Research Article

Novel Degree-Based Topological Descriptors of Carbon Nanotubes

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Received 27 July 2021; Accepted 27 August 2021; Published 8 September 2021

1. Introduction

The applications of graph theory are diversified in every field, but chemistry is the major area of the implementation of graph theory. In chemical graph theory, topological index plays a vital role which facilitates the chemists with a treasure of data that correlate with the structure of the chemical compound. The topological index is a numerical descriptor, defines the graph topology of the molecule, and predicts an extensive range of molecular properties [5–6].

From the last two decades, topological indices (TIs) are identified and used in pharmacological medicine, bio-inorganic chemistry, toxicity, and theoretical chemistry and are also used for correlation analysis [7–11].

Topological descriptors are frequently used in the discovery of drugs as they have rich datasets that give high predictive values. These descriptors give the information depending on the arrangement of atoms and their bonds of a chemical compound. They are studied for chemical compounds where, generally, the hydrogen atoms are suppressed. The originality of QSAR/QSPR models depends on physicochemical properties for chemical compounds with high degree of precision. These models depend on various factors such as selecting the suitable compounds, suitable descriptors, and suitable algorithms or tools used in model development [12]. The QSAR/QSPR analysis is based on the data obtained by the numerical descriptors. These data are used to verify whether the compound under the study is suitable for drug making as the TIs provide computational data about the compound. Considering the information of the compound, QSAR/QSPR/QSTR analyses are carried out.

The TIs have increasing popularity in the field of research as they involve only computation without performing any physical experiment. Recent years have proved considerable attention in TIs as the effects of an atomic type and group efforts are considered in QSAR/QSPR modelling [13–15]. Distance-based TIs are used in QSAR analysis,
while chirality descriptors are introduced based on molecular graphs [16].

Alkanes are acyclic saturated hydrocarbons in which carbons and hydrogens are arranged in a tree-like structure. The main use of alkanes is found in crude oil such as petroleum, cooking gas, pesticides, and drug synthesis. The compounds that contain absolutely the same number of atoms but their arrangement differs are termed as isomers. A study is carried out for eighteen octane isomers (refer Figure 1).

A structure whose size is between the microscopic and molecular structure is referred to as a nanostructure. There are different types of nanostructures, namely, nanocages, nanocomposites, nanoparticles, nanofabrics, etc. In the recent years, nanostructures have attracted lot of researchers in the areas of biology, chemistry, and medicines. Topological indices of nanostructures can be studied from [17–24]. The nanostructures made of carbons with cylindrical shape are carbon nanotubes (CNTs). They have a similar structure to that of a fullerene and graphene except their cylindrical shape. The shape of fullerene is as that of a football or basketball design where hexagons are connected.

In 1991, Iijima [25] used carbon nanotubes that have attracted many researchers in nanoscience and nanotechnology worldwide. As they have exotic properties, they are widely used in both research and applications. Nanotubes have a distinctive structure with remarkable mechanical and electrical properties. In case of carbon nanotubes, the hexagons are surrounded by squares, and each of these patterns is linearly arranged. Carbon nanotubes reveal exceptional electrical conductivity and possess wonderful tensile strength and thermal conductivity as they have nanostructures in which the carbon atoms are strongly connected.

Carbon nanotubes have applications in orthopaedic implants, especially in total hip replacement and other treatments pertaining to bone-related ailments. They are used as a grouting agent placed between the prosthesis and the bone as a part of their therapeutic use. The CNTs are used in biomedical fields because of their structural stiffness and effective optical absorption from UV to IR. Also, they can be altered chemically which are expected to be useful in many fields of technology such as electronics, composites materials, and carbon fibres. They have incredible applications in the field of materials science [26]. When the hexagonal lattice is rolled in different directions, it looks like single-wall carbon nanotubes have spiral shape and translational symmetry along the tube axis. It has rotational symmetry along its own axis. Even though nanotubes have favourable applications in a variety of fields, their large-scale production has been restricted. The main constraint that obstructs their use lies in difficulty in controlling their structure, impurities, and poor process ability. To enhance their usage, they have grabbed the attention especially in the formation of composites with polymers.

