

Research Article

Computation of Topological Indices of Graphene

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We compute ABC index, ABC_4 index, Randic connectivity index, Sum connectivity index, GA index, and GA_5 index of Graphene.

1. Introduction

Graphene is an atomic scale honeycomb lattice made of carbon atoms. It is the world's first 2D material which was isolated from graphite in the year 2004 by Professor Andre Geim and Professor Kostya Novoselov. Graphene is 200 times stronger than steel, one million times thinner than a human hair, and world's most conductive material. So it has captured the attention of scientists, researchers, and industries worldwide. It is one of the most promising nanomaterials because of its unique combination of superb properties, which opens a way for its exploitation in a wide spectrum of applications ranging from electronics to optics, sensors, and biodevices. Also it is the most effective material for electromagnetic interference (EMI) shielding.

Topological indices are the molecular descriptors that describe the structures of chemical compounds and they help us to predict certain physicochemical properties like boiling point, enthalpy of vaporization, stability, and so forth. In this paper, we determine the topological indices like atom-bond connectivity index, fourth atom-bond connectivity index, Sum connectivity index, Randic connectivity index, geometric-arithmetic connectivity index, and fifth geometric-arithmetic connectivity index of Graphene.

All molecular graphs considered in this paper are finite, connected, loopless, and without multiple edges. Let $G = (V, E)$ be a graph with n vertices and m edges. The degree of a vertex $u \in V(G)$ is denoted by d_u and is the number of vertices that are adjacent to u . The edge connecting the vertices u

and v is denoted by uv . Using these terminologies, certain topological indices are defined in the following manner.

The atom-bond connectivity index, ABC index, is one of the degree based molecular descriptors, which was introduced by Estrada et al. [1] in late 1990s, and it can be used for modelling thermodynamic properties of organic chemical compounds; it is also used as a tool for explaining the stability of branched alkanes [2]. Some upper bounds for the atom-bond connectivity index of graphs can be found in [3]. The atom-bond connectivity index of chemical bicyclic graphs and connected graphs can be seen in [4, 5]. For further results on ABC index of trees, see the papers [6–9] and the references cited therein.

Definition 1. Let $G = (V, E)$ be a molecular graph, and d_u is the degree of the vertex u ; then ABC index of G is defined as $ABC(G) = \sum_{uv \in E} \sqrt{(d_u + d_v - 2)/d_u d_v}$.

The fourth atom-bond connectivity index, $ABC_4(G)$ index, was introduced by Ghorbani and Hosseinzadeh [10] in 2010. Further studies on $ABC_4(G)$ index can be found in [11, 12].

Definition 2. Let G be a graph; then its fourth ABC index is defined as $ABC_4(G) = \sum_{uv \in E(G)} \sqrt{(S_u + S_v - 2)/S_u S_v}$, where S_u is sum of the degrees of all neighbours of vertex u in G . In other words, $S_u = \sum_{uv \in E(G)} d_v$, similarly for S_v .

The first and oldest degree based topological index is Randic index [13] denoted by $\chi(G)$ and it was introduced by

Milan Randic in 1975. It provides a quantitative assessment of branching of molecules.

Definition 3. For the graph G Randic index is defined as $\chi(G) = \sum_{uv \in E(G)} (1/\sqrt{d_u d_v})$.

Sum connectivity index belongs to a family of Randic like indices and it was introduced by Zhou and Trinajstić [14]. Further studies on Sum connectivity index can be found in [15].

Definition 4. For a simple connected graph G , its Sum connectivity index $S(G)$ is defined as $S(G) = \sum_{uv \in E(G)} (1/\sqrt{d_u + d_v})$.

The geometric-arithmetic index, $GA(G)$ index, of a graph G was introduced by Vukičević and Furtula [16]. Further studies on GA index can be found in [17–19].

Definition 5. Let G be a graph and let $e = uv$ be an edge of G ; then, $GA(G) = \sum_{e=uv \in E(G)} (2\sqrt{d_u d_v}/d_u + d_v)$.

The fifth geometric-arithmetic index, $GA_5(G)$, was introduced by Graovac et al. [20] in 2011.

Definition 6. For a graph G , the fifth geometric-arithmetic index is defined as $GA_5(G) = \sum_{uv \in E(G)} (2\sqrt{S_u S_v}/(S_u + S_v))$, where S_u is the sum of the degrees of all neighbors of the vertex u in G , similarly S_v .

