figure 1, the structure of silicon carbide $\text{Si}_2\text{C}_3\text{-III}[n, m]$ is presented, where silicon (Si) and carbon (C) are shown by blue and brown colors, respectively. By graphical visualization of silicon carbide, we fix some notations, that is, here n represents the number of connected unit cells in a row and m show the number of connected rows each with n number of cell. Figure 2 demonstrates the connections of cell in a row and connection of row with another row. In Figure 2(a), we have one row with $n = 5$

Figure 1: (a) Unit cell of $\text{Si}_2\text{C}_3\text{-III}[n, m]$, (b) $\text{Si}_2\text{C}_3\text{-III}[5,4]$.

Figure 2: (a) 2D structure of $\text{Si}_2\text{C}_3\text{-III}[5,1]$, (b) 2D structure of $\text{Si}_2\text{C}_3\text{-III}[5,2]$.

and $m = 1$ and red edges show the connection between the unit cell in a row. In Figure 2(b), we presented $\text{Si}_2\text{C}_3\text{-III}[5,2]$, green edges show the connection of the upper and lower rows. Hence, the number of vertices $\text{Si}_2\text{C}_3\text{-III}[n, m]$ is $10mn$ and the number of edges are $15mn - 2n - 3m$. For further details of silicon carbide, we refer [17,21–23].

To compute the topological indices, we defined the partitions of vertices and edges of $\text{Si}_2\text{C}_3\text{-III}[n, m]$. In $\text{Si}_2\text{C}_3\text{-III}[n, m]$, for $n, m \geq 1$, we partitioned the vertex set into three subsets depending upon the degrees of vertices. Let $V_1 = \{v \in V(G) | d(v) = 1\}$ and it has only two elements, and $V_2 = \{v \in V(G) | d(v) = 2\}$ and it has $4n + 3m - 1$ elements. Similarly, the set $V_3 = \{v \in V(G) | d(v) = 3\}$ and it has $10mn - 4n - 3m - 1$ elements. In a similar way, according to the degrees of the end vertices of the elements of $E(G)$, the set $E(G)$ of $\text{Si}_2\text{C}_3\text{-III}[n, m]$ may also be partitioned into its four subsets E_1, E_2, E_3 , and E_4 . Let $uv \in E_1$, if $d(u) = 1$, $d(v) = 3$, then E_1 contains 2 edges. If $uv \in E_2$, then $d(u) = 2$ and $d(v) = 2$, then by simple counting, we observe that E_2 contains $2m + 2$ edges. The set E_3 contains $8n + 8m - 12$ edges uv , where $d(u) = 2$ and $d(v) = 3$. The set E_4 contains $15mn - 10n - 13m + 8$ edges uv , where $d(u) = d(v) = 3$. Table 1 gives the details of partition of edges of $\text{Si}_2\text{C}_3\text{-III}[n, m]$ for $m, n \geq 1$ depending upon degrees.

Table 1: Degree-based partition of edges of $\text{Si}_2\text{C}_3\text{-III}[n, m]$

$(d(u), d(v))$	Number of edges	$d(e)$
(1, 3)	2	2
(2, 2)	$2m + 2$	2
(2, 3)	$8n + 8m - 12$	3
(3, 3)	$15mn - 10n - 13m + 8$	4

To establish our results, we adopt an approach for combinatorial enrolling, an edge allocate, a vertex portion strategy, enlist hypothetical instruments, and degree counting procedure for vertices and edges. Moreover, we use Matlab and Maple for the estimations, attestation and plotting the obtained results. For further details, see refs. [8,24–27].

3 Main results

In this section, we computed the formulas for the first and second K-Banhatti, modified K-Banhatti, K-hyper Banhatti, and hyper Revan indices of silicon carbide $\text{Si}_2\text{C}_3\text{-III}[n, m]$.