There are two types of configurations in the arrangement of nanotubes, namely, zigzag and armchair. In the zigzag configuration, the hexagons are placed one below the other linearly, whereas in the armchair configuration, they are placed next to each other. This gives two different types of configurations with different terminologies discussed now. To explain the structure of a nanotube that is infinitely long, we imagine it to be cut open by a parallel axis and placed on a plane. Then, the atoms and bonds coincide with an imaginary graphene sheet. The length of the two atoms on opposite edges of the strip corresponds to circumference of the cylindrical graphene sheet [27–29].

The main objectives of this work are as follows:

To define novel indices
To discuss the physical and chemical applicability of octane isomers using regression models
To compute defined indices for carbon nanotubes such as \( C_4C_8(S) \), \( C_4C_8(R) \), and H-naphthalenic nanosheets

Let \( G = (V, E) \) be a graph with a vertex set \( V(G) \) and an edge set \( E(G) \) such that \( |V(G)| = n \) and \( |E(G)| = m \). For standard graph terminologies and notations, refer to [30, 31], where \((u,v)\) is an element of \( E(G) \), \( d_u \) represents the degree of the vertex \( u \), and \( S_u \) represents the neighborhood degree of the vertex \( u \).

**Definition 1.** Recently, Usha et al. [32] defined the geometric-harmonic (GH) index, inspired by Vukicevic and Furtula [33] in designing the GA index:

\[
GH(G) = \sum \frac{(d_u + d_v)\sqrt{d_u \cdot d_v}}{2}
\]

Motivated by the above work, in this paper, an attempt is made to define three novel indices based on degree and neighborhood degree, namely, harmonic-geometric (HG), neighborhood geometric-harmonic (NGH), and neighborhood harmonic-geometric (NHG) indices. They are defined as follows:

\[
HG(G) = \sum \frac{2}{(d_u + d_v)\sqrt{d_u \cdot d_v}}
\]

\[
NGH(G) = \sum \frac{2}{(S_u + S_v)\sqrt{S_u \cdot S_v}}
\]

\[
NHG(G) = \sum \frac{2}{(S_u + S_v)\sqrt{S_u \cdot S_v}}
\]

1.1. Chemical Applicability of GH, NGH, HG, and NHG Indices. In this section, a linear regression model of four physical properties is presented for GH, NGH, HG, and NHG indices. The physical properties such as entropy \((S)\), acentric factor \((AF)\), enthalpy of vaporization \((HVAP)\), and standard enthalpy of vaporization \((DHVAP)\) of octane isomers have shown good correlation with the indices considered in the study. The GH, HG, NGH, and NHG indices are tested for the octane isomers' database available at https://www.moleculardescriptors.eu/dataset.htm. The GH, HG, NGH, and NHG indices are computed and tabulated in columns 6, 7, 8, and 9 of Table 1.
Figure 1: (a) $n$-Octane, (b) 2-methylheptane, (c) 3-methylheptane, (d) 4-methylheptane, (e) 3-ethylhexane, (f) 2,2-dimethylhexane, (g) 2,3-dimethylhexane, (h) 2,4-dimethylhexane, (i) 2,5-dimethylhexane, (j) 3,3-dimethylhexane, (k) 3,4-dimethylhexane, (l) 3-ethyl-2-methylpentane, (m) 3-ethyl-3-methylpentane, (n) 2,2,3-trimethylpentane, (o) 2,2,4-trimethylpentane, (p) 2,3,3-trimethylpentane, (q) 2,3,4-trimethylpentane, and (r) 2,2,3,3-trimethylbutane.

Table 1: Experimental values of S, AF, HVAP, and DHVAP and the corresponding values of the GH index, HG index, NGH index, and NHG index of octane isomers.