2. Main Results

Theorem 7. The atom-bond connectivity index of Graphene with “ t ” rows of benzene rings and “ s ” benzene rings in each row is given by

$$ABC(G) = \begin{cases} \frac{(12 + 2\sqrt{2})s + (6 - 2\sqrt{2})}{3\sqrt{2}}, & \text{if } t = 1, \\ \frac{(12 - 4\sqrt{2})s + (9 - 2\sqrt{2})t + 6\sqrt{2}ts - 2\sqrt{2}}{3\sqrt{2}}, & \text{if } t \neq 1. \end{cases} \quad (1)$$

Proof. Consider a Graphene with “ t ” rows and “ s ” benzene rings in each row. Let $m_{i,j}$ denote the number of edges connecting the vertices of degrees d_i and d_j . Two-dimensional structure of Graphene (as shown in Figure 1) contains only $m_{2,2}$, $m_{2,3}$, and $m_{3,3}$ edges. In Figure 1 $m_{2,2}$ and $m_{3,3}$ edges are colored in green and red, respectively. The number of $m_{2,2}$, $m_{2,3}$, and $m_{3,3}$ edges in each row is mentioned in Table 1.

∴ Graphene contains $m_{2,2} = (t + 4)$ edges, $m_{2,3} = (4s + 2t - 4)$ edges, and $m_{3,3} = (3ts - 2s - t - 1)$ edges.

Case 1. The atom-bond connectivity index of Graphene for $t \neq 1$ is

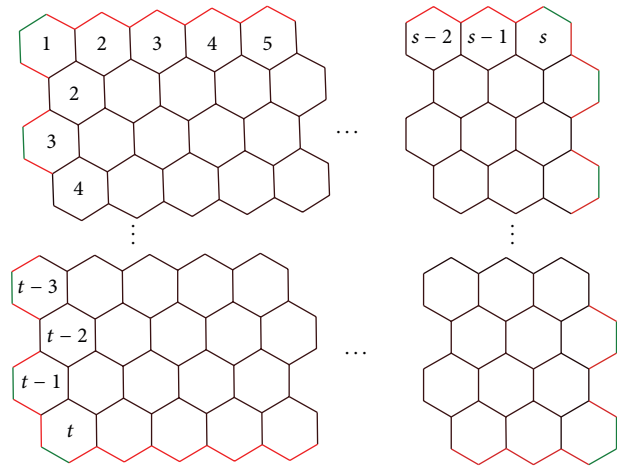


FIGURE 1

TABLE 1

Row	$m_{2,2}$	$m_{2,3}$	$m_{3,3}$
1	3	$2s$	$3s - 2$
2	1	2	$3s - 1$
3	1	2	$3s - 1$
4	1	2	$3s - 1$
⋮	⋮	⋮	⋮
t	3	$2s$	$s - 1$
Total	$t + 4$	$4s + 2t - 4$	$3ts - 2s - t - 1$

$$\begin{aligned} ABC(G) &= \sum_{uv \in E} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}} \\ &= m_{2,2} \sqrt{\frac{2 + 2 - 2}{2 \cdot 2}} + m_{2,3} \sqrt{\frac{2 + 3 - 2}{2 \cdot 3}} \\ &\quad + m_{3,3} \sqrt{\frac{3 + 3 - 2}{3 \cdot 3}} \\ &= (t + 4) \left(\frac{1}{\sqrt{2}} \right) + (4s + 2t - 4) \left(\frac{1}{\sqrt{2}} \right) \\ &\quad + (3ts - 2s - t - 1) \left(\frac{2}{3} \right) \\ &= \left(\frac{1}{\sqrt{2}} \right) (t + 4 + 4s + 2t - 4) \\ &\quad + (6ts - 4s - 2t - 2) \left(\frac{1}{3} \right) \\ &= \left(\frac{1}{\sqrt{2}} \right) (3t + 4s) + (6ts - 4s - 2t - 2) \left(\frac{1}{3} \right) \\ &= \frac{9t + 12s + 6\sqrt{2}ts - 4\sqrt{2}s - 2\sqrt{2}t - 2\sqrt{2}}{3\sqrt{2}} \end{aligned}$$

