Computing some Novel Closed Neighborhood Degree-Based Topological Indices of Graphene Structures

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Abstract: Chemical graph theory (CGT) is a crucial part of mathematical chemistry, which characterizes the chemical compounds as molecular graphs using graph-theoretical tools. By IUPAC terminology, a numerical parameter that represents the topology of a molecular graph is known as a topological index (TI). In this scenario, our research interest is to employ newly defined seven TIs, namely closed neighborhood first Zagreb index (CM1(G)), modified closed neighborhood first Zagreb index (CM1*(G)), closed neighborhood second Zagreb index (CM2(G)), closed neighborhood Forgotten index (CF(G)), modified closed neighborhood Forgotten index (CF*(G)), closed neighborhood first hyper Zagreb index (CHM1(G)) and closed neighborhood second hyper Zagreb index (CHM2(G)) as well as explore them mathematically. Without applying quantum mechanics, these TIs could obtain the maximum information behind the graphene structures.

Keywords: topological index; graphene structure; closed neighborhood degree; Zagreb; Forgotten.

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1. Introduction

Let G be a graph with node and link sets as V(G) and E(G), respectively. Consider |E(G)| = τ and |V(G)| = h. The link sw connects the nodes s and w. The number of nodes adjacent to s is the degree of a node s ∈ V(G), represented dG(s). Let N[w] be the closed neighborhood set of node w that includes w and its neighbors [1]. All the graphs discussed in this article are finite, undirected, connected, loopless with no parallel links.

1.1. Basics.

The industry is thriving today due to interdisciplinary approaches in various fields. This enables one to comprehend the applications of several disciplines. CGT combines chemistry and mathematics, which play a vital role in CGT. Chemistry develops a molecular structure for a specific compound, while graph theory translates that structure into a molecular graph, then investigated by various characteristic tools such as TIs [2]. Moreover, TIs are currently gaining attention in computational chemistry due to their application in non-empirical QSAR and QSPR studies [3]. To date, several degree-based TIs have been established to describe molecules' physical and chemical characteristics [4]. The Randic [5], Zagreb [6], hyper Zagreb [7], and forgotten [8] indices were proposed by respective authors in their work. We suggest the interested reader to the literature [9-23].
1.2. Overview of graphene.

Graphene is a class of carbon allotrope, which is the strongest substance ever tested. It is composed of a single sheet of carbon atoms arranged on a honeycomb grid [24]. It ranks as a good conductor of heat and electricity. Compared to graphite, its property of magnetism stands as stronger and nonlinear. At normal temperature, it possesses excellent electron mobility. It is one such functional nanomaterial featuring potential applications in optics, electronics, bio-sensors, and so on [24]. As a result, it has sparked the interest of researchers globally.

1.3. Suggested TIs.

In this day and age, several mathematicians and chemists are striving to build novel indices for predicting chemical compounds' physicochemical and biological behavior [25]. For this objective, herein, we employ newly defined seven TIs, expressly closed neighborhood first Zagreb index (CM\textsubscript{1}(G)), modified closed neighborhood first Zagreb index (CM\textsubscript{1}*(G)), closed neighborhood second Zagreb index (CM\textsubscript{2}(G)), closed neighborhood Forgotten index (CF(G)), modified closed neighborhood Forgotten index (CF\textsuperscript{*}(G)), closed neighborhood first hyper Zagreb index (CHM\textsubscript{1}(G)), and closed neighborhood second hyper Zagreb index (CHM\textsubscript{2}(G)). Closed neighborhood degree-sum of the node \(s\) in \(V(G)\) and the newly defined TIs are expressed as follows,

\[
\Omega_G(s) = \sum_{w \in N(s)} d_G(w).
\]

(1)

\[
CM_1(G) = \sum_{s \in V(G)} (\Omega_G(s) + \Omega_G(w)).
\]

(2)

\[
CM_1^*(G) = \sum_{s \in V(G)} \Omega_G(s)^2.
\]

(3)

\[
CM_2(G) = \sum_{s \in V(G)} (\Omega_G(s) \Omega_G(w)).
\]

(4)

\[
CF(G) = \sum_{s \in V(G)} (\Omega_G(s)^2 + \Omega_G(w)^2).
\]

(5)

\[
CF^*(G) = \sum_{s \in V(G)} \Omega_G(s)^3.
\]

(6)

\[
CHM_1(G) = \sum_{s \in V(G)} (\Omega_G(s) + \Omega_G(w))^2.
\]

(7)

\[
CHM_2(G) = \sum_{s \in V(G)} (\Omega_G(s) \Omega_G(w))^2.
\]

(8)