| Alkane                | S    | AF  | HVAP | DHVAP | GH   | NGH  | HG   | NHG  |
|-----------------------|------|-----|------|-------|------|------|------|------|
| $n$-Octane            | 111.7| 0.39| 73.19| 9.915 | 24.42| 84.49| 2.19 | 0.68 |
| 2-Methylheptane       | 109.8| 0.38| 70.30| 9.484 | 27.17| 98.74| 1.96 | 0.57 |
| 3-Methylheptane       | 111.3| 0.37| 71.30| 9.521 | 27.95| 107.4| 1.96 | 0.56 |
| 4-Methylheptane       | 109.3| 0.37| 70.91| 9.483 | 27.95| 113.3| 2.05 | 0.60 |
| 3-Ethylhexane         | 109.4| 0.36| 71.70| 9.476 | 28.73| 131.9| 2.15 | 0.47 |
| 2,2-Dimethylhexane    | 103.4| 0.34| 67.70| 8.915 | 33.60| 122.9| 1.68 | 0.47 |
| 2,3-Dimethylhexane    | 108.0| 0.34| 70.20| 9.272 | 31.63| 110.6| 1.86 | 0.49 |
| 2,4-Dimethylhexane    | 107.0| 0.34| 68.50| 9.029 | 30.88| 123.3| 1.82 | 0.47 |
| 2,5-Dimethylhexane    | 105.7| 0.35| 68.60| 9.051 | 32.24| 133.2| 1.73 | 0.46 |
| 3,3-Dimethylhexane    | 104.7| 0.32| 68.50| 8.973 | 35.21| 151.3| 1.82 | 0.49 |
| 3,4-Dimethylhexane    | 106.6| 0.34| 70.20| 9.316 | 32.41| 117.7| 1.95 | 0.57 |
| 2-Methyl-3-ethylpentane| 106.1| 0.32| 69.70| 9.209 | 32.41| 176.1| 1.95 | 0.34 |
| 3-Methyl-3-ethylpentane| 101.5| 0.30| 69.30| 9.081 | 36.82| 149.3| 1.96 | 0.37 |
| 2,2,3-Trimethylpentane| 101.3| 0.30| 67.30| 8.826 | 38.83| 164.3| 1.60 | 0.33 |
| 2,2,4-Trimethylpentane| 104.1| 0.30| 64.87| 8.402 | 36.53| 155.8| 1.45 | 0.35 |
| 2,3,3-Trimethylpentane| 102.1| 0.29| 68.10| 8.897 | 39.66| 141.6| 1.64 | 0.46 |
| 2,3,4-Trimethylpentane| 102.4| 0.31| 68.37| 9.014 | 35.32| 168.7| 1.66 | 0.39 |
| 2,2,3,3-Trimethylbutane| 93.0| 0.25| 66.20| 8.410 | 46.00| 223.6| 1.26 | 0.22 |

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Using the method of least squares, the linear regression models for $S$, $AF$, $HVAP$, and $DHVAP$ are fitted using the data of Table 1.

The fitted models for the GH index are

$$S = 133.078 (\pm 1.82) - 0.833 (\pm 0.054)GH, \quad (3)$$
aentric factor $= 0.557 (\pm 0.009) - 0.007 (\pm 0.000)GH, \quad (4)$

$$HVAP = 79.613 (\pm 1.878) - 0.315 (\pm 0.056)GH, \quad (5)$$
$$DHVAP = 11.273 (\pm 0.285) - 0.065 (\pm 0.008)GH. \quad (6)$$

The fitted models for the HG index are

$$S = 76.608 (\pm 4.486) + 15.766 (\pm 2.435)HG, \quad (7)$$
aentric factor $= 0.114 (\pm 0.037) + 0.121 (\pm 0.020)HG, \quad (8)$

$$HVAP = 54.960 (\pm 1.356) + 7.773 (\pm 0.736)HG, \quad (9)$$
$$DHVAP = 6.428 (\pm 0.249) + 1.477 (\pm 0.135)HG. \quad (10)$$

The fitted models for the NGH index are

$$S = 121.77 (\pm 2.35) - 0.119 (\pm 0.017)NGH, \quad (11)$$
aentric factor $= 0.465 (\pm 0.018) - 0.001 (\pm 0.000)NGH, \quad (12)$

$$HVAP = 75.007 (\pm 1.552) - 0.043 (\pm 0.011)NGH, \quad (13)$$
$$DHVAP = 10.363 (\pm 0.257) - 0.009 (\pm 0.002)NGH. \quad (14)$$

The fitted models for the NHG index are

$$S = 89.524 (\pm 2.505) + 34.35 (\pm 5.271)NHG, \quad (15)$$
aentric factor $= 0.207 (\pm 0.018) + 0.277 (\pm 0.038)NHG, \quad (16)$

$$HVAP = 62.667 (\pm 1.352) + 14.044 (\pm 2.846)NHG, \quad (17)$$
$$DHVAP = 7.793 (\pm 0.219) + 2.882 (\pm 0.460)NHG. \quad (18)$$

Note: in equations (3)–(18), the errors of the regression coefficients are represented within brackets.