Theorem 1. Let $G \cong \text{Si}_2\text{C}_3\text{-III}[n, m]$ be the graph of silicon carbide. Then,

$$B_1[G] = 210mn - 52n - 78m + 12,$$

$$B_2[G] = 360mn - 120n - 176m + 44.$$

Proof. Let $G \cong \text{Si}_2\text{C}_3\text{-III}[n, m]$ be the graph of silicon carbide. The edge partition of $\text{Si}_2\text{C}_3\text{-III}[n, m]$ based on degrees of edges is given in Table 1. Then by using Table 1 the first K-Banhatti index of G is calculated as

$$\begin{aligned}
 B_1[G] &= \sum_{ue} [d(u) + d(e)] \\
 &= \sum_{uv=e} [d(u) + d(e) + d(v) + d(e)] \\
 &= 2[(1 + 2) + (3 + 2)] + (2m + 2)[(2 + 2) + (2 + 2)] \\
 &\quad + (8n + 8m - 12)[(2 + 3) + (3 + 3)] \\
 &\quad + (15mn - 10n - 13m + 8)[(3 + 4) + (3 + 4)] \\
 &= 210mn - 52n - 78m + 12.
 \end{aligned}$$

Second K-Banhatti index of G is calculated as

$$\begin{aligned}
 B_2[G] &= \sum_{ue} [d(u)d(v)] \\
 &= \sum_{uv=e} [d(u) \times d(e) + d(v) \times d(e)] \\
 &= 2[(1 \times 2) + (3 \times 2)] + (2m + 2)[(2 \times 2) + (2 \times 2)] \\
 &\quad + (8n + 8m - 12)[(2 \times 3) + (3 \times 3)] \\
 &\quad + (15mn - 10n - 13m + 8)[(3 \times 4) + (3 \times 4)] \\
 &= 360mn - 120n - 176m + 44. \quad \square
 \end{aligned}$$

Theorem 2. Let $G \cong \text{Si}_2\text{C}_3\text{-III}[n, m]$ be the graph of silicon carbide. Then,

$$\begin{aligned}
 {}^m B_1[G] &= \frac{30}{7}mn - \frac{8}{105}n - \frac{23}{105}m - \frac{1}{21}, \\
 {}^m B_2[G] &= \frac{5}{2}mn - \frac{5}{9}n - \frac{19}{18}m - \frac{1}{3}.
 \end{aligned}$$

Proof. Let $G \cong \text{Si}_2\text{C}_3\text{-III}[n, m]$ be the graph of silicon carbide. Then, by definition of ${}^mB_1[G]$, we have

$$\begin{aligned} {}^mB_1[G] &= \sum_{ue} \frac{1}{d(u) + d(e)} \\ &= \sum_{uv=e} \frac{1}{d(u) + d(e)} + \frac{1}{d(v) + d(e)} \\ &= 2 \left[\frac{1}{3} + \frac{1}{5} \right] + (2m + 2) \left[\frac{1}{4} + \frac{1}{4} \right] \\ &\quad + (8n + 8m - 12) \left[\frac{1}{5} + \frac{1}{6} \right] \\ &\quad + (15mn - 10n - 13m + 8) \left[\frac{1}{7} + \frac{1}{7} \right] \\ &= \frac{30}{7}mn - \frac{8}{105}n - \frac{23}{105}m - \frac{1}{21}. \end{aligned}$$

Moreover, from the definition ${}^mB_2[G]$, we have

$$\begin{aligned} {}^mB_2[G] &= \sum_{ue} \frac{1}{d(u) \times d(e)} \\ &= \sum_{uv=e} \frac{1}{d(u) \times d(e)} + \frac{1}{d(v) \times d(e)} \\ &= 2 \left[\frac{1}{2} + \frac{1}{6} \right] + (2m + 2) \left[\frac{1}{4} + \frac{1}{4} \right] \\ &\quad + (8n + 8m - 12) \left[\frac{1}{6} + \frac{1}{9} \right] \\ &\quad + (15mn - 10n - 13m + 8) \left[\frac{1}{12} + \frac{1}{12} \right] \\ &= \frac{5}{2}mn - \frac{5}{9}n - \frac{19}{18}m - \frac{1}{3}. \end{aligned} \quad \square$$

