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QSAR analysis for the class of silicon-carbide structures

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Graph theory has many applications in the chemistry and analysis of molecular structures and has grown popular. Topological descriptors are numeric numbers that contain chemical information and provide structural features of compounds relevant to the chemical approach. The most important components in topological indices are the physical-chemical properties of essential chemical substances. The molecular graph of $2D$ silicon-carbide structures is investigated in this paper. The scope of this paper is to determine the bond-breaking energy and the stability measure of silicon-carbides with topological indices.

KEYWORDS
QSAR/QSPR, Molecular descriptor, Topological indices, Degree, Silicon-Caribe, Energy, Stability

1 | INTRODUCTION

Chemical graph theory is an exciting topic of mathematics that combines graph theory and chemistry. Chemical graphs are studied using a schematic diagram with atoms as vertices and covalent bonds as edges. The mathematical area of chemistry known as chemical graph theory is a topological field of chemistry; it uses graph theory to chemical structure modeling. In addition, it is used to represent molecules mathematically and investigate the physico-chemical properties of molecular graphs.

Mathematical chemistry is a branch of physical chemistry in which we evaluate and estimate a molecular structure of a chemical compound using mathematical methods. In mathematical chemistry, notably in QSPR/QSAR

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studies, molecular descriptors show a vital part [1, 2]. In [3] from a molecular graph, the development of molecular descriptors is to determine numbers and using those numbers, we can describe the molecular graph. The calculation of a topological index for a molecular graph is a kind of molecular descriptor of chemical phenomena in this sense.

Chemical graph theory is a simple connected graph that begins with molecular graphs, the fundamental models. Chemical graph theory is an area of mathematical chemistry that combines graph theory, chemistry, and mathematics into one discipline [4, 5, 6]. In chemistry, the idea of valence and the concept of degree in a graph are related in some way.

Topological indices are numerical parameters obtained mathematically for a molecular graph. (For this concept, the term graph-theoretical index is more accurate than the topological index). It correlates chemical structure with biological reaction or chemical reactivity (octane numbers and other reactivity data). Since isomorphic graphs have identical values for any given topological index, these indices are referred to as graph invariant. Moreover, topological indices frequently represent the size and as well as shape of molecules.

In QSAR studies and related topics, the application of topological indices has become increasingly crucial in predicting the physicochemical properties of chemical compounds, see [7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17]. Graph theoretical and topological models have found applications in many scientific fields over the last two decades, including theoretical chemistry, toxicology, pharmacology and pharmaceutical chemistry, and others.

Graph theoretical concepts have been used in chemical physics, polymer chemistry, rationalization of physical chemistry additivity principle, computation of chemical structure quantum mechanical parameters, and documentation on chemicals. An interesting methodological framework called chemometric methods appears to provide for a good understanding of topological descriptors.

The process of this system is formalised as follows: This paper initially starts with section 1 as the introduction. Section 2, consists of a preliminary dealing with the underlying information of the silicon-carbide structures and topological indices. In section 3, we discourse some applications of the silicon-carbide. Section 4 discusses linear regression model for the topological indices. The study of section 5, encloses the discussion based on the derivation of indices for the class of silicon-carbide structures. Section 6, includes a discussion and comparison for the consider structures. And then finally, we end with the conclusion in section 7.

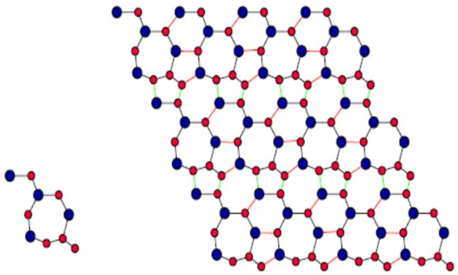
2 | PRELIMINARIES

This section deals with basic details of silicon-carbide structures. Moreover, it states some of the topological indices which we use later.

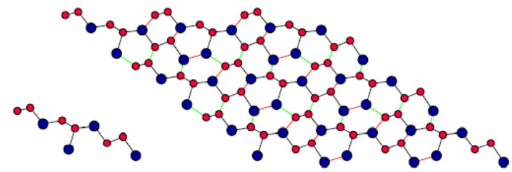
2.1 | Silicon-Carbide ($Si_2C_3 - I, II, III$)

Carbon is abundant in all three $Si - C$ 2D alloys with varying stoichiometric compositions. As a result, their more stable formations may correspond to the honeycomb structure of graphene. Our worldwide search indicates that many of these 2D $Si - C$ compounds have structures that differ significantly from graphene, as shown in Fig. 1. The low-energy $Si_2C_3 - I$ sheet has a planar structure composed of pentagonal, hexagonal and heptagonal rings. Also, each hexagonal ring is encircled by four heptagonal and two pentagonal rings.

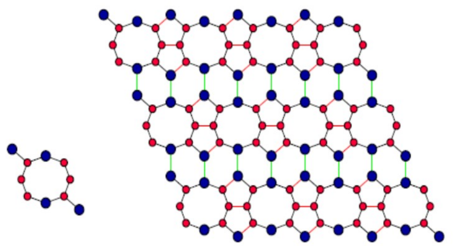
Each hexagonal ring comprises three Si atoms and three C atoms, with the Si and C atoms alternating at the vertices. Pentagonal rings are of two types: one with four C and one Si atom and the other with three C and two Si atoms. Three Si and four C atoms make up each of the heptagonal rings. Each Si atom in all polyhedral rings is attached to three C atoms in the same plane, indicating a preference for Sp^2 planar bonding. No $Si - Si$ bonds in the $Si_2C_3 - I$ sheet structure, see Fig. 1 (a).



(a) $Si_2C_3 - I$



(b) $Si_2C_3 - II$



(c) $Si_2C_3 - III$

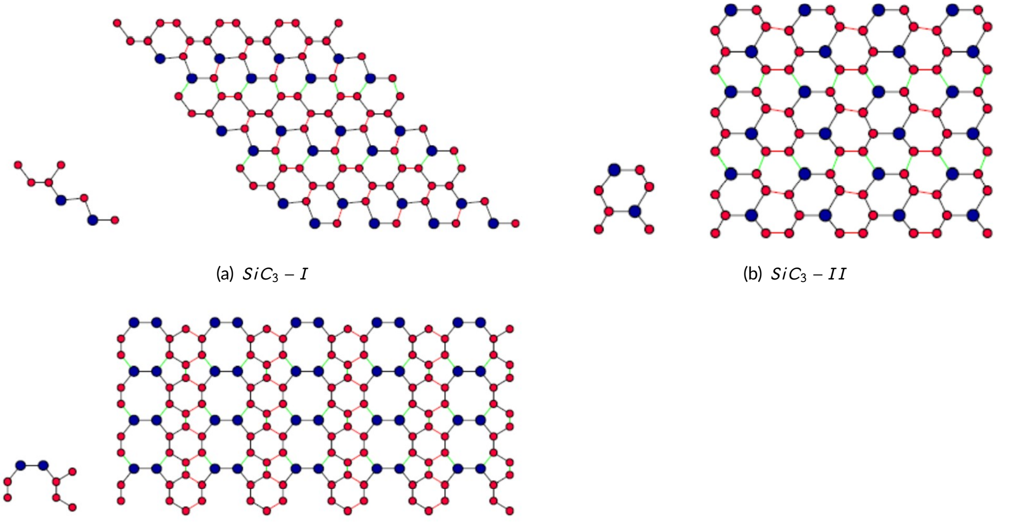
FIGURE 1 Silicon-Carbide (Si_2C_3) with unit cell on the left

The $Si_2C_3 - II$ sheet possesses more energy than the $Si_2C_3 - I$ sheet, although the polygon rings in the $Si_2C_3 - II$ sheet are entirely hexagonal, see Fig. 1 (b). Remarkably, this $Si_2C_3 - II$ sheet can be regarded as silicon-doped graphene. In contrast to the $Si_2C_3 - I$ sheet, where all Si atoms are individually placed in the sheet (no $Si - Si$ bonds), the $Si_2C_3 - II$ sheet contains discretely distributed Si atoms and Si dimers. Since silicon $Si - Si$ bonds do not favour the sp^2 hybridization, a planar structure should be energetically unfavourable, which may be a remarkable reason why $Si_2C_3 - II$ is less stable than $Si_2C_3 - I$.

$Si_2C_3 - III$ sheet contains more energy than $Si_2C_3 - I$ sheet, and it is the third lowest energy structure of Si_2C_3. The $Si_2C_3 - III$ sheet is made up of pentagonal, hexagonal, and octagonal rings, with four pentagonal and four hexagonal rings surrounding each octagonal ring, see Fig. 1 (c). Because all of the Si atoms in this system form Si dimers, the energy of the system is larger than that of the $Si_2C_3 - I$ or $Si_2C_3 - II$ sheets.

2.2 | Silicon-Carbide ($SiC_3 - I, II, III$)

A close energy range is observed for three $2D$ structures of SiC_3. As shown in Fig. 2 (a), $SiC_3 - I$ has a graphene-like hexagonal-ring structure. Each Si atom in the $SiC_3 - I$ sheet, like the $Si_2C_3 - I$ sheet, is connected to three C atoms but not to Si atoms. Chair $Si - C$ chains are formed by Si atoms and C atoms bound to Si, whereas armchair C chains are formed by other C atoms. The $SiC_3 - I$ sheet structure is formed by the interconnection of $Si - C$ chains with C chains. The $SiC_3 - I$ sheet can be thought of as silicon-doped graphene.



(a) $SiC_3 - I$ (b) $SiC_3 - II$

(c) $SiC_3 - III$

FIGURE 2 Silicon-Carbide (SiC_3) with unit cell on the left

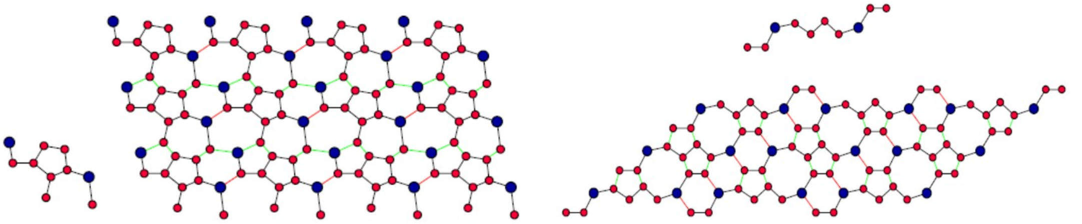
A $SiC_3 - II$ sheet is similar to a graphene sheet in structure. As in the $SiC_3 - I$ sheet, the Si atoms in $SiC_3 - II$ are also located separately, see Fig. 2 (b). As a result, the $SiC_3 - II$ sheet energy is higher than the $SiC_3 - I$ sheet energy. $SiC_3 - I$ and $SiC_3 - II$ sheets have the same structure, except for the two Si atoms in each hexagonal ring that are located differently. In $SiC_3 - I$, there are more interconnected C atoms due to the different location distribution of Si atoms compared to $SiC_3 - II$, so the $SiC_3 - I$ sheet should have a lower energy than $SiC_3 - II$. The structure of the $SiC_3 - II$ sheet cannot be broken into C chains and $Si - C$ chains because to the differing Si distributions, but the $SiC_3 - I$ sheet can.

$SiC_3 - III$ sheet structure is substantially different from $SiC_3 - I$ and $SiC_3 - II$ sheets. $SiC_3 - III$ sheets have higher symmetry than $SiC_3 - I$ and $SiC_3 - II$ sheet and it is made up of octagonal, hexagonal, and pentagonal rings, see Fig. 2 (c). In the $SiC_3 - III$ sheet, the Si atoms form dimers, whereas the C atoms form full hexagonal rings. Si dimers in a planar form are known to be energetically disfavored, whereas C hexagonal rings are favoured. As a result, despite the presence of $Si - Si$ bonds, the total energy of the $SiC_3 - III$ sheet is slightly larger than that of the $SiC_3 - II$ sheet.

2.3 | Silicon-Carbide ($SiC_4 - I, II$)

$SiC_4 - I$ sheet has pentagonal, hexagonal, and heptagonal rings, identical to $Si_2C_3 - I$ sheet. $SiC_4 - I$ sheet is the lowest-energy structure of SiC_4. Four heptagonal rings and two pentagonal rings surround each hexagonal ring. The SiC_4 structure, is illustrated in Fig. 3 (a), can be seen as an alternate arrangement of two separate chains: one made by heptagonal rings and the other by pentagonal and hexagonal rings.

The structure of the $SiC_4 - II$ sheet is similar to that of the $Si_2C_3 - III$ and $SiC_3 - III$ sheets, consisting of pentagonal, hexagonal, and octagonal rings, see Fig. 3 (b). The $SiC_4 - II$ sheet, unlike the other two forms, does not



(a) $SiC_4 - I$ (b) $SiC_4 - II$

FIGURE 3 Silicon-Carbide (SiC_4) with unit cell on the left

include silicon dimers. Because of the unfavourable octagonal rings in $2D$ carbon structures, the cohesive energy of $SiC_4 - II$ sheet is higher than that of $SiC_4 - I$ sheet.

Let $G = (V, E)$ be a graph with V as the vertex set and E as the edge set. The number of edges of G connecting with t is the degree d_t of a vertex t.

The fourth version of the atom - bond connectivity index ABC_4 was introduced by Ghorbhani et al [18, 19] as follows

$$ABC_4(G) = \sum_{st \in E(G)} \sqrt{\frac{\delta_s + \delta_t - 2}{\delta_s \delta_t}}, \tag{1}$$

where $\delta_s = \sum_{st \in E(G)} \delta_t$ and $\delta_t = \sum_{st \in E(G)} \delta_s$. See [20, 21, 22, 23, 24], the fourth version of the atom - bond connectivity index for further information on its features.

The fifth version of the geometric arithmetic index GA_5 was introduced by Graovoc et al. [25, 19] as

$$GA_5(G) = \sum_{st \in E(G)} \frac{2\sqrt{\delta_s \times \delta_t}}{\delta_s + \delta_t}. \tag{2}$$

The Neighborhood Inverse sum index [26, 27, 28] is calculated as follows

$$NI(G) = \sum_{st \in E(G)} \frac{\delta_s \times \delta_t}{\delta_s + \delta_t}. \tag{3}$$

The Neighborhood Harmonic index [26, 27, 28] is defined as

$$NH(G) = \sum_{st \in E(G)} \frac{2}{\delta_s + \delta_t}. \tag{4}$$

The Neighborhood second modified Zagreb index [29, 26] is defined as,

$$M_2^{mn}(G) = \sum_{st \in E(G)} \frac{1}{\delta_s \times \delta_t}. \tag{5}$$

The Fifth ND_e index [26, 27, 28] is given by

$$ND_5(G) = \sum_{st \in E(G)} \frac{\delta_s^2 + \delta_t^2}{\delta_s \times \delta_t}. \tag{6}$$

3 | APPLICATIONS OF $Si - C$

Silicon is an organic material that is prominent for compiling new organic molecules, including the ultra-high protons catalyst and conductivity analysis. Silicon-Carbide (SiC) is a popular non-oxide ceramic engineering material. Silicon-Carbide is a reliable material that exhibits excellent properties in the optical, mechanical, chemical and electronic fields, making it ideal for industrial applications. SiC is lightweight and typically has low dimensionality; hence it is generally used in nanoscale devices.