From Table 2 and Figure 2, it is obvious that the GH index highly correlates with the aentric factor and the correlation coefficient $|r| = 0.987$. Also, the GH index has good correlation coefficient $|r| = 0.968$ with entropy, $|r| = 0.815$ with $HVAP$, and $|r| = 0.885$ with $DHVAP$.

From Table 3 and Figure 3, it is noticed that the HG index highly correlates with $DHVAP$ and the correlation coefficient $r = 0.939$. Also, the HG index has good correlation coefficient $r = 0.85$ with entropy, $r = 0.833$ with the aentric factor, and $r = 0.935$ with $HVAP$.

From Table 4 and Figure 4, it is clear that the NGH index highly correlates with the aentric factor and the correlation coefficient $|r| = 0.877$. Also, the NGH index has good correlation coefficient $|r| = 0.873$ with entropy, $|r| = 0.695$ with $HVAP$, and $|r| = 0.778$ with $DHVAP$.

From Table 5 and Figure 5, it is clear that the NHG index highly correlates with the aentric factor and the correlation coefficient $r = 0.877$. Also, the NHG index has good correlation coefficient $r = 0.852$ with entropy, $r = 0.777$ with $HVAP$, and $r = 0.843$ with $DHVAP$.

2. GH, NGH, HG, and NHG Indices of $C_4C_8(S)$, $C_4C_8(R)$, and H-Naphthalenic Nanosheets

2.1. Results for the $C_4C_8(S)$ Nanosheet. The alternating pattern of 4 carbon atoms forming squares and 8 carbon atoms forming octagons constitutes the TUC$_4$C$_8(S)[a,b]$ nanosheet.

In this section, GH, HG, NGH, and NHG indices of the $C_4C_8(S)$ nanosheet are computed. The pattern of carbon atoms gives rise to two types of nanosheets, namely, $T^1[a,b]$ and $T^2[a,b]$. The 2-dimensional nanosheet is represented by $T^1[a,b]$, where $a$ and $b$ are parameters (Figure 6). In $T^1[a,b]$, $C_4$ acts as a square, while $C_8$ is an octagon in which $a$ and $b$ represent the column and row, respectively. Figure 7 depicts the type $1-C_4C_8(S)$ nanosheet. The number of vertices of the $C_4C_8(S)$ nanosheet is $8ab$, and the number of edges is $12ab - 2a - 2b$.

The edge partition of the $T^1[a,b]$ nanosheet based on the degree of vertices is detailed in Table 6.

Theorem 1. Let $T^1[a,b]$ be an $(a,b)$-dimensional nanosheet; then, GH and HG indices are equal to

$$GH(T^1[a,b]) = \frac{108ab}{125} - \frac{4938}{125}a + \frac{4938}{125}b + \frac{376}{125}, \quad (19)$$

$$HG(T^1[a,b]) = \frac{4}{3}a + \frac{33}{125}a + \frac{33}{125}b + \frac{69}{500}$$

Proof. Using Table 6, the definitions of GH and HG indices are as follows:
Table 2: Parameters of regression models for the GH index.

| Physical properties | Value of the correlation coefficient | Residual standard error |
|---------------------|--------------------------------------|-------------------------|
| Entropy             | −0.968                               | 1.17                    |
| Acentric factor     | −0.987                               | 0.0059                  |
| HVAP                | −0.815                               | 1.21                    |
| DHVAP               | −0.885                               | 0.184                   |

Table 3: Parameters of regression models for the HG index.

| Physical properties | Value of the correlation coefficient | Residual standard error |
|---------------------|--------------------------------------|-------------------------|
| Entropy             | 0.85                                 | 2.448                   |
| Acentric factor     | 0.833                                | 0.020                   |
| HVAP                | 0.935                                | 0.74                    |
| DHVAP               | 0.939                                | 0.136                   |

Table 4: Parameters of regression models for the NGH index.