1.4. Motivation and scheme.

Mathematically, the correlation coefficient \(|R|\) is determined to measure the effectiveness of a TI in predicting the physicochemical behavior of a chemical substance. TIs with a significant \(|R|\) value (greater than 0.8) are highly appreciable in QSPR/QSAR analysis. The suggested TIs CM\textsubscript{1}(G), CM\textsubscript{1}*(G), CM\textsubscript{2}(G), CF(G), CF\textsuperscript{*}(G), CHM\textsubscript{1}(G), and CHM\textsubscript{2}(G) exhibit strong correlations (\(|R| > 0.8\)) with acentric factor, critical pressure, density, entropy,
heats of vaporization, standard enthalpy of vaporization and mean radius of octane isomers as reported in [26]. Moreover, these TIs show excellent linear relationships with a boiling point, molecular weight, n-octanol air partition coefficient, and n-octanol water partition coefficient of priority PAHs (Polycyclic Aromatic Hydrocarbons) demonstrated in [27]. As a result, the indices listed above are efficient in QSAR/QSPR analysis and strong statistical accuracy. In addition, when compared to previously established degree-based TIs, the mean isomer degeneracy of these indices is exceptional, indicating that they have superior isomer discrimination capacity (exactly 1) [26]. Therefore, computing these indices for various chemically significant networks is worthwhile. At this juncture of the research, we compute these indices for the graphene network to reveal its mathematical aspects.

Section 1 deals with some basic concepts and introduces the suggested indices. Section 2 discusses the methodology of the work. Section 3 delves into the main results obtained from the study. The outcomes of the research are provided concisely in Section 4.

2. Materials and Methods

2.1. Methodology.

This section first describes the closed neighborhood degree sum-based partitioning of graphene molecular structure with respect to nodes and links. We get the seven TIs for the graphene structure by adopting these partitions. Assume a graphene structure with \( u \) rows and \( v \) rings of benzene in each row. For node and link partitions, we reserve the symbols \( V_\alpha \) and \( E_{(\beta,\gamma)} \), respectively.

\[
V_\alpha = \{ s \in V(G) : \Omega_G(s) = \alpha \},
\]
\[
E_{(\beta,\gamma)} = \{ s w \in E(G) : \Omega_G(s) = \beta, \Omega_G(w) = \gamma \}.
\]

We explore four distinct cases for the topological characteristics of graphene molecular structure based on the count of rows and the number of benzene rings in every row. Figures (1-4) depict the molecular graph of graphene structure.

2.1. Case 1: \( u > 1; \ v > 1 \).

we get the following partitions from Figure 1 and Tables (1, 5).

\[
V(G) = V_6 \cup V_7 \cup V_8 \cup V_{10} \cup V_{11} \cup V_{12}.
\]
\[
E(G) = E_{(6,7)} \cup E_{(7,7)} \cup E_{(7,10)} \cup E_{(7,11)} \cup E_{(8,10)} \cup E_{(10,12)} \cup E_{(11,11)} \cup E_{(11,12)} \cup E_{(12,12)}.
\]

2.2. Case 2: \( u = 1; \ v > 1 \).

From Figure 2 and Tables (2, 6), one can obtain the partitions as follows.

\[
V(G) = V_6 \cup V_7 \cup V_8 \cup V_{10}.
\]
\[
E(G) = E_{(6,6)} \cup E_{(6,7)} \cup E_{(7,10)} \cup E_{(8,10)} \cup E_{(10,10)}.
\]
2.3. Case 3: \( u > 1; \ v = 1 \).

We arrive at the partitions of graphene as below, from Figure 3 and Tables (3, 7).

\[
V(G) = V_6 \cup V_7 \cup V_{10} \cup V_{11}.
\]

\[
E(G) = E_{(6,6)} \cup E_{(6,7)} \cup E_{(7,7)} \cup E_{(7,10)} \cup E_{(7,11)} \cup E_{(10,11)} \cup E_{(11,11)}.
\]

2.4. Case: 4. \( u = 1; \ v = 1 \).

In this case, we have the following partitions from Figure 4 and Tables (4, 8).

\[
V(G) = V_6.
\]

\[
E(G) = E_{(6,6)}.
\]

We used combinatorial computation, analytic methods, statistical approach, graph-theoretical terminologies, counting degrees, link and node partition techniques to obtain our key results. GNU-OCTAVE 5.2.0 has been used for 3D surface plotting. The computational results were compared graphically using MATLAB 2017.