In [30], it has numerous industrial applications, including high temperature, voltage, and frequency semiconductor device applications. Several physical properties of silicon-carbide have been studied, including its wide bandgap, high melting temperature, high thermal conductivity, high electron drift velocity, high Young's modulus and hardness, high breakdown electric field, excellent ability to resist oxidation and corrosion, good thermal shock resistance, high strength at elevated temperatures, and excellent chemical and physical stability.

4 | REGRESSION MODELS

In our regression analysis study, we tested the following linear model.

$$P = A(TI) + B, \tag{7}$$

where P is the Physical property of Silicon-Carbide, A is a constant and B is the regression coefficient and TI represents the topological index.

A correlation between the physical property of silicon carbide structures and six topological indices can be calculated using $SPSS$ software. Using Table 1 and equation (7), we can obtain a linear model for the topological indices, they are the following,

$$eV = 9.365 - 0.154[ABC_4(G)] \tag{8}$$

$$eV = 7.526 + 0.005[GA_5(G)] \tag{9}$$

$$eV = 8.015 - 0.092[NH(G)] \tag{10}$$

$$eV = 8.086 - 0.009[NI(G)] \tag{11}$$

$$eV = 7.660 - 0.00007[ND_5(G)] \tag{12}$$

$$eV = 7.687 - 0.041[M_2^{nm}(G)] \tag{13}$$

S. No	Silicon Carbides	Cohesive energy (eV per atom)
1	$Si_2C_3 - I$	7.2660
2	$Si_2C_3 - II$	7.1712
3	$Si_2C_3 - III$	7.1446
4	$SiC_3 - I$	7.8561
5	$SiC_3 - II$	7.8409
6	$SiC_3 - III$	7.8365
7	$SiC_4 - I$	8.0631
8	$SiC_4 - II$	8.0434

TABLE 1 Predicted values of Cohesive energy

5 | TOPOLOGICAL INDICES

In this section, we will figure out how to calculate the ABC_4 index, GA_5 index, Neighborhood inverse sum index, Neighborhood Harmonic index, Fifth NDe index and Neighborhood second modified Zagreb index for the class of Silicon-Carbide. Furthermore, the characteristics of silicon-carbide molecular structures are discussed and evaluated to obtain closely related formulas.

We categorize p as the number of unit cells attached in a row. The number of rows attached with p unit cells is referred by q. From the figures, one can see how the cells are connected to other cells and also they are differentiated individually. We represent red as carbon atoms and blue as silicon atoms. For detailed information refer [31, 32, 33].

Theorem 1 *Let the Silicon-Carbide is represented by $Si_2C_3 - I[p, q]$. Then,*

1. $ABC_4(Si_2C_3 - I[p, q]) = 6.6667pq - 0.2373p - 0.3566q - 0.1730.$

2. $GA_5(Si_2C_3 - I[p, q]) = 15pq - 2.0850p - 3.1310q - 0.0382.$

3. $NH(Si_2C_3 - I[p, q]) = 1.6667pq + 0.1779p + 0.2717q + 0.0499.$

4. $NI(Si_2C_3 - I[p, q]) = 67.5pq - 21.0775p - 31.3780q + 7.6755.$

5. $ND_5(Si_2C_3 - I[p, q]) = 135pq - 3.9667p - 5.8675q + 0.5333.$

6. $M_2^{nm}(Si_2C_3 - I[p, q]) = 0.1852pq + 0.0875p + 0.1357q + 0.1020.$

Proof Consider the graph $Si_2C_3 - I[p, q]$ for $p, q \geq 2$ of silicon-carbide. According to the degrees of the vertices, the vertex is divided into three groups. The collection of vertices of degree i is designated by the symbol V_i. For $Si_2C_3 - I[p, q]$, we have $|V_1| = 2$, $|V_2| = 4p + 6q - 4$ and $|V_3| = 10pq - 4p - 6q + 2$. The edge set divides into the following sections corresponding to their neighbourhood degree sum, which are

$$\begin{aligned}
E_1 &= \{uv \in E(Si_2C_3 - I[p,q]) \mid d_u = 2 \ and \ d_v = 4\}\\
E_2 &= \{uv \in E(Si_2C_3 - I[p,q]) \mid d_u = 3 \ and \ d_v = 5\}\\
E_3 &= \{uv \in E(Si_2C_3 - I[p,q]) \mid d_u = 4 \ and \ d_v = 5\}\\
E_4 &= \{uv \in E(Si_2C_3 - I[p,q]) \mid d_u = 4 \ and \ d_v = 7\}\\
E_5 &= \{uv \in E(Si_2C_3 - I[p,q]) \mid d_u = 5 \ and \ d_v = 5\}\\
E_6 &= \{uv \in E(Si_2C_3 - I[p,q]) \mid d_u = 5 \ and \ d_v = 6\}\\
E_7 &= \{uv \in E(Si_2C_3 - I[p,q]) \mid d_u = 5 \ and \ d_v = 7\}\\
E_8 &= \{uv \in E(Si_2C_3 - I[p,q]) \mid d_u = 5 \ and \ d_v = 8\}\\
E_9 &= \{uv \in E(Si_2C_3 - I[p,q]) \mid d_u = 6 \ and \ d_v = 7\}\\
E_{10} &= \{uv \in E(Si_2C_3 - I[p,q]) \mid d_u = 6 \ and \ d_v = 8\}\\
E_{11} &= \{uv \in E(Si_2C_3 - I[p,q]) \mid d_u = 7 \ and \ d_v = 8\}\\
E_{12} &= \{uv \in E(Si_2C_3 - I[p,q]) \mid d_u = 7 \ and \ d_v = 9\}\\
E_{13} &= \{uv \in E(Si_2C_3 - I[p,q]) \mid d_u = 8 \ and \ d_v = 8\}\\
E_{14} &= \{uv \in E(Si_2C_3 - I[p,q]) \mid d_u = 8 \ and \ d_v = 9\}\\
E_{15} &= \{uv \in E(Si_2C_3 - I[p,q]) \mid d_u = 9 \ and \ d_v = 9\}
\end{aligned}$$

From the graph $Si_2C_3 - I[p,q]$, we can see that $\mid E_1 \mid = 1$, $\mid E_2 \mid = 1$, $\mid E_3 \mid = 2$, $\mid E_4 \mid = 1$, $\mid E_5 \mid = p + 2q - 1$, $\mid E_6 \mid = 1$, $\mid E_7 \mid = 2q + 2$, $\mid E_8 \mid = 2p + 2q - 5$, $\mid E_9 \mid = 4p + 2q - 7$, $\mid E_{10} \mid = 2q - 2$, $\mid E_{11} \mid = 1$, $\mid E_{12} \mid = 2p + 2q - 3$, $\mid E_{13} \mid = p + 2q - 4$, $\mid E_{14} \mid = 2p + 4q - 7$, and $\mid E_{15} \mid = 15pq - 14p - 21q + 20$.
Then, by definition ABC_4 index of $Si_2C_3 - I[p,q]$ is calculated as follows by using the edge partition,

$$\begin{aligned}
ABC_4(Si_2C_3 - I[p,q]) &= \sum_{st \in E(G)} \sqrt{\frac{\delta_s + \delta_t - 2}{\delta_s \times \delta_t}}\\
&= \sqrt{\frac{2+4-2}{2\times 4}} + \sqrt{\frac{3+5-2}{3\times 5}} + 2\sqrt{\frac{4+5-2}{4\times 5}} + \sqrt{\frac{4+7-2}{4\times 7}} + (p+2q-1)\sqrt{\frac{5+5-2}{5\times 5}}\\
&+ \sqrt{\frac{5+6-2}{5\times 6}} + (2q+2)\sqrt{\frac{5+7-2}{5\times 7}} + (2p+2q-5)\sqrt{\frac{5+8-2}{5\times 8}} + (4p+2q-7)\sqrt{\frac{6+7-2}{6\times 7}}\\
&+ (2p-2)\sqrt{\frac{6+8-2}{6\times 8}} + \sqrt{\frac{7+8-2}{7\times 8}} + (2p+2q-3)\sqrt{\frac{7+9-2}{7\times 9}} + (p+2q-4)\sqrt{\frac{8+8-2}{8\times 8}}\\
&+ (2p+4q-7)\sqrt{\frac{8+9-2}{8\times 9}} + (15pq-14p-21q+20)\sqrt{\frac{9+9-2}{9\times 9}}
\end{aligned}$$

After an easy computation, we arrive at

$$ABC_4(Si_2C_3 - I[p,q]) = 6.6667pq - 0.2373p - 0.3566q - 0.1730.$$

By definition, GA_5 index of $Si_2C_3-I[p,q]$ is calculated as follows by using the edge partition,

$$\begin{aligned}
GA_5(Si_2C_3-I[p,q]) &= \sum_{st\in E(G)} \frac{2\sqrt{\delta_s\times\delta_t}}{\delta_s+\delta_t} \\
&= \frac{2\sqrt{2\times 4}}{2+4}+\frac{2\sqrt{3\times 5}}{3+5}+2\left(\frac{2\sqrt{4\times 5}}{4+5}\right)+\frac{2\sqrt{4\times 7}}{4+7}+(p+2q-1)\left(\frac{2\sqrt{5\times 5}}{5+5}\right)+\frac{2\sqrt{5\times 6}}{5+6} \\
&+(2q+2)\left(\frac{2\sqrt{5\times 7}}{5+7}\right)+(2p+2q-5)\left(\frac{2\sqrt{5\times 8}}{5+8}\right)+(4p+2q-7)\left(\frac{2\sqrt{6\times 7}}{6+7}\right) \\
&+(2q-2)\left(\frac{2\sqrt{6\times 8}}{6+8}\right)+\frac{2\sqrt{7\times 8}}{7+8}+(2p+2q-3)\left(\frac{2\sqrt{7\times 9}}{7+9}\right)+(p+2q-4)\left(\frac{2\sqrt{8\times 8}}{8+8}\right) \\
&+(2p+4q-7)\left(\frac{2\sqrt{8\times 9}}{8+9}\right)+(15pq-14p-21q+20)\left(\frac{2\sqrt{9\times 9}}{9+9}\right)
\end{aligned}$$

We obtain our desired outcome after simplifying the above form,

$$GA_5(Si_2C_3-I[p,q]) = 15pq-2.0850p-3.1310q-0.0382.$$

By definition, NH index of $Si_2C_3-I[p,q]$ is calculated as follows by using the edge partition,

$$\begin{aligned}
NH(Si_2C_3-I[p,q]) &= \sum_{st\in E(G)} \frac{2}{\delta_s+\delta_t} \\
&= \frac{2}{2+4}+\frac{2}{3+5}+\frac{2\times 2}{4+5}+\frac{2}{4+7}+(p+2q-1)\left(\frac{2}{5+5}\right)+\left(\frac{2}{5+6}\right)+(2q+2)\left(\frac{2}{5+7}\right) \\
&+(2p+2q-5)\left(\frac{2}{5+8}\right)+(4p+2q-7)\left(\frac{2}{6+7}\right)+(2q-2)\left(\frac{2}{6+8}\right)+\left(\frac{2}{7+8}\right)+(2p+2q-3)\left(\frac{2}{7+9}\right) \\
&+(p+2q-4)\left(\frac{2}{8+8}\right)+(2p+4q-7)\left(\frac{2}{8+9}\right)+(15pq-14p-21q+20)\left(\frac{2}{9+9}\right)
\end{aligned}$$

After an easy computation, we arrive at

$$NH(Si_2C_3-II[p,q]) = 1.6667pq+0.1779p+0.2717q+0.0499.$$

By definition, NI index of $Si_2C_3-II[p,q]$ is calculated as follows by using the edge partition,

$$\begin{aligned}
NI(Si_2C_3-I[p,q]) &= \sum_{st\in E(G)} \frac{\delta_s\times\delta_t}{\delta_s+\delta_t} \\
&= \left(\frac{2\times 4}{2+4}\right)+\left(\frac{3\times 5}{3+5}\right)+2\left(\frac{4\times 5}{4+5}\right)+\left(\frac{4\times 7}{4+7}\right)+(p+2q-2)\left(\frac{5\times 5}{5+5}\right)+\left(\frac{5\times 6}{5+6}\right) \\
&+(2q+2)\left(\frac{5\times 7}{5+7}\right)+(2p+2q-5)\left(\frac{5\times 8}{5+8}\right)+(4p+2q-7)\left(\frac{6\times 7}{6+7}\right)+(2q-2)\left(\frac{6\times 8}{6+8}\right) \\
&+\left(\frac{7\times 8}{7+8}\right)+(2p+2q-3)\left(\frac{7\times 9}{7+9}\right)+(p+2q-4)\left(\frac{8\times 8}{8+8}\right)+(2p+4q-7)\left(\frac{8\times 9}{8+9}\right) \\
&+(15pq-14p-21q+20)\left(\frac{9\times 9}{9+9}\right)
\end{aligned}$$

We obtain our desired outcome after simplifying the above form,

$$NI(Si_2C_3-I[p,q]) = 67.5pq - 21.0775p - 31.3780q + 7.6755.$$

By definition, ND_5 index of $Si_2C_3-I[p,q]$ is calculated as follows by using the edge partition,

$$\begin{aligned}
ND_5(Si_2C_3-I[p,q]) &= \sum_{st\in E(G)} \frac{\delta_s^2+\delta_t^2}{\delta_s\times\delta_t} \\
&= \left(\frac{2^2+4^2}{2\times 4}\right) + \left(\frac{3^2+5^2}{3\times 5}\right) + 2\left(\frac{4^2+5^2}{4\times 5}\right) + \left(\frac{4^2+7^2}{4\times 7}\right) + (p+2q-1)\left(\frac{5^2+5^2}{5\times 5}\right) \\
&+ \left(\frac{5^2+6^2}{5\times 6}\right) + (2q+2)\left(\frac{5^2+7^2}{5\times 7}\right) + (2p+2q-5)\left(\frac{5^2+8^2}{5\times 8}\right) + (4p+2q-7)\left(\frac{6^2+7^2}{6\times 7}\right) \\
&+ (2q-2)\left(\frac{6^2+8^2}{6\times 8}\right) + \left(\frac{7^2+8^2}{7\times 8}\right) + (2p+2q-3)\left(\frac{7^2+9^2}{7\times 9}\right) + (p+2q-4)\left(\frac{8^2+8^2}{8\times 8}\right) \\
&+ (2p+4q-7)\left(\frac{8^2+9^2}{8\times 9}\right) + (15pq-14p-21q+20)\left(\frac{9^2+9^2}{9\times 9}\right)
\end{aligned}$$

After an easy computation, we arrive at

$$ND_5(Si_2C_3-I[p,q]) = 135pq - 3.9667p - 5.8675q + 0.5333.$$

By definition, M_2^{nm} index of $Si_2C_3-I[p,q]$ is calculated as follows by using the edge partition,

$$\begin{aligned}
M_2^{mn}(Si_2C_3-I[p,q]) &= \sum_{st\in E(G)} \frac{1}{\delta_s\times\delta_t} \\
&= \frac{1}{2\times 4} + \frac{1}{3\times 5} + \frac{2}{4\times 5} + \frac{1}{4\times 7} + (p+2q-1)\left(\frac{1}{5\times 5}\right) + \frac{1}{5\times 6} + (2q+2)\left(\frac{1}{5\times 7}\right) \\
&+ (2p+2q-5)\left(\frac{1}{5\times 8}\right) + (4p+2q-7)\left(\frac{1}{6\times 7}\right) + (2q-2)\left(\frac{1}{6\times 8}\right) + \left(\frac{1}{7\times 8}\right) \\
&+ (2p+2q-3)\left(\frac{1}{7\times 9}\right) + (p+2q-4)\left(\frac{1}{8\times 8}\right) + (2p+4q-7)\left(\frac{1}{8\times 9}\right) \\
&+ (15pq-14p-21q+20)\left(\frac{1}{9\times 9}\right)
\end{aligned}$$