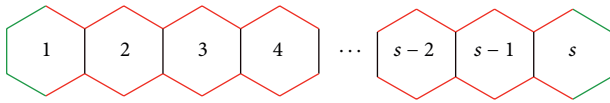


FIGURE 2

∴ ABC(G)

$$= \frac{(12 - 4\sqrt{2})s + (9 - 2\sqrt{2})t + 6\sqrt{2}ts - 2\sqrt{2}}{3\sqrt{2}}, \quad t \neq 1. \tag{2}$$

Case 2. For $t = 1, m_{2,2} = 6, m_{2,3} = (4s - 4),$ and $m_{3,3} = (s - 1)$ edges as shown in Figure 2:

$$\begin{aligned} \text{ABC}(G) &= \sum_{uv \in E} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}} \\ &= m_{2,2} \sqrt{\frac{2+2-2}{2 \cdot 2}} + m_{2,3} \sqrt{\frac{2+3-2}{2 \cdot 3}} \end{aligned}$$

$$\begin{aligned} &+ m_{3,3} \sqrt{\frac{3+3-2}{3 \cdot 3}} \\ &= 6 \left(\frac{1}{\sqrt{2}} \right) + (4s - 4) \left(\frac{1}{\sqrt{2}} \right) \\ &+ (s - 1) \left(\frac{2}{3} \right) \\ &= (6 + 4s - 4) \left(\frac{1}{\sqrt{2}} \right) + (s - 1) \left(\frac{2}{3} \right) \\ &= (4s + 2) \left(\frac{1}{\sqrt{2}} \right) + (s - 1) \left(\frac{2}{3} \right) \\ &= \frac{12s + 6 + 2\sqrt{2}s - 2\sqrt{2}}{3\sqrt{2}} \end{aligned}$$

$$\therefore \text{ABC}(G) = \frac{(12 + 2\sqrt{2})s + (6 - 2\sqrt{2})}{3\sqrt{2}}, \quad \text{for } t = 1. \tag{3}$$

□

Theorem 8. The fourth atom-bond connectivity index of Graphene is

$$\text{ABC}_4(G) = \begin{cases} \frac{3\sqrt{6}}{2}, & \text{if } t = 1, s = 1, \\ 2.541937s + 1.140265, & \text{if } t = 1, s > 1, \\ (1.217295)t + (1.212097)s + (1.333333)ts - (0.088070), & \text{if } t \neq 1. \end{cases} \tag{4}$$

Proof. Let $e_{i,j}$ denote the number of edges of Graphene with $i = S_u$ and $j = S_v$. It is easy to see that the summation of degrees of edge endpoints of Graphene has nine edge types $e_{4,5}, e_{5,5}, e_{5,7}, e_{5,8}, e_{6,7}, e_{7,9}, e_{8,8}, e_{8,9},$ and $e_{9,9}$ that are enumerated in Table 2. For convenience these edge types are colored by grey, yellow, red, purple, blue, green, lightblue, brown, and black, respectively, as shown in Figure 3.

Case 1. The fourth atom-bond connectivity index of Graphene for $t \neq 1$ is

$$\begin{aligned} \text{ABC}_4(G) &= \sum_{uv \in E(G)} \sqrt{\frac{S_u + S_v - 2}{S_u S_v}} = e_{4,5} \left(\sqrt{\frac{7}{20}} \right) \\ &+ e_{5,5} \left(\frac{\sqrt{8}}{5} \right) + e_{5,7} \left(\sqrt{\frac{2}{7}} \right) + e_{5,8} \left(\sqrt{\frac{11}{40}} \right) \\ &+ e_{6,7} \left(\sqrt{\frac{11}{42}} \right) + e_{7,9} \left(\sqrt{\frac{14}{63}} \right) + e_{8,8} \left(\frac{\sqrt{14}}{8} \right) \\ &+ e_{9,8} \left(\sqrt{\frac{15}{72}} \right) + e_{9,9} \left(\frac{4}{9} \right) = 4 \left(\sqrt{\frac{7}{20}} \right) + t \left(\frac{\sqrt{8}}{5} \right) \end{aligned}$$