![Figure 1](https://biointerfaceresearch.com/)

**Figure 1.** Molecular graph of graphene when \( u > 1 \) and \( v > 1 \).

![Figure 2](https://biointerfaceresearch.com/)

**Figure 2.** Molecular graph of graphene when \( u = 1 \) and \( v > 1 \).

![Figure 3](https://biointerfaceresearch.com/)

**Figure 3.** Molecular graph of graphene when \( u > 1 \) and \( v = 1 \).
Figure 4. Molecular graph of graphene when \( u = 1 \) and \( v = 1 \).

| Table 1. Node Partition when \( u > 1 \) \( v > 1 \). |
|-----------------------------------------------|
| Types of node \( V_\alpha \) | \( V_6 \) | \( V_7 \) | \( V_8 \) | \( V_{10} \) | \( V_{11} \) | \( V_{12} \) |
| Number of nodes \( V_\alpha \) | 2 | \( 2u+4 \) | \( 2v - 4 \) | \( 2v \) | \( 2u - 4 \) | \( (2v - 2)(u - 1) \) |

| Table 2. Node Partition when \( u = 1 \) \( v > 1 \). |
|-----------------------------------------------|
| Types of node \( V_\alpha \) | \( V_6 \) | \( V_7 \) | \( V_8 \) | \( V_{10} \) |
| Number of nodes \( V_\alpha \) | 4 | 4 | \( 2v - 4 \) | \( 2v - 2 \) |

| Table 3. Node Partition when \( u > 1 \) \( v = 1 \). |
|-----------------------------------------------|
| Types of node \( V_\alpha \) | \( V_6 \) | \( V_7 \) | \( V_{10} \) | \( V_{11} \) |
| Number of nodes \( V_\alpha \) | 4 | \( 2u \) | 2 | \( 2u - 4 \) |

| Table 4. Node Partition when \( u = 1 \) \( v = 1 \). |
|-----------------------------------------------|
| Types of node \( V_\alpha \) | \( V_6 \) |
| Number of nodes \( V_\alpha \) | 6 |

| Table 5. Link Partition when \( u > 1 \) \( v > 1 \). |
|-----------------------------------------------|
| Types of link \( E(\beta,\gamma) \) | \( E_{(6,7)} \) | \( E_{(7,7)} \) | \( E_{(7,10)} \) | \( E_{(7,11)} \) | \( E_{(8,10)} \) | \( E_{(10,12)} \) | \( E_{(11,11)} \) | \( E_{(12,12)} \) |
| Number of links \( E(\beta,\gamma) \) | 4 | \( u \) | 8 | \( 2u - 4 \) | \( 4v - 8 \) | \( 2v \) | \( u - 2 \) | \( 2u - 4 \) | \( 3uv - 4u - 4v + 5 \) |

| Table 6. Link Partition when \( u = 1 \) \( v > 1 \). |
|-----------------------------------------------|
| Types of link \( E(\beta,\gamma) \) | \( E_{(6,6)} \) | \( E_{(6,7)} \) | \( E_{(7,10)} \) | \( E_{(8,10)} \) | \( E_{(10,10)} \) |
| Number of links \( E(\beta,\gamma) \) | 2 | 4 | 4 | \( 4v - 8 \) | \( v - 1 \) |

| Table 7. Link Partition when \( u > 1 \) \( v = 1 \). |
|-----------------------------------------------|
| Types of link \( E(\beta,\gamma) \) | \( E_{(6,6)} \) | \( E_{(6,7)} \) | \( E_{(7,7)} \) | \( E_{(7,10)} \) | \( E_{(10,11)} \) | \( E_{(11,11)} \) |
| Number of links \( E(\beta,\gamma) \) | 2 | 4 | \( u - 2 \) | 4 | \( 2u - 4 \) | \( 2 \) | \( 2u - 5 \) |

| Table 8. Link Partition when \( u = 1 \) \( v = 1 \). |
|-----------------------------------------------|
| Types of link \( E(\beta,\gamma) \) | \( E_{(6,6)} \) |
| Number of links \( E(\beta,\gamma) \) | 6 |

3. Results and Discussion

Theorem 3.1: The CM\(_1\)(G) index of graphene with \( u \) rows and \( v \) benzene rings per row is
Proof: For each of the four cases, we present the proof.