We obtain our desired outcome after simplifying the above form,

$$M_2^{nm}(Si_2C_3-I[p,q]) = 0.1852pq + 0.0875p + 0.1357q + 0.1020.$$

Theorem 2 *Let the Silicon-Carbide is represented by $Si_2C_3-II[p,q]$. Then,*

1. $ABC_4(Si_2C_3-II[p,q]) = 6.6667pq - 0.3566p - 0.3566q - 0.2996.$

2. $GA_5(Si_2C_3-II[p,q]) = 15pq - 3.1310p - 3.1310q + 0.1080.$

3. $NH(Si_2C_3-II[p,q]) = 1.6667pq + 0.2717p + 0.2717q + 0.2079.$

4. $NI(Si_2C_3 - II[p,q]) = 67.5pq - 31.3780p - 31.3780q + 12.1758.$

5. $ND_5(Si_2C_3 - II[p,q]) = 30pq - 4.9246p - 4.9246q - 0.8214.$

6. $M_2^{nm}(Si_2C_3 - II[p,q]) = 0.1852pq + 0.1357p + 0.1357q + 0.2675.$

Proof Consider the graph $Si_2C_3 - II[p,q]$ for $p,q \geq 2$ of silicon-carbide. According to the degrees of the vertices, the vertex is divided into three groups. The collection of vertices of degree i is designated by the symbol V_i. For $Si_2C_3 - II[p,q]$, we have $|V_1| = 2$, $|V_2| = 6p + 6q - 6$ and $|V_3| = 10pq - 6p - 6q + 4$. The edge set divides into the following sections corresponding to their neighbourhood degree sum, which are

$$E_1 = \{uv \in E(Si_2C_3 - II[p,q]) \mid d_u = 2 \ and \ d_v = 3\}$$
$$E_2 = \{uv \in E(Si_2C_3 - II[p,q]) \mid d_u = 3 \ and \ d_v = 7\}$$
$$E_3 = \{uv \in E(Si_2C_3 - II[p,q]) \mid d_u = 3 \ and \ d_v = 4\}$$
$$E_4 = \{uv \in E(Si_2C_3 - II[p,q]) \mid d_u = 4 \ and \ d_v = 5\}$$
$$E_5 = \{uv \in E(Si_2C_3 - II[p,q]) \mid d_u = 5 \ and \ d_v = 5\}$$
$$E_6 = \{uv \in E(Si_2C_3 - II[p,q]) \mid d_u = 5 \ and \ d_v = 7\}$$
$$E_7 = \{uv \in E(Si_2C_3 - II[p,q]) \mid d_u = 5 \ and \ d_v = 8\}$$
$$E_8 = \{uv \in E(Si_2C_3 - II[p,q]) \mid d_u = 6 \ and \ d_v = 7\}$$
$$E_9 = \{uv \in E(Si_2C_3 - II[p,q]) \mid d_u = 6 \ and \ d_v = 8\}$$
$$E_{10} = \{uv \in E(Si_2C_3 - II[p,q]) \mid d_u = 7 \ and \ d_v = 8\}$$
$$E_{11} = \{uv \in E(Si_2C_3 - II[p,q]) \mid d_u = 7 \ and \ d_v = 9\}$$
$$E_{12} = \{uv \in E(Si_2C_3 - II[p,q]) \mid d_u = 8 \ and \ d_v = 8\}$$
$$E_{13} = \{uv \in E(Si_2C_3 - II[p,q]) \mid d_u = 8 \ and \ d_v = 9\}$$
$$E_{14} = \{uv \in E(Si_2C_3 - II[p,q]) \mid d_u = 9 \ and \ d_v = 9\}$$

From the graph $Si_2C_3 - II[p,q]$, we can see that $|E_1| = 2$, $|E_2| = 1$, $|E_3| = 2$, $|E_4| = 2$, $|E_5| = 2p + 2q - 4$, $|E_6| =$ 2p+2q, $|E_7| = 2p + 2q - 6$, $|E_8| = 2p + 2q - 2$, $|E_9| = 2p + 2q - 6$, $|E_{10}| = 4$, $|E_{11}| = 2p + 2q - 3$, $|E_{12}| = 2p + 2q - 8$, $|E_{13}| = 4p + 4q - 12$, and $|E_{14}| = 15pq - 21p - 21q + 30$.
Then, by definition ABC_4 index of $Si_2C_3 - II[p,q]$ is calculated as follows by using the edge partition,

$$\begin{aligned} ABC_4(Si_2C_3 - II[p,q]) &= \sum_{st \in E(G)} \sqrt{\frac{\delta_s + \delta_t - 2}{\delta_s \times \delta_t}} \\ &= 2\sqrt{\frac{2+3-2}{2\times 3}} + \sqrt{\frac{3+7-2}{3\times 7}} + 2\sqrt{\frac{3+4-2}{3\times 4}} + 2\sqrt{\frac{4+5-2}{4\times 5}} + (2p+2q-4)\sqrt{\frac{5+5-2}{5\times 5}} \\ &+ (2p+2q)\sqrt{\frac{5+7-2}{5\times 7}} + (2p+2q-6)\sqrt{\frac{5+8-2}{5\times 8}} + (2p+2q-2)\sqrt{\frac{6+7-2}{6\times 7}} + (2p+2q-6)\sqrt{\frac{6+8-2}{6\times 8}} \\ &+ 4\sqrt{\frac{7+8-2}{7\times 8}} + (2p+2q-3)\sqrt{\frac{7+9-2}{7\times 9}} + (2p+2q-8)\sqrt{\frac{8+8-2}{8\times 8}} + (4p+4q-12)\sqrt{\frac{8+9-2}{8\times 9}} \end{aligned}$$

$$+ (15pq - 21p - 21q + 30)\sqrt{\frac{9+9-2}{9\times 9}}$$

After an easy computation, we arrive at

$$ABC_4(Si_2C_3 - II[p,q]) = 6.6667pq - 0.3566p - 0.3566q - 0.2996.$$

By definition, GA_5 index of $Si_2C_3 - II[p,q]$ is calculated as follows by using the edge partition,

$$\begin{aligned}
GA_5(Si_2C_3 - II[p,q]) &= \sum_{st\in E(G)} \frac{2\sqrt{\delta_s \times \delta_t}}{\delta_s + \delta_t} \\
&= \frac{4\sqrt{2\times 3}}{2+3} + \frac{2\sqrt{3\times 7}}{3+7} + \frac{4\sqrt{3\times 4}}{3+4} + \frac{4\sqrt{4\times 5}}{4+5} + (2p+2q-4)\left(\frac{2\sqrt{5\times 5}}{5+5}\right) + (2p+2q)\frac{2\sqrt{5\times 7}}{5+7} \\
&+ (2p+2q-6)\left(\frac{2\sqrt{5\times 8}}{5+8}\right) + (2p+2q-2)\left(\frac{2\sqrt{6\times 7}}{6+7}\right) + (2p+2q-6)\left(\frac{2\sqrt{6\times 8}}{6+8}\right) \\
&+ \frac{8\sqrt{7\times 8}}{7+8} + (2p+2q-3)\left(\frac{2\sqrt{7\times 9}}{7+9}\right) + (2p+2q-8)\left(\frac{2\sqrt{8\times 8}}{8+8}\right) + (4p+4q-12)\left(\frac{2\sqrt{8\times 9}}{8+9}\right) \\
&+ (15pq - 21p - 21q + 30)\left(\frac{2\sqrt{9\times 9}}{9+9}\right)
\end{aligned}$$

We obtain our desired outcome after simplifying the above form,

$$GA_5(Si_2C_3 - II[p,q]) = 15pq - 3.1310p - 3.1310q + 0.1080.$$

By definition, NH index of $Si_2C_3 - II[p,q]$ is calculated as follows by using the edge partition,

$$\begin{aligned}
NH(Si_2C_3 - II[p,q]) &= \sum_{st\in E(G)} \frac{2}{\delta_s + \delta_t} \\
&= \frac{2\times 2}{2+3} + \frac{2}{3+7} + \frac{2\times 2}{3+4} + \frac{2\times 2}{4+5} + (2p+2q-4)\left(\frac{2}{5+5}\right) + (2p+2q)\left(\frac{2}{5+7}\right) + (2p+2q-6)\left(\frac{2}{5+8}\right) \\
&+ (2p+2q-2)\left(\frac{2}{6+7}\right) + (2p+2q-6)\left(\frac{2}{6+8}\right) + \left(\frac{4\times 2}{7+8}\right) + (2p+2q-3)\left(\frac{2}{7+9}\right) \\
&+ (2p+2q-8)\left(\frac{2}{8+8}\right) + (4p+4q-12)\left(\frac{2}{8+9}\right) + (15pq - 21p - 21q + 30)\left(\frac{2}{9+9}\right)
\end{aligned}$$

After an easy computation, we arrive at

$$NH(Si_2C_3 - II[p,q]) = 1.6667pq + 0.2717p + 0.2717q + 0.2079.$$

By definition, NI index of $Si_2C_3 - II[p,q]$ is calculated as follows by using the edge partition,

$$NI(Si_2C_3 - II[p,q]) = \sum_{st\in E(G)} \frac{\delta_s \times \delta_t}{\delta_s + \delta_t}$$

$$= 2\left(\frac{2\times 3}{2+3}\right) + \left(\frac{3\times 7}{3+7}\right) + 2\left(\frac{3\times 4}{3+4}\right) + 2\left(\frac{4\times 5}{4+5}\right) + (2p+2q-4)\left(\frac{5\times 5}{5+5}\right) + (2p+2q)\left(\frac{5\times 7}{5+7}\right)$$
$$+ (2p+2q-6)\left(\frac{5\times 8}{5+8}\right) + (2p+2q-2)\left(\frac{6\times 7}{6+7}\right) + (2p+2q-6)\left(\frac{6\times 8}{6+8}\right) + 4\left(\frac{7\times 8}{7+8}\right)$$
$$+ (2p+2q-3)\left(\frac{7\times 9}{7+9}\right) + (2p+2q-8)\left(\frac{8\times 8}{8+8}\right) + (4p+4q-12)\left(\frac{8\times 8}{8+8}\right) + (15pq-21p-21q+30)\left(\frac{9\times 9}{9+9}\right)$$

We obtain our desired outcome after simplifying the above form,

$$NI(Si_2C_3 - II[p,q]) = 67.5pq - 31.3780p - 31.3780q + 12.1758.$$

By definition, ND_5 index of $Si_2C_3 - II[p,q]$ is calculated as follows by using the edge partition,

$$ND_5(Si_2C_3 - II[p,q]) = \sum_{st\in E(G)} \frac{\delta_s^2 + \delta_t^2}{\delta_s \times \delta_t}$$
$$= 2\left(\frac{2^2+3^2}{2\times 3}\right) + \left(\frac{3^2+7^2}{3\times 7}\right) + 2\left(\frac{3^2+4^2}{3\times 4}\right) + 2\left(\frac{4^2+5^2}{4\times 5}\right) + (2p+2q-4)\left(\frac{5^2+5^2}{5\times 5}\right)$$
$$+ (2p+2q)\left(\frac{5^2+7^2}{5\times 7}\right) + (2p+2q-6)\left(\frac{5^2+8^2}{5\times 8}\right) + (2p+2q-2)\left(\frac{6^2+7^2}{6\times 7}\right) + (2p+2q-6)\left(\frac{6^2+8^2}{6\times 8}\right)$$
$$+ 4\left(\frac{7^2+8^2}{7\times 8}\right) + (2p+2q-3)\left(\frac{7^2+9^2}{7\times 9}\right) + (2p+2q-8)\left(\frac{8^2+8^2}{8\times 8}\right) + (4p+4q-12)\left(\frac{8^2+9^2}{8\times 9}\right)$$
$$+ (15pq-21p-21q+30)\left(\frac{9^2+9^2}{9\times 9}\right)$$

After an easy computation, we arrive at

$$ND_5(Si_2C_3 - II[p,q]) = 30pq - 4.9246p - 4.9246q - 0.8214.$$

By definition, M_2^{nm} index of $Si_2C_3 - II[p,q]$ is calculated as follows by using the edge partition,

$$M_2^{mn}(Si_2C_3 - II[p,q]) = \sum_{st\in E(G)} \frac{1}{\delta_s \times \delta_t}$$
$$= \frac{2}{2\times 3} + \frac{1}{3\times 7} + \frac{2}{3\times 4} + \frac{2}{4\times 5} + (2p+2q-4)\left(\frac{1}{5\times 5}\right) + (2p+2q)\left(\frac{1}{5\times 7}\right) + (2p+2q-6)\left(\frac{1}{5\times 8}\right)$$
$$+ (2p+2q-2)\left(\frac{1}{6\times 7}\right) + (2p+2q-6)\left(\frac{1}{6\times 8}\right) + 4\left(\frac{1}{7\times 8}\right) + (2p+2q-3)\left(\frac{1}{7\times 9}\right)$$
$$+ (2p+2q-8)\left(\frac{1}{8\times 8}\right) + (4p+4q-12)\left(\frac{1}{8\times 9}\right) + (15pq-21p-21q+30)\left(\frac{1}{9\times 9}\right)$$

We obtain our desired outcome after simplifying the above form,

$$M_2^{nm}(Si_2C_3 - II[p,q]) = 0.1852pq + 0.1357p + 0.1357q + 0.2675.$$

Theorem 3 *Let the Silicon-Carbide is represented by $Si_2C_3 - III[p,q]$. Then,*

1. $ABC_4(Si_2C_3 - III[p,q]) = 6.6667pq - 0.2425p - 0.3534q - 0.1671.$

2. $GA_5(Si_2C_3 - III[p,q]) = 15pq + 2.9057p - 3.0992q + 0.0356.$

3. $NH(Si_2C_3 - III[p,q]) = 1.6667pq + 0.2085p + 0.2932q + 0.0431.$

4. $NI(Si_2C_3 - III[p,q]) = 67.5pq - 21.4038p - 31.1603q + 7.5293.$

5. $ND_5(Si_2C_3 - III[p,q]) = 30pq - 3.5556p - 5.1937q - 0.2698.$

6. $M_2^{nm}(Si_2C_3 - III[p,q]) = 0.1851pq + 0.0811p + 0.1431q + 0.0801.$

Proof Consider the graph $Si_2C_3 - III[p,q]$ for $p,q \geq 2$ of silicon-carbide. According to the degrees of the vertices, the vertex is divided into three groups. The collection of vertices of degree i is designated by the symbol V_i. For $Si_2C_3 - II[p,q]$, we have $|V_1| = 2$, $|V_2| = 4p + 6q - 4$ and $|V_3| = 10pq - 4p - 6q + 2$. The edge set divides into the following sections corresponding to their neighbourhood degree sum, which are

$$\begin{aligned}
E_1 &= \{uv \in E(Si_2C_3 - III[p,q]) \mid d_u = 3 \ and \ d_v = 5\} \\
E_2 &= \{uv \in E(Si_2C_3 - III[p,q]) \mid d_u = 4 \ and \ d_v = 5\} \\
E_3 &= \{uv \in E(Si_2C_3 - III[p,q]) \mid d_u = 5 \ and \ d_v = 5\} \\
E_4 &= \{uv \in E(Si_2C_3 - III[p,q]) \mid d_u = 5 \ and \ d_v = 6\} \\
E_5 &= \{uv \in E(Si_2C_3 - III[p,q]) \mid d_u = 5 \ and \ d_v = 7\} \\
E_6 &= \{uv \in E(Si_2C_3 - III[p,q]) \mid d_u = 6 \ and \ d_v = 7\} \\
E_7 &= \{uv \in E(Si_2C_3 - III[p,q]) \mid d_u = 7 \ and \ d_v = 9\} \\
E_8 &= \{uv \in E(Si_2C_3 - III[p,q]) \mid d_u = 9 \ and \ d_v = 9\}
\end{aligned}$$

From the graph $Si_2C_3 - III[p,q]$, we can see that $\mid E_1 \mid = 2$, $\mid E_2 \mid = 4$, $\mid E_3 \mid = 2q$, $\mid E_4 \mid = 2$, $\mid E_5 \mid = 4q - 2$, $\mid E_6 \mid = 8p + 4q - 14$, $\mid E_7 \mid = 4p + 4q - 8$, and $\mid E_8 \mid = 15pq - 14p - 17q + 16$.

Then, by definition ABC_4 index of $Si_2C_3 - III[p,q]$ is calculated as follows by using the edge partition,

$$\begin{aligned}
ABC_4(Si_2C_3 - III[p,q]) &= \sum_{st \in E(G)} \sqrt{\frac{\delta_s + \delta_t - 2}{\delta_s \times \delta_t}} \\
&= 2\sqrt{\frac{3+5-2}{3 \times 5}} + 4\sqrt{\frac{4+5-2}{4 \times 5}} + 2q\sqrt{\frac{5+5-2}{5 \times 5}} + 2\sqrt{\frac{5+6-2}{5 \times 6}} + (4q-2)\sqrt{\frac{5+7-2}{5 \times 7}} \\
&+ (8p + 4q - 14)\sqrt{\frac{6+7-2}{6 \times 7}} + (4p + 4q - 8)\sqrt{\frac{7+9-2}{7 \times 9}} + (15pq - 14p - 17q + 16)\sqrt{\frac{9+9-2}{9 \times 9}}
\end{aligned}$$

After an easy computation, we arrive at

$$ABC_4(Si_2C_3 - III[p,q]) = 6.6667pq - 0.2425p - 0.3534q - 0.1671.$$

By definition, GA_5 index of $Si_2C_3-III[p,q]$ is calculated as follows by using the edge partition,

$$\begin{aligned}GA_5(Si_2C_3-III[p,q]) &= \sum_{st\in E(G)} \frac{2\sqrt{\delta_s\times\delta_t}}{\delta_s+\delta_t}\\ &= \frac{4\sqrt{3\times5}}{3+5}+\frac{8\sqrt{4\times5}}{4+5}+2q\left(\frac{2\sqrt{5\times5}}{5+5}\right)+\frac{4\sqrt{5\times6}}{5+6}+(4q-2)\left(\frac{2\sqrt{5\times7}}{5+7}\right)+(8p+4q-14)\frac{2\sqrt{6\times7}}{6+7}\\ &+(4p+4q-8)\left(\frac{2\sqrt{7\times9}}{7+9}\right)+(15pq-14p-17q+16)\left(\frac{2\sqrt{9\times9}}{9+9}\right)\end{aligned}$$

We obtain our desired outcome after simplifying the above form,

$$GA_5(Si_2C_3-III[p,q]) = 15pq+2.9057p-3.0992q+0.0356.$$

By definition, NH index of $Si_2C_3-III[p,q]$ is calculated as follows by using the edge partition,

$$\begin{aligned}NH(Si_2C_3-III[p,q]) &= \sum_{st\in E(G)} \frac{2}{\delta_s+\delta_t}\\ &= \frac{2\times2}{3+5}+\frac{4\times2}{4+5}+2q\left(\frac{2}{5+5}\right)+\frac{2\times2}{5+6}+(4q-2)\left(\frac{2}{5+7}\right)+(8p+4q-14)\left(\frac{2}{6+7}\right)\\ &+(4p+4q-8)\left(\frac{2}{7+9}\right)+(15pq-14p-17q+16)\left(\frac{2}{9+9}\right)\end{aligned}$$

After an easy computation, we arrive at

$$NH(Si_2C_3-III[p,q]) = 1.6667pq+0.2085p+0.2932q+0.0431.$$

By definition, NI index of $Si_2C_3-III[p,q]$ is calculated as follows by using the edge partition,

$$\begin{aligned}NI(Si_2C_3-III[p,q]) &= \sum_{st\in E(G)} \frac{\delta_s\times\delta_t}{\delta_s+\delta_t}\\ &= 2\left(\frac{3\times5}{3+5}\right)+4\left(\frac{4\times5}{4+5}\right)+2q\left(\frac{5\times5}{5+5}\right)+2\left(\frac{5\times6}{5+6}\right)+(4q-2)\left(\frac{5\times7}{5+7}\right)+(8p+4q-14)\left(\frac{6\times7}{6+7}\right)\\ &+(4p+4q-8)\left(\frac{7\times9}{7+9}\right)+(15pq-14p-17q+16)\left(\frac{9\times9}{9+9}\right)\end{aligned}$$

We obtain our desired outcome after simplifying the above form,

$$NI(Si_2C_3-III[p,q]) = 67.5pq-21.4038p-31.1603q+7.5293.$$

By definition, ND_5 index of $Si_2C_3-III[p,q]$ is calculated as follows by using the edge partition,

$$ND_5(Si_2C_3-III[p,q]) = \sum_{st\in E(G)} \frac{\delta_s^2+\delta_t^2}{\delta_s\times\delta_t}$$

$$= 2\left(\frac{3^2+5^2}{3\times 5}\right)+4\left(\frac{4^2+5^2}{4\times 5}\right)+2q\left(\frac{5^2+5^2}{5\times 5}\right)+2\left(\frac{5^2+6^2}{5\times 6}\right)+(4q-2)\left(\frac{5^2+7^2}{5\times 7}\right)$$
$$+(8p+4q-14)\left(\frac{6^2+7^2}{6\times 7}\right)+(4p+4q-8)\left(\frac{7^2+9^2}{7\times 9}\right)+(15pq-14p-17q+16)\left(\frac{9^2+9^2}{9\times 9}\right)$$

After an easy computation, we arrive at

$$ND_5(Si_2C_3-III[p,q]) = 30pq-3.5556p-5.1937q-0.2698.$$

By definition, M_2^{nm} index of $Si_2C_3-III[p,q]$ is calculated as follows by using the edge partition,

$$M_2^{mn}(Si_2C_3-III[p,q]) = \sum_{st\in E(G)}\frac{1}{\delta_s\times\delta_t}$$
$$= \frac{2}{3\times 5}+\frac{4}{4\times 5}+\frac{2q}{5\times 5}+\frac{2}{5\times 6}+(4q-2)\left(\frac{1}{5\times 7}\right)+(8p+4q-14)\left(\frac{1}{6\times 7}\right)$$
$$+(4p+4q-8)\left(\frac{1}{7\times 9}\right)+(15pq-14p-17q+16)\left(\frac{1}{9\times 9}\right)$$

We obtain our desired outcome after simplifying the above form,

$$M_2^{nm}(Si_2C_3-III[p,q]) = 0.1851pq+0.0811p+0.1431q+0.0801.$$

Theorem 4 *Let the Silicon-Carbide is represented by $SiC_3-I[p,q]$. Then,*

1. $ABC_4(SiC_3-I[p,q]) = 5.3566pq-0.3019p-0.3890q-0.2011.$
2. $GA_5(SiC_3-I[p,q]) = 12pq-2.1149p-3.1332q+0.0658.$
3. $NH(SiC_3-I[p,q]) = 1.3472pq+0.1388p+0.2522q+0.1060.$
4. $NI(SiC_3-I[p,q]) = 53.5pq-19.2511p-30.6446q+8.2757.$
5. $ND_5(SiC_3-I[p,q]) = 24pq-3.0444p-4.9067q-0.45.$
6. $M_2^{nm}(SiC_3-I[p,q]) = 0.1514pq+0.0841p+0.1313q+0.1718.$

Proof Consider the graph $SiC_3-I[p,q]$ for $p,q\geq 2$ of silicon-carbide. According to the degrees of the vertices, the vertex is divided into three groups. The collection of vertices of degree i is designated by the symbol V_i. For $SiC_3-I[p,q]$, we have $|V_1|=3$, $|V_2|=4p+6q-6$ and $|V_3|=8pq-4p-6q+3$. The edge set divides into the following sections corresponding to their sum of the degrees of the neighbourhood, which are

$$\begin{aligned}
E_1 &= \{uv \in E(SiC_3 - I[p,q]) \mid d_u = 2 \; and \; d_v = 4\}\\
E_2 &= \{uv \in E(SiC_3 - I[p,q]) \mid d_u = 2 \; and \; d_v = 3\}\\
E_3 &= \{uv \in E(SiC_3 - I[p,q]) \mid d_u = 3 \; and \; d_v = 7\}\\
E_4 &= \{uv \in E(SiC_3 - I[p,q]) \mid d_u = 3 \; and \; d_v = 5\}\\
E_5 &= \{uv \in E(SiC_3 - I[p,q]) \mid d_u = 5 \; and \; d_v = 5\}\\
E_6 &= \{uv \in E(SiC_3 - I[p,q]) \mid d_u = 4 \; and \; d_v = 6\}\\
E_7 &= \{uv \in E(SiC_3 - I[p,q]) \mid d_u = 5 \; and \; d_v = 6\}\\
E_8 &= \{uv \in E(SiC_3 - I[p,q]) \mid d_u = 5 \; and \; d_v = 7\}\\
E_9 &= \{uv \in E(SiC_3 - I[p,q]) \mid d_u = 5 \; and \; d_v = 8\}\\
E_{10} &= \{uv \in E(SiC_3 - I[p,q]) \mid d_u = 6 \; and \; d_v = 6\}\\
E_{11} &= \{uv \in E(SiC_3 - I[p,q]) \mid d_u = 6 \; and \; d_v = 7\}\\
E_{12} &= \{uv \in E(SiC_3 - I[p,q]) \mid d_u = 6 \; and \; d_v = 8\}\\
E_{13} &= \{uv \in E(SiC_3 - I[p,q]) \mid d_u = 7 \; and \; d_v = 8\}\\
E_{14} &= \{uv \in E(SiC_3 - I[p,q]) \mid d_u = 7 \; and \; d_v = 9\}\\
E_{15} &= \{uv \in E(SiC_3 - I[p,q]) \mid d_u = 8 \; and \; d_v = 8\}\\
E_{16} &= \{uv \in E(SiC_3 - I[p,q]) \mid d_u = 8 \; and \; d_v = 9\}\\
E_{17} &= \{uv \in E(SiC_3 - I[p,q]) \mid d_u = 9 \; and \; d_v = 9\}
\end{aligned}$$

From the graph $SiC_3 - I[p,q]$, we can see that $\mid E_1 \mid = 1$, $\mid E_2 \mid = 1$, $\mid E_3 \mid = 1$, $\mid E_4 \mid = 1$, $\mid E_5 \mid = 2p + 2q - 4$, $\mid E_6 \mid = 1$, $\mid E_7 \mid = 1$, $\mid E_8 \mid = 2q + 1$, $\mid E_9 \mid = 4p + 2q - 9$, $\mid E_{10} \mid = 1$, $\mid E_{11} \mid = 2q - 1$, $\mid E_{12} \mid = 2q - 2$, $\mid E_{13} \mid = q$, $\mid E_{14} \mid = 2q - 1$, $\mid E_{15} \mid = pq - p - q + 3$, $\mid E_{16} \mid = 4p + 4q - 13$, and $\mid E_{17} \mid = 11pq - 11p - 19q + 19$.

Then, by definition ABC_4 index of $SiC_3 - I[p,q]$ is calculated as follows by using the edge partition,

$$\begin{aligned}
ABC_4(SiC_3 - I[p,q]) &= \sum_{st \in E(G)} \sqrt{\frac{\delta_s + \delta_t - 2}{\delta_s \delta_t}}\\
&= \sqrt{\frac{2+4-2}{2\times 4}} + \sqrt{\frac{2+3-2}{2\times 3}} + \sqrt{\frac{3+7-2}{3\times 7}} + \sqrt{\frac{3+5-2}{3\times 5}} + (2p+2q-4)\sqrt{\frac{5+5-2}{5\times 5}}\\
&+ \sqrt{\frac{4+6-2}{4\times 6}} + \sqrt{\frac{5+6-2}{5\times 6}} + (2q+1)\sqrt{\frac{5+7-2}{5\times 7}} + (4p+2q-9)\sqrt{\frac{5+8-2}{5\times 8}} + \sqrt{\frac{6+6-2}{6\times 6}}\\
&+ (2q-1)\sqrt{\frac{6+7-2}{6\times 7}} + (2q-2)\sqrt{\frac{6+8-2}{6\times 8}} + q\sqrt{\frac{7+8-2}{7\times 8}} + (2q-1)\sqrt{\frac{7+9-2}{7\times 9}}\\
&+ (pq-p-q+3)\sqrt{\frac{8+8-2}{8\times 8}} + (4p+4q-13)\sqrt{\frac{8+9-2}{8\times 9}} + (11pq-11p-19q+19)\sqrt{\frac{9+9-2}{9\times 9}}
\end{aligned}$$

After an easy computation, we arrive at

$$ABC_4(SiC_3 - I[p,q]) = 5.3566pq - 0.3019p - 0.3890q - 0.2011.$$

By definition, GA_5 index of $SiC_3 - I[p,q]$ is calculated as follows by using the edge partition,

$$\begin{aligned}
GA_5(SiC_3 - I[p,q]) &= \sum_{st\in E(G)} \frac{2\sqrt{\delta_s \times \delta_t}}{\delta_s + \delta_t} \\
&= \left(\frac{2\sqrt{2\times 4}}{2+4}\right) + \left(\frac{2\sqrt{2\times 3}}{2+3}\right) + \left(\frac{2\sqrt{3\times 7}}{3+7}\right) + \left(\frac{2\sqrt{3\times 5}}{3+5}\right) + (2p+2q-4)\left(\frac{2\sqrt{5\times 5}}{5+5}\right) \\
&+ \left(\frac{2\sqrt{6\times 4}}{6+4}\right) + \left(\frac{2\sqrt{5\times 6}}{5+6}\right) + (2q+1)\left(\frac{2\sqrt{5\times 7}}{5+7}\right) + (4p+2q-9)\left(\frac{2\sqrt{5\times 8}}{5+8}\right) + \left(\frac{2\sqrt{6\times 6}}{6+6}\right) \\
&+ (2q-1)\left(\frac{2\sqrt{6\times 7}}{6+7}\right) + (2q-2)\left(\frac{2\sqrt{6\times 8}}{6+8}\right) + q\left(\frac{2\sqrt{7\times 8}}{7+8}\right) + (2q-1)\left(\frac{2\sqrt{7\times 9}}{7+9}\right) \\
&+ (pq-p-q+3)\left(\frac{2\sqrt{8\times 8}}{8+8}\right) + (4p+4q-13)\left(\frac{2\sqrt{8\times 9}}{8+9}\right) + (11pq-11p-19q+19)\left(\frac{2\sqrt{9\times 9}}{9+9}\right)
\end{aligned}$$

We obtain our desired outcome after simplifying the above form,

$$GA_5(SiC_3 - I[p,q]) = 12pq - 2.1149p - 3.1332q + 0.0658.$$

By definition, NH index of $SiC_3 - I[p,q]$ is calculated as follows by using the edge partition,

$$\begin{aligned}
NH(SiC_3 - I[p,q]) &= \sum_{st\in E(G)} \frac{2}{\delta_s + \delta_t} \\
&= \frac{2}{2+4} + \frac{2}{2+3} + \frac{2}{3+7} + \frac{2}{3+5} + (2p+2q-4)\left(\frac{2}{5+5}\right) + \frac{2}{4+6} + \frac{2}{5+6} + (2q+1)\frac{2}{5+7} \\
&+ (4p+2q-9)\left(\frac{2}{5+8}\right) + \frac{2}{6+6} + (2q-1)\left(\frac{2}{6+7}\right) + (2q-2)\left(\frac{2}{6+8}\right) + q\left(\frac{2}{7+8}\right) \\
&+ (2q-1)\left(\frac{2}{7+9}\right) + (pq-p-q+3)\left(\frac{2}{8+8}\right) + (4p+4q-13)\left(\frac{2}{8+9}\right) + (11pq-11p-19q+19)\left(\frac{2}{9+9}\right)
\end{aligned}$$

After an easy computation, we arrive at

$$NH(SiC_3 - I[p,q]) = 1.3472pq + 0.1388p + 0.2522q + 0.1060.$$

By definition, NI index of $SiC_3 - I[p,q]$ is calculated as follows by using the edge partition,

$$\begin{aligned}
NI(SiC_3 - I[p,q]) &= \sum_{st\in E(G)} \frac{\delta_s \times \delta_t}{\delta_s + \delta_t} \\
&= \left(\frac{2\times 4}{2+4}\right) + \left(\frac{2\times 3}{2+3}\right) + \left(\frac{3\times 7}{3+7}\right) + \left(\frac{3\times 5}{3+5}\right) + (2p+2q-4)\left(\frac{5\times 5}{5+5}\right) + \left(\frac{4\times 6}{4+6}\right) + \left(\frac{5\times 6}{5+6}\right) \\
&+ (2q+1)\left(\frac{5\times 7}{5+7}\right) + (4p+2q-9)\left(\frac{5\times 8}{5+8}\right) + \left(\frac{6\times 6}{6+6}\right) + (2q-1)\left(\frac{6\times 7}{6+7}\right) + (2q-2)\left(\frac{6\times 8}{6+8}\right) \\
&+ q\left(\frac{7\times 8}{7+8}\right) + (2q-1)\left(\frac{7\times 9}{7+9}\right) + (pq-p-q+3)\left(\frac{8\times 8}{8+8}\right) + (4p+4q-13)\left(\frac{8\times 9}{8+9}\right) \\
&+ (11pq-11p-19q+19)\left(\frac{9\times 9}{9+9}\right)
\end{aligned}$$

We obtain our desired outcome after simplifying the above form,

$$NI(SiC_3 - I[p,q]) = 53.5pq - 19.2511p - 30.6446q + 8.2757.$$

By definition, ND_5 index of $SiC_3 - I[p,q]$ is calculated as follows by using the edge partition,

$$\begin{aligned}
ND_5(SiC_3 - I[p,q]) &= \sum_{st\in E(G)} \frac{\delta_s^2+\delta_t^2}{\delta_s\times\delta_t} \\
&= \left(\frac{2^2+4^2}{2\times 4}\right) + \left(\frac{2^2+3^2}{2\times 3}\right) + \left(\frac{3^2+7^2}{3\times 7}\right) + \left(\frac{3^2+5^2}{3\times 5}\right) + (2p+2q-4)\left(\frac{5^2+5^2}{5\times 5}\right) + \left(\frac{4^2+6^2}{4\times 6}\right) \\
&+ \left(\frac{5^2+6^2}{5\times 6}\right) + (2q+1)\left(\frac{5^2+7^2}{5\times 7}\right) + (4p+2q-9)\left(\frac{5^2+8^2}{5\times 8}\right) + \left(\frac{6^2+6^2}{6\times 6}\right) + (2q-1)\left(\frac{6^2+7^2}{6\times 7}\right) \\
&+ (2q-2)\left(\frac{6^2+8^2}{6\times 8}\right) + q\left(\frac{7^2+8^2}{7\times 8}\right) + (2q-1)\left(\frac{7^2+9^2}{7\times 9}\right) + (pq-p-q+3)\left(\frac{8^2+8^2}{8\times 8}\right) \\
&+ (4p+4q-13)\left(\frac{8^2+9^2}{8\times 9}\right) + (11pq-11p-19q+19)\left(\frac{9^2+9^2}{9\times 9}\right)
\end{aligned}$$

After an easy computation, we arrive at

$$ND_5(SiC_3 - I[p,q]) = 24pq - 3.0444p - 4.9067q - 0.45.$$

By definition, M_2^{nm} index of $SiC_3 - I[p,q]$ is calculated as follows by using the edge partition,

$$\begin{aligned}
M_2^{mn}(SiC_3 - I[p,q]) &= \sum_{st\in E(G)} \frac{1}{\delta_s\times\delta_t} \\
&= \frac{1}{2\times 4} + \frac{1}{2\times 3} + \frac{1}{3\times 7} + \frac{1}{3\times 5} + \frac{2p+2q-4}{5\times 5} + \frac{1}{4\times 6} + \frac{1}{5\times 6} + \frac{2q+1}{5\times 7} + \frac{4p+2q-9}{5\times 8} \\
&+ \frac{1}{6\times 6} + \frac{2q-1}{6\times 7} + \frac{2q-2}{6\times 8} + \frac{q}{7\times 8} + \frac{2q-1}{7\times 9} + \frac{pq-p-q+3}{8\times 8} + \frac{4p+4q-13}{8\times 9} \\
&+ (11pq-11p-19q+19)\left(\frac{1}{9\times 9}\right)
\end{aligned}$$

We obtain our desired outcome after simplifying the above form,

$$M_2^{nm}(SiC_3 - I[p,q]) = 0.1514pq + 0.0841p + 0.1313q + 0.1718.$$

Theorem 5 *Let the Silicon-Carbide is represented by $SiC_3 - II[p,q]$. Then,*

1. $ABC_4(SiC_3 - II[p,q]) = 5.333pq - 0.232p - 0.242q - 0.179.$

2. $GA_5(SiC_3 - II[p,q]) = 12pq - 2.115p - 2.055q - 0.012.$

3. $NH(SiC_3 - II[p,q]) = 1.333pq + 0.180p + 0.175q - 0.036.$

4. $NI(SiC_3 - II[p,q]) = 54pq - 20.751p - 21.404q + 6.733.$

5. $ND_5(SiC_3 - II[p,q]) = 24pq - 3.044p - 3.556q + 0.148.$

6. $M_2^{nm}(SiC_3 - II[p,q]) = 0.148pq + 0.093p + 0.081q + 0.039.$

Proof Consider the graph $SiC_3 - II[p,q]$ for $p, q \geq 2$ of silicon-carbide. According to the degrees of the vertices, the vertex is divided into three groups. The collection of vertices of degree i is designated by the symbol V_i. For $SiC_3 - II[p,q]$, we have $|V_1| = 2$, $|V_2| = 4p + 4q - 4$ and $|V_3| = 8pq - 4p - 4q + 2$. The edge set divides into the following sections corresponding to their sum of the degrees of the neighbourhood, which are

$$
\begin{aligned}
E_1 &= \{uv \in E(SiC_3 - II[p,q]) \mid d_u = 3 \; and \; d_v = 6\} \\
E_2 &= \{uv \in E(SiC_3 - II[p,q]) \mid d_u = 4 \; and \; d_v = 5\} \\
E_3 &= \{uv \in E(SiC_3 - II[p,q]) \mid d_u = 5 \; and \; d_v = 5\} \\
E_4 &= \{uv \in E(SiC_3 - II[p,q]) \mid d_u = 5 \; and \; d_v = 7\} \\
E_5 &= \{uv \in E(SiC_3 - II[p,q]) \mid d_u = 5 \; and \; d_v = 8\} \\
E_6 &= \{uv \in E(SiC_3 - II[p,q]) \mid d_u = 6 \; and \; d_v = 6\} \\
E_7 &= \{uv \in E(SiC_3 - II[p,q]) \mid d_u = 6 \; and \; d_v = 7\} \\
E_8 &= \{uv \in E(SiC_3 - II[p,q]) \mid d_u = 6 \; and \; d_v = 8\} \\
E_9 &= \{uv \in E(SiC_3 - II[p,q]) \mid d_u = 7 \; and \; d_v = 9\} \\
E_{10} &= \{uv \in E(SiC_3 - II[p,q]) \mid d_u = 8 \; and \; d_v = 8\} \\
E_{11} &= \{uv \in E(SiC_3 - II[p,q]) \mid d_u = 8 \; and \; d_v = 9\} \\
E_{12} &= \{uv \in E(SiC_3 - II[p,q]) \mid d_u = 9 \; and \; d_v = 9\}
\end{aligned}
$$

From the graph $SiC_3 - II[p,q]$, we can see that $|E_1| = 2$, $|E_2| = 4$, $|E_3| = 2p - 3$, $|E_4| = 2$, $|E_5| = 4(p-1)$, $|E_6| = 2$, $|E_7| = 8q - 10$, $|E_8| = 2$, $|E_9| = 4(q-1)$, $|E_{10}| = 2p - 3$, $|E_{11}| = 4(p-1)$, and $|E_{12}| = 12pq - 14p - 14q + 16$.

Then, by definition ABC_4 index of $SiC_3 - II[p,q]$ is calculated as follows by using the edge partition,

$$
\begin{aligned}
ABC_4(SiC_3 - II[p,q]) &= \sum_{st \in E(G)} \sqrt{\frac{\delta_s + \delta_t - 2}{\delta_s \delta_t}} \\
&= 2\sqrt{\frac{3+6-2}{3\times 6}} + 4\sqrt{\frac{4+5-2}{4\times 5}} + (2p-3)\sqrt{\frac{5+5-2}{5\times 5}} + 2\sqrt{\frac{5+7-2}{5\times 7}} \\
&+ (4p-4)\sqrt{\frac{5+8-2}{5\times 8}} + 2\sqrt{\frac{6+6-2}{6\times 6}} + (8q-10)\sqrt{\frac{6+7-2}{6\times 7}} + 2\sqrt{\frac{6+8-2}{6\times 8}} \\
&+ (4q-4)\sqrt{\frac{7+9-2}{7\times 9}} + (2p-3)\sqrt{\frac{8+8-2}{8\times 8}} + (4p-4)\sqrt{\frac{8+9-2}{8\times 9}} \\
&+ (12pq - 14p - 14q + 16)\sqrt{\frac{9+9-2}{9\times 9}}
\end{aligned}
$$

After an easy computation, we arrive at

$$ABC_4(SiC_3 - II[p,q]) = 5.333pq - 0.232p - 0.242q - 0.179.$$

By definition, GA_5 index of $SiC_3 - II[p,q]$ is calculated as follows by using the edge partition,

$$\begin{aligned}
GA_5(SiC_3 - II[p,q]) &= \sum_{st \in E(G)} \frac{2\sqrt{\delta_s \times \delta_t}}{\delta_s + \delta_t} \\
&= 2\left(\frac{2\sqrt{3\times 6}}{3+6}\right) + 4\left(\frac{2\sqrt{4\times 5}}{4+5}\right) + (2p-3)\left(\frac{2\sqrt{5\times 5}}{5+5}\right) + 2\left(\frac{2\sqrt{5\times 7}}{5+7}\right) \\
&+ (4p-4)\left(\frac{2\sqrt{5\times 8}}{5+8}\right) + 2\left(\frac{2\sqrt{6\times 6}}{6+6}\right) + (8q-10)\left(\frac{2\sqrt{6\times 7}}{6+7}\right) + 2\left(\frac{2\sqrt{6\times 8}}{6+8}\right) \\
&+ (4q-4)\left(\frac{2\sqrt{7\times 9}}{7+9}\right) + (2p-3)\left(\frac{2\sqrt{8\times 8}}{8+8}\right) + (4p-4)\left(\frac{2\sqrt{8\times 9}}{8+9}\right) \\
&+ (12pq - 14p - 14q + 16)\left(\frac{2\sqrt{9\times 9}}{9+9}\right)
\end{aligned}$$

We obtain our desired outcome after simplifying the above form,

$$GA_5(SiC_3 - II[p,q]) = 12pq - 2.115p - 2.055q - 0.012.$$

By definition, NH index of $SiC_3 - II[p,q]$ is calculated as follows by using the edge partition,

$$\begin{aligned}
NH(SiC_3 - II[p,q]) &= \sum_{st \in E(G)} \frac{2}{\delta_s + \delta_t} \\
&= \frac{2\times 2}{3+6} + \frac{4\times 2}{4+5} + (2p-3)\left(\frac{2}{5+5}\right) + \frac{2\times 2}{5+7} + (4p-4)\left(\frac{2}{5+8}\right) \\
&+ \frac{2\times 2}{6+6} + (8q-10)\left(\frac{2}{6+7}\right) + \frac{2\times 2}{6+8} + (4q-4)\left(\frac{2}{7+9}\right) \\
&+ (2p-3)\left(\frac{2}{8+8}\right) + (4p-4)\left(\frac{2}{8+9}\right) + (12pq - 14p - 14q + 16)\left(\frac{2}{9+9}\right)
\end{aligned}$$

After an easy computation, we arrive at

$$NH(SiC_3 - II[p,q]) = 1.333pq + 0.180p + 0.175q - 0.036.$$

By definition, NI index of $SiC_3 - II[p,q]$ is calculated as follows by using the edge partition,

$$\begin{aligned}
NI(SiC_3 - II[p,q]) &= \sum_{st \in E(G)} \frac{\delta_s \times \delta_t}{\delta_s + \delta_t} \\
&= 2\left(\frac{3\times 6}{3+6}\right) + 4\left(\frac{4\times 5}{4+5}\right) + (2p-3)\left(\frac{5\times 5}{5+5}\right) + 2\left(\frac{5\times 7}{5+7}\right) + (4p-4)\left(\frac{5\times 8}{5+8}\right) \\
&+ 2\left(\frac{6\times 6}{6+6}\right) + (8q-10)\left(\frac{6\times 7}{6+7}\right) + 2\left(\frac{6\times 8}{6+8}\right) + (4q-4)\left(\frac{7\times 9}{7+9}\right) \\
&+ (2p-3)\left(\frac{8\times 8}{8+8}\right) + (4p-4)\left(\frac{8\times 9}{8+9}\right) + (12pq - 14p - 14q + 16)\left(\frac{9\times 9}{9+9}\right)
\end{aligned}$$

We obtain our desired outcome after simplifying the above form,

$$NI(SiC_3-II[p,q]) = 54pq - 20.751p - 21.404q + 6.733.$$

By definition, ND_5 index of $SiC_3-II[p,q]$ is calculated as follows by using the edge partition,

$$\begin{aligned}
ND_5(SiC_3-II[p,q]) &= \sum_{st\in E(G)} \frac{\delta_s^2+\delta_t^2}{\delta_s\times\delta_t} \\
&= 2\left(\frac{3^2+6^2}{3\times 6}\right) + 4\left(\frac{4^2+5^2}{4\times 5}\right) + (2p-3)\left(\frac{5^2+5^2}{5\times 5}\right) + 2\left(\frac{5^2+7^2}{5\times 7}\right) \\
&+ (4p-4)\left(\frac{5^2+8^2}{5\times 8}\right) + 2\left(\frac{6^2+6^2}{6\times 6}\right) + (8q-10)\left(\frac{6^2+7^2}{6\times 7}\right) + 2\left(\frac{6^2+8^2}{6\times 8}\right) \\
&+ (4q-4)\left(\frac{7^2+9^2}{7\times 9}\right) + (2p-3)\left(\frac{8^2+8^2}{8\times 8}\right) + (4p-4)\left(\frac{8^2+9^2}{8\times 9}\right) \\
&+ (12pq-14p-14q+16)\left(\frac{9^2+9^2}{9\times 9}\right)
\end{aligned}$$

After an easy computation, we arrive at

$$ND_5(SiC_3-II[p,q]) = 24pq - 3.044p - 3.556q + 0.148.$$

By definition, M_2^{nm} index of $SiC_3-II[p,q]$ is calculated as follows by using the edge partition,

$$\begin{aligned}
M_2^{mn}(SiC_3-II[p,q]) &= \sum_{st\in E(G)} \frac{1}{\delta_s\times\delta_t} \\
&= \frac{2}{3\times 6} + \frac{4}{4\times 5} + (2p-3)\left(\frac{1}{5\times 5}\right) + \frac{2}{5\times 7} + (4p-4)\left(\frac{1}{5\times 8}\right) + \frac{2}{6\times 6} \\
&+ (8q-10)\left(\frac{1}{6\times 7}\right) + \frac{2}{6\times 8} + (4q-4)\left(\frac{1}{7\times 9}\right) + (2p-3)\left(\frac{1}{8\times 8}\right) \\
&+ (4p-4)\left(\frac{1}{8\times 9}\right) + (12pq-14p-14q+16)\left(\frac{1}{9\times 9}\right)
\end{aligned}$$

We obtain our desired outcome after simplifying the above form,

$$M_2^{nm}(SiC_3-II[p,q]) = 0.148pq + 0.093p + 0.081q + 0.039.$$

Theorem 6 *Let the Silicon-Carbide is represented by $SiC_3-III[p,q]$. Then,*

1. $ABC_4(SiC_3-III[p,q]) = 5.3333pq - 0.3412p - 0.2321q - 0.2878.$

2. $GA_5(SiC_3-III[p,q]) = 12pq - 3.1229p - 2.0933q - 0.0371.$

3. $NH(SiC_3-III[p,q]) = 1.3333pq + 0.3138p + 0.1930q - 0.0399.$

4. $NI(SiC_3-III[p,q]) = 54pq - 47.4512p - 20.6047q + 9.8785.$

5. $ND_5(SiC_3 - III[p,q]) = 24pq - 4.9913p - 3.2302q + 0.4056.$

6. $M_2^{nm}(SiC_3 - III[p,q]) = 0.1481pq + 0.1599p + 0.1191q + 0.1088.$

Proof Consider the graph $SiC_3 - III[p,q]$ for $p,q \geq 2$ of silicon-carbide. According to the degrees of the vertices, the vertex is divided into three groups. The collection of vertices of degree i is designated by the symbol V_i. For $SiC_3 - II[p,q]$, we have $|V_1| = 3$, $|V_2| = 6p + 4q - 6$ and $|V_3| = 8pq - 6p - 4q - 1$. The edge set divides into the following sections corresponding to their sum of the degrees of the neighbourhood, which are

$$E_1 = \{uv \in E(SiC_3 - III[p,q]) \mid d_u = 2 \; and \; d_v = 4\}$$
$$E_2 = \{uv \in E(SiC_3 - III[p,q]) \mid d_u = 3 \; and \; d_v = 6\}$$
$$E_3 = \{uv \in E(SiC_3 - III[p,q]) \mid d_u = 4 \; and \; d_v = 4\}$$
$$E_4 = \{uv \in E(SiC_3 - III[p,q]) \mid d_u = 4 \; and \; d_v = 5\}$$
$$E_5 = \{uv \in E(SiC_3 - III[p,q]) \mid d_u = 5 \; and \; d_v = 5\}$$
$$E_6 = \{uv \in E(SiC_3 - III[p,q]) \mid d_u = 4 \; and \; d_v = 7\}$$
$$E_7 = \{uv \in E(SiC_3 - III[p,q]) \mid d_u = 5 \; and \; d_v = 6\}$$
$$E_8 = \{uv \in E(SiC_3 - III[p,q]) \mid d_u = 5 \; and \; d_v = 7\}$$
$$E_9 = \{uv \in E(SiC_3 - III[p,q]) \mid d_u = 5 \; and \; d_v = 8\}$$
$$E_{10} = \{uv \in E(SiC_3 - III[p,q]) \mid d_u = 6 \; and \; d_v = 7\}$$
$$E_{11} = \{uv \in E(SiC_3 - III[p,q]) \mid d_u = 7 \; and \; d_v = 9\}$$
$$E_{12} = \{uv \in E(SiC_3 - III[p,q]) \mid d_u = 8 \; and \; d_v = 6\}$$
$$E_{13} = \{uv \in E(SiC_3 - III[p,q]) \mid d_u = 8 \; and \; d_v = 9\}$$
$$E_{14} = \{uv \in E(SiC_3 - III[p,q]) \mid d_u = 8 \; and \; d_v = 8\}$$
$$E_{15} = \{uv \in E(SiC_3 - III[p,q]) \mid d_u = 9 \; and \; d_v = 9\}$$

From the graph $SiC_3 - III[p,q]$, we can see that $|E_1| = 2$, $|E_2| = 1$, $|E_3| = 1$, $|E_4| = 2p$, $|E_5| = p + 2q - 4$, $|E_6| = 2$, $|E_7| = 1$, $|E_8| = 2p + 2q - 4$, $|E_9| = 2p + 2q - 5$, $|E_{10}| = 2p - 2$, $|E_{11}| = 2p + q - 2$, $|E_{12}| = 1$, $|E_{13}| = 4p + 2q - 7$, $|E_{14}| = q - 2$, and $|E_{15}| = 12pq - 18p - 12q + 18$.
Then, by definition ABC_4 index of $SiC_3 - III[p,q]$ is calculated as follows by using the edge partition,

$$\begin{aligned}
ABC_4(SiC_3 - III[p,q]) &= \sum_{st \in E(G)} \sqrt{\frac{\delta_s + \delta_t - 2}{\delta_s \delta_t}} \\
&= 2\sqrt{\frac{2+4-2}{2\times 4}} + \sqrt{\frac{3+6-2}{3\times 6}} + \sqrt{\frac{4+4-2}{4\times 4}} + (2p)\sqrt{\frac{4+5-2}{4\times 5}} + (p+2q-4)\sqrt{\frac{5+5-2}{5\times 5}} \\
&+ 2\sqrt{\frac{4+7-2}{4\times 7}} + \sqrt{\frac{5+6-2}{5\times 6}} + (2p+2q-4)\sqrt{\frac{5+7-2}{5\times 7}} + (2p+2q-5)\sqrt{\frac{5+8-2}{5\times 8}} \\
&+ (2p-2)\sqrt{\frac{6+7-2}{6\times 7}} + (2p+q-2)\sqrt{\frac{7+9-2}{7\times 9}} + \sqrt{\frac{8+6-2}{8\times 6}} + (4p+2q-7)\sqrt{\frac{8+9-2}{8\times 9}}
\end{aligned}$$

$$+ (q-2)\sqrt{\frac{8+8-2}{8\times 8}} + (12pq-18p-12q+18)\sqrt{\frac{9+9-2}{9\times 9}}$$

After an easy computation, we arrive at

$$ABC_4(SiC_3 - III[p,q]) = 5.3333pq - 0.3412p - 0.2321q - 0.2878.$$

By definition, GA_5 index of $SiC_3 - III[p,q]$ is calculated as follows by using the edge partition,

$$\begin{aligned} GA_5(SiC_3 - III[p,q]) &= \sum_{st\in E(G)} \frac{2\sqrt{\delta_s\times\delta_t}}{\delta_s+\delta_t} \\ &= 2\left(\frac{2\sqrt{2\times 4}}{2+4}\right) + \left(\frac{2\sqrt{3\times 6}}{3+6}\right) + \left(\frac{2\sqrt{4\times 4}}{4+4}\right) + (2p)\left(\frac{2\sqrt{4\times 5}}{4+5}\right) + (p+2q-4)\left(\frac{2\sqrt{5\times 5}}{5+5}\right) \\ &+ 2\left(\frac{2\sqrt{4\times 7}}{4+7}\right) + \left(\frac{2\sqrt{5\times 6}}{5+6}\right) + (2p+2q-4)\left(\frac{2\sqrt{5\times 7}}{5+7}\right) + (2p+2q-5)\left(\frac{2\sqrt{5\times 8}}{5+8}\right) \\ &+ (2p-2)\left(\frac{2\sqrt{6\times 7}}{6+7}\right) + (2p+q-2)\left(\frac{2\sqrt{7\times 9}}{7+9}\right) + \left(\frac{2\sqrt{8\times 6}}{8+6}\right) + (4p+2q-7)\left(\frac{2\sqrt{8\times 9}}{8+9}\right) \\ &+ (q-2)\left(\frac{2\sqrt{8\times 8}}{8+8}\right) + (12pq-18p-12q+18)\left(\frac{2\sqrt{9\times 9}}{9+9}\right) \end{aligned}$$

We obtain our desired outcome after simplifying the above form,

$$GA_5(SiC_3 - III[p,q]) = 12pq - 3.1229p - 2.0933q - 0.0371.$$

By definition, NH index of $SiC_3 - III[p,q]$ is calculated as follows by using the edge partition,

$$\begin{aligned} NH(SiC_3 - III[p,q]) &= \sum_{st\in E(G)} \frac{2}{\delta_s+\delta_t} \\ &= \frac{2\times 2}{2+4} + \frac{2}{3+6} + \frac{2}{4+4} + (2p)\left(\frac{2}{4+5}\right) + (p+2q-4)\left(\frac{2}{5+5}\right) + \frac{4}{4+7} + \left(\frac{2}{5+6}\right) \\ &+ (2p+2q-4)\left(\frac{2}{5+7}\right) + (2p+2q-5)\left(\frac{2}{5+8}\right) + (2p-2)\left(\frac{2}{6+7}\right) + (2p+q-2)\left(\frac{2}{7+9}\right) \\ &+ \left(\frac{2}{8+6}\right) + (4p+2q-7)\left(\frac{2}{8+9}\right) + (q-2)\left(\frac{2}{8+8}\right) + (12pq-14p-14q+16)\left(\frac{2}{9+9}\right) \end{aligned}$$

After an easy computation, we arrive at

$$NH(SiC_3 - III[p,q]) = 1.3333pq + 0.3138p + 0.1930q - 0.0399.$$

By definition, NI index of $SiC_3 - III[p,q]$ is calculated as follows by using the edge partition,

$$NI(SiC_3 - III[p,q]) = \sum_{st\in E(G)} \frac{\delta_s\times\delta_t}{\delta_s+\delta_t}$$

$$= 2\left(\frac{2\times4}{2+4}\right)+\left(\frac{3\times6}{3+6}\right)+\left(\frac{4\times4}{4+4}\right)+(2p)\left(\frac{4\times5}{4+5}\right)+(p+2q-4)\left(\frac{5\times5}{5+5}\right)+2\left(\frac{4\times7}{4+7}\right)+\left(\frac{5\times6}{5+6}\right)$$
$$+(2p+2q-4)\left(\frac{5\times7}{5+7}\right)+(2p+2q-5)\left(\frac{5\times8}{5+8}\right)+(2p-2)\left(\frac{6\times7}{6+7}\right)+(2p+q-2)\left(\frac{7\times9}{7+9}\right)$$
$$+\left(\frac{8\times6}{8+6}\right)+(4p+2q-7)\left(\frac{8\times9}{8+9}\right)+(q-2)\left(\frac{8\times8}{8+8}\right)+(12pq-18p-12q+18)\left(\frac{9\times9}{9+9}\right)$$

We obtain our desired outcome after simplifying the above form,

$$NI(SiC_3-III[p,q]) = 54pq-47.4512p-20.6047q+9.8785.$$

By definition, ND_5 index of $SiC_3-III[p,q]$ is calculated as follows by using the edge partition,

$$ND_5(SiC_3-III[p,q]) = \sum_{st\in E(G)}\frac{\delta_s^2+\delta_t^2}{\delta_s\times\delta_t}$$
$$= 2\left(\frac{2^2+4^2}{2\times4}\right)+\left(\frac{3^2+6^2}{3\times6}\right)+\left(\frac{4^2+4^2}{4\times4}\right)+(2p)\left(\frac{4^2+5^2}{4\times5}\right)+(p+2q-4)\left(\frac{5^2+5^2}{5\times5}\right)$$
$$+2\left(\frac{4^2+7^2}{4\times7}\right)+\left(\frac{5^2+6^2}{5\times6}\right)+(2p+q-4)\left(\frac{5^2+7^2}{5\times7}\right)+(2p+2q-5)\left(\frac{5^2+8^2}{5\times8}\right)$$
$$+(2p-2)\left(\frac{6^2+7^2}{6\times7}\right)+(2p+q-2)\left(\frac{7^2+9^2}{7\times9}\right)+\left(\frac{8^2+6^2}{8\times6}\right)+(4p+2q-7)\left(\frac{8^2+9^2}{8\times9}\right)$$
$$+(q-2)\left(\frac{8^2+8^2}{8\times8}\right)+(12pq-18p-12q+18)\left(\frac{9^2+9^2}{9\times9}\right)$$

After an easy computation, we arrive at

$$ND_5(SiC_3-III[p,q]) = 24pq-4.9913p-3.2302q+0.4056.$$

By definition, M_2^{nm} index of $SiC_3-III[p,q]$ is calculated as follows by using the edge partition,

$$M_2^{mn}(SiC_3-III[p,q]) = \sum_{st\in E(G)}\frac{1}{\delta_s\times\delta_t}$$
$$= \frac{2}{2\times4}+\frac{1}{3\times6}+\frac{1}{4\times4}+\frac{2p}{4\times5}+\left(\frac{p+2q-4}{5\times5}\right)+\frac{2}{4\times7}+\frac{1}{5\times6}+\frac{2p+2q-5}{5\times7}$$
$$+\left(\frac{2p+2q-5}{5\times8}\right)+\left(\frac{2p-2}{6\times7}\right)+\left(\frac{2p+q-2}{7\times9}\right)+\frac{1}{8\times6}+\left(\frac{4p+2q-7}{8\times9}\right)$$
$$+\left(\frac{q-2}{8\times8}\right)+\left(\frac{12pq-18p-12q+18}{9\times9}\right)$$