$$\begin{aligned} &+ 8 \left(\sqrt{\frac{2}{7}} \right) + (2t - 4) \left(\sqrt{\frac{11}{40}} \right) + (4s - 8) \left(\sqrt{\frac{11}{42}} \right) \\ &+ 2s \left(\sqrt{\frac{14}{63}} \right) + (t - 2) \left(\frac{\sqrt{14}}{8} \right) + (2t - 4) \left(\sqrt{\frac{15}{72}} \right) \\ &+ (3ts - 4s - 4t + 5) \left(\frac{4}{9} \right) = 4 \left(\frac{\sqrt{7}}{2\sqrt{5}} \right) + t \left(\frac{\sqrt{8}}{5} \right) \\ &+ 8 \left(\sqrt{\frac{2}{7}} \right) + 2(t - 2) \left(\frac{\sqrt{11}}{2\sqrt{10}} \right) + (4s - 8) \left(\sqrt{\frac{11}{42}} \right) \\ &+ 2s \left(\frac{\sqrt{2}}{3} \right) + (t - 2) \left(\frac{\sqrt{14}}{8} \right) + (2t - 4) \left(\frac{\sqrt{5}}{2\sqrt{6}} \right) \\ &+ (3ts - 4s - 4t + 5) \left(\frac{4}{9} \right) = \left(\frac{\sqrt{8}}{5} + \sqrt{\frac{11}{10}} + \frac{\sqrt{14}}{8} \right. \\ &+ \left. \sqrt{\frac{5}{6}} - \frac{16}{9} \right) t + \left(4\sqrt{\frac{11}{42}} + \frac{2\sqrt{2}}{3} - \frac{16}{9} \right) s + \frac{4}{3} ts \\ &+ \left(2\sqrt{\frac{7}{5}} + 8\sqrt{\frac{2}{7}} - 2\sqrt{\frac{11}{10}} - 8\sqrt{\frac{11}{42}} - \frac{\sqrt{14}}{4} - 2\sqrt{\frac{5}{6}} \right) \end{aligned}$$

TABLE 2

Rows	$e_{4,5}$	$e_{5,5}$	$e_{5,7}$	$e_{5,8}$	$e_{6,7}$	$e_{7,9}$	$e_{8,8}$	$e_{8,9}$	$e_{9,9}$
1	2	1	3	1	$2s - 4$	s	0	1	$2s - 3$
2	0	1	1	1	0	0	1	2	$3s - 4$
3	0	1	0	2	0	0	1	2	$3s - 4$
4	0	1	0	2	0	0	1	2	$3s - 4$
\vdots	\vdots	\vdots	\vdots	\vdots	\vdots	\vdots	\vdots	\vdots	\vdots
$t - 2$	0	1	0	2	0	0	1	2	$3s - 4$
$t - 1$	0	1	1	1	0	0	1	1	$3s - 4$
t	2	1	3	1	$2s - 4$	s	0	0	0
Total	4	t	8	$2t - 4$	$4s - 8$	$2s$	$t - 2$	$2t - 4$	$3ts - 4s - 4t + 5$

$$+ \frac{20}{9}),$$

$$ABC_4(G) = (1.217295)t + (1.212097)s + (1.333333) \cdot ts - (0.088070), \quad t \neq 1.$$

(5)

Case 2. For $t = 1$ and $s > 1$, Graphene has five types of edges, namely, $e_{4,4}$, $e_{4,5}$, $e_{5,7}$, $e_{6,7}$, and $e_{7,7}$. These edges are colored in orange, pink, red, blue, and lavender, respectively, as shown in Figure 4. The number of edges of these types is shown in Table 3:

$$\begin{aligned} ABC_4(G) &= e_{4,4} \left(\frac{\sqrt{6}}{4} \right) + e_{4,5} \left(\sqrt{\frac{7}{20}} \right) + e_{5,7} \left(\sqrt{\frac{2}{7}} \right) \\ &\quad + e_{6,7} \left(\sqrt{\frac{11}{42}} \right) + e_{7,7} \left(\frac{\sqrt{12}}{7} \right) \\ &= 2 \left(\frac{\sqrt{6}}{4} \right) + 4 \left(\sqrt{\frac{7}{20}} \right) + 4 \left(\sqrt{\frac{2}{7}} \right) \\ &\quad + (4s - 8) \sqrt{\frac{11}{42}} + (s - 1) \left(\frac{\sqrt{12}}{7} \right) \\ &= \left(4\sqrt{\frac{11}{42}} + \frac{\sqrt{12}}{7} \right) s \\ &\quad + \left(\frac{\sqrt{6}}{2} + 4\sqrt{\frac{7}{20}} + 4\sqrt{\frac{2}{7}} - 8\sqrt{\frac{11}{42}} - \frac{\sqrt{12}}{7} \right) \end{aligned}$$

$$\therefore ABC_4(G) = (2.541937)s + 1.140265.$$

Case 3. For $t = 1$ and $s = 1$, we have only 6 edges of the type $e_{4,4}$ as shown in Figure 5:

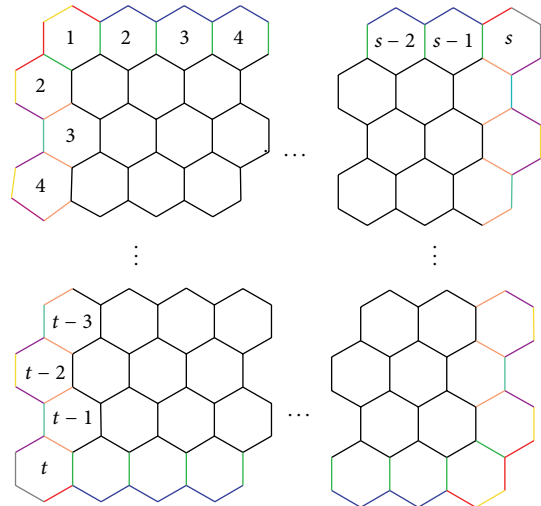


FIGURE 3

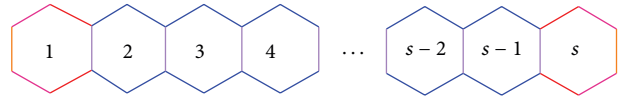


FIGURE 4

$$ABC_4(G) = e_{4,4} \left(\frac{\sqrt{6}}{4} \right) = \frac{6\sqrt{6}}{4},$$

(7)

$$\therefore ABC_4(G) = \frac{3\sqrt{6}}{2}.$$

□

Theorem 9. The Randic connectivity index of Graphene is

$$\chi(G) = \begin{cases} \frac{(2\sqrt{6} + 1)s + (8 - 2\sqrt{6})}{3}, & \text{if } t = 1, \\ \frac{(1 + 2\sqrt{6})t - 4(1 - \sqrt{6})s + 6ts + (10 - 4\sqrt{6})}{6}, & \text{if } t \neq 1. \end{cases} \quad (8)$$

Proof.

Case 1. For $t \neq 1$,

$$\begin{aligned} \chi(G) &= \sum_{e=uv \in E(G)} \frac{1}{\sqrt{d_u d_v}} \\ &= m_{2,2} \left(\frac{1}{\sqrt{2.2}} \right) + m_{2,3} \left(\frac{1}{\sqrt{3.2}} \right) + m_{3,3} \left(\frac{1}{\sqrt{3.3}} \right) \end{aligned}$$



FIGURE 5

$$\begin{aligned}
 &= (t+4) \left(\frac{1}{2}\right) + (4s+2t-4) \left(\frac{1}{\sqrt{6}}\right) \\
 &\quad + (3ts-2s-t-1) \left(\frac{1}{3}\right) \\
 &= \left(\frac{3t+12+6ts-4s-2t-2}{6}\right) \\
 &\quad + (4s+2t-4) \left(\frac{1}{\sqrt{6}}\right) \\
 &= \left(\frac{t-4s+6ts+10}{6}\right) + (4s+2t-4) \left(\frac{1}{\sqrt{6}}\right) \\
 &= \frac{(t-4s+6ts+10) + \sqrt{6}(4s+2t-4)}{6} \\
 &= \frac{t-4s+6ts+10+4\sqrt{6}s+2\sqrt{6}t-4\sqrt{6}}{6} \\
 \therefore \chi(G) &= \frac{(1+2\sqrt{6})t-4(1-\sqrt{6})s+6ts+(10-4\sqrt{6})}{6}.
 \end{aligned} \tag{9}$$

Case 2. For $t = 1$,

$$\begin{aligned}
 \chi(G) &= \sum_{e=uv \in E(G)} \frac{1}{\sqrt{d_u d_v}} \\
 &= m_{2,2} \left(\frac{1}{\sqrt{2.2}}\right) + m_{2,3} \left(\frac{1}{\sqrt{3.2}}\right) \\
 &\quad + m_{3,3} \left(\frac{1}{\sqrt{3.3}}\right) \\
 &= 6 \left(\frac{1}{2}\right) + (4s-4) \left(\frac{1}{\sqrt{6}}\right) + (s-1) \left(\frac{1}{3}\right) \\
 &= 3 + (4s-4) \left(\frac{1}{\sqrt{6}}\right) + (s-1) \left(\frac{1}{3}\right) \\
 &= \frac{9\sqrt{6} + 12s - 12 + \sqrt{6}s - \sqrt{6}}{3\sqrt{6}} \\
 \therefore \chi(G) &= \frac{(2\sqrt{6}+1)s + (8-2\sqrt{6})}{3}.
 \end{aligned} \tag{10}$$