Case 1: Equation (2) yields the following result to the link partition for \( u > 1, v > 1 \) given in Table 5.

\[
CM_1(G) = \sum_{s \in V(G)} (\Omega_G(s) + \Omega_G(w))
\]

\[
= |E(6,7)| (6 + 7) + |E(7,7)| (7 + 7) + |E(7,10)| (7 + 10) + |E(7,11)| (7 + 11) + |E(8,10)| (8 + 10)
+ |E(10,12)| (10 + 12) + |E(11,11)| (11 + 11) + |E(11,12)| (11 + 12) + |E(12,12)| (12 + 12).
\]

\[
= 4(13) + 14u + 8(17) + (2u - 4)(18) + (4v - 8)(18) + 2v(22) + (u - 2)(22)
+ (2u - 4)(23) + 24(3uv - 4u - 4v + 5).
\]

\[
= 72uv + 22u + 20v - 44.
\]

Case 2: Using the link partition for \( u = 1, v > 1 \) provided in Table 6, Eq. (2) will be

\[
CM_1(G) = \sum_{s \in V(G)} (\Omega_G(s) + \Omega_G(w))
\]

\[
= |E(6,6)| (6 + 6) + |E(6,7)| (6 + 7) + |E(7,10)| (7 + 10) + |E(7,11)| (7 + 11) + |E(8,10)| (8 + 10)
+ |E(10,12)| (10 + 12) + |E(11,11)| (11 + 11).
\]

\[
= 2(12) + 4(13) + (u - 2)(14) + 4(17) + (2u - 4)(18) + 2(21) + (2u - 5)(22).
\]

\[
= 94u - 24.
\]

Case 3: To the link partition for \( u > 1, v = 1 \) given in Table 7, Eq.(2) exhibits the following outcome.

\[
CM_1(G) = \sum_{s \in V(G)} (\Omega_G(s) + \Omega_G(w))
\]

\[
= |E(6,6)| (6 + 6) + |E(6,7)| (6 + 7) + |E(7,7)| (7 + 7) + |E(7,10)| (7 + 10) + |E(7,11)| (7 + 11)
+ |E(10,11)| (10 + 11) + |E(11,11)| (11 + 11).
\]

\[
= 2(12) + 4(13) + (u - 2)(14) + 4(17) + (2u - 4)(18) + 2(21) + (2u - 5)(22).
\]

\[
= 94u - 24.
\]

Case 4: From Table 8, we apply the link partition for \( u = 1, v = 1 \) in Eq. (2) to obtain,

\[
CM_1(G) = \sum_{s \in V(G)} (\Omega_G(s) + \Omega_G(w)) = |E(6,6)| (6 + 6) = 6(6 + 6) = 72.
\]

Theorem 3.2: The CM\(_1^*(G)\) index of graphene with \( u \) rows and \( v \) benzene rings in each row is

\[
CM_1^*(G) = \begin{cases} 
288uv + 52u + 40v - 184, & \text{if } u > 1, v > 1 \\
328v - 116, & \text{if } u = 1, v > 1 \\
340u - 140, & \text{if } u > 1, v = 1 \\
216, & \text{if } u = 1, v = 1 
\end{cases}
\]

Proof: We present the proof for the four cases.
Case 1: For node partition $u > 1$, $v > 1$, we are moving forward applying Table 1 on Eq. (3).

$$CM_1'(G) = \sum_{s \in V(G)} (\Omega_G(s))^2$$

$$= |V_6|(6)^2 + |V_7|(7)^2 + |V_8|(8)^2 + |V_{10}|(10)^2 + |V_{11}|(11)^2 + |V_{12}|(12)^2.$$

$$= 2(36) + 49(2u + 4) + 64(2v - 4) + 2v(100) + (2u - 4)(121) + 144(2v - 2)(u - 1).$$

$$= 288uv + 52u + 40v - 184.$$ 

Case 2: For $u = 1$, $v > 1$, using Table 2 on Eq. (3), we obtain,

$$CM_1'(G) = \sum_{s \in V(G)} (\Omega_G(s))^2$$

$$= |V_6|(6)^2 + |V_7|(7)^2 + |V_8|(8)^2 + |V_{10}|(10)^2.$$

$$= 4(36) + 4(49) + (2v - 4)(64) + (2v - 2)(100).$$

$$= 328v - 116.$$ 

Case 3: we are presenting the following result to the node partition for $u > 1$, $v = 1$ given in Table 3 on Eq. (3).

$$CM_1'(G) = \sum_{s \in V(G)} (\Omega_G(s))^2$$

$$= |V_6|(6)^2 + |V_7|(7)^2 + |V_{10}|(10)^2 + |V_{11}|(11)^2.$$

$$= 4(36) + 2u(49) + 2(100) + (2u - 4)(121).$$

$$= 340u - 140.$$ 

Case 4: For $u = 1$, $v = 1$, using Table 4 on Eq. (3), we obtain,

$$CM_1'(G) = \sum_{s \in V(G)} (\Omega_G(s))^2 = |V_6|(6)^2 = 6(36) = 216.$$ 

Theorem 3.3: The $CM_2(G)$ index of graphene with $u$ rows and $v$ benzene rings per row is

$$CM_2(G) = \begin{cases} 
432uv + 12u - 16v - 270, & \text{if } u > 1, v > 1 \\
420v - 220, & \text{if } u = 1, v > 1 \\
445u - 271, & \text{if } u > 1, v = 1 \\
216, & \text{if } u = 1, v = 1 
\end{cases}$$

Proof: We provide proof for each of the four cases.

