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Some topological indices of fluorographene

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Abstract. ABC index, ABC_4 index, Randić connectivity index, sum connectivity index, GA index, GA_5 index, harmonic index, second zagreb index and AZI of fluorographene are computed.

Keywords. vertex degree, neighborhood vertex, topological index.

1 Introduction

Graphene is a potential candidate material used in building of next-generation nanoelectronic and optoelectronic devices due to its unique properties, such as optical, mechanical flexibility and high carrier mobility [21]. Layer of graphene is typically used to build field effective transistors (FETs) on oxidized silicon wafers (insulator). Graphene oxide (GO), one type of graphene-based insulator, is often applied as a gate dielectric material in electronic devices, such as resistive random-access memory (RRAM) and thin film transistors. However, GC is having major drawbacks in having the low thermal stability, this reduces its dielectric resistivity. Thus, it is of great challenge to find new suitable dielectric materials for use in the fabrication of nano-scale devices. The exposure of graphene to atomic flourine(F) results in a stoichiometric derivative that is an excellent insulator with high thermal and chemical stability results in fluorographene. Fluorinated graphene(FG), one of the thinnest insulators known, is an attractive 2D material. The optical and electrical properties of FG are radically different from those of graphene, graphene oxide and hydrogenated graphene, due to a wide gap opened in the electronic spectrum. Mechanically, FG is remarkably stiff but stretchable, similar to its record-breaking parent, graphene.

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Topological indices are numbers associated with molecular graphs for the purpose of allowing quantitative structure activity/property/toxicity relationships. 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, Randić connectivity index, geometric-arithmetic connectivity index, fifth geometric-arithmetic connectivity index, harmonic index, second zagreb index and augmented zagreb index of Fluorographene.

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 introduced by Estrada et al. [7] 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 [8]. 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 [1,29]. For further results on ABC index of trees, see the papers [14, 19, 28, 30] and the references cited therein.

Definition 1.1. ([7]) *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*

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{(d_u + d_v - 2)}{d_u d_v}}.$$

The fourth atom-bond connectivity index, $ABC_4(G)$ index, was introduced by Ghorbani and Hosseinzadeh [16] in 2010. Further studies on $ABC_4(G)$ index can be found in [10, 11].

Definition 1.2. ([16]) *Let G be a graph, then the fourth atom-bond connectivity index of G is defined as*

$$ABC_4(G) = \sum_{uv \in E(G)} \sqrt{\frac{(S_u + S_v - 2)}{S_u S_v}},$$

where S_u is sum of the degrees of all neighbors 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 Randić index [24] denoted by $\chi(G)$ and it was introduced by Milan Randić in 1975. It provides a quantitative assessment of the branching of molecules.

Definition 1.3. ([24]) *For the graph G, Randić index is defined as*

$$\chi(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}.$$

Sum connectivity index belongs to a family of Randić like indices and it was introduced by Zhou and Trinajstić [31]. Further studies on Sum connectivity index can be found in [32].

Definition 1.4. ([31]) *For a graph (G), Sum connectivity index $S(G)$ is defined as*

$$S(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u + d_v}}.$$

The geometric-arithmetic index, $GA(G)$ index, of a graph G was introduced by Vukicević and Furtula in [25]. Further studies on GA index can be found in [2,5,17,27].

Definition 1.5. ([25]) *For a graph (G), geometric-arithmetic index $GA(G)$ is defined as*

$$GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}.$$

The fifth geometric-arithmetic index, $GA_5(G)$, was introduced by Graovać et al. [17] in 2011.

Definition 1.6. ([17]) *For a graph G, the fifth geometric-arithmetic index is defined as*

$$GA_5(G) = \sum_{uv \in E(G)} \frac{2\sqrt{S_u S_v}}{S_u + S_v},$$

where S_u is sum of the degrees of all neighbors of vertex u in G, similarly for S_v.

The harmonic index first appeared in [9]. Favaron et al. in [13] considered the relation between the harmonic index and the eigenvalues of graphs. The relation between harmonic index and chromatic number is found in [6]. For further results on harmonic index see the papers [23,33].

Definition 1.7. ([9]) *For a graph G, the harmonic index is defined as*

$$H(G) = \sum_{uv \in E(G)} \frac{2}{d_u + d_v}.$$

The first and second Zagreb index of a graph were first introduced by I. Gutman and N. Trinajstic in [18]. Some properties of the second zagreb index are found in [4]. The first Zagreb index, second Zagreb index, first Zagreb polynomial and second Zagreb polynomial of a family of hydrocarbon structures "Polycyclic Aromatic Hydrocarbons" (PAH) are found in [12]. For further results on Zagreb indices see the papers [22,26].

Definition 1.8. ([18]) *For a graph G, the second Zagreb index is defined as*

$$M_2(G) = \sum_{uv \in E(G)} d_u d_v.$$

The augmented Zagreb index (AZI) was first introduced by Furtula et al. in [15] and they showed that AZI index is a valuable predictive index in the study of the heat of formation in octanes and heptanes, whose prediction power is better than atom-bond connectivity index.

Definition 1.9. ([15]) *For a graph G, the augmented Zagreb index is defined as*

$$AZI(G) = \sum_{uv \in E(G)} \left(\frac{d_u d_v}{d_u + d_v - 2} \right)^3.$$

2 Main Results

Theorem 2.1. *The atom-bond connectivity index of fluorographene with t rows and s fluorine attached benzene rings in each row is given by*

$$ABC(G) = \begin{cases} \frac{1}{12}((11\sqrt{6} + 8\sqrt{15} + 3\sqrt{3})s + (13\sqrt{6} - 8\sqrt{15} - 12\sqrt{3} + 12)), & \text{if } t = 1; \\ 5.4397s + 2.9783t + 3.5692st - 0.62675, & \text{if } t \neq 1. \end{cases}$$

Proof. Consider a fluorographene with t rows and s fluorine attached 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 fluorographene (as shown in Figure 1) contains only $m_{1,3}, m_{3,3}, m_{3,4}$, $m_{4,4}$ and $m_{1,4}$ edges. In Figure 1. $m_{1,3}, m_{3,3}, m_{3,4}, m_{4,4}$ and $m_{1,4}$ edges are colored in blue, cyan, black, red and green, respectively. The number of $m_{1,3}, m_{3,3}, m_{3,4}, m_{4,4}$ and $m_{1,4}$ edges in each row is mentioned in Table 1. Therefore, fluorographene contains $m_{1,3} = 2(s + t + 1)$ edges, $m_{3,3} = t + 4$ edges, $m_{3,4} = 4s + 2t - 4$ edges, $m_{4,4} = 3st - 2s - t - 1$ edges and $m_{1,4} = 2(st - 1)$ edges.

Case 1: $t \neq 1$. The atom-bond connectivity index of fluorographene is

$$
\begin{aligned}
ABC(G) &= \sum_{uv \in E(G)} \sqrt{\frac{(d_u + d_v - 2)}{d_u d_v}} \\
&= m_{1,3}\sqrt{\frac{(1+3-2)}{1 \cdot 3}} + m_{3,3}\sqrt{\frac{(3+3-2)}{3 \cdot 3}} + m_{3,4}\sqrt{\frac{(3+4-2)}{3 \cdot 4}} