Chemical Applicability of Newly Introduced Topological Invariants and Their Relation with Polycyclic Compounds

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Received 2 May 2022; Revised 27 May 2022; Accepted 2 June 2022; Published 31 July 2022

1. Introduction and Preliminaries

To reduce the consumption of time and cost during examining the biological, physical, and chemical properties of millions of newly invented nanomaterials, crystalline materials, and drugs, chemists study the quantitative structure-property relationship (QSPR) and the quantitative structure-activity relationship (QSAR) [1–4]. Topological indices (TIs), numeric invariants describing properties of particular molecular structures, are used as a fundamental tool in the QSPR and QSAR. These indices help in production of different chemicals with desired characteristics and estimation of physiochemical properties of existing compounds [5–9]. Another dominant benefit of the TIs is their effectiveness during investigation of different aspects of chemical compounds and new drugs, which is the fundamental requirement of the medical sciences and industry. Consequently, studying and computing the behavior of the TIs of the molecular structures is a significant source to provide qualitative and quantitative information and therefore is one of the trends in modern research. Along with drug design, isomer discrimination, chemical documentation, and biological characterization, different applications of TIs in mathematical chemistry are described in [10–15].

Silicon carbides, which occur as incredibly abundant minerals in nature containing covalent bonds between carbon and silicon atoms, are biatomic compounds with tetrahedrally oriented layers of carbon and silicon atoms. Because of these strongly packed layers and short-length covalent bonds, SiC as consequences of nonoxidizing behavior, high melting points, high erosion resistance, thermal, and chemical stability, silicon carbides have vital industrial applications [16–18]. These electrical properties and low-cost production methodologies give superiority to silicon carbides among other metals and semiconductors. Being one of the most extensively used wide bandgap materials, SiC performs a vital role in power industries by setting new principles in power savings as rectifiers or switches in the system for data centers, wind turbines, solar cells, and electric vehicles along with high radiation and temperature-
tolerant electronic appliances. Several papers have been devoted to the study of silicon and carbon-based structures, for details, see [19–23]. Some silicon carbides variants such as $Si_2C_3 - I[a, b], Si_2C_3 - II[a, b], Si_2C_3 - III[a, b]$ and $SiC_3 - I[a, b]$ are studied in this article.

The main objective of our work is to inaugurate some novel indices, discuss the physical and chemical applicability of octane isomers using regression models, and compute defined indices for different variants of silicon carbides mentioned earlier. This process provides an accurate estimation of physicochemical properties, i.e., boiling point, melting point, bond energy, and intermolecular forces. Particularly, these indices are helpful in predicting the properties of chemical compounds having polymerization such as silicon carbides, benzenoid hydrocarbons, and carbon nanotubes widely used in nanotech equipment.

Now, we provide some preliminary concepts, while standard notations [24] are referred. Consider $G(\mathcal{V}, E)$ be a graph with a vertex set $\mathcal{V}$ and an edge set $E$, the number of different edges that are incident to a vertex $v$ is the degree of the vertex $v$ denoted by $d_v$. Furthermore, a subset $\mathcal{N} \subseteq \mathcal{V}$ of all vertices which are adjacent to a vertex $v$ is known as open neighborhood of $v$ denoted by $\mathcal{N}(v)$. If we include the vertex $v$ to the set $\mathcal{N}(v)$, then we obtain the closed neighborhood of $v$, denoted by $\mathcal{N}'[v]$. The ev-degree of the edge $e = uv \in E$ is denoted by $\lambda_{e,v}$ and the number of vertices of the union of the closed neighborhoods of $u$ and $v$.

A number of topological indices have been introduced in the last decade such as the vertex connectivity index, edge connectivity index, geometric index, wiener index, harmonic index, Randić’s molecular connectivity index, and face index [25–30]. The concept of neighborhood degrees was introduced by Chellali [31], and then, numerous articles have been published elaborating on these concepts [32–34]. Lately, Usha et al. [35] introduced the geometric-harmonic index combining geometric and harmonic indices, inspired by Furtula and Vukičević [36] in designing the GHI.

