Closed Neighborhood Degree Sum-Based Topological Descriptors of Graphene Structures

Vignesh Ravi 1, Kalyani Desikan 1*

1 Division of Mathematics, School of Advanced Sciences, Vellore Institute of Technology, Chennai; rvignesh.2018@vitstudent.ac.in (V.R.), kalyanidesikan@vit.ac.in (K.D.);
2 Correspondence: kalyanidesikan@vit.ac.in (K.D);
Scopus Author ID 7005615253

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Abstract: Topological descriptors defined on chemical structures enable understanding the properties and activities of chemical molecules. In this paper, we compute closed neighborhood degree sum-based indices for four different Graphene structures. The cardinality of closed neighborhood degree-based edge partitions for four different Graphene structures is used to compute the closed neighborhood degree sum-based indices.

Keywords: Graphene structure; closed neighborhood degree; closed neighborhood degree-based topological indices; reciprocal indices.

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1. Introduction

Cheminformatics is a field of study that employs quantitative structure behavior and structure-property relationships to study chemical compounds' bioactivities and properties [1, 2]. In research findings, physicochemical properties and topological indices are used to predict the bioactivity of organic compounds [3]. Nodes represent atoms or molecules in a chemical graph, while the links denote the chemical bond between the atoms or molecules.

Topological descriptors defined on chemical structures play a crucial role in understanding the properties and activities of chemical molecules. The degree of a vertex is indicated by $d_v$ or $d(u)$ [4], and it denotes the number of edges that are incident on that vertex. The closed neighborhood degree of a node $u \in V$, indicated as $\delta[u]$, is the sum of degrees of all the nodes in the neighborhood of the node $u$ and $d(u)$.

Graphene, a carbon allotrope with a honeycomb grid structure, is the most enduring compound material. It has excellent thermal and electric conductivity properties. It has a high nonlinear magnetic property compared to graphite.

Numerous researchers have described and evaluated various topological descriptors of many compounds, such as Graphene, Graphene transformations, and their applications [5 - 34].

Open neighborhood degree sum-based topological indices were studied recently by Vignesh and Kalyani Desikan [35]. They proposed some new open neighborhood degree sum based indices, namely $SK_N^2, SK1_N, SK2_N, mR_N, ISI_N$. Vignesh et al. [36] proposed the reciprocal versions of the indices mentioned in [35]. Further, Vignesh and Kalyani Desikan [37] proposed the closed neighborhood versions of the aforesaid topological indices denoted as $SK_N^2(G), SK1_N^c(G), SK2_N^c(G), mR_N^c(G), ISI_N^c(G)$ along with their reciprocal versions as follows:
\[
SK_N^c(G) = \sum_{uv \in E(G)} \left[ \frac{\delta[u] + \delta[v]}{2} \right]
\]
(1)

\[
SK1_N^c(G) = \sum_{uv \in E(G)} \left[ \frac{\delta[u] \cdot \delta[v]}{2} \right]
\]
(2)

\[
SK2_N^c(G) = \sum_{uv \in E(G)} \left[ \frac{\delta[u] + \delta[v]}{2} \right]^2
\]
(3)

\[
mR_N^c(G) = \sum_{uv \in E(G)} \left[ \frac{1}{\max(\delta[u], \delta[v])} \right]
\]
(4)

\[
I SI_N^c(G) = \sum_{uv \in E(G)} \left[ \frac{\delta[u] \cdot \delta[v]}{\delta[u] + \delta[v]} \right]
\]
(5)

\[
RSK_N^c(G) = \sum_{uv \in E(G)} \left[ \frac{2}{\delta[u] + \delta[v]} \right]
\]
(6)

\[
RSK1_N^c(G) = \sum_{uv \in E(G)} \left[ \frac{2}{\delta[u] + \delta[v]} \right]
\]
(7)

\[
RSK2_N^c(G) = \sum_{uv \in E(G)} \left[ \frac{2}{\delta[u] + \delta[v]} \right]^2
\]
(8)

\[
RmR_N^c(G) = \sum_{uv \in E(G)} \left[ \max \{ \delta[u], \delta[v] \} \right]
\]
(9)

\[
RISI_N^c(G) = \sum_{uv \in E(G)} \left[ \frac{\delta[u] + \delta[v]}{\delta[u] \cdot \delta[v]} \right]
\]
(10)

where \( \delta[u] = \left[ \sum_{v \in N(u)} \deg(v) \right] + \deg(u) \). \( N(u) \) is the Neighborhood set of the vertex \( u \).

In this paper, we estimate the closed neighborhood topological descriptors \( SK_N^c(G), SK1_N^c(G), SK2_N^c(G), mR_N^c(G), ISI_N^c(G) \) as well as their reciprocal versions. The results are obtained by ascertaining the cardinality of edge partitions of the four distinct Graphene structures. For the Graphene structures, refer to [29].