| Physical properties | Value of the correlation coefficient | Residual standard error |
|---------------------|--------------------------------------|-------------------------|
| Entropy             | −0.873                               | 2.274                   |
| Acentric factor     | −0.877                               | 0.0176                  |
| HVAP                | −0.695                               | 1.502                   |
| DHVAP               | −0.778                               | 0.248                   |

Table 5: Parameters of regression models for the NHG index.

| Physical properties | Value of the correlation coefficient | Residual standard error |
|---------------------|--------------------------------------|-------------------------|
| Entropy             | 0.852                                | 2.436                   |
| Acentric factor     | 0.877                                | 0.018                   |
| HVAP                | 0.777                                | 1.315                   |
| DHVAP               | 0.843                                | 0.213                   |

Figure 2: Scatter diagram of physical properties S, AF, HVAP, and DHVAP with the GH index.
Figure 3: Scatter diagram of physical properties S, AF, HVAP, and DHVAP with the HG index.

Figure 4: Scatter diagram of physical properties S, AF, HVAP, and DHVAP with the NGH index.
Figure 5: Scatter diagram of physical properties $S$, $AF$, $HVAP$, and $DHVAP$ with the NHG index.

Figure 6: A TUC$_4$C$_8$($S$)$[a,b]$ nanotube.

Figure 7: Type I-C$_4$C$_8$($S$) nanosheet $T^1[a,b]$. 
The edge partition of the $T^1[a,b]$ nanosheet based on the neighborhood degree of vertices is detailed in Table 7.

**Theorem 2.** Let $T^1[a,b]$ be an $(a,b)$-dimensional nanosheet; then, NGH and NHG indices are equal to

\[
\text{NGH}(T^1[a,b]) = 972ab - \frac{251531}{500}a + \frac{251531}{500}b + \frac{159121}{1000},
\]

\[
\text{NHG}(T^1[a,b]) = \frac{37}{250}ab + \frac{91}{1000}a + \frac{91}{1000}b + \frac{157}{1000}.
\]
Table 7: Edge partition of $T^1[a,b]$ for neighborhood degree-based vertices.

| $(S_u, S_v)$ with $uv \in E(G)$ | Number of edges |
|---------------------------------|----------------|
| $(4,4)$ | 4 |
| $(4,5)$ | 8 |
| $(5,5)$ | $2a + 2b - 8$ |
| $(5,8)$ | $4a + 4b - 8$ |
| $(8,8)$ | $2a + 2b - 4$ |
| $(8,9)$ | $4a + 4b - 8$ |
| $(9,9)$ | $12ab - 14a - 14b + 16$ |

$$NGH(T^1[a,b]) = \sum_{uv \in E(G)} \frac{(S_u + S_v)\sqrt{S_u \times S_v}}{2}$$

$$= 4 \left\{ \frac{(4 + 4)(\sqrt{4 \times 4})}{2} \right\} + 8 \left\{ \frac{(4 + 5)(\sqrt{4 \times 5})}{2} \right\} + (2a + 2b - 8) \left\{ \frac{(5 + 5)(\sqrt{5 \times 5})}{2} \right\} + (4a + 4b - 8) \left\{ \frac{(5 + 8)(\sqrt{5 \times 8})}{2} \right\} + (2a + 2b - 4) \left\{ \frac{(8 + 8)(\sqrt{8 \times 8})}{2} \right\} + (4a + 4b - 8) \left\{ \frac{(8 + 9)(\sqrt{8 \times 9})}{2} \right\}$$

$$+ (12ab - 14a - 14b + 16) \left\{ \frac{(9 + 9)(\sqrt{9 \times 9})}{2} \right\}$$

$$NGH(T^1[a,b]) = 972ab - \frac{251531}{500}a - \frac{251531}{500}b + \frac{159121}{1000}$$

$$NHG(T^1[a,b]) = \sum_{uv \in E(G)} \frac{(S_u + S_v)\sqrt{S_u \times S_v}}{2}$$

$$= 4 \left\{ \frac{2}{(4 + 4)(\sqrt{4 \times 4})} \right\} + 8 \left\{ \frac{2}{(4 + 5)(\sqrt{4 \times 5})} \right\} + (2a + 2b - 8) \left\{ \frac{2}{(5 + 5)(\sqrt{5 \times 5})} \right\} + (4a + 4b - 8) \left\{ \frac{2}{(5 + 8)(\sqrt{5 \times 8})} \right\} + (2a + 2b - 4) \left\{ \frac{2}{(8 + 8)(\sqrt{8 \times 8})} \right\} + (4a + 4b - 8) \left\{ \frac{2}{(8 + 9)(\sqrt{8 \times 9})} \right\}$$

$$+ (12ab - 14a - 14b + 16) \left\{ \frac{2}{(9 + 9)(\sqrt{9 \times 9})} \right\}$$

$$NHG(T^1[a,b]) = \frac{37}{250}ab + \frac{91}{1000}a + \frac{91}{1000}b + \frac{157}{1000}$$