Case 1: From Table 5, using the link partition for $u > 1$, $v > 1$ in Eq. (4) we obtain,

$$CM_2(G) = \sum_{s \in E(G)} (\Omega_G(s) \cdot \Omega_G(w))$$

$$= |E_{(6,7)}|(6 \times 7) + |E_{(7,7)}|(7 \times 7) + |E_{(7,10)}|(7 \times 10) + |E_{(7,11)}|(7 \times 11) + |E_{(8,10)}|(8 \times 10) + |E_{(10,12)}|(10 \times 12) + |E_{(11,11)}|(11 \times 11) + |E_{(11,12)}|(11 \times 12) + |E_{(12,12)}|(12 \times 12).$$

$$= 4(42) + 49u + 8(70) + (2u - 4)(77) + (4v - 8)(80) + 2v(120) + (u - 2)(121) + (2u - 4)(132) + 144(3uv - 4u - 4v + 5).$$

$$= 432uv + 12u - 16v - 270.$$
Case 2: For \( u = 1, v > 1 \), we are looking forward to applying Table 6 on Eq. (4).

\[
CM_2 (G) = \sum_{s, w \in E(G)} (\Omega_G (s) \cdot \Omega_G (w))
\]

\[
= |E_{(6,6)}|(6 \times 6) + |E_{(6,7)}|(6 \times 7) + |E_{(7,10)}|(7 \times 10) + |E_{(8,10)}|(8 \times 10) + |E_{(10,10)}|(10 \times 10)
\]

\[
= 2(36) + 4(42) + 4(70) + (4v - 8)(80) + (v - 1)(100).
\]

\[
= 420v - 220.
\]

Case 3: Equation (4) yields the following result to the link partition for \( u > 1, v = 1 \) given in Table 7.

\[
CM_2 (G) = \sum_{s, w \in E(G)} (\Omega_G (s) \cdot \Omega_G (w))
\]

\[
= |E_{(6,6)}|(6 \times 6) + |E_{(6,7)}|(6 \times 7) + |E_{(7,7)}|(7 \times 7) + |E_{(7,10)}|(7 \times 10) + |E_{(7,11)}|(7 \times 11)
\]

\[
+ |E_{(10,10)}|(10 \times 11) + |E_{(11,10)}|(11 \times 11).
\]

\[
= 2(36) + 4(42) + (u - 2)(49) + 4(70) + (2u - 4)(77) + 2(110) + (2u - 5)(121).
\]

\[
= 445u - 271.
\]

Case 4: For \( u = 1, v = 1 \), using Table 8 on Eq. (4), we obtain,

\[
CM_2 (G) = \sum_{s, w \in E(G)} (\Omega_G (s) \cdot \Omega_G (w)) = |E_{(6,6)}|(6 \times 6) = 6(36) = 216.
\]

Theorem 3.4: The \( CF(G) \) index of graphene with \( u \) rows and \( v \) benzene rings in each row is

\[
CF(G) = \begin{cases} 
864uv - 5lu - 8v - 346 & \text{if } u > 1, v > 1 \\
856v - 432 & \text{if } u = 1, v > 1 \\
922u - 564 & \text{if } u > 1, v = 1 \\
432 & \text{if } u = 1, v = 1
\end{cases}
\]

Proof: We build the proof for the four cases.

Case 1: For \( u > 1, v > 1 \), we are looking forward to applying Table 5 on Eq. (5).

\[
CF (G) = \sum_{s, w \in E(G)} (\Omega_G (s)^2 + \Omega_G (w)^2)
\]

\[
= |E_{(6,7)}|(6^2 + 7^2) + |E_{(7,7)}|(7^2 + 7^2) + |E_{(7,10)}|(7^2 + 10^2) + |E_{(7,11)}|(7^2 + 11^2)
\]

\[
+ |E_{(8,10)}|(8^2 + 10^2) + |E_{(10,10)}|(10^2 + 12^2) + |E_{(10,11)}|(11^2 + 11^2) + |E_{(11,11)}|(11^2 + 12^2)
\]

\[
+ |E_{(12,12)}|(12^2 + 12^2).
\]

\[
= 4(85) + 98u + 8(149) + (2u - 4)(170) + (4v - 8)(164) + 2v(244) + (u - 2)(133)
\]

\[
+ (2u - 4)(265) + 288(3uv - 4u - 4v + 5).
\]

\[
= 864uv - 5lu - 8v - 346.
\]