Graphene structures can be classified into four based on the number of layers and benzene rings. The edge types for the four structures are indicated by (\( \delta[u], \delta[v] \)). The edge partitions for the four structures are presented in the tables below:

**Table 1.** Edge Partition when \( a > 1 \ b > 1 \).

| Edge Type | Number of Edges |
|-----------|-----------------|
| (6, 7)    | 4               |
| (7, 7)    | a               |
| (7, 10)   | 8               |
| (7, 11)   | 2a-4            |
| (8, 10)   | 4b-8            |
| (10, 12)  | 2b              |
| (11, 11)  | a-2             |
| (11, 11)  | 2a-4            |
| (12, 12)  | 3a-b – 4a-4b – 5 |

**Table 2.** Edge Partition when \( a = 1 \ b > 1 \).

| Edge Type | Number of Edges |
|-----------|-----------------|
| \( E(\delta_u, \delta_v) \) | [6, 6] |
| \( E(\delta_u, \delta_v) \) | [6, 7] |
| \( E(\delta_u, \delta_v) \) | [7, 10] |
| \( E(\delta_u, \delta_v) \) | [8, 10] |
| \( E(\delta_u, \delta_v) \) | [10, 10] |

**Table 3.** Edge Partition when \( a > 1 \ b = 1 \).

| Edge Type | Number of Edges |
|-----------|-----------------|
| (6, 6)    | 2               |
| (6, 7)    | 4               |
| (7, 7)    | a-2             |
| (7, 10)   | 4               |
| (7, 11)   | 4a-8            |
| (10, 11)  | b-1             |
| (11, 11)  |                 |

**Table 4.** Edge Partition when \( a = 1 \ b = 1 \).

| Edge Type | Number of Edges |
|-----------|-----------------|
| (6, 6)    | 6               |

where \( a \) and \( b \) denote the rows and number of benzene rings, respectively.
2. Materials and Methods

The closed neighborhood degree sum-based topological descriptors of Graphene structures have been computed. To obtain our results, we adopted the closed neighborhood degree sum-based edge partition method.

3. Results on Closed Neighborhood Degree Based Topological Descriptors

In this section, we compute closed neighborhood degree-based topological indices, namely, $SK_N^c, SK1_N^c, SK2_N^c, mR_N^c, ISI_N^c$, of Graphene structures.

Theorem 3.1: $SK_N^c$ index of Graphene with $a$ rows and $b$ benzene rings is given by

$$ SK_N^c = \begin{cases} 11a + 10b + 36ab - 22 & \text{if } a > 1, b > 1 \\ 46b - 10 & \text{if } a = 1, b > 1 \\ 47a - 12 & \text{if } a > 1, b = 1 \\ 36 & \text{if } a = 1, b = 1 \end{cases} $$

Proof: We provide the proof for the four cases,

Case 1: From Table 1, we use the edge partition for $a > 1, b > 1$ in equation 1 to obtain,

$$ SK_N^c = \sum_{uv \in E_1} \left[ \frac{6 + 7}{2} \right] + \sum_{uv \in E_2} \left[ \frac{7 + 7}{2} \right] + \sum_{uv \in E_3} \left[ \frac{7 + 10}{2} \right] + \sum_{uv \in E_4} \left[ \frac{7 + 11}{2} \right] $$

$$ + \sum_{uv \in E_5} \left[ \frac{8 + 10}{2} \right] + \sum_{uv \in E_6} \left[ \frac{10 + 12}{2} \right] + \sum_{uv \in E_7} \left[ \frac{11 + 11}{2} \right] + \sum_{uv \in E_8} \left[ \frac{11 + 12}{2} \right] $$

$$ + \sum_{uv \in E_9} \left[ \frac{12 + 12}{2} \right] $$

$$ = 11a + 10b + 36ab - 22. $$

Case 2: From Table 2, we use the edge partition for $a = 1, b > 1$ in equation 1 to obtain,

$$ SK_N^c = \sum_{uv \in E_1} \left[ \frac{6 + 6}{2} \right] + \sum_{uv \in E_2} \left[ \frac{6 + 7}{2} \right] + \sum_{uv \in E_3} \left[ \frac{7 + 10}{2} \right] + \sum_{uv \in E_4} \left[ \frac{8 + 10}{2} \right] $$

$$ + \sum_{uv \in E_5} \left[ \frac{10 + 10}{2} \right] $$

$$ = 46b - 10. $$

Case 3: From Table 3, we use the edge partition for $a > 1, b = 1$ in equation 1 to obtain,

$$ SK_N^c = \sum_{uv \in E_1} \left[ \frac{6 + 6}{2} \right] + \sum_{uv \in E_2} \left[ \frac{6 + 7}{2} \right] + \sum_{uv \in E_3} \left[ \frac{7 + 7}{2} \right] + \sum_{uv \in E_4} \left[ \frac{7 + 10}{2} \right] + \sum_{uv \in E_5} \left[ \frac{7 + 11}{2} \right] $$

$$ + \sum_{uv \in E_6} \left[ \frac{10 + 11}{2} \right] + \sum_{uv \in E_7} \left[ \frac{11 + 11}{2} \right] $$

$$ = 47a - 12. $$
Case 4: From Table 4, we use the edge partition for \( a = 1, b = 1 \) in equation 1 to obtain,

\[
SK_N^e = \sum_{uv \in E_1} \left[ \frac{6+6}{2} \right] = 36.
\]