$$GHI(G) = \sum \frac{(d_u + d_v) \sqrt{d_u \cdot d_v}}{2}$$

Shanmukha [37] et al. introduced three degree and neighborhood degree-based novel indices, namely, harmonic-geometric (HGI), neighborhood harmonic-geometric (NHGI), and neighborhood geometric-harmonic (NGHI) indices motivated by the above work. They are defined as follows:

$$\text{HGI}(G) = \sum \frac{2}{(d_u + d_v) \sqrt{d_u \cdot d_v}}$$

$$\text{NGHI}(G) = \sum \frac{(\lambda_u + \lambda_v) \sqrt{\lambda_u \cdot \lambda_v}}{2}$$

$$\text{NHGI}(G) = \sum \frac{2}{(\lambda_u + \lambda_v) \sqrt{\lambda_u \cdot \lambda_v}}$$

To compute our results, we utilize the edge parcel technique, vertex segment strategy, graph hypothetical devices, degree checking strategy, expository strategies, the whole of degrees of the neighbor technique, and combinatorial techniques. In addition, MATLAB is utilized for mathematical calculations and verifications, whereas Maple is used for graphical analysis and plotting these scientific results.

2. Regression Models and Chemical Applicability

In this section, linear regression models of newly introduced topological indices and four physical properties of octane isomers as shown in Figure 1 are presented. These models describe that physical properties, i.e., anacentric factor (AF), entropy (S), enthalpy of vaporization (HVAP), and standard enthalpy of vaporization (DHVAP) have excellent correlation with the GHI, NGHI, HGI, and NHGI.

The linear regression models for $S, AF, HVAP,$ and DHVAP are generated utilizing the method of least squares and given data in Table 1. The regression models for the GHI with mentioned physical properties are given as follows:

$$S = 133.0781 (\pm 1.8201) - 0.8332 (\pm 0.0540)GHI,$$

$$AF = 0.5571 (\pm 0.0093) - 0.0069 (\pm 0.0000)GHI,$$

$$HVAP = 79.613 (\pm 1.878) - 0.315 (\pm 0.056)GHI,$$

$$DHVAP = 11.273 (\pm 0.285) - 0.065 (\pm 0.008)GHI.$$ (3)

The regression models for the HGI with mentioned physical properties are given as follows:

$$S = 76.6079 (\pm 4.4860) + 15.7661 (\pm 2.4350)HGI,$$

$$AF = 0.1143 (\pm 0.0371) + 0.1211 (\pm 0.0202)HGI,$$

$$HVAP = 54.9601 (\pm 1.3559) + 7.7728 (\pm 0.7360)HGI,$$

$$DHVAP = 6.4280 (\pm 0.2491) + 1.4772 (\pm 0.1350)HGI.$$ (4)

The regression models for the NHGI with mentioned physical properties are given as follows:

$$S = 121.7701 (\pm 2.3500) - 0.1189 (\pm 0.0170)NHGI,$$

$$AF = 0.4650 (\pm 0.01803) - 0.0011 (\pm 0.0000)NHGI,$$

$$HVAP = 75.0071 (\pm 1.5522) - 0.0431 (\pm 0.0110)NHGI,$$

$$DHVAP = 10.3631 (\pm 0.2570) - 0.0094 (\pm 0.0021)NHGI.$$ (5)

The regression models for the NGHI with mentioned physical properties are given as follows:

$$S = 89.5241 (\pm 2.5052) + 34.3521 (\pm 5.2711)NGHI,$$

$$AF = 0.2072 (\pm 0.0182) + 0.2770 (\pm 0.0380)NGHI,$$

$$HVAP = 62.6671 (\pm 1.3520) + 14.0441 (\pm 2.8460)NGHI,$$

$$DHVAP = 7.7929 (\pm 0.2188) + 2.8821 (\pm 0.4600)NGHI.$$ (6)
In the above equations, the errors of regression coefficients are written within brackets. The residual standard (RS) error and the correlation coefficient for the regression models of GHI, NGHI, HGI, and NHGI with four physical properties are presented in Figures 2–5 and Tables 2–5 which clarify a significant association between these parameters.

3. Results for \( \text{Si}_2\text{C}_3 - II[a, b] \)

Utilizing edge partition strategies, degree, and ev-degree based frequencies of different edges, two-dimensional molecular structure of \( \text{Si}_2\text{C}_3 - II[a, b] \) is analyzed in Tables 6 and 7 whereas Figure 6 describes the unit molecular cell and \( \text{Si}_2\text{C}_3 - II[4, 1] \) having 1 row and 4 molecules in each row.
Figure 2: Correlation of GH (x-axis) and physical properties S, AF, HVAP, and DHVAP (y-axis).

Figure 3: Correlation of HG (x-axis) and physical properties S, AF, HVAP, and DHVAP (y-axis).
**Figure 4:** Correlation of NGH (x-axis) and physical properties S, AF, HVAP, and DHVAP (y-axis).