Theorem 3. Let $G \cong \text{Si}_2\text{C}_3\text{-III}[n, m]$ be the graph of silicon carbide. Then,

$$\begin{aligned} HB_1[G] &= 1470mn - 492n - 722m + 184, \\ HB_2[G] &= 4320mn - 1944n - 2744m + 1044. \end{aligned}$$

Proof. Let $G \cong \text{Si}_2\text{C}_3\text{-III}[n, m]$ be the graph of silicon carbide. Then, the first K-hyper Bhanhatti index of G is calculated as

$$\begin{aligned} HB_1[G] &= \sum_{ue} [d(u) + d(e)]^2 \\ &= \sum_{uv=e} [(d(u) + d(e))^2 + (d(v) + d(e))^2] \\ &= 2[(1 + 2)^2 + (3 + 2)^2] + (2m + 2)[(2 + 2)^2 + (2 + 2)^2] \\ &\quad + (8n + 8m - 12)[(2 + 3)^2 + (3 + 3)^2] \\ &\quad + (15mn - 10n - 13m + 8)[(3 + 4)^2 + (3 + 4)^2] \\ &= 1470mn - 492n - 722m + 184. \end{aligned}$$

Second K-hyper Bhanhatti index of G is calculated as

$$\begin{aligned} HB_2[G] &= \sum_{ue} [d(u)d(v)]^2 \\ &= \sum_{uv=e \in E} [(d(u) \times d(e))^2 + (d(v) \times d(e))^2] \\ &= 2[(1 \times 3)^2 + (3 \times 2)^2] + (2m + 2)[(2 \times 2)^2 + (2 \times 2)^2] \\ &\quad + (8n + 8m - 12)[(2 \times 3)^2 + (3 \times 3)^2] \\ &\quad + (15mn - 10n - 13m + 8)[(3 \times 4)^2 + (3 \times 4)^2] \\ &= 4320mn - 1944n - 2744m + 1044. \end{aligned} \quad \square$$

Table 2 shows partition of edges of $\text{Si}_2\text{C}_3\text{-III}[n, m]$ for $m, n \geq 1$ based on degrees along with $r_G(u)$ and $r_G(v)$.

Theorem 4. Let $G \cong \text{Si}_2\text{C}_3\text{-III}[n, m]$ be the graph of silicon carbide. Then,

$$\begin{aligned} HR_1[G] &= 60mn + 32n + 52m - 12, \\ HR_2[G] &= 60mn - 8n + 12m + 34. \end{aligned}$$

Proof. Let $G \cong \text{Si}_2\text{C}_3\text{-III}[n, m]$ be the graph of silicon carbide. Then, by definition of $HR_1[G]$, we have

$$\begin{aligned} HR_1[G] &= \sum_{uv \in E} [r_G(u) + r_G(v)]^2 \\ &= 2[3 + 1]^2 + (2m + 2)[2 + 2]^2 \\ &\quad + (8n + 8m - 12)[2 + 1]^2 \\ &\quad + (15mn - 10n - 13m + 8)[1 + 1]^2 \\ &= 60mn + 32n + 52m - 12. \end{aligned}$$

Moreover, from the definition of $HR_2[G]$, we have

$$\begin{aligned} HR_2[G] &= \sum_{uv \in E} [r_G(u)r_G(v)]^2 \\ &= 2[3 \times 1]^2 + (2m + 2)[2 \times 2]^2 \\ &\quad + (8n + 8m - 12)[2 \times 1]^2 \\ &\quad + (15mn - 10n - 13m + 8)[1 \times 1]^2 \\ &= 60mn - 8n + 12m + 34. \end{aligned} \quad \square$$

Table 2: Edge partition of $\text{Si}_2\text{C}_3\text{-III}[n, m]$ silicon carbide

$(d(u), d(v))$	Number of edges	$r_G(u)$	$r_G(v)$
(1, 3)	2	3	1
(2, 2)	$2m + 2$	2	2
(2, 3)	$8n + 8m - 12$	2	1
(3, 3)	$15mn - 10n - 13m + 8$	1	1

Figure 3: Comparison of K-Banhatti B_1 and K-Banhatti B_2 indices.