Theorem 3.2: \( SK1_N^e \) index of Graphene with \( a \) rows and \( b \) benzene rings is given by

\[
SK1_N^e = \begin{cases} 
6a - 8b + 216ab - 135 & \text{if } a > 1, b > 1 \\
210b - 110 & \text{if } a = 1, b > 1 \\
445a - 271 & \text{if } a > 1, b = 1 \\
108 & \text{if } a = 1, b = 1
\end{cases}
\]

Proof: We provide the proof for the four cases,

Case 1: From Table 1, we use the edge partition for \( a > 1, b > 1 \) in equation 2 to obtain,

\[
SK1_N^e = \sum_\{uv \in E_1\} \left[ \frac{6*7}{2} \right] + \sum_\{uv \in E_2\} \left[ \frac{7*7}{2} \right] + \sum_\{uv \in E_3\} \left[ \frac{7*10}{2} \right] + \sum_\{uv \in E_4\} \left[ \frac{7*11}{2} \right] + \sum_\{uv \in E_5\} \left[ \frac{8*10}{2} \right] + \sum_\{uv \in E_6\} \left[ \frac{10*12}{2} \right] + \sum_\{uv \in E_7\} \left[ \frac{11*11}{2} \right] + \sum_\{uv \in E_8\} \left[ \frac{11*12}{2} \right] + \sum_\{uv \in E_9\} \left[ \frac{12*12}{2} \right] = 6a - 8b + 216ab - 135.
\]

Case 2: From Table 2, we use the edge partition for \( a = 1, b > 1 \) in equation 2 to obtain,

\[
SK1_N^e = \sum_\{uv \in E_1\} \left[ \frac{6*6}{2} \right] + \sum_\{uv \in E_2\} \left[ \frac{6*7}{2} \right] + \sum_\{uv \in E_3\} \left[ \frac{7*10}{2} \right] + \sum_\{uv \in E_4\} \left[ \frac{8*10}{2} \right] + \sum_\{uv \in E_5\} \left[ \frac{10*10}{2} \right] = 210b - 110.
\]

Case 3: From Table 3, we use the edge partition for \( a > 1, b = 1 \) in equation 2 to obtain,

\[
SK1_N^e = \sum_\{uv \in E_1\} \left[ \frac{6*6}{2} \right] + \sum_\{uv \in E_2\} \left[ \frac{6*7}{2} \right] + \sum_\{uv \in E_3\} \left[ \frac{7*7}{2} \right] + \sum_\{uv \in E_4\} \left[ \frac{7*10}{2} \right] + \sum_\{uv \in E_5\} \left[ \frac{7*11}{2} \right] + \sum_\{uv \in E_6\} \left[ \frac{10*11}{2} \right] + \sum_\{uv \in E_7\} \left[ \frac{11*11}{2} \right] = 445a - 271.
\]

Case 4: From Table 4, we use the edge partition for \( a = 1, b = 1 \) in equation 2 to obtain,

\[
SK1_N^e = \sum_{uv \in E_1} \left[ \frac{6*6}{2} \right] = 108.
\]

Theorem 3.3: \( SK2_N^e \) index of Graphene with \( a \) rows and \( b \) benzene rings is given by
\[ SK_{N^c}^2 = \begin{cases} 
\frac{41a - 20b + 864ab - 552}{2} & \text{if } a > 1, b > 1 \\
\frac{424b - 218}{906a - 553} & \text{if } a = 1, b > 1 \\
\frac{216}{2} & \text{if } a > 1, b = 1 \\
\frac{216}{2} & \text{if } a = 1, b = 1 
\end{cases} \]

Proof: We provide the proof for the four cases,

Case 1: From Table 1, we use the edge partition for \( a > 1, b > 1 \) in equation 3 to obtain,

\[
SK_{N^c}^2 = \sum_{uv \in E_1} \left[ \frac{6 + 7}{2} \right]^2 + \sum_{uv \in E_2} \left[ \frac{7 + 7}{2} \right]^2 + \sum_{uv \in E_3} \left[ \frac{7 + 10}{2} \right]^2 + \sum_{uv \in E_4} \left[ \frac{7 + 11}{2} \right]^2
+ \sum_{uv \in E_5} \left[ \frac{8 + 10}{2} \right]^2 + \sum_{uv \in E_6} \left[ \frac{10 + 12}{2} \right]^2 + \sum_{uv \in E_7} \left[ \frac{11 + 11}{2} \right]^2
+ \sum_{uv \in E_8} \left[ \frac{11 + 12}{2} \right]^2 + \sum_{uv \in E_9} \left[ \frac{12 + 12}{2} \right]^2
= \frac{41a - 20b + 864ab - 552}{2}.
\]