**Figure 5:** Correlation of NHG (x-axis) and physical properties S, AF, HVAP, and DHVAP (y-axis).
By the definition of the degree-based geometric-harmonic index, harmonic-geometric index, and edge frequency of $Si_2C_3-II[a, b]$ given in Table 6, we compute following results:

$$GHI^d(Si_2C_3-II) = \sum_{e \in E(Si_2C_3-II)} \frac{(d_u + d_v)\sqrt{d_u \cdot d_v}}{2} = 2 \times \frac{3\sqrt{2}}{2} + 1 \times \frac{4\sqrt{3}}{2} + (2a + 2b + 1) \times \frac{4\sqrt{2}}{2}$$

$$+ (8a + 8b - 14) \times \frac{5\sqrt{6}}{2} + (15ab - 13a - 13b + 11) \times \frac{6\sqrt{9}}{2}$$

$$= 135ab - \frac{7501}{125}a - \frac{7501}{125}b - \frac{3122}{125}.$$  

$$HGI^d(Si_2C_3-II) = \sum_{e \in E(Si_2C_3-II)} \frac{(d_u + d_v)\sqrt{d_u \cdot d_v}}{2} = 2 \times \frac{2}{3\sqrt{2}} + 1 \times \frac{2}{4\sqrt{3}} + (2a + 2b + 1) \times \frac{2}{4\sqrt{4}}$$

$$+ (8a + 8b - 14) \times \frac{2}{5\sqrt{6}} + (15ab - 13a - 13b + 11) \times \frac{2}{6\sqrt{9}}$$

$$= \frac{208}{125}ab + \frac{45}{125}a + \frac{45}{125}b + \frac{16}{125}.$$  

By the definition of the ev-degree-based geometric harmonic index, harmonic geometric index, and edge frequency of $Si_2C_3-II[a, b]$ given in Table 7, we compute following results:

| Physical properties | Correlation coefficient | RS Error |
|---------------------|-------------------------|----------|
| Entropy             | -0.9680                 | 1.1700   |
| Acentric factor     | -0.9870                 | 0.0059   |
| HVAP                | -0.8150                 | 1.2100   |
| DHVAP               | -0.8850                 | 0.1840   |

| Physical properties | Correlation coefficient | RS Error |
|---------------------|-------------------------|----------|
| Entropy             | 0.8500                  | 2.4480   |
| Acentric factor     | 0.8330                  | 0.0200   |
| HVAP                | 0.9350                  | 0.7400   |
| DHVAP               | 0.9390                  | 0.1360   |

| Physical properties | Correlation coefficient | RS Error |
|---------------------|-------------------------|----------|
| Entropy             | -0.8730                 | 2.2740   |
| Acentric factor     | -0.8770                 | 0.01760  |
| HVAP                | -0.6950                 | 1.5020   |
| DHVAP               | -0.7780                 | 0.2480   |

| Physical properties | Correlation coefficient | RS Error |
|---------------------|-------------------------|----------|
| Entropy             | 0.8520                  | 2.4360   |
| Acentric factor     | 0.8770                  | 0.0180   |
| HVAP                | 0.7770                  | 1.3150   |
| DHVAP               | 0.8430                  | 0.2130   |

| $(d_u, d_v)$         | Frequency               |
|---------------------|-------------------------|
| (1, 2)              | 2                       |
| (1, 3)              | 1                       |
| (2, 2)              | $2a + 2b + 1$           |
| (2, 3)              | $8a + 8b - 14$          |
| (3, 3)              | $15ab - 13a - 13b + 11$ |
Table 7: The number of edges of $\text{Si}_2\text{C}_3 - \text{II}[a,b]$.

| $(\lambda_u, \lambda_v)$ | Frequency |
|-------------------------|-----------|
| (2, 3)                  | $2a + 2b - 4$ |
| (3, 4)                  | $4a - 4$ for $a = 1$ |
| (4, 5)                  | $2a + 2b - 2$ for $a \geq 2$ |
| (5, 5)                  | $4a - 5$ for $a = 1$ |
| (6, 5)                  | $2a - 2b$ for $a \geq 2$ |
| (7, 6)                  | $1$ for $a = 1$ |
| (5, 7)                  | $0$ for $a \geq 2$ |
| (3, 6)                  | $1$ for $a = 1$ |
| (6, 6)                  | $0$ for $a \geq 2$ |
| (7, 7)                  | $2a - 3$ for $a = 1$ |
| (7, 8)                  | $0$ for $a = 1$ |
| (9, 9)                  | $4$ for $a \geq 2$ |