Figure 5: Comparison of K-hyper Bhanhatti HB_1 and K-hyper Bhanhatti HB_2 indices.

4 Graphical analysis

In Figure 3, K-Banhatti B_1 index is represented by blue color and K-Banhatti B_2 index is represented by cyan color. From this graph, we observe that number of unit cells in K-Banhatti B_2 index is greater than K-Banhatti B_1 index.

In Figure 4, modified K-Banhatti mB_1 index is represented by green color and modified K-Banhatti mB_2 index is represented by yellow color. From this graph, we observe that number of unit cells in modified K-Banhatti mB_1 index is greater than modified K-Banhatti mB_2 index.

In Figure 5, K-hyper Bhanhatti HB_1 index is represented by purple color and K-hyper Bhanhatti HB_2 index is represented by red color. From this graph, we observe that number of unit cells in K-hyper Bhanhatti HB_2 index is greater than K-hyper Bhanhatti HB_1 index.

Figure 4: Comparison of modified K-Banhatti mB_1 and modified K-Banhatti mB_2 indices.

5 Discussion

In reticular chemistry, it is very difficult to investigate the physico-chemical properties and characterization of large chemical structures. However, topological indices are very useful in order to study such properties of large networks. The structural characteristics of the molecules are numerically represented by using the topological indices which may be obtained by applying the theoretical concept on these large networks. In this article, we gave precise formulas of some well-known topological

Figure 6: Comparison of first K-Banhattis indices.

Figure 7: Comparison of second K-Banhattis indices.

indices for silicon carbide. In Figures 3–5, we have compared K-Banhatti B_1 and K-Banhatti B_2 indices, modified first K-Banhatti mB_1 and modified second K-Banhatti mB_2 indices, and first K-hyper Bhanhatti HB_1 and second K-hyper Bhanhatti HB_2 indices, graphically. Similarly, Figure 6(a) represents a comparison of K-Banhatti B_1 , modified K-Banhatti mB_1 and K-hyper Bhanhatti HB_1 indices, and Figure 6(b) represents a comparison of K-Banhatti B_2 , modified K-Banhatti mB_2 and K-hyper Bhanhatti HB_2 indices. Therefore, these results show that the number of unit cells in modified K-Banhatti mB_1 index and modified K-Banhatti mB_2 index is smaller than among all the above indices.

6 Conclusion and future work

Topological indices are helpful in predicting several physico-chemical properties of the chemical compound. The applications of silicon carbide $\text{Si}_2\text{C}_3\text{-III}[n, m]$ have a vital role in chemistry, especially it helps in assembly procedures and host–guest reaction. Moreover, silicon carbide is also used in bullet proof vests, car clutches, car breaks, LED lights, and detectors. We have computed topological indices, namely first and second K-Banhatti, modified K-Banhatti, K-hyper Bhanhatti, Revan, and hyper Revan indices of silicon carbide $\text{Si}_2\text{C}_3\text{-III}[n, m]$. These formulas may help to correlate the silicon carbide $\text{Si}_2\text{C}_3\text{-III}[n, m]$ structure with chemical engineering. This work motivates to explore much more about silicon carbide and raise many questions in the minds of relevant researchers, which may lead to new know more facts about it. Furthermore, the topological indices considered in this article can be computed for crystal cubic carbon

structure, benzenoid systems, or some other chemical structures.

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