Case 2: From Table 2, we use the edge partition for \( a = 1, b > 1 \) in equation 3 to obtain,

\[
SK_{N^c}^2 = \sum_{uv \in E_1} \left[ \frac{6 + 6}{2} \right]^2 + \sum_{uv \in E_2} \left[ \frac{6 + 7}{2} \right]^2 + \sum_{uv \in E_3} \left[ \frac{7 + 10}{2} \right]^2 + \sum_{uv \in E_4} \left[ \frac{8 + 10}{2} \right]^2
+ \sum_{uv \in E_5} \left[ \frac{10 + 10}{2} \right]^2
= 424b - 218.
\]

Case 3: From Table 3, we use the edge partition for \( a > 1, b = 1 \) in equation 3 to obtain,

\[
SK_{N^c}^2 = \sum_{uv \in E_1} \left[ \frac{6 + 6}{2} \right]^2 + \sum_{uv \in E_2} \left[ \frac{6 + 7}{2} \right]^2 + \sum_{uv \in E_3} \left[ \frac{7 + 7}{2} \right]^2 + \sum_{uv \in E_4} \left[ \frac{7 + 10}{2} \right]^2
+ \sum_{uv \in E_5} \left[ \frac{7 + 11}{2} \right]^2 + \sum_{uv \in E_6} \left[ \frac{10 + 11}{2} \right]^2 + \sum_{uv \in E_7} \left[ \frac{11 + 11}{2} \right]^2
+ \sum_{uv \in E_8} \left[ \frac{11 + 12}{2} \right]^2 + \sum_{uv \in E_9} \left[ \frac{12 + 12}{2} \right]^2
= \frac{906a - 553}{2}.
\]

Case 4: From Table 4, we use the edge partition for \( a = 1, b = 1 \) in equation 3 to obtain,

\[
SK_{N^c}^2 = \sum_{uv \in E_1} \left[ \frac{6 + 6}{2} \right]^2 = 216.
\]

Theorem 3.4: \( mR_{N^c} \) index of Graphene with \( a \) rows and \( b \) benzene rings is given by
\[ m_{Nc} = \begin{cases} 
\frac{1150a + 1078b + 1155ab - 1505}{4620} & \text{if } a > 1, b > 1 \\
\frac{21b + 17}{42} & \text{if } a = 1, b > 1 \\
13 \frac{[45a + 34]}{1155} & \text{if } a > 1, b = 1 \\
1 & \text{if } a = 1, b = 1 
\end{cases} \]

Proof: We provide the proof for the four cases,

Case 1: From Table 1, we use the edge partition for \( a > 1, b > 1 \) in equation 4 to obtain,

\[
m_{Nc} = \sum_{uv \in E_1} \left[ \frac{1}{\max\{6,7\}} \right] + \sum_{uv \in E_2} \left[ \frac{1}{\max\{7,7\}} \right] + \sum_{uv \in E_3} \left[ \frac{1}{\max\{7,10\}} \right] + \sum_{uv \in E_4} \left[ \frac{1}{\max\{7,11\}} \right] + \sum_{uv \in E_5} \left[ \frac{1}{\max\{8,10\}} \right] + \sum_{uv \in E_6} \left[ \frac{1}{\max\{10,12\}} \right] + \sum_{uv \in E_7} \left[ \frac{1}{\max\{11,11\}} \right] + \sum_{uv \in E_8} \left[ \frac{1}{\max\{11,12\}} \right] + \sum_{uv \in E_9} \left[ \frac{1}{\max\{12,12\}} \right] = \frac{1150a + 1078b + 1155ab - 1505}{4620}.
\]

Case 2: From Table 2, we use the edge partition for \( a = 1, b > 1 \) in equation 4 to obtain,

\[
m_{Nc} = \sum_{uv \in E_1} \left[ \frac{1}{\max\{6,7\}} \right] + \sum_{uv \in E_2} \left[ \frac{1}{\max\{7,7\}} \right] + \sum_{uv \in E_3} \left[ \frac{1}{\max\{7,10\}} \right] + \sum_{uv \in E_4} \left[ \frac{1}{\max\{8,10\}} \right] + \sum_{uv \in E_5} \left[ \frac{1}{\max\{8,10\}} \right] = \frac{21b + 17}{42}.
\]

Case 3: From Table 3, we use the edge partition for \( a > 1, b = 1 \) in equation 4 to obtain,

\[
m_{Nc} = \sum_{uv \in E_1} \left[ \frac{1}{\max\{6,6\}} \right] + \sum_{uv \in E_2} \left[ \frac{1}{\max\{6,7\}} \right] + \sum_{uv \in E_3} \left[ \frac{1}{\max\{7,7\}} \right] + \sum_{uv \in E_4} \left[ \frac{1}{\max\{7,10\}} \right] + \sum_{uv \in E_5} \left[ \frac{1}{\max\{7,11\}} \right] + \sum_{uv \in E_6} \left[ \frac{1}{\max\{10,11\}} \right] + \sum_{uv \in E_7} \left[ \frac{1}{\max\{11,11\}} \right] + \sum_{uv \in E_8} \left[ \frac{1}{\max\{11,12\}} \right] = 13 \frac{[45a + 34]}{1155}.
\]