Case 2: To the link partition for \( u = 1, v > 1 \) given in Table 6, Eq.(5) exhibits the following result.
\[
CF(G) = \sum_{s, w \in E(G)} \left( \Omega_G(s)^2 + \Omega_G(w)^2 \right) \\
= |E_{(6,6)}|[6^2 + 2^2] + |E_{(6,7)}|[6^2 + 7^2] + |E_{(7,10)}|[7^2 + 10^2] \\
+ |E_{(8,10)}|[8^2 + 2^2] + |E_{(10,10)}|[10^2 + 2^2] \\
= 2(72) + 4(85) + 4(149) + (4v - 8)(164) + (v - 1)(200). \\
= 856v - 432.
\]

Case 3: From Table 7, using the link partition for \( u > 1, v = 1 \) in Eq. (5) we attain,
\[
CF(G) = \sum_{s, w \in E(G)} \left( \Omega_G(s)^2 + \Omega_G(w)^2 \right) \\
= |E_{(6,6)}|[6^2 + 6^2] + |E_{(6,7)}|[6^2 + 7^2] + |E_{(7,10)}|[7^2 + 10^2] \\
+ |E_{(7,11)}|[7^2 + 11^2] + |E_{(10,11)}|[10^2 + 11^2] + |E_{(11,11)}|[11^2 + 11^2] \\
= 2(72) + 4(85) + (u - 2)(98) + 4(149) + (2u - 4)(170) + 2(221) + (2u - 5)(242). \\
= 922u - 564.
\]

Case 4: From Table 8, we use the link partition for \( u = 1, v > 1 \) to get,
\[
CF(G) = \sum_{s, w \in E(G)} \left( \Omega_G(s)^2 + \Omega_G(w)^2 \right) \\
= |E_{(6,6)}|[6^2 + 6^2] + |E_{(6,7)}|[6^2 + 7^2] + |E_{(7,10)}|[7^2 + 10^2] \\
+ |E_{(7,11)}|[7^2 + 11^2] + |E_{(10,11)}|[10^2 + 11^2] + |E_{(11,11)}|[11^2 + 11^2] \\
= 2(72) + 4(85) + (u - 2)(98) + 4(149) + (2u - 4)(170) + 2(221) + (2u - 5)(242). \\
= 922u - 564.
\]

Theorem 3.5: The CF*(\( G \)) index of graphene with \( u \) rows and \( v \) benzene rings in each row is
\[
CF^*(G) = \begin{cases} 
3456uv - 108u - 432v - 2112, & \text{if } u > 1, v > 1 \\
3024v - 1812, & \text{if } u = 1, v > 1 \\
3348u - 2460, & \text{if } u > 1, v = 1 \\
7776, & \text{if } u = 1, v = 1
\end{cases}
\]

Proof: We provide proof for all four cases.

Case 1: Equation (6) yields the following result to the link partition for \( u > 1, v > 1 \) given in Table 1.
\[
CF^*(G) = \sum_{s \in V(G)} (\Omega_G(s))^3 \\
= |V_6|[6^3] + |V_7|[7^3] + |V_8|[8^3] + |V_{10}|[10^3] + |V_{11}|[11^3] + |V_{12}|[12^3]. \\
= 2(216) + 343(2u + 4) + 512(2v - 4) + 2v(1000) + (2u - 4)(1331) + 1728(2v - 2)(u - 1). \\
= 3456uv - 108u - 432v - 2112.
\]

Case 2: For \( u = 1, v > 1 \), We are looking forward to applying Table 2 on Eq. (6).
\[
CF^*(G) = \sum_{s \in V(G)} (\Omega_G(s))^3 \\
= |V_6|[6^3] + |V_7|[7^3] + |V_8|[8^3] + |V_{10}|[10^3].
\]
\[=4(216) + 4(343) + (2v - 4)(512) + (2v - 2)(1000).\]

\[=3024v - 1812.\]

Case 3: From Table 3, we use the link partition for \(u > 1, v = 1\) in Eq. (6) to arrive,

\[
\text{CF }^*(G) = \sum_{s \in V(G)} \left( \Omega_G(s) \right)^3
\]

\[
= |V_6| \left( 6 \right)^3 + |V_7| \left( 7 \right)^3 + |V_{10}| \left( 10 \right)^3 + |V_{11}| \left( 11 \right)^3.
\]

\[
= 4(216) + 2u(343) + 2(1000) + (2u - 4)(1331).
\]

\[
= 3348 + 2460.
\]