□

Theorem 10. The Sum connectivity index of Graphene is

$$S(G) = \begin{cases} \frac{(\sqrt{5} + 4\sqrt{6})s + (3\sqrt{30} - \sqrt{5} - 4\sqrt{6})}{\sqrt{30}}, & \text{if } t = 1, \\ \frac{(\sqrt{30} + 4\sqrt{6} - 2\sqrt{5})t + (8\sqrt{6} - 4\sqrt{5})s + 6\sqrt{5}ts + (4\sqrt{30} - 8\sqrt{6} - 2\sqrt{5})}{2\sqrt{30}}, & \text{if } t \neq 1. \end{cases} \tag{11}$$

Proof.

Case 1. For $t \neq 1$,

$$\begin{aligned}
 S(G) &= \sum_{e=uv \in E(G)} \frac{1}{\sqrt{d_u + d_v}} = m_{2,2} \left(\frac{1}{\sqrt{2+2}}\right) + m_{2,3} \left(\frac{1}{\sqrt{2+3}}\right) + m_{3,3} \left(\frac{1}{\sqrt{3+3}}\right) \\
 &= (t+4) \left(\frac{1}{2}\right) + (4s+2t-4) \left(\frac{1}{\sqrt{5}}\right) + (3ts-2s-t-1) \left(\frac{1}{\sqrt{6}}\right) \\
 &= \frac{t\sqrt{30} + 4\sqrt{30} + 8\sqrt{6}s + 4\sqrt{6}t - 8\sqrt{6} + 6\sqrt{5}ts - 4\sqrt{5}s - 2\sqrt{5}t - 2\sqrt{5}}{2\sqrt{30}} \\
 \therefore S(G) &= \frac{(\sqrt{30} + 4\sqrt{6} - 2\sqrt{5})t + (8\sqrt{6} - 4\sqrt{5})s + 6\sqrt{5}ts + (4\sqrt{30} - 8\sqrt{6} - 2\sqrt{5})}{2\sqrt{30}}, \quad t \neq 1.
 \end{aligned} \tag{12}$$

TABLE 3

Number of benzene rings (s)	e _{4,4}	e _{4,5}	e _{5,7}	e _{6,7}	e _{7,7}
2	2	4	4	0	1
3	2	4	4	4	2
4	2	4	4	8	3
5	2	4	4	12	4
⋮	⋮	⋮	⋮	⋮	⋮
s - 1	2	4	4	4s - 12	s - 2
s	2	4	4	4s - 8	s - 1

Case 2. For t = 1,

$$\begin{aligned}
 S(G) &= \sum_{e=uv \in E(G)} \frac{1}{\sqrt{d_u + d_v}} \\
 &= m_{2,2} \left(\frac{1}{2}\right) + m_{2,3} \left(\frac{1}{\sqrt{5}}\right) + m_{3,3} \left(\frac{1}{\sqrt{6}}\right) \\
 &= 6 \left(\frac{1}{2}\right) + (4s - 4) \left(\frac{1}{\sqrt{5}}\right) + (s - 1) \left(\frac{1}{\sqrt{6}}\right) \\
 &= 3 + (4s - 4) \left(\frac{1}{\sqrt{5}}\right) + (s - 1) \left(\frac{1}{\sqrt{6}}\right) \tag{13} \\
 &= \left(\frac{3\sqrt{6} + (s - 1)}{\sqrt{6}}\right) + \left(\frac{4s - 4}{\sqrt{5}}\right) \\
 &= \frac{3\sqrt{30} + \sqrt{5}s - \sqrt{5} + 4\sqrt{6}s - 4\sqrt{6}}{\sqrt{30}} \\
 \therefore S(G) &= \frac{(\sqrt{5} + 4\sqrt{6})s + (3\sqrt{30} - \sqrt{5} - 4\sqrt{6})}{\sqrt{30}}.
 \end{aligned}$$

□

Theorem 11. The geometric-arithmetic index of Graphene with “t” rows and “s” benzene rings in each row is given by

$$GA(G) = \begin{cases} \frac{(5 + 8\sqrt{6})s + (25 - 8\sqrt{6})}{5}, & \text{if } t = 1, \\ \frac{(8\sqrt{6} - 10)s + 4\sqrt{6}t + 15ts + (15 - 8\sqrt{6})}{5}, & \text{if } t \neq 1. \end{cases} \tag{14}$$

Proof.