Case 4: From Table 4, we use the edge partition for \( a = 1, b = 1 \) in equation 4 to obtain,

\[
m_{Nc} = \sum_{uv \in E_1} \left[ \frac{1}{\max\{6,6\}} \right] = 1.
\]

Theorem 3.5: \( ISI_{Nc} \) index of Graphene structure with \( a \) rows and \( b \) benzene rings is given by
Proof: We provide the proof for the four cases,

Case 1: From Table 1, we use the edge partition for \( a > 1, b > 1 \) in equation 5 to obtain,

\[
ISI_{N^c} = \sum_{uv \in E_1} \left( \frac{6+7}{6+7} \right) + \sum_{uv \in E_2} \left( \frac{7+7}{7+7} \right) + \sum_{uv \in E_3} \left( \frac{7+10}{7+10} \right) + \sum_{uv \in E_4} \left( \frac{7+11}{7+11} \right) + \\
\sum_{uv \in E_5} \left( \frac{8+10}{8+10} \right) + \sum_{uv \in E_6} \left( \frac{10+12}{10+12} \right) + \sum_{uv \in E_7} \left( \frac{11+11}{11+11} \right) + \sum_{uv \in E_8} \left( \frac{11+12}{11+12} \right) + \sum_{uv \in E_9} \left( \frac{12+12}{12+12} \right)
\]

\[
= \frac{2533102a + 2358512b + 9057906ab - 5414079}{503217}.
\]

Case 2: From Table 2, we use the edge partition for \( a = 1, b > 1 \) in equation 5 to obtain,

\[
ISI_{N^c} = \sum_{uv \in E_1} \left( \frac{6+6}{6+6} \right) + \sum_{uv \in E_2} \left( \frac{6+7}{6+7} \right) + \sum_{uv \in E_3} \left( \frac{7+10}{7+10} \right) + \sum_{uv \in E_4} \left( \frac{8+10}{8+10} \right) + \\
\sum_{uv \in E_5} \left( \frac{7+11}{7+11} \right) + \sum_{uv \in E_6} \left( \frac{10+11}{10+11} \right) + \sum_{uv \in E_7} \left( \frac{11+11}{11+11} \right)
\]

\[
= \frac{45305b - 10267}{1989}.
\]

Case 3: From Table 3, we use the edge partition for \( a > 1, b = 1 \) in equation 5 to obtain,

\[
ISI_{N^c} = \sum_{uv \in E_1} \left( \frac{6+6}{6+6} \right) + \sum_{uv \in E_2} \left( \frac{6+7}{6+7} \right) + \sum_{uv \in E_3} \left( \frac{7+7}{7+7} \right) + \sum_{uv \in E_4} \left( \frac{7+10}{7+10} \right) + \\
\sum_{uv \in E_5} \left( \frac{7+11}{7+11} \right) + \sum_{uv \in E_6} \left( \frac{10+11}{10+11} \right) + \sum_{uv \in E_7} \left( \frac{11+11}{11+11} \right)
\]

\[
= \frac{642005a - 159871}{27846}.
\]

Case 4: From Table 4, we use the edge partition for \( a = 1, b = 1 \) in equation 5 to obtain,

\[
ISI_{N^c} = \sum_{uv \in E_1} \left( \frac{6+6}{6+6} \right) = 18.
\]

4. Results on Reciprocal Closed Neighborhood Degree

In this section, we compute the reciprocal closed neighborhood degree-based topological indices, namely \( RSK_{N^c}, RSK1_{N^c}, RSK2_{N^c}, RmR_{N^c}, RISI_{N^c} \) of Graphene structures.

Theorem 4.1: \( RSK_{N^c} \) index of Graphene with \( a \) rows and \( b \) benzene rings is given by
Proof: We provide the proof for the four cases,

Case 1: From Table 1, we use the edge partition for $a > 1, b > 1$ in equation 6 to obtain,

$$RSK_{Nc} = \frac{4178668a + 4127396b + 3522519ab + 1553433}{14090076} \quad \text{if} \quad a > 1, b > 1$$

$$= 7 \left[ \frac{1547b + 1223}{19890} \right] \quad \text{if} \quad a = 1, b > 1$$

$$= \frac{83759a + 65102}{153153} \quad \text{if} \quad a > 1, b = 1$$

$$= \frac{1}{1} \quad \text{if} \quad a = 1, b = 1$$

Case 2: From Table 2, we use the edge partition for $a = 1, b > 1$ in equation 6 to obtain,

$$RSK_{Nc} = \frac{4178668a + 4127396b + 3522519ab + 1553433}{14090076} \quad \text{if} \quad a > 1, b > 1$$