We obtain our desired outcome after simplifying the above form,

$$M_2^{nm}(SiC_3-III[p,q]) = 0.1481pq+0.1599p+0.1191q+0.1088.$$

Theorem 7 *Let the Silicon-Carbide is represented by $SiC_4-I[p,q]$. Then,*

1. $ABC_4(SiC_4-I[p,q]) = 5.778pq+1.008p+1.546q-3.425.$

2. $GA_5(SiC_4-I[p,q]) = 55.154pq - 8.710p + 2.384q - 26.004.$

3. $NH(SiC_4-I[p,q]) = 1.444pq + 0.552p + 0.624q - 0.800.$

4. $NI(SiC_4-I[p,q]) = 58.5pq - 16.419p - 2.780q - 23.277.$

5. $ND_5(SiC_4-I[p,q]) = 26pq + 3.113p + 4.983q - 15.260.$

6. $M_2^{nm}(SiC_4-I[p,q]) = 0.160pq + 0.187p + 0.143q - 0.010.$

Proof Consider the graph $SiC_4-I[p,q]$ for $p,q \geq 2$ of silicon-carbide. According to the degrees of the vertices, the vertex is divided into three groups. The collection of vertices of degree i is designated by the symbol V_i. For $SiC_3-II[p,q]$, we have $|V_1| = 3p$, $|V_2| = 2p+4q-2$ and $|V_3| = 10pq-5p-4q+2$. The edge set divides into the following sections corresponding to their sum of the degrees of the neighbourhood, which are

$$
\begin{aligned}
E_1 &= \{uv \in E(SiC_4-I[p,q]) \mid d_u = 2 \; and \; d_v = 4\}\\
E_2 &= \{uv \in E(SiC_4-I[p,q]) \mid d_u = 3 \; and \; d_v = 7\}\\
E_3 &= \{uv \in E(SiC_4-I[p,q]) \mid d_u = 5 \; and \; d_v = 5\}\\
E_4 &= \{uv \in E(SiC_4-I[p,q]) \mid d_u = 4 \; and \; d_v = 7\}\\
E_5 &= \{uv \in E(SiC_4-I[p,q]) \mid d_u = 4 \; and \; d_v = 8\}\\
E_6 &= \{uv \in E(SiC_4-I[p,q]) \mid d_u = 5 \; and \; d_v = 7\}\\
E_7 &= \{uv \in E(SiC_4-I[p,q]) \mid d_u = 5 \; and \; d_v = 8\}\\
E_8 &= \{uv \in E(SiC_4-I[p,q]) \mid d_u = 7 \; and \; d_v = 8\}\\
E_9 &= \{uv \in E(SiC_4-I[p,q]) \mid d_u = 7 \; and \; d_v = 9\}\\
E_{10} &= \{uv \in E(SiC_4-I[p,q]) \mid d_u = 8 \; and \; d_v = 8\}\\
E_{11} &= \{uv \in E(SiC_4-I[p,q]) \mid d_u = 8 \; and \; d_v = 9\}\\
E_{12} &= \{uv \in E(SiC_4-I[p,q]) \mid d_u = 9 \; and \; d_v = 9\}
\end{aligned}
$$

From the graph $SiC_4-I[p,q]$, we can see that $|E_1| = 2$, $|E_2| = 3p-2$, $|E_3| = 1$, $|E_4| = 1$, $|E_5| = p+2q-2$, $|E_6| = 3$, $|E_7| = 2p+4q-7$, $|E_8| = p+1$, $|E_9| = 5p-3$, $|E_{10}| = q-1$, $|E_{11}| = 3p+6q-11$, and $|E_{12}| = 13pq-15p-11q+11$.

Then, by definition ABC_4 index of $SiC_4-I[p,q]$ is calculated as follows by using the edge partition,

$$
\begin{aligned}
ABC_4(SiC_4-I[p,q]) &= \sum_{st\in E(G)} \sqrt{\frac{\delta_s+\delta_t-2}{\delta_s\delta_t}}\\
&= 2\sqrt{\frac{2+4-2}{2\times 4}} + (3p-2)\sqrt{\frac{3+7-2}{3\times 7}} + \sqrt{\frac{4+7-2}{4\times 7}} + \sqrt{\frac{4+8-2}{4\times 8}}\\
&+ (p+2q-2)\sqrt{\frac{5+5-2}{5\times 5}} + 3\sqrt{\frac{5+7-2}{5\times 7}} + (2p+4q-7)\sqrt{\frac{5+8-2}{5\times 8}}
\end{aligned}
$$

$$+ (p+1)\sqrt{\frac{7+8-2}{7\times 8}} + (5p-3)\sqrt{\frac{7+9-2}{7\times 9}} + (q-1)\sqrt{\frac{8+8-2}{8\times 8}}$$
$$+ (3p+6q-11)\sqrt{\frac{8+9-2}{8\times 9}} + (13pq-15p-11q+11)\sqrt{\frac{9+9-2}{9\times 9}}$$

After an easy computation, we arrive at

$$ABC_4(SiC_4 - I[p,q]) = 5.778pq + 1.008p + 1.546q - 3.425.$$

By definition, GA_5 index of $SiC_4 - I[p,q]$ is calculated as follows by using the edge partition,

$$\begin{aligned}
GA_5(SiC_4 - I[p,q]) &= \sum_{st\in E(G)} \frac{2\sqrt{\delta_s \times \delta_t}}{\delta_s + \delta_t} \\
&= 2\left(\frac{2\sqrt{2\times 4}}{2+4}\right) + (3p-2)\left(\frac{2\sqrt{3\times 7}}{3+7}\right) + \left(\frac{2\sqrt{4\times 7}}{4+7}\right) + \left(\frac{2\sqrt{4\times 8}}{4+8}\right) \\
&+ (p+2q-2)\left(\frac{2\sqrt{5\times 5}}{5+5}\right) + 3\left(\frac{2\sqrt{5\times 7}}{5+7}\right) + (2p+4q-7)\left(\frac{2\sqrt{5\times 8}}{5+8}\right) \\
&+ (p+1)\left(\frac{2\sqrt{7\times 8}}{7+8}\right) + (5p-3)\left(\frac{2\sqrt{7\times 9}}{7+9}\right) + (q-1)\left(\frac{2\sqrt{8\times 8}}{8+8}\right) \\
&+ (3p+6q-11)\left(\frac{2\sqrt{8\times 9}}{8+9}\right) + (13pq-15p-11q+11)\left(\frac{2\sqrt{9\times 9}}{9+9}\right)
\end{aligned}$$

We obtain our desired outcome after simplifying the above form,

$$GA_5(SiC_4 - I[p,q]) = 55.154pq - 8.710p + 2.384q - 26.004.$$

By definition, NH index of $SiC_4 - I[p,q]$ is calculated as follows by using the edge partition,

$$\begin{aligned}
NH(SiC_4 - I[p,q]) &= \sum_{st\in E(G)} \frac{2}{\delta_s + \delta_t} \\
&= \frac{2\times 2}{2+4} + (3p-2)\left(\frac{2}{3+7}\right) + \frac{2}{4+7} + \frac{2}{4+8} + (p+2q-2)\left(\frac{2}{5+5}\right) \\
&+ \frac{3\times 2}{5+7} + (2p+4q-7)\left(\frac{2}{5+8}\right) + (p+1)\left(\frac{2}{7+8}\right) + (5p-3)\left(\frac{2}{7+9}\right) \\
&+ (q-1)\left(\frac{2}{8+8}\right) + (3p+6q-11)\left(\frac{2}{8+9}\right) + (13pq-15p-11q+11)\left(\frac{2}{9+9}\right)
\end{aligned}$$

After an easy computation, we arrive at

$$NH(SiC_4 - I[p,q]) = 1.444pq + 0.552p + 0.624q - 0.800.$$

By definition, NI index of $SiC_4 - I[p,q]$ is calculated as follows by using the edge partition,

$$NI(SiC_4 - I[p,q]) = \sum_{st\in E(G)} \frac{\delta_s \times \delta_t}{\delta_s + \delta_t}$$

$$
\begin{aligned}
&= 2\left(\frac{2\times 4}{2+4}\right) + (3p-2)\left(\frac{3\times 7}{3+7}\right) + \left(\frac{4\times 7}{4+7}\right) + \left(\frac{4\times 8}{4+8}\right) + (p+2q-2)\left(\frac{5\times 5}{5+5}\right)\\
&+ 3\left(\frac{5\times 7}{5+7}\right) + (2p+4q-7)\left(\frac{5\times 8}{5+8}\right) + (p+1)\left(\frac{7\times 8}{7+8}\right) + (5p-3)\left(\frac{7\times 9}{7+9}\right)\\
&+ (q-1)\left(\frac{8\times 8}{8+8}\right) + (3p+6q-11)\left(\frac{8\times 9}{8+9}\right) + (13pq-15p-11q+11)\left(\frac{9\times 9}{9+9}\right)
\end{aligned}
$$

We obtain our desired outcome after simplifying the above form,

$$NI(SiC_4 - I[p,q]) = 58.5pq - 16.419p - 2.780q - 23.277.$$

By definition, ND_5 index of $SiC_4 - I[p,q]$ is calculated as follows by using the edge partition,

$$
\begin{aligned}
ND_5(SiC_4 - I[p,q]) &= \sum_{st\in E(G)} \frac{\delta_s^2 + \delta_t^2}{\delta_s \times \delta_t}\\
&= 2\left(\frac{2^2+4^2}{2\times 4}\right) + (3p-2)\left(\frac{3^2+7^2}{3\times 7}\right) + \left(\frac{4^2+7^2}{4\times 7}\right) + \left(\frac{4^2+8^2}{4\times 8}\right)\\
&+ (p+2q-2)\left(\frac{5^2+5^2}{5\times 5}\right) + 3\left(\frac{5^2+7^2}{5\times 7}\right) + (2p+4q-7)\left(\frac{5^2+8^2}{5\times 8}\right)\\
&+ (p+1)\left(\frac{7^2+8^2}{7\times 8}\right) + (5p-3)\left(\frac{7^2+9^2}{7\times 9}\right) + (q-1)\left(\frac{8^2+8^2}{8\times 8}\right)\\
&+ (3p+6q-11)\left(\frac{8^2+9^2}{8\times 9}\right) + (13pq-15p-11q+11)\left(\frac{9^2+9^2}{9\times 9}\right)
\end{aligned}
$$

After an easy computation, we arrive at

$$ND_5(SiC_4 - I[p,q]) = 26pq + 3.113p + 4.983q - 15.260.$$

By definition, M_2^{nm} index of $SiC_4 - I[p,q]$ is calculated as follows by using the edge partition,

$$
\begin{aligned}
M_2^{mn}(SiC_4 - I[p,q]) &= \sum_{st\in E(G)} \frac{1}{\delta_s \times \delta_t}\\
&= \frac{2}{2\times 4} + (3p-2)\left(\frac{1}{3\times 7}\right) + \frac{1}{4\times 7} + \frac{1}{4\times 8} + (p+2q-2)\left(\frac{1}{5\times 5}\right) + \frac{3}{5\times 7}\\
&+ (2p+4q-7)\left(\frac{1}{5\times 8}\right) + (p+1)\left(\frac{1}{7\times 8}\right) + (5p-3)\left(\frac{1}{7\times 9}\right) + (q-1)\left(\frac{1}{8\times 8}\right)\\
&+ (3p+6q-11)\left(\frac{1}{8\times 9}\right) + (13pq-15p-11q+11)\left(\frac{1}{9\times 9}\right)
\end{aligned}
$$

We obtain our desired outcome after simplifying the above form,

$$M_2^{nm}(SiC_4 - I[p,q]) = 0.160pq + 0.187p + 0.143q - 0.010.$$

Theorem 8 *Let the Silicon-Carbide is represented by $SiC_4 - II[p,q]$. Then,*

1. $ABC_4(SiC_4 - II[p,q]) = 6.6667pq - 0.4778p - 0.2425q - 0.1815.$

2. $GA_5(SiC_4 - II[p,q]) = 15pq - 4.1585p - 2.0551q + 0.6342.$

3. $NH(SiC_4 - II[p,q]) = 1.6667pq + 0.3593p + 0.8002q + 0.2550.$

4. $NI(SiC_4 - II[p,q]) = 67.5pq - 42.0799p - 21.4038q + 10.0819.$

5. $ND_5(SiC_4 - II[p,q]) = 135pq - 6.7024p - 3.5556q - 0.1294.$

6. $M_2^{nm}(SiC_4 - II[p,q]) = 0.1852pq + 0.1763p + 0.0811q + 0.2659.$

Proof Consider the graph $SiC_4 - II[p,q]$ for $p,q \geq 2$ of silicon-carbide. According to the degrees of the vertices, the vertex is divided into three groups. The collection of vertices of degree i is designated by the symbol V_i. For $SiC_4 - II[p,q]$, we have $|V_1| = 2$, $|V_2| = 8p + 4q - 4$ and $|V_3| = 10pq - 8p - 4q + 2$. The edge set divides into the following sections corresponding to their sum of the degrees of the neighbourhood, which are

$$
\begin{aligned}
E_1 &= \{uv \in E(SiC_4 - II[p,q]) \mid d_u = 2 \; and \; d_v = 3\} \\
E_2 &= \{uv \in E(SiC_4 - II[p,q]) \mid d_u = 5 \; and \; d_v = 3\} \\
E_3 &= \{uv \in E(SiC_4 - II[p,q]) \mid d_u = 5 \; and \; d_v = 5\} \\
E_4 &= \{uv \in E(SiC_4 - II[p,q]) \mid d_u = 5 \; and \; d_v = 6\} \\
E_5 &= \{uv \in E(SiC_4 - II[p,q]) \mid d_u = 5 \; and \; d_v = 7\} \\
E_6 &= \{uv \in E(SiC_4 - II[p,q]) \mid d_u = 5 \; and \; d_v = 8\} \\
E_7 &= \{uv \in E(SiC_4 - II[p,q]) \mid d_u = 6 \; and \; d_v = 6\} \\
E_8 &= \{uv \in E(SiC_4 - II[p,q]) \mid d_u = 6 \; and \; d_v = 7\} \\
E_9 &= \{uv \in E(SiC_4 - II[p,q]) \mid d_u = 6 \; and \; d_v = 8\} \\
E_{10} &= \{uv \in E(SiC_4 - II[p,q]) \mid d_u = 7 \; and \; d_v = 7\} \\
E_{11} &= \{uv \in E(SiC_4 - II[p,q]) \mid d_u = 7 \; and \; d_v = 9\} \\
E_{12} &= \{uv \in E(SiC_4 - II[p,q]) \mid d_u = 8 \; and \; d_v = 8\} \\
E_{13} &= \{uv \in E(SiC_4 - II[p,q]) \mid d_u = 8 \; and \; d_v = 9\} \\
E_{14} &= \{uv \in E(SiC_4 - II[p,q]) \mid d_u = 9 \; and \; d_v = 9\}
\end{aligned}
$$

From the graph $SiC_4 - II[p,q]$, we can see that $|E_1| = 2$, $|E_2| = 2$, $|E_3| = 2p$, $|E_4| = 2$, $|E_5| = 2p+2$, $|E_6| = 2p-2$, $|E_7| = 4$, $|E_8| = 6p + 8q - 18$, $|E_9| = 2p - 2$, $|E_{10}| = 2$, $|E_{11}| = 4p + 4q - 12$, $|E_{12}| = 2p - 2$, $|E_{13}| = 4p - 4$, and $|E_{14}| = 15pq - 28p - 14q + 26$.