2.2 Results for the $C_4C_8(R)$ Nanosheet. This structure is formed by 4 carbon atoms forming a rhombus that are linearly bridged by edges whose sequence looks like 4 rhombuses connected by 4 edges row and column wise resulting in an alternating pattern of rhombuses and octagons and is represented as $T^2[a,b]$. The 2-dimensional lattice of the TUC$_4$C$_8(R)[a,b]$ nanosheet, where $a$ and $b$ are parameters, is shown in Figure 8. Figure 9 shows the type $2 - C_4C_8(R)$ nanosheet. In the following theorem, GH, HG, and NHG indices of this nanosheet are computed. The number of vertices of the type-2 structure is $4ab + 4(a + b) + 4$, and the number of edges is $6ab + 5a + 5b + 4$.

The edge partition of the $T^2[a,b]$ nanosheet for degree-based vertices is detailed in Table 8.

**Theorem 3.** Let $T^2[a,b]$ be an $(a,b)$-dimensional nanosheet; then, GH and HG indices are equal to

$$GH(T^2[a,b]) = 54ab + \frac{669}{20}a + \frac{669}{20}b + 16$$

$$HG(T^2[a,b]) = \frac{2}{3}ab + \frac{191}{250}a + \frac{191}{250}b + 1.$$
Proof. Using Table 8, the definitions of GH and HG indices are as follows:

\[
GH\left(T^2[a,b]\right) = \sum_{uv \in E(G)} \frac{(d_u + d_v)\sqrt{d_u \times d_v}}{2}
\]

\[
= 4 \left\{ \frac{(2 + 2)(\sqrt{2 \times 2})}{2} \right\} + (4a + 4b) \left\{ \frac{(2 + 3)(\sqrt{2 \times 3})}{2} \right\} + (6ab + a + b) \left\{ \frac{(3 + 3)(\sqrt{3 \times 3})}{2} \right\}
\]

\[
GH\left(T^2[a,b]\right) = 54ab + \frac{669}{20}a + \frac{669}{20}b + 16.
\]

\[
HG\left(T^2[a,b]\right) = \sum_{uv \in E(G)} \frac{2}{(d_u + d_v)\sqrt{d_u \times d_v}}
\]

\[
= 2 \left\{ \frac{2}{(2 + 2)(\sqrt{2 \times 2})} \right\} + (4a + 4b) \left\{ \frac{2}{(2 + 3)(\sqrt{2 \times 3})} \right\} + (6ab + a + b) \left\{ \frac{2}{(3 + 3)(\sqrt{3 \times 3})} \right\}
\]

\[
HG\left(T^2[a,b]\right) = \frac{2}{3}ab + \frac{191}{250}a + \frac{191}{250}b + 1.
\]
The edge partition of the $T^2 [a, b]$ nanosheet based on the neighborhood degree of vertices is detailed in Table 9.

**Theorem 4.** Let $T^2 [a, b]$ be an $(a, b)$-dimensional nanosheet; then, NGH and NHG indices are equal to

$$\text{NGH}(T^2 [a, b]) = 486ab + \frac{20549}{100} a + \frac{20549}{100} b + \frac{21549}{500},$$

$$\text{NHG}(T^2 [a, b]) = \frac{37}{500} ab + \frac{107}{1000} a + \frac{107}{1000} b + \frac{19}{100}.$$

(25)