$$= 7 \left[ \frac{1547b + 1223}{19890} \right] \quad \text{if} \quad a = 1, b > 1$$

$$= \frac{83759a + 65102}{153153} \quad \text{if} \quad a > 1, b = 1$$

$$= \frac{1}{1} \quad \text{if} \quad a = 1, b = 1$$

Case 3: From Table 3, we use the edge partition for $a > 1, b = 1$ in equation 6 to obtain,

$$RSK_{Nc} = \frac{4178668a + 4127396b + 3522519ab + 1553433}{14090076} \quad \text{if} \quad a > 1, b > 1$$

$$= 7 \left[ \frac{1547b + 1223}{19890} \right] \quad \text{if} \quad a = 1, b > 1$$

$$= \frac{83759a + 65102}{153153} \quad \text{if} \quad a > 1, b = 1$$

$$= \frac{1}{1} \quad \text{if} \quad a = 1, b = 1$$

Case 4: From Table 4, we use the edge partition for $a = 1, b = 1$ in equation 6 to obtain,

$$RSK_{Nc} = \frac{4178668a + 4127396b + 3522519ab + 1553433}{14090076} \quad \text{if} \quad a > 1, b > 1$$

$$= 7 \left[ \frac{1547b + 1223}{19890} \right] \quad \text{if} \quad a = 1, b > 1$$

$$= \frac{83759a + 65102}{153153} \quad \text{if} \quad a > 1, b = 1$$

$$= \frac{1}{1} \quad \text{if} \quad a = 1, b = 1$$

Theorem 4.2: $RSK_{1c}$ index of Graphene with $a$ rows and $b$ benzene rings is given by

$$RSK_{1c} = \begin{cases} 
2 \left[ \frac{179380a + 166012b + 88935ab + 194089}{4268880} \right] & \text{if} \quad a > 1, b > 1 \\
8 \left[ \frac{378b + 617}{25200} \right] & \text{if} \quad a = 1, b > 1 \\
4 \left[ \frac{33570a + 49109}{1067220} \right] & \text{if} \quad a > 1, b = 1 \\
1 & \text{if} \quad a = 1, b = 1 
\end{cases}$$

Proof: We provide the proof for the four cases,
Case 1: From Table 1, we use the edge partition for \( a > 1, b > 1 \) in equation 7 to obtain,
\[
RSK_{1}^{Nc} = \sum_{uv \in E_1} \left[ \frac{2}{6*7} \right] + \sum_{uv \in E_2} \left[ \frac{2}{7*7} \right] + \sum_{uv \in E_3} \left[ \frac{2}{7*10} \right] + \sum_{uv \in E_4} \left[ \frac{2}{7*11} \right] + \sum_{uv \in E_5} \left[ \frac{2}{8*10} \right] + \sum_{uv \in E_6} \left[ \frac{2}{10*12} \right] + \sum_{uv \in E_7} \left[ \frac{2}{11*11} \right] + \sum_{uv \in E_8} \left[ \frac{2}{11*12} \right] + \sum_{uv \in E_9} \left[ \frac{2}{12*12} \right]
\]
\[
= 2 \left[ \frac{179380a + 166012b + 88935ab + 194089}{4268880} \right].
\]

Case 2: From Table 2, we use the edge partition for \( a = 1, b > 1 \) in equation 7 to obtain,
\[
RSK_{1}^{Nc} = \sum_{uv \in E_1} \left[ \frac{2}{6*6} \right] + \sum_{uv \in E_2} \left[ \frac{2}{6*7} \right] + \sum_{uv \in E_3} \left[ \frac{2}{7*10} \right] + \sum_{uv \in E_4} \left[ \frac{2}{8*10} \right] + \sum_{uv \in E_5} \left[ \frac{2}{10*10} \right]
\]
\[
= 8 \left[ \frac{378b+617}{25200} \right].
\]

Case 3: From Table 3, we use the edge partition for \( a > 1, b = 1 \) in equation 7 to obtain,
\[
RSK_{1}^{Nc} = \sum_{uv \in E_1} \left[ \frac{2}{6*6} \right] + \sum_{uv \in E_2} \left[ \frac{2}{6*7} \right] + \sum_{uv \in E_3} \left[ \frac{2}{7*7} \right] + \sum_{uv \in E_4} \left[ \frac{2}{7*10} \right] + \sum_{uv \in E_5} \left[ \frac{2}{7*11} \right] + \sum_{uv \in E_6} \left[ \frac{2}{10*11} \right] + \sum_{uv \in E_7} \left[ \frac{2}{11*11} \right]
\]
\[
= 4 \left[ \frac{33570a + 49109}{1067220} \right].
\]

Case 4: From Table 4, we use the edge partition for \( a = 1, b = 1 \) in equation 7 to obtain,
\[
RSK_{1}^{Nc} = \sum_{uv \in E_1} \left[ \frac{2}{6*6} \right] = \frac{1}{3}.
\]