Case 1. For t ≠ 1,

$$\begin{aligned}
 GA(G) &= \sum_{e=uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v} \\
 &= m_{2,2} \left(\frac{2\sqrt{2.2}}{2 + 2}\right) + m_{2,3} \left(\frac{2\sqrt{2.3}}{2 + 3}\right)
 \end{aligned}$$

$$\begin{aligned}
 &+ m_{3,3} \left(\frac{2\sqrt{3.3}}{3 + 3}\right) \\
 &= m_{2,2} + m_{2,3} \left(\frac{2\sqrt{6}}{2 + 3}\right) + m_{3,3} \left(\frac{2(3)}{6}\right) \\
 &= m_{2,2} + m_{2,3} \left(\frac{2\sqrt{6}}{5}\right) + m_{3,3} \\
 &= (t + 4) + (4s + 2t - 4) \left(\frac{2\sqrt{6}}{5}\right) \\
 &\quad + (3ts - 2s - t - 1) \\
 &= \frac{(8\sqrt{6} - 10)s + 4\sqrt{6}t + 15ts + (15 - 8\sqrt{6})}{5},
 \end{aligned}$$

GA(G)

$$= \frac{(8\sqrt{6} - 10)s + 4\sqrt{6}t + 15ts + (15 - 8\sqrt{6})}{5},$$

t ≠ 1. (15)

Case 2. For t = 1,

$$\begin{aligned}
 GA(G) &= \sum_{e=uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v} \\
 &= m_{2,2} \left(\frac{2\sqrt{2.2}}{2 + 2}\right) + m_{2,3} \left(\frac{2\sqrt{2.3}}{2 + 3}\right) \\
 &\quad + m_{3,3} \left(\frac{2\sqrt{3.3}}{3 + 3}\right) \\
 &= 6(1) + (4s - 4) \left(\frac{2\sqrt{6}}{5}\right) + (s - 1)(1) \tag{16} \\
 &= (s + 5) + (8s - 8) \left(\frac{\sqrt{6}}{5}\right) \\
 &= \frac{5s + 25 + 8\sqrt{6}s - 8\sqrt{6}}{5} \\
 GA(G) &= \frac{(5 + 8\sqrt{6})s + (25 - 8\sqrt{6})}{5}, \quad \text{for } t = 1.
 \end{aligned}$$

□

Theorem 12. The fifth geometric-arithmetic index of Graphene is

$$GA_5(G) = \begin{cases} 6, & \text{if } t = 1, s = 1, \\ (4.988148)s + 0.942989, & \text{if } t = 1, s > 1, \\ (1.942554)t + (1.972462)s + 3ts - 0.998066, & \text{if } t \neq 1. \end{cases} \tag{17}$$

Proof.