\[ \text{NGHI}^{\text{TV}}(\text{Si}_2\text{C}_3 - \text{II}) = \sum_{\mathcal{E}(\text{Si}_2\text{C}_3 - \text{II})} (\lambda_u + \lambda_v) \sqrt{\lambda_u \cdot \lambda_v} \]

\[ = 2 \times \frac{5\sqrt{6}}{2} + 2 \times \frac{7\sqrt{12}}{2} + 2 \times \frac{9\sqrt{20}}{2} + (2a + 2b + 4) \times \frac{10\sqrt{25}}{2} + (2a + 2b - 2) \times \frac{13\sqrt{42}}{2} + (2a + 2b) \times \frac{12\sqrt{35}}{2} + 4 \times \frac{15\sqrt{56}}{2} + (15ab - 21a + 21b + 30) \]

\[ \times \frac{18\sqrt{81}}{2} + (2a + 2b - 6) \times \frac{14\sqrt{48}}{2} + (4a + 4b - 12) \times \frac{17\sqrt{72}}{2} \]

\[ + (2a + 2b - 6) \times \frac{13\sqrt{40}}{2} + 1 \times \frac{10\sqrt{21}}{2} + (2a + 2b - 3) \times \frac{16\sqrt{63}}{2} + (2a + 2b - 8) \times \frac{16\sqrt{64}}{2} \]

\[ = 765ab + \frac{5232}{25}a + \frac{54860}{25}b + \frac{12857}{25} \]

\[ \text{NHGI}^{\text{TV}}(\text{Si}_2\text{C}_3 - \text{II}) = \sum_{\mathcal{E}(\text{Si}_2\text{C}_3 - \text{II})} \frac{2}{(\lambda_u + \lambda_v) \sqrt{\lambda_u \cdot \lambda_v}} \]
\[ GHI_d(SiC_3 - III) = \sum_{e \in E(SiC_3 - III)} \frac{(d_u + d_v)\sqrt{d_u \cdot d_v}}{2} \]
\[ = 2 \times \frac{2}{\sqrt{2}} + 2 \times \frac{2}{\sqrt{12}} + 2 \times \frac{2}{9\sqrt{20}} + (2a + 2b + 4) \times \frac{2}{10\sqrt{25}} + (2a + 2b - 2) \]
\[ \times \frac{2}{13\sqrt{42}} + (2a + 2b) \times \frac{2}{12\sqrt{56}} + (4) \times \frac{2}{15\sqrt{56}} + (15ab - 21a + 21b + 30) \]
\[ \times \frac{2}{18\sqrt{81}} + (2a + 2b - 6) \times \frac{2}{14\sqrt{48}} + (4a + 4b - 12) \times \frac{2}{17\sqrt{72}} + (2a + 2b - 6) \]
\[ \times \frac{2}{13\sqrt{40}} + 1 \times \frac{2}{10\sqrt{21}} + (2a + 2b - 3) \times \frac{2}{16\sqrt{63}} + (2a + 2b - 8) \times \frac{2}{16\sqrt{64}} \]
\[ = \frac{108ab - 7407}{125} + \frac{4938}{125} a + \frac{2340}{125} b + \frac{7}{25} \]

\[ HGI_d(SiC_3 - III) = \sum_{e \in E(SiC_3 - III)} \frac{2}{(d_u + d_v)\sqrt{d_u \cdot d_v}} \]
\[ = 2 \times \frac{2}{3\sqrt{2}} + (1) \times \frac{2}{4\sqrt{3}} + (3a + 2b - 3) \times \frac{2}{4\sqrt{4}} + (6a + 4b - 8) \]
\[ \times \frac{2}{5\sqrt{6}} + (12ab - 12a - 8b + 8) \times \frac{2}{6\sqrt{9}} \]
\[ = \frac{167ab + 2}{125} a + \frac{33}{125} b + \frac{8}{125} \]

4. Results for \(SiC_3 - III\) \([a, b]\)

Utilizing edge partition strategies, degree, and ev-degree-based frequencies of different edges, two-dimensional molecular structure of \(SiC_3 - III\) \([a, b]\) is analyzed in Tables 8 and 9 whereas Figure 7 describes the unit molecular cell and \(SiC_3 - III\) \([5, 2]\) having 2 rows and 5 unit molecules in each row.