Theorem 4.3: RSK2_{Nc} index of Graphene with \( a \) rows and \( b \) benzene rings is given by
\[
RSK_{2}^{Nc} = \begin{cases} 
0.0407a + 0.0381b + \left( \frac{ab}{48} \right) + 0.0452 & \text{if } a > 1, b > 1 \\
0.0594b + 0.0968 & \text{if } a = 1, b > 1 \\
0.0616a + 0.0922 & \text{if } a > 1, b = 1 \\
\frac{1}{6} & \text{if } a = 1, b = 1
\end{cases}
\]

Proof: We provide the proof for the four cases,

Case 1: From Table 1, we use the edge partition for \( a > 1, b > 1 \) in equation 8 to obtain,
Case 1: From Table 1, we use the edge partition for \(a > 1, b > 1\) in equation 9 to obtain,
\[
RSK2_{N^c} = \sum_{u \in E_1} \left[ \frac{2}{6+7} \right]^2 + \sum_{u \in E_2} \left[ \frac{2}{7+7} \right]^2 + \sum_{u \in E_3} \left[ \frac{2}{7+10} \right]^2 + \sum_{u \in E_4} \left[ \frac{2}{7+11} \right]^2
\]
\[
+ \sum_{u \in E_5} \left[ \frac{2}{8+10} \right]^2 + \sum_{u \in E_6} \left[ \frac{2}{10+12} \right]^2 + \sum_{u \in E_7} \left[ \frac{2}{11+11} \right]^2
\]
\[
= 0.0407a + 0.0381b + \left( \frac{ab}{48} \right) + 0.0452.
\]
Case 2: From Table 2, we use the edge partition for \(a = 1, b > 1\) in equation 8 to obtain,
\[
RSK2_{N^c} = \sum_{u \in E_1} \left[ \frac{2}{6+6} \right]^2 + \sum_{u \in E_2} \left[ \frac{2}{6+7} \right]^2 + \sum_{u \in E_3} \left[ \frac{2}{7+7} \right]^2 + \sum_{u \in E_4} \left[ \frac{2}{7+10} \right]^2 + \sum_{u \in E_5} \left[ \frac{2}{10+10} \right]^2
\]
\[
= 0.0594b + 0.0968.
\]
Case 3: From Table 3, we use the edge partition for \(a > 1, b = 1\) in equation 8 to obtain,
\[
RSK2_{N^c} = \sum_{u \in E_1} \left[ \frac{2}{6+6} \right]^2 + \sum_{u \in E_2} \left[ \frac{2}{6+7} \right]^2 + \sum_{u \in E_3} \left[ \frac{2}{7+7} \right]^2 + \sum_{u \in E_4} \left[ \frac{2}{7+10} \right]^2 + \sum_{u \in E_5} \left[ \frac{2}{7+11} \right]^2 + \sum_{u \in E_6} \left[ \frac{2}{10+11} \right]^2 + \sum_{u \in E_7} \left[ \frac{2}{11+11} \right]^2
\]
\[
= 0.0616a + 0.0922.
\]
Case 4: From Table 4, we use the edge partition for \(a = 1, b = 1\) in equation 8 to obtain,
\[
RSK2_{N^c} = \sum_{u \in E_1} \left[ \frac{2}{6+6} \right]^2 = \frac{1}{6}
\]
Theorem 4.4: \(RmR_{N^c}\) index of Graphene with \(a\) rows and \(b\) benzene rings is given by
\[
RmR_{N^c} = \begin{cases} 
16a + 16b + 36ab - 26 & \text{if } a > 1, b > 1 \\
50b - 10 & \text{if } a = 1, b > 1 \\
51a - 11 & \text{if } a > 1, b = 1 \\
36 & \text{if } a = 1, b = 1 
\end{cases}
\]
Proof: We provide the proof for the four cases,
Case 1: From Table 1, we use the edge partition for \(a > 1, b > 1\) in equation 9 to obtain,
\[
RmR_{N^c} = \sum_{u \in E_1} \left[ \max\{6,7\} \right] + \sum_{u \in E_2} \left[ \max\{7,7\} \right] + \sum_{u \in E_3} \left[ \max\{7,10\} \right]
\]
\[
+ \sum_{u \in E_4} \left[ \max\{7,11\} \right] + \sum_{u \in E_5} \left[ \max\{8,10\} \right] + \sum_{u \in E_6} \left[ \max\{10,12\} \right]
\]
\[
+ \sum_{u \in E_7} \left[ \max\{11,11\} \right] + \sum_{u \in E_8} \left[ \max\{11,12\} \right]
\]
Case 2: From Table 2, we use the edge partition for \( a = 1, b > 1 \) in equation 9 to obtain,

\[
RmR_{N^c} = \sum_{uv \in E_1} [\max\{6,6\}] + \sum_{uv \in E_2} [\max\{6,7\}] + \sum_{uv \in E_3} [\max\{7,10\}]
+ \sum_{uv \in E_4} [\max\{8,10\}] + \sum_{uv \in E_5} [\max\{10,10\}]
= 50b - 10.
\]