**Proof.** Using Table 9, the definitions of NGH and NHG indices are as follows:

$$\text{NGH}(T^2 [a, b]) = \sum_{uv \in E(G)} \frac{(S_u + S_v) \sqrt{S_u S_v}}{2}$$

$$= 4 \left\{ \frac{5 + 8}{2} \right\} + 8 \left\{ \frac{5 + 8}{2} \right\} + (4a + 4b - 8) \left\{ \frac{6 + 8}{2} \right\} + (2a + 2b + 4)$$

$$\cdot \left\{ \frac{8 + 9}{2} \right\} + (4a + 4b - 8) \left\{ \frac{8 + 9}{2} \right\} + (6ab - 5a - 5b + 4) \left\{ \frac{9 + 9}{2} \right\}$$

$$\text{NHG}(T^2 [a, b]) = \frac{20549}{100} a + \frac{20549}{100} b + \frac{21549}{500},$$

$$\text{NHG}(T^2 [a, b]) = \sum_{uv \in E(G)} \frac{2}{(S_u + S_v) \sqrt{S_u S_v}}$$

$$= 4 \left\{ \frac{5 + 8}{2} \right\} + 8 \left\{ \frac{5 + 8}{2} \right\} + (4a + 4b - 8) \left\{ \frac{6 + 8}{2} \right\} + (2a + 2b + 4)$$

$$\cdot \left\{ \frac{8 + 9}{2} \right\} + (4a + 4b - 8) \left\{ \frac{8 + 9}{2} \right\} + (6ab - 5a - 5b + 4) \left\{ \frac{9 + 9}{2} \right\}$$

(26)

2.3. **Results for the H-Naphthalenic Nanosheet.** Carbon atoms bonded in the form of a hexagonal structure constitute carbon nanotubes. They are peri-condensed benzenoids which mean three or more rings share the same atoms. H-Naphthalenic nanosheet is constituted by the alternating sequence of squares $C_4$, hexagons $C_6$, and octagons $C_8$ and is represented as $T^3 [a, b]$, where $a$ and $b$ are the parameters. The number of vertices of the H-naphthalenic nanosheet is $10ab$, and the edges are $15ab - 2a - 2b$. The GH, HG, NGH, and NHG indices of this nanosheet are computed; see Figure 10.

| $S_u, S_v$ with $uv \in E(G)$ | Number of edges |
|-----------------------------|-----------------|
| (5, 5)                      | 4               |
| (5, 8)                      | 8               |
| (6, 8)                      | $4a + 4b - 8$   |
| (8, 8)                      | $2a + 2b + 4$   |
| (8, 9)                      | $4a + 4b - 8$   |
| (9, 9)                      | $6ab - 5a - 5b + 4$ |

Table 9: Edge partition of $T^2 [a, b]$. |  

(27)
Proof. Using Table 10, the definitions of GH and HG indices are as follows:

\[
\text{GH}(T^3[a,b]) = \sum_{uv \in E(G)} \frac{(d_u + d_v) \sqrt{d_u \times d_v}}{2}
\]

\[
= (2b + 4) \left\{ \frac{(2 + 2) (\sqrt{2 \times 2})}{2}\right\} + (8a + 8b - 8) \left\{ \frac{(2 + 3) (\sqrt{2 \times 3})}{2}\right\}
\]

\[
+ (15ab - 10a - 8b + 4) \left\{ \frac{(3 + 3) (\sqrt{3 \times 3})}{2}\right\}
\]

\[
\text{GH}(T^3[a,b]) = 135ab - \frac{4101}{100}a - \frac{7901}{200}b + \frac{301}{100}
\]

\[
\text{HG}(T^3[a,b]) = \sum_{uv \in E(G)} \frac{2}{(d_u + d_v) \sqrt{d_u \times d_v}}
\]

\[
= (2b + 4) \left\{ \frac{2}{(2 + 2) (\sqrt{2 \times 2})}\right\} + (8a + 8b - 8) \left\{ \frac{2}{(2 + 3) (\sqrt{2 \times 3})}\right\}
\]

\[
+ (15ab - 10a - 8b + 4) \left\{ \frac{2}{(3 + 3) (\sqrt{3 \times 3})}\right\}
\]

\[
\text{HG}(T^3[a,b]) = \frac{1667}{1000}ab + \frac{39}{200}a + \frac{33}{125}b + \frac{69}{1500}
\]
The edge partition of the $T^3[a, b]$ nanosheet based on the neighborhood degree of vertices is detailed in Table 11.