By the definition of the degree-based geometric-harmonic index, harmonic-geometric index, and edge frequency of \(SiC_3 - III\) \([a, b]\) given in Table 8, we compute following results:
Table 8: The number of edges of $SiC_3 - III[a, b]$.

| $(d_u, d_v)$ | Frequency |
|-------------|-----------|
| (1, 2)      | 2         |
| (1, 3)      | 1         |
| (2, 2)      | $3a + 2b - 3$ |
| (2, 3)      | $6a + 4b - 8$ |
| (3, 3)      | $12ab - 12a - 8b + 8$ |

Table 9: The number of edges of $SiC_3 - III[a, b]$.

| $(\lambda_u, \lambda_v)$ | Frequency |
|--------------------------|-----------|
| (4, 5)                   | $2a$      |
| (3, 4)                   | $\begin{cases} 1 & \text{for } a = 1 \\ 0 & \text{for } a \geq 2 \end{cases}$ |
| (5, 5)                   | $\begin{cases} a & \text{for } a = 1 \\ a + 2b - 4 & \text{for } a \geq 2 \end{cases}$ |
| (3, 5)                   | $\begin{cases} 1 & \text{for } a = 1 \\ 0 & \text{for } a \geq 2 \end{cases}$ |
| (2, 3)                   | $\begin{cases} 1 & \text{for } a = 1 \\ 0 & \text{for } a \geq 2 \end{cases}$ |
| (4, 2)                   | $\begin{cases} 1 & \text{for } a = 1 \\ 2 & \text{for } a \geq 2 \end{cases}$ |
| (5, 6)                   | $\begin{cases} 4a - 4 & \text{for } a = 1 \\ 1 & \text{for } a \geq 2 \end{cases}$ |
| (6, 6)                   | $\begin{cases} 2a - 2 & \text{for } a = 1 \\ 0 & \text{for } a \geq 2 \end{cases}$ |
| (4, 7)                   | $\begin{cases} 0 & \text{for } a = 1 \\ 2 & \text{for } a \geq 2 \end{cases}$ |
| (7, 5)                   | $\begin{cases} 0 & \text{for } a = 1 \\ 2a - 2b - 4 & \text{for } a \geq 2 \end{cases}$ |
| (4, 4)                   | $\begin{cases} 0 & \text{for } a = 1 \\ 1 & \text{for } a \geq 2 \end{cases}$ |
| (6, 3)                   | $\begin{cases} 0 & \text{for } a = 1 \\ 1 & \text{for } a \geq 2 \end{cases}$ |
| (6, 8)                   | $\begin{cases} 0 & \text{for } a = 1 \\ 1 & \text{for } a \geq 2 \end{cases}$ |
| (8, 9)                   | $\begin{cases} 0 & \text{for } a = 1 \\ 4a + 2b - 7 & \text{for } a \geq 2 \end{cases}$ |
| (8, 5)                   | $\begin{cases} 0 & \text{for } a = 1 \\ 2a + 2b - 5 & \text{for } a \geq 2 \end{cases}$ |
| (7, 9)                   | $\begin{cases} 0 & \text{for } a = 1 \\ 2a + b - 2 & \text{for } a \geq 2 \end{cases}$ |
| (9, 9)                   | $\begin{cases} 0 & \text{for } a = 1 \\ 12ab - 18a - 12b + 18 & \text{for } a \geq 2 \end{cases}$ |
| (6, 7)                   | $\begin{cases} 0 & \text{for } a = 1 \\ 2a - 2 & \text{for } a \geq 2 \end{cases}$ |
| (8, 8)                   | $\begin{cases} 0 & \text{for } 1 \leq a \leq 2 \\ b - 2 & \text{for } a \geq 3 \end{cases}$ |
NGHII\textsuperscript{77} (SiC\textsubscript{3} – III) = \sum_{e \in \text{E(SiC}_{3} – III)} \frac{(\lambda_u + \lambda_v)\sqrt{\lambda_u \cdot \lambda_v}}{2} \\
= 2a \times \frac{9\sqrt{20}}{2} + (a + 2b - 4) \times \frac{10\sqrt{25}}{2} + 2 \times \frac{6\sqrt{8}}{2} + \frac{11\sqrt{30}}{2} + 2 \times \frac{11\sqrt{28}}{2} \\
+ (2a + 2b - 4) \times \frac{(12)\sqrt{(35)}}{2} + \frac{8\sqrt{16}}{2} + \frac{9\sqrt{18}}{2} + \frac{14\sqrt{48}}{2} + (4a + 2b - 7) \\
\times \frac{17\sqrt{72}}{2} + (2a + 2b - 5) \times \frac{13\sqrt{40}}{2} + (2a + b - 2) \times \frac{16\sqrt{63}}{2} + (12ab - 18a - 12b + 18) \\
\times \frac{18\sqrt{81}}{2} + (2a - 2) \times \frac{13\sqrt{42}}{2} + (b - 2) \times \frac{16\sqrt{16}}{2} \\
= 972ab - \frac{18383}{25} a - \frac{13476}{25} b + \frac{13881}{25}, \\
(10) \\
NHGII\textsuperscript{77} (SiC\textsubscript{3} – III) = \sum_{e \in \text{E(SiC}_{3} – III)} \frac{2}{(\lambda_u + \lambda_v)\sqrt{\lambda_u \cdot \lambda_v}} \\
= 2a \times \frac{2}{9\sqrt{20}} + (a + 2b - 4) \times \frac{2}{10\sqrt{25}} + 2 \times \frac{2}{6\sqrt{8}} + \frac{2}{11\sqrt{30}} + 2 \times \frac{2}{11\sqrt{28}} \\
+ (2a + 2b - 4) \times \frac{2}{(12)\sqrt{(35)}} + \frac{2}{8\sqrt{16}} + \frac{2}{9\sqrt{18}} + \frac{2}{14\sqrt{48}} + (4a + 2b - 7) \\
\times \frac{2}{17\sqrt{72}} + (2a + 2b - 5) \times \frac{2}{13\sqrt{40}} + (2a + b - 2) \times \frac{2}{16\sqrt{63}} + (12ab - 18a - 12b + 18) \\
\times \frac{2}{18\sqrt{81}} + (2a - 2) \times \frac{2}{13\sqrt{42}} + (b - 2) \times \frac{2}{16\sqrt{16}} \\
= \frac{4}{25} ab + \frac{304}{25} a + \frac{171}{25} b + \frac{320}{25}.
5. Results for $\text{Si}_2\text{C}_3-\text{III} \{a,b\}$