Case 3: From Table 3, we use the edge partition for \( a > 1, b = 1 \) in equation 9 to obtain,

\[
RmR_{N^c} = \sum_{uv \in E_1} [\max\{6,6\}] + \sum_{uv \in E_2} [\max\{6,7\}] + \sum_{uv \in E_3} [\max\{7,7\}] + \sum_{uv \in E_4} [\max\{7,10\}]
+ \sum_{uv \in E_5} [\max\{7,11\}] + \sum_{uv \in E_6} [\max\{10,11\}] + \sum_{uv \in E_7} [\max\{11,11\}]
= 51a - 11.
\]

Case 4: From Table 4, we use the edge partition for \( a = 1, b = 1 \) in equation 9 to obtain,

\[
RmR_{N^c} = \sum_{uv \in E_1} [\frac{1}{\max\{6,6\}}] = 36.
\]

Theorem 4.5: \( RISI_{N^c} \) index of Graphene with \( a \) rows and \( b \) benzene rings is given by

\[
RISI_{N^c} = \begin{cases} 
24 \left[ \frac{1425a + 1386b + 1155ab + 505}{55440} \right] & \text{if } a > 1, b > 1 \\
120 \left[ \frac{231b + 184}{25200} \right] & \text{if } a = 1, b > 1 \\
12 \left[ \frac{1290a + 973}{13860} \right] & \text{if } a > 1, b = 1 \\
2 & \text{if } a = 1, b = 1 
\end{cases}
\]

Proof: We provide the proof for the four cases,

Case 1: From Table 1, we use the edge partition for \( a > 1, b > 1 \) in equation 10 to obtain,

\[
RISI_{N^c} = \sum_{uv \in E_1} \left[ \frac{(6 + 7)}{(6 * 7)} \right] + \sum_{uv \in E_2} \left[ \frac{(7 + 7)}{(7 * 7)} \right] + \sum_{uv \in E_3} \left[ \frac{(7 + 10)}{(7 * 10)} \right] + \sum_{uv \in E_4} \left[ \frac{(7 + 11)}{(7 * 11)} \right]
+ \sum_{uv \in E_5} \left[ \frac{(8 + 10)}{(8 * 10)} \right] + \sum_{uv \in E_6} \left[ \frac{(10 + 12)}{(10 * 12)} \right] + \sum_{uv \in E_7} \left[ \frac{(11 + 11)}{(11 * 11)} \right]
+ \sum_{uv \in E_8} \left[ \frac{(11 + 12)}{(11 * 12)} \right] + \sum_{uv \in E_9} \left[ \frac{(12 + 12)}{(12 * 12)} \right]
= 24 \left[ \frac{1425a + 1386b + 1155ab + 505}{55440} \right].
\]

Case 2: From Table 2, we use the edge partition for \( a = 1, b > 1 \) in equation 10 to obtain,
\[ RISI_{Nc} = \sum_{uv \in E_1} \frac{(6 + 6)}{(6 \times 6)} + \sum_{uv \in E_2} \frac{(6 + 7)}{(6 \times 7)} + \sum_{uv \in E_3} \frac{(7 + 10)}{(7 \times 10)} + \sum_{uv \in E_4} \frac{(8 + 10)}{(8 \times 10)} + \sum_{uv \in E_5} \frac{(10 + 10)}{(10 \times 10)} \]

\[ = 120 \left[ \frac{231b+184}{25200} \right]. \]

Case 3: From Table 3, we use the edge partition for \( a > 1, b = 1 \) in equation 10 to obtain,

\[ RISI_{Nc} = \sum_{uv \in E_1} \frac{(6 + 6)}{(6 \times 6)} + \sum_{uv \in E_2} \frac{(6 + 7)}{(6 \times 7)} + \sum_{uv \in E_3} \frac{(7 + 7)}{(7 \times 7)} + \sum_{uv \in E_4} \frac{(7 + 10)}{(7 \times 10)} + \sum_{uv \in E_5} \frac{(7 + 11)}{(7 \times 11)} + \sum_{uv \in E_6} \frac{(10 + 11)}{(10 \times 11)} + \sum_{uv \in E_7} \frac{(11 + 11)}{(11 \times 11)} \]

\[ = 12 \left[ \frac{1290a+973}{13860} \right]. \]

Case 4: From Table 4, we use the edge partition for \( a = 1, b = 1 \) in equation 10 to obtain,

\[ RISI_{Nc} = \sum_{uv \in E_1} \frac{(6+6)}{(6+6)} = 2. \]

4. Conclusions

The analysis of chemical molecules and the study of how the indices relate to the molecular properties is made possible by computing numerous topological indices of chemical graphs. We determined the cardinality of closed neighborhood degree edge partitions corresponding to four distinct Graphene structures and computed 10 closed neighborhood degree sum-based topological indices. In our future work, we plan to apply these descriptors to various transformations of Graphene structures.

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Conflicts of Interest

The authors declare no conflict of interest.

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