**Theorem 6.** Let $T^3[a, b]$ be an $(a, b)$-dimensional nanosheet; then, NGH and NHG indices are equal to

\[
\text{NGH}(T^3[a, b]) = 1215ab - \frac{11199}{20} a - \frac{251531}{500} b + \frac{17382}{125},
\]

\[
\text{NHG}(T^3[a, b]) = \frac{37}{200}ab + \frac{15}{200}a + \frac{91}{1000}b + \frac{249}{2500}
\]

(29)

**Proof.** Using Table 11, the definitions of NGH and NHG indices are as follows:

\[
\text{NGH}(T^3[a, b]) = \sum_{uv \in E(G)} \frac{(S_u + S_v) \sqrt{S_u \times S_v}}{2}
\]

\[
= 8 \left( \frac{(4+5)\sqrt{4 \times 5}}{2} \right) + (2b - 4) \left( \frac{(5+5)\sqrt{5 \times 5}}{2} \right) + 4 \left( \frac{(5+7)\sqrt{7 \times 7}}{2} \right) + (4b - 4)
\]

\[
\cdot \left( \frac{(5+8)\sqrt{5 \times 8}}{2} \right) + (4a - 4) \left( \frac{(6+7)\sqrt{6 \times 7}}{2} \right) + (4a - 4) \left( \frac{(6+8)\sqrt{6 \times 8}}{2} \right)
\]

\[
+ 2a \left( \frac{(7+9)\sqrt{7 \times 9}}{2} \right) + (2a + 2b - 4) \left( \frac{(8+8)\sqrt{8 \times 8}}{2} \right) + (4a + 4b - 8)
\]

\[
\cdot \left( \frac{(8+9)\sqrt{8 \times 9}}{2} \right) + (15ab - 18a - 14b + 16) \left( \frac{(9+9)\sqrt{9 \times 9}}{2} \right)
\]

(30)

\[
\text{NHG}(T^3[a, b]) = \sum_{uv \in E(G)} \frac{(S_u + S_v) \sqrt{S_u \times S_v}}{2}
\]

\[
= 8 \left( \frac{2(4+5)\sqrt{4 \times 5}}{2} \right) + (2b - 4) \left( \frac{2(5+5)\sqrt{5 \times 5}}{2} \right) + 4 \left( \frac{2(5+7)\sqrt{7 \times 7}}{2} \right) + (4b - 4)
\]

\[
\cdot \left( \frac{2(5+8)\sqrt{5 \times 8}}{2} \right) + (4a - 4) \left( \frac{2(6+7)\sqrt{6 \times 7}}{2} \right) + (4a - 4) \left( \frac{2(6+8)\sqrt{6 \times 8}}{2} \right)
\]

\[
+ 2a \left( \frac{2(7+9)\sqrt{7 \times 9}}{2} \right) + (2a + 2b - 4) \left( \frac{2(8+8)\sqrt{8 \times 8}}{2} \right) + (4a + 4b - 8)
\]

\[
\cdot \left( \frac{2(8+9)\sqrt{8 \times 9}}{2} \right) + (15ab - 18a - 14b + 16) \left( \frac{2(9+9)\sqrt{9 \times 9}}{2} \right)
\]

□
3. Conclusion

This paper is devoted to defining NGH, HG, and NHG indices, and the chemical applicability is studied for some physical and chemical properties of octane isomers using regression models including the recently introduced GH index. The GH index has a high negative correlation with acentric factor having $r = 0.987$ with a residual standard error of 0.0059. The HG index has a high positive correlation with DHVAP having $r = 0.939$ with a residual standard error of 0.136. The NGH index has a high negative correlation with acentric factor having $r = 0.877$ with a residual standard error of 0.0176. The NHG index has a high positive correlation with acentric factor having $r = 0.877$ with a residual standard error of 0.018. The applications of carbon nanotubes have considerably increased because of their excellent mechanical, thermal, and electrical properties. The novel indices introduced in this paper would be of great help to understand the physicochemical and biological properties of various compounds in addition to the existing degree-based indices.

**Data Availability**

The data used to support the findings of this study are cited at relevant places within the text as references.

**Conflicts of Interest**

The authors declare that they have no conflicts of interest.

**Authors’ Contributions**

All authors contributed equally to this work.

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