Then, by definition ABC_4 index of $SiC_4 - II[p,q]$ is calculated as follows by using the edge partition,

$$ABC_4(SiC_4 - II[p,q]) = \sum_{st \in E(G)} \sqrt{\frac{\delta_s + \delta_t - 2}{\delta_s \delta_t}}$$

$$= 2\sqrt{\frac{2+3-2}{2\times 3}} + 2\sqrt{\frac{5+3-2}{5\times 3}} + (2p)\sqrt{\frac{5+5-2}{5\times 5}} + 2\sqrt{\frac{5+6-2}{5\times 6}} + (2p+2)\sqrt{\frac{5+7-2}{5\times 7}}$$
$$+ (2p-2)\sqrt{\frac{5+8-2}{5\times 8}} + 4\sqrt{\frac{6+6-2}{6\times 6}} + (6p+8q-18)\sqrt{\frac{6+7-2}{6\times 7}} + (2p-2)\sqrt{\frac{6+8-2}{6\times 8}}$$
$$+ 2\sqrt{\frac{7+7-2}{7\times 7}} + (4p+4q-12)\sqrt{\frac{7+9-2}{7\times 9}} + (2p-2)\sqrt{\frac{8+8-2}{8\times 8}} + (4p-4)\sqrt{\frac{8+9-2}{8\times 9}}$$
$$+ (15pq-28p-14q+26)\sqrt{\frac{9+9-2}{9\times 9}}$$

After an easy computation, we arrive at

$$ABC_4(SiC_4 - II[p,q]) = 6.6667pq - 0.4778p - 0.2425q - 0.1815.$$

By definition, GA_5 index of $SiC_4 - II[p,q]$ is calculated as follows by using the edge partition,

$$GA_5(SiC_4 - II[p,q]) = \sum_{st\in E(G)} \frac{2\sqrt{\delta_s\times\delta_t}}{\delta_s+\delta_t}$$
$$= \left(\frac{4\sqrt{2\times 3}}{2+3}\right) + \left(\frac{4\sqrt{5\times 3}}{5+3}\right) + (2p)\left(\frac{2\sqrt{5\times 5}}{5+5}\right) + \left(\frac{4\sqrt{5\times 6}}{5+6}\right) + (2p+2)\left(\frac{2\sqrt{5\times 7}}{5+7}\right)$$
$$+ (2p-2)\left(\frac{2\sqrt{5\times 8}}{5+8}\right) + \left(\frac{8\sqrt{6\times 6}}{6+6}\right) + (6p+8q-18)\left(\frac{2\sqrt{6\times 7}}{6+7}\right) + (2p-2)\left(\frac{2\sqrt{6\times 8}}{6+8}\right)$$
$$+ \left(\frac{4\sqrt{7\times 7}}{7+7}\right) + (4p+4q-12)\left(\frac{2\sqrt{7\times 9}}{7+9}\right) + (2p-2)\left(\frac{2\sqrt{8\times 8}}{8+8}\right) + (4p-4)\left(\frac{2\sqrt{8\times 9}}{8+9}\right)$$
$$+ (15pq-28p-14q+26)\left(\frac{2\sqrt{9\times 9}}{9+9}\right)$$

We obtain our desired outcome after simplifying the above form,

$$GA_5(SiC_4 - II[p,q]) = 15pq - 4.1585p - 2.0551q + 0.6342.$$

By definition, NH index of $SiC_4 - II[p,q]$ is calculated as follows by using the edge partition,

$$NH(SiC_4 - II[p,q]) = \sum_{st\in E(G)} \frac{2}{\delta_s+\delta_t}$$
$$= \frac{2\times 2}{2+3} + \left(\frac{2\times 2}{5+3}\right) + (2p)\left(\frac{2}{5+5}\right) + \frac{2\times 2}{5+6} + (2p+2)\left(\frac{2}{5+7}\right) + (2p-2)\left(\frac{2}{5+8}\right) + \left(\frac{4\times 2}{6+6}\right)$$
$$+ (6p+8q-18)\left(\frac{2}{6+7}\right) + (2p-2)\left(\frac{2}{6+8}\right) + \left(\frac{4}{7+7}\right) + (4p+4q-12)\left(\frac{2}{7+9}\right)$$
$$+ (2p-2)\left(\frac{2}{8+8}\right) + (4p-4)\left(\frac{2}{8+9}\right) + (15pq-28p-14q+26)\left(\frac{2}{9+9}\right)$$

After an easy computation, we arrive at

$$NH(SiC_4 - II[p,q]) = 1.6667pq + 0.3593p + 0.8002q + 0.2550.$$

By definition, NI index of $SiC_4 - II[p,q]$ is calculated as follows by using the edge partition,

$$\begin{aligned}
NI(SiC_4 - II[p,q]) &= \sum_{st\in E(G)} \frac{\delta_s \times \delta_t}{\delta_s + \delta_t} \\
&= 2\left(\frac{2\times 3}{2+3}\right) + 2\left(\frac{5\times 3}{5+3}\right) + (2p)\left(\frac{5\times 5}{5+5}\right) + 2\left(\frac{5\times 6}{5+6}\right) + (2p+2)\left(\frac{5\times 7}{5+7}\right) + (2p-2)\left(\frac{5\times 8}{5+8}\right) \\
&+ 4\left(\frac{6\times 6}{6+6}\right) + (6p+8q-18)\left(\frac{6\times 7}{6+7}\right) + (2p-2)\left(\frac{6\times 8}{6+8}\right) + 2\left(\frac{7\times 7}{7+7}\right) + (4p+4q-12)\left(\frac{7\times 9}{7+9}\right) \\
&+ (2p-2)\left(\frac{8\times 8}{8+8}\right) + (4p-4)\left(\frac{8\times 9}{8+9}\right) + (15pq-28p-14q+26)\left(\frac{9\times 9}{9+9}\right)
\end{aligned}$$

We obtain our desired outcome after simplifying the above form,

$$NI(SiC_4 - II[p,q]) = 67.5pq - 42.0799p - 21.4038q + 10.0819.$$

By definition, ND_5 index of $SiC_4 - II[p,q]$ is calculated as follows by using the edge partition,

$$\begin{aligned}
ND_5(SiC_4 - II[p,q]) &= \sum_{st\in E(G)} \frac{\delta_s^2 + \delta_t^2}{\delta_s \times \delta_t} \\
&= 2\left(\frac{2^2+3^2}{2\times 3}\right) + 2\left(\frac{5^2+3^2}{5\times 3}\right) + (2p)\left(\frac{5^2+5^2}{5\times 5}\right) + 2\left(\frac{5^2+6^2}{5\times 6}\right) + (2p+2)\left(\frac{5^2+7^2}{5\times 7}\right) \\
&+ (2p-2)\left(\frac{5^2+8^2}{5\times 8}\right) + 4\left(\frac{6^2+6^2}{6\times 6}\right) + (6p+8q-18)\left(\frac{6^2+7^2}{6\times 7}\right) + (2p-2)\left(\frac{6^2+8^2}{6\times 8}\right) \\
&+ 2\left(\frac{7^2+7^2}{7\times 7}\right) + (4p+4q-12)\left(\frac{7^2+9^2}{7\times 9}\right) + (2p-2)\left(\frac{8^2+8^2}{8\times 8}\right) + (4p-4)\left(\frac{8^2+9^2}{8\times 9}\right) \\
&+ (15pq-28p-14q+26)\left(\frac{9^2+9^2}{9\times 9}\right)
\end{aligned}$$

After an easy computation, we arrive at

$$ND_5(SiC_4 - II[p,q]) = 135pq - 6.7024p - 3.5556q - 0.1294.$$

By definition, M_2^{nm} index of $SiC_4 - II[p,q]$ is calculated as follows by using the edge partition,

$$\begin{aligned}
M_2^{mn}(SiC_4 - II[p,q]) &= \sum_{st\in E(G)} \frac{1}{\delta_s \times \delta_t} \\
&= \frac{2}{2\times 3} + \frac{2}{5\times 3} + \frac{2p}{5\times 5} + \frac{2}{5\times 6} + \left(\frac{2p+2}{5\times 7}\right) + \frac{2p-2}{5\times 8} + \left(\frac{4}{6\times 6}\right) \\
&+ \left(\frac{6p+8q-18}{6\times 7}\right) + \left(\frac{2p-2}{6\times 8}\right) + \left(\frac{2}{7\times 7}\right) + \left(\frac{4p+4q-12}{7\times 9}\right) + \left(\frac{2p-2}{8\times 8}\right) \\
&+ \left(\frac{4p-4}{8\times 9}\right) + \left(\frac{15pq-28p-14q+26}{9\times 9}\right)
\end{aligned}$$

We obtain our desired outcome after simplifying the above form,

$$M_2^{nm}(SiC_4 - II[p,q]) = 0.1852pq + 0.1763p + 0.0811q + 0.2659.$$

Silicon Carbides	ABC_4	GA_5	NH	NI	ND_5	M_2^{nm}
Si_2C_3-I	12.3292	22.6608	4.0108	69.1425	256.7324	0.7831
Si_2C_3-II	11.9640	20.7150	4.3564	53.0418	44.4048	1.0450
Si_2C_3-III	12.3279	32.7478	4.0867	68.5614	47.4253	0.7556
SiC_3-I	9.5193	16.7028	3.3302	46.1289	36.5545	0.7741
SiC_3-II	9.7810	17.7030	3.1650	51.8270	38.5040	0.6020
SiC_3-III	9.4643	15.6238	3.4473	2.3714	35.1928	0.8439
SiC_4-I	11.6930	69.2680	3.8160	58.1050	47.9490	0.8270
SiC_4-II	11.9538	20.2621	5.1072	39.5183	252.9102	1.0700

TABLE 2 Computed TI values for $p=2$ and $q=1$

Topological indices	N	A	B	r	F	p	Indicator
ABC_4	6	-0.154	9.365	-0.510	2.106	<0.001	Significant
GA_5	6	0.005	7.526	0.215	0.292	<0.001	Significant
NH	6	-0.092	8.015	-0.149	0.136	<0.001	Significant
NI	6	-0.009	8.086	-0.485	1.848	<0.001	Significant
ND_5	6	-0.00007	7.660	-0.019	0.002	<0.001	Significant
M_2^{nm}	6	-0.041	7.687	-0.016	0.002	<0.001	Significant

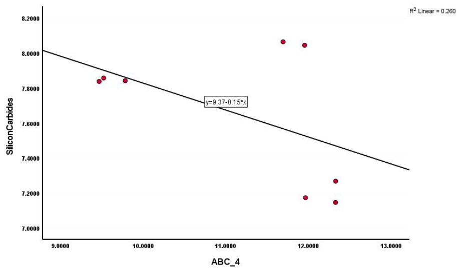
TABLE 3 Statistical parameters for the linear QSPR model for Topological indices

6 | DISCUSSION AND GRAPH COMPARISON

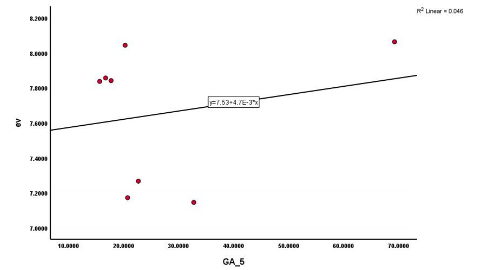
In this paper, we evaluated some topological indices to a class of $2D$ molecular structures of silicon carbide for certain value of $p=2$ and $q=1$ Table. 2 and Table: 3 shows the computation of statistical parameters of the linear model for defined topological indices. In particular, we obtain closely related formulas of all topological indices for some p and q values. One can observe that as the values of p and q increase, the value of all indices increases accordingly.

Topological indices usually correlate with the physical-chemical properties of a molecule. In physical chemistry, cohesive energy is a physical property that measures the energy required to break all the bonds associated with one of its constituent molecules. With this motivation, we compared the values of topological indices with energy and stability measures for silicon carbide compounds.

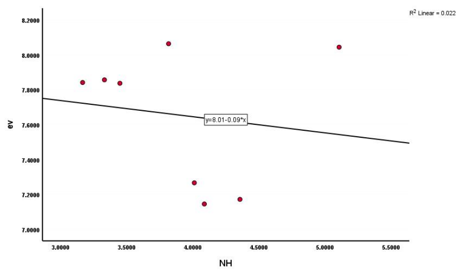
Fig. 4 shows the correlation graphs between topological indices and physical property (eV) for silicon carbide structures. Besides all the indices, the bond-breaking energy for the atom of silicon carbide structures can be predicted by the GA_5 index since it is positively correlated. Furthermore, from a thermodynamic point of view, the low stability of silicon carbide structures is a also predicted by the GA_5 index, see Fig. 5.



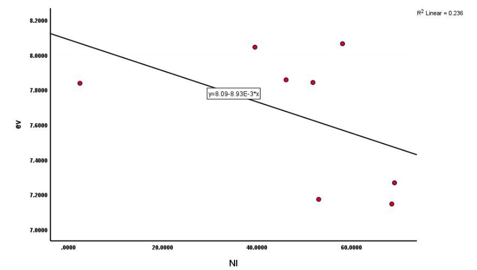
(a) ABC_5



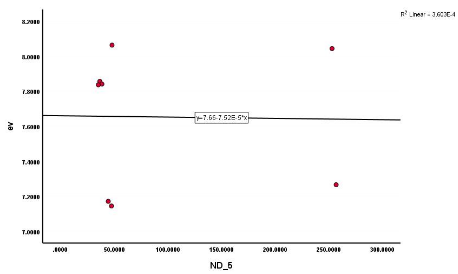
(b) GA_5



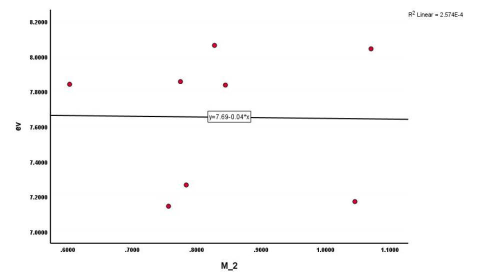
(c) NH



(d) NI



(e) ND_5



(f) M_2^{nm}

FIGURE 4 Correlation graphs for Silicon-Carbide structures

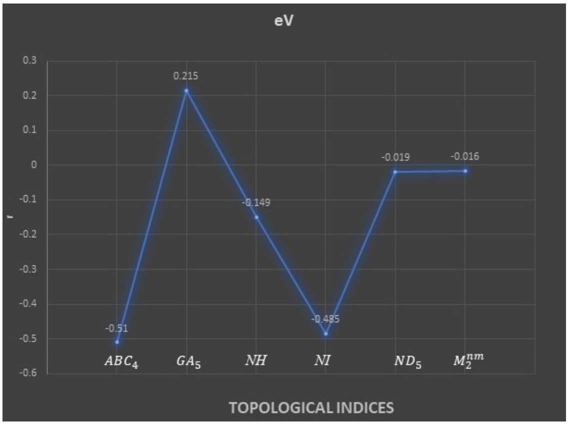


FIGURE 5 Correlation graphs for Silicon-Carbide structures

7 | CONCLUSION

In this analysis, we examine all 2D $Si - C$ compounds, and although they are C-rich, they are mostly lowest-energy and low-energy metastable structures. A heptagonal or a pentagonal ring can occasionally form in a low-energy structure, and an octagonal ring typically appears in a metastable structure. We compute topological indices for $Si - C$ structures with these features. Moreover, we visualize the correlation graph for all the indices. Consequently, this paper presents a prediction of energy and stability measured by topological indices. Our future aim is to find out which index correlates well with the rest of the traits.

Conflict of interest

The authors declare that there is no conflict of interest.

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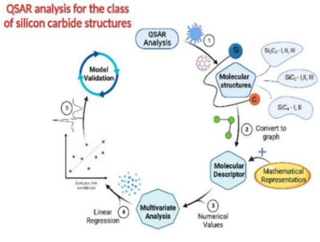
GRAPHICAL ABSTRACT



In this paper, topological indices have been used for a class of silicon-carbon structures to analyze their bond-breaking energy and stability measures.