Utilizing edge partition strategies, degree, and ev-degree based frequencies of different edges, two-dimensional molecular structure of $\text{Si}_2\text{C}_3-\text{III} \{a,b\}$ is analyzed in Tables 10 and 11, whereas Figure 8 describes the unit molecular cell and $\text{Si}_2\text{C}_3-\text{III} [5,4]$ having 4 rows and 5 unit molecules in each row. By the definition of the degree-based geometric-harmonic index, harmonic-geometric index, and edge frequency of $\text{Si}_2\text{C}_3-\text{III} \{a,b\}$ given in Table 10, we compute following results:

$$\text{GHI}^d (\text{Si}_2\text{C}_3-\text{III}) = \sum_{e \in E (\text{Si}_2\text{C}_3-\text{III})} \frac{(d_u + d_v)\sqrt{d_u \cdot d_v}}{2}$$

$$= 2 \times \frac{4\sqrt{3}}{2} + (8a + 8b - 12) \times \frac{5\sqrt{6}}{2} + (2b + 2) \times \frac{4\sqrt{4}}{2} + (15ab - 10a - 13b + 8) \times \frac{6\sqrt{9}}{2}$$

$$= 135ab - 41a - 60b + \frac{336}{25}$$

(11)

$$\text{HGI}^d (\text{Si}_2\text{C}_3-\text{III}) = \sum_{e \in E (\text{Si}_2\text{C}_3-\text{III})} \frac{2}{(d_u + d_v)\sqrt{d_u \cdot d_v}}$$

$$= 2 \times \frac{2}{4\sqrt{3}} + (8a + 8b - 12) \times \frac{2}{5\sqrt{6}} + (2b + 2) \times \frac{2}{4\sqrt{4}} + (15ab - 10a - 13b + 8) \times \frac{2}{6\sqrt{9}}$$

$$= \frac{208}{125}ab + \frac{24}{125}a + \frac{45}{125}b + \frac{1}{100}$$

By the definition of the ev-degree-based geometric-harmonic index, harmonic-geometric index, and edge frequency of $\text{Si}_2\text{C}_3-\text{III} \{a,b\}$ given in Table 11, we compute following results:

$$\text{NGHI}^{ev} (\text{Si}_2\text{C}_3-\text{III}) = \sum_{e \in E (\text{Si}_2\text{C}_3-\text{III})} \frac{(\lambda_u + \lambda_v)\sqrt{\lambda_u \cdot \lambda_v}}{2}$$