Case 4: For \(u = 1, v = 1\), using Table 4 on Eq. (6), we obtain,

\[
\text{CF }^*(G) = \sum_{s \in V(G)} \left( \Omega_G(s) \right)^3 = |V_6| \left( 6 \right)^3 = 6(216) = 7776.
\]

Theorem 3.6: The CHM\(_1\)(G) index of graphene with \(u\) rows and \(v\) benzene rings in each row is

\[
\text{CHM}_1(G) = \begin{cases} 
1728uv + 82u - 40v - 1104 , & \text{if } u > 1, v > 1 \\
1696v - 872 , & \text{if } u = 1, v > 1 \\
1812u - 1106 , & \text{if } u > 1, v = 1 \\
864 , & \text{if } u = 1, v = 1
\end{cases}
\]

Proof: We derive the proof for the four cases.

Case 1: For \(u > 1, v > 1\), using Table 5 on Eq. (7), we achieve,

\[
\text{CHM}_1(G) = \sum_{s \in E(G)} \left( \Omega_G(s) + \Omega_G(w) \right)^2
\]

\[
= |E_{(6,7)}| \left( 6 + 7 \right)^2 + |E_{(7,7)}| \left( 7 + 7 \right)^2 + |E_{(7,10)}| \left( 7 + 10 \right)^2 + |E_{(7,11)}| \left( 7 + 11 \right)^2
\]

\[
+ |E_{(8,10)}| \left( 8 + 10 \right)^2 + |E_{(10,12)}| \left( 10 + 12 \right)^2 + |E_{(11,11)}| \left( 11 + 11 \right)^2 + |E_{(11,12)}| \left( 11 + 12 \right)^2
\]

\[
+ |E_{(12,12)}| \left( 12 + 12 \right)^2.
\]

\[
= 4(169) + 196u + 8(289) + (2u - 4)(324) + (4v - 8)(324) + 2v(484) + (u - 2)(484)
\]

\[
+ (2u - 4)(529) + 576(3uv - 4u - 4v + 5).
\]

\[
= 1728uv + 82u - 40v - 1104.
\]

Case 2: From Table 6, we use the link partition for \(u = 1, v > 1\) in Eq. (7) to obtain,

\[
\text{CHM}_1(G) = \sum_{s \in E(G)} \left( \Omega_G(s) + \Omega_G(w) \right)^2
\]

\[
= |E_{(6,6)}| \left( 6 + 6 \right)^2 + |E_{(6,7)}| \left( 6 + 7 \right)^2 + |E_{(7,10)}| \left( 7 + 10 \right)^2 + |E_{(8,10)}| \left( 8 + 10 \right)^2
\]

\[
+ |E_{(10,12)}| \left( 10 + 10 \right)^2
\]

\[
= 2(144) + 4(169) + 4(289) + (4v - 8)(324) + (v - 1)(400).
\]

\[
= 1696v - 872.
\]

Case 3: For \(u > 1, v = 1\), we are looking forward to applying Table 7 on Eq. (7).
\[ CHM_1(G) = \sum_{s \in E(G)} (\Omega_G(s) + \Omega_G(w))^2 \]
\[ = |E_{(6,6)}|(6+6)^2 + |E_{(6,7)}|(6+7)^2 + |E_{(7,7)}|(7+7)^2 + |E_{(7,10)}|(7+10)^2 \]
\[ + |E_{(7,11)}|(7+11)^2 + |E_{(10,11)}|(10+11)^2 + |E_{(11,11)}|(11+11)^2. \]
\[ = 2(144) + 4(169) + (u-2)(196) + 4(289) + (2u-4)(324) + 2(441) + (2u-5)(484). \]
\[ = 1812u - 1106. \]

Case 4: For \( u = 1, v = 1 \), using Table 8 on Eq. (7), we have,
\[ CHM_1(G) = \sum_{s \in E(G)} (\Omega_G(s) + \Omega_G(w))^2 = |E_{(6,6)}|(6+6)^2 = 6(144) = 864. \]

Theorem 3.7: The CHM_{2}(G) index of graphene with \( u \) rows and \( v \) benzene rings per row is
\[ CHM_2(G) = \begin{cases} 
62208uv - 19196u - 28544v - 23958 & \text{if } u > 1, v > 1 \\
35600v - 31952 & \text{if } u = 1, v > 1 \\
43541u - 48275 & \text{if } u > 1, v = 1 \\
7776 & \text{if } u = 1, v = 1 
\end{cases} \]

Proof: We present the proof for all four cases.