Case 1. For $t \neq 1$,

$$\begin{aligned}
 GA_5(G) &= \sum_{uv \in E(G)} \frac{2\sqrt{S_u S_v}}{S_u + S_v} = e_{4,5} \left(\frac{4\sqrt{5}}{9} \right) + e_{5,5} (1) \\
 &+ e_{5,7} \left(\frac{\sqrt{35}}{6} \right) + e_{5,8} \left(\frac{2\sqrt{40}}{13} \right) + e_{6,7} \left(\frac{2\sqrt{42}}{13} \right) \\
 &+ e_{7,9} \left(\frac{3\sqrt{7}}{8} \right) + e_{8,8} (1) + e_{9,8} \left(\frac{12\sqrt{2}}{17} \right) + e_{9,9} (1) \\
 &= 4 \left(\frac{4\sqrt{5}}{9} \right) + t(1) + 8 \left(\frac{\sqrt{35}}{6} \right) + (2t - 4) \\
 &\cdot \left(\frac{2\sqrt{40}}{13} \right) + (4s - 8) \left(\frac{2\sqrt{42}}{13} \right) + 2s \left(\frac{3\sqrt{7}}{8} \right) + (t \\
 &- 2)(1) + (2t - 4) \left(\frac{12\sqrt{2}}{17} \right) + (3ts - 4s - 4t + 5) \\
 &\cdot (1) = 16 \left(\frac{\sqrt{5}}{9} \right) + t + 4 \left(\frac{\sqrt{35}}{3} \right) + (4t - 8) \\
 &\cdot \left(\frac{\sqrt{40}}{13} \right) + (8s - 16) \left(\frac{\sqrt{42}}{13} \right) + \left(\frac{3\sqrt{7}}{4} \right) s + (t \\
 &- 2) + (24t - 48) \left(\frac{\sqrt{2}}{17} \right) + (3ts - 4s - 4t + 5) \\
 &= \left[1 + 4 \left(\frac{\sqrt{40}}{13} \right) + 1 + 24 \left(\frac{\sqrt{2}}{17} \right) - 4 \right] t \\
 &+ \left[8 \left(\frac{\sqrt{42}}{13} \right) + 3 \left(\frac{\sqrt{7}}{4} \right) - 4 \right] s + 3ts \\
 &+ \left[16 \left(\frac{\sqrt{5}}{9} \right) + 4 \left(\frac{\sqrt{35}}{3} \right) - 8 \left(\frac{\sqrt{40}}{13} \right) \right. \\
 &\left. - 16 \left(\frac{\sqrt{42}}{13} \right) - 2 - 48 \left(\frac{\sqrt{2}}{17} \right) + 5 \right] = \left[\frac{4\sqrt{40}}{13} \right. \\
 &\left. + \frac{24\sqrt{2}}{17} - 2 \right] t + \left[\frac{8\sqrt{42}}{13} + \frac{3\sqrt{7}}{4} - 4 \right] s + 3ts \\
 &+ \left[\frac{16\sqrt{5}}{9} + \frac{4\sqrt{35}}{3} - \frac{8\sqrt{40}}{13} - \frac{16\sqrt{42}}{13} - \frac{48\sqrt{2}}{17} \right. \\
 &\left. + 3 \right]. \\
 \therefore GA_5(G) &= (1.942554)t + (1.972462)s + 3ts \\
 &- 0.998066, \quad t \neq 1.
 \end{aligned}$$

Case 2. For $t = 1$ and $s > 1$, Graphene has five types of edges, namely, $e_{4,4}$, $e_{4,5}$, $e_{5,7}$, $e_{6,7}$, and $e_{7,7}$ as shown in Figure 4:

$$\begin{aligned}
 GA_5(G) &= e_{4,4} (1) + e_{4,5} \left(\frac{4\sqrt{5}}{9} \right) + e_{5,7} \left(\frac{\sqrt{35}}{6} \right) \\
 &+ e_{6,7} \left(\frac{2\sqrt{42}}{13} \right) + e_{7,7} (1) \\
 &= 2(1) + 4 \left(\frac{4\sqrt{5}}{9} \right) + 4 \left(\frac{\sqrt{35}}{6} \right) \\
 &+ (4s - 8) \left(\frac{2\sqrt{42}}{13} \right) + (s - 1)(1) \\
 &= \left(8 \frac{\sqrt{42}}{13} + 1 \right) s \\
 &+ \left(2 + 16 \frac{\sqrt{5}}{9} + 4 \frac{\sqrt{35}}{6} - 16 \frac{\sqrt{42}}{13} - 1 \right) \\
 &= \left(\frac{8\sqrt{42}}{13} + 1 \right) s \\
 &+ \left(\frac{16\sqrt{5}}{9} + \frac{4\sqrt{35}}{6} - \frac{16\sqrt{42}}{13} + 1 \right) \\
 \therefore GA_5(G) &= (4.988148)s + 0.942989.
 \end{aligned} \tag{19}$$

Case 3. For $t = 1$ and $s = 1$, we have only 6 edges of the type $e_{4,4}$ as shown in Figure 5:

$$\begin{aligned}
 GA_5(G) &= e_{4,4} (1) = 6(1) \\
 \therefore GA_5(G) &= 6.
 \end{aligned} \tag{20}$$

□

3. Conclusion

The problem of finding the general formula for ABC index, ABC_4 index, Randic connectivity index, Sum connectivity index, GA index, and GA_5 index of Graphene is solved here analytically without using computers.

Conflict of Interests

The authors declare that there is no conflict of interests regarding the publication of this paper.

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