$$= 2 \times \frac{8\sqrt{15}}{2} + 2b \times \frac{10\sqrt{25}}{2} + 4 \times \frac{9\sqrt{20}}{2} + (4b - 2) \times \frac{(12)\sqrt{35}}{2}$$

$$+ (8a + 4b - 14) \times \frac{13\sqrt{42}}{2} + 2 \times \frac{11\sqrt{30}}{2} + (4a + 8b - 8) \times \frac{16\sqrt{63}}{2} + (15ab - 14a - 17b + 16) \times \frac{18\sqrt{81}}{2}$$

$$= 1215ab + \frac{67876}{125}a + \frac{95315}{125}b + \frac{37376}{125}$$

(12)

$$\text{NHGI}^{ev} (\text{Si}_2\text{C}_3-\text{III}) = \sum_{e \in E (\text{Si}_2\text{C}_3-\text{III})} \frac{2}{(\lambda_u + \lambda_v)\sqrt{\lambda_u \cdot \lambda_v}}$$

$$= 2 \times \frac{2}{8\sqrt{15}} + 2b \times \frac{2}{10\sqrt{25}} + 4 \times \frac{2}{9\sqrt{20}} + (4b - 2) \times \frac{2}{12\sqrt{35}}$$

$$+ (8a + 4b - 14) \times \frac{2}{13\sqrt{42}} + (2) \times \frac{11\sqrt{30}}{2} + (4a + 8b - 8) \times \frac{16\sqrt{63}}{2}$$

$$\times \frac{18\sqrt{81}}{2} + (15ab - 14a - 17b + 16) \times \frac{2}{18\sqrt{81}}$$

$$= \frac{1}{5}ab + \frac{295}{25}a + \frac{294}{25}b - \frac{241}{25}.$$
6. Results for $Si_2C_3 - I[a, b]$

Utilizing edge partition strategies, degree, and ev-degree-based frequencies of different edges, two-dimensional molecular structure of $Si_2C_3 - I[a, b]$ is analyzed in Tables 12 and 13, whereas Figure 9 describes the unit molecular cell and $Si_2C_3 - III[3, 4]$ having 3 rows and 4 unit molecules in each row.

By the definition of the degree-based geometric-harmonic index, harmonic-geometric index, and edge frequency of $Si_2C_3 - I[a, b]$ given in Table 12, we compute following results:

### Table 10: The number of edges of $Si_2C_3 - III[a, b]$.

| $(d_u, d_v)$ | Frequency |
|-------------|-----------|
| (1, 3)      | 2         |
| (2, 2)      | $2b + 2$  |
| (2, 3)      | $8a + 8b - 12$ |
| (3, 3)      | $15ab - 10a - 13b + 8$ |

### Table 11: The number of edges of $Si_2C_3 - III[a, b]$.

| $(\lambda_u, \lambda_v)$ | Frequency |
|--------------------------|-----------|
| (3, 5)                   | 2         |
| (5, 5)                   | $2b$      |
| (5, 4)                   | 4         |
| (5, 7)                   | $4b - 2$  |
| (6, 7)                   | $8a + 4b - 14$ |
| (6, 5)                   | 2         |
| (7, 9)                   | $4a + 4b - 8$ |
| (9, 9)                   | $15ab - 14a - 17b + 16$ |

Figure 8: The unit cell and $Si_2C_3 - III[5, 4]$, respectively.
Table 12: The number of edges of $\text{Si}_2\text{C}_3 - I[a,b]$.

| $(d_{uv}, d_{uv})$ | Frequency   |
|-------------------|-------------|
| (1, 2)            | 2           |
| (1, 3)            | 1           |
| (2, 2)            | $6a + 8b - 9$ |
| (2, 3)            | $a + 2b$    |
| (3, 3)            | $15ab - 9a - 13b + 7$ |

Table 13: The number of edges of $\text{Si}_2\text{C}_3 - I[a,b]$.

| $(\lambda_u, \lambda_v)$ | Frequency   |
|--------------------------|-------------|
| (2, 4)                   | 1           |
| (3, 5)                   | 1           |
| (5, 5)                   | 1           |
| (4, 5)                   | 2           |
| (7, 5)                   | $a + 2b - 1$ |
| (7, 6)                   | $2b + 2$    |
| (7, 9)                   | $4a + 2b - 7$ |
| (7, 8)                   | $2a + 2b - 3$ |
| (4, 7)                   | 1           |
| (8, 5)                   | 1           |
| (8, 9)                   | $2a + 4b - 7$ |
| (8, 8)                   | $a + 2b - 4$ |
| (9, 9)                   | $15ab - 5a - 21b + 20$ |
| (6, 8)                   | $2b - 2$    |