Case 1: To the link partition for \( u > 1, v > 1 \) given in Table 5, Eq.(8) exhibits the following outcome.
\[ CHM_2(G) = \sum_{s \in E(G)} (\Omega_G(s) \Omega_G(w))^2 \]
\[ = |E_{(6,7)}|(6 \times 7)^2 + |E_{(7,7)}|(7 \times 7)^2 + |E_{(7,10)}|(7 \times 10)^2 + |E_{(7,11)}|(7 \times 11)^2 \]
\[ + |E_{(8,10)}|(8 \times 10)^2 + |E_{(10,12)}|(10 \times 12)^2 + |E_{(11,11)}|(11 \times 11)^2 \]
\[ + |E_{(11,12)}|(11 \times 12)^2 + |E_{(12,12)}|(12 \times 12)^2. \]
\[ = 4(1764) + 2401u + 8(4900) + (2u-4)(5929) + (4v-8)(6400) + 2v(14400) \]
\[ + (u-2)(14641) + (2u-4)(17424) + 20736(3uv - 4u - 4v + 5). \]
\[ = 62208uv - 19196u - 28544v - 23958. \]

Case 2: For \( u = 1, v > 1 \), We are looking forward to applying Table 6 on Eq. (8).
\[ CHM_2(G) = \sum_{s \in E(G)} (\Omega_G(s) \Omega_G(w))^2 \]
\[ = |E_{(6,6)}|(6 \times 6)^2 + |E_{(6,7)}|(6 \times 7)^2 + |E_{(7,10)}|(7 \times 10)^2 + |E_{(8,10)}|(8 \times 10)^2 \]
\[ + |E_{(10,10)}|(10 \times 10)^2 \]
\[ = 2(1296) + 4(1764) + 4(4900) + (4v-8)(6400) + (v-1)(10000). \]
\[ = 35600v - 31952. \]

Case 3: For \( u > 1, v = 1 \), we apply Table 7 on Eq. (8).
\[ CHM_2(G) = \sum_{(s,w) \in E(G)} (\Omega_G(s) \Omega_G(w))^2 \]

\[ = |E_{(6,6)}|(6 \times 6)^2 + |E_{(6,7)}|(6 \times 7)^2 + |E_{(7,7)}|(7 \times 7)^2 + |E_{(7,10)}|(7 \times 10)^2 + |E_{(7,11)}|(7 \times 11)^2 + |E_{(10,11)}|(10 \times 11)^2 + |E_{(11,11)}|(11 \times 11)^2. \]

\[ = 2(1296) + 4(1764) + (u-2)(2401) + 4(4900) + (2u-4)(5929) + 2(12100) + (2u-5)(14641). \]

\[ = 43541u - 48275. \]

Case 4: From Table 8, using the link partition for \( u = 1, v = 1 \) in Eq. (8), we attain,

\[ CHM_2(G) = \sum_{(s,w) \in E(G)} (\Omega_G(s) \Omega_G(w))^2 = |E_{(6,6)}|(6 \times 6)^2 = 6(1296) = 7776. \]

Novel TIs for graphene are pictorially depicted in Fig. (5–11). The first case is displayed in (a) segment of the figure, while the next two cases are depicted in (b) segment of the figure, applying various colors.

![Figures 5, 6, and 7](https://biointerfaceresearch.com/)
Figure 8. The $CF(G)$ index of graphene for (a) $u > 1; v > 1$ and (b) $u = 1; v > 1; u > 1; v = 1$.

Figure 9. The $CF^*(G)$ index of graphene for (a) $u > 1; v > 1$ and (b) $u = 1; v > 1; u > 1; v = 1$.

Figure 10. The $CHM_1(G)$ index of graphene for (a) $u > 1; v > 1$ and (b) $u = 1; v > 1; u > 1; v = 1$.

Figure 11. The $CHM_2(G)$ index of graphene for (a) $u > 1; v > 1$ and (b) $u = 1; v > 1; u > 1; v = 1$. 
4. Conclusions

In summary, we have computed accurate expressions of certain closed neighborhood versions of TIs for graphene structure. Moreover, the values of TIs for graphene are compared graphically (Figure 12). The behavior of suggested TIs for graphene is approached nearer (except CHM\(_2\)(G)) at the beginning of a given domain and after that found to be progressed higher. Among the seven TIs, CHM\(_2\)(G) has the greatest dominating power for graphene. On the other hand, CM\(_1\)(G) grows more slowly than other indices. The nature of CM\(_1^*\)(G) is closer to CM\(_2\)(G) index. The indices CHM\(_1\)(G), CF\(_1^*\)(G), and CF(G) increase gradually and develop a ‘Trident pattern’. The obtained results could provide new insights in the field of structural chemistry and also offer potential applications in predicting the properties of novel nanomaterials at the preliminary investigation.

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**Conflicts of Interest**

The authors declare no conflict of interest.
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