Figure 9: The unit cell and $\text{Si}_2\text{C}_3 - I[5,4]$, respectively.
By the definition of the degree-based geometric-harmonic index, harmonic-geometric index, and edge frequency of $S_i C_3 - I[a, b]$ given in Table 13, we compute following results:

$$\text{NGHI}^{(d)} (S_i C_3 - I) = \sum_{e \in E} \frac{(\lambda_u + \lambda_v) \sqrt{\lambda_u \cdot \lambda_v}}{2}$$

$$= \frac{6 \sqrt{2}}{2} + \frac{8 \sqrt{15}}{2} + \frac{11 \sqrt{30}}{2} + 2 \times \frac{9 \sqrt{20}}{2} + (a + 2b - 1) \times \frac{10 \sqrt{25}}{2} + (2b + 2)$$

$$\times \frac{12 \sqrt{35}}{2} + (4a + 2b - 7) \times \frac{13 \sqrt{42}}{2} + (2a + 2b - 3) \times \frac{16 \sqrt{63}}{2} + \frac{15 \sqrt{56}}{2}$$

$$\times \frac{28 \sqrt{28}}{2} + (2a + 2b - 5) \times \frac{13 \sqrt{40}}{2} + (2a + 4b - 7) \times \frac{17 \sqrt{72}}{2} + (a + 2b - 4)$$

$$\times \frac{64 \sqrt{64}}{2} + (15ab - 5a - 21b + 20) \times \frac{18 \sqrt{81}}{2} + (2b - 2) \times \frac{14 \sqrt{48}}{2}$$

$$= \frac{1}{5} ab + \frac{226}{25} a + \frac{342}{25} b - \frac{414}{25}.$$

$$\text{NHGI}^{(d)} (S_i C_3 - I) = \sum_{e \in E} \frac{(\lambda_u + \lambda_v) \sqrt{\lambda_u \cdot \lambda_v}}{2}$$

$$= \frac{2}{6 \sqrt{2}} + \frac{2 \sqrt{8}}{2 \sqrt{15}} + \frac{2 \sqrt{11 \sqrt{30}}}{2} + 2 \times \frac{2 \sqrt{9 \sqrt{20}}}{2} + (a + 2b - 1) \times \frac{2}{10 \sqrt{25}} + (2b + 2)$$

$$\times \frac{2 \sqrt{12 \sqrt{35}}}{2} + (4a + 2b - 7) \times \frac{2 \sqrt{13 \sqrt{42}}}{2} + (2a + 2b - 3) \times \frac{2}{16 \sqrt{63}} + \frac{2}{15 \sqrt{56}}$$

$$\times \frac{2 \sqrt{11 \sqrt{28}}}{2} + (2a + 2b - 5) \times \frac{2 \sqrt{13 \sqrt{40}}}{2} + (2a + 4b - 7) \times \frac{2}{17 \sqrt{72}} + (a + 2b - 4)$$

$$\times \frac{2 \sqrt{16 \sqrt{64}}}{2} + (15ab - 5a - 21b + 20) \times \frac{2 \sqrt{18 \sqrt{81}}}{2} + (2b - 2) \times \frac{2}{14 \sqrt{48}}$$

$$= \frac{19}{100} ab + \frac{19}{100} a + \frac{14}{100} b - \frac{11}{100}.$$
7. Conclusions

In this article, we discussed the regression models of newly introduced topological descriptors of the geometric-harmonic index, harmonic-geometric index, neighborhood geometric-harmonic index, and neighborhood harmonic-geometric index. We analyzed extraordinary correlation coefficients for these indices with different physical properties of octane isomers which represent the strong prediction abilities of the GHI, NGHI, HGI, and NHGI. Analytical values of these molecular variants are calculated to estimate physiochemical properties of silicon carbides. Our work allows researchers to calculate TIs for different polymeric compounds to elaborate on their chemical topologies and characteristics in the future. Also, we analyze the computed information and result graphically to understand their behavior with increasing molecular units in chemical structure of silicon carbides as shown in Figures 10 and 11.

Data Availability

The data used to support the findings of this study are included within the article.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

Acknowledgments

The authors would like to thank the Deanship of Scientific Research of King Abdulaziz University, Jeddah, Saudi Arabia, for technical and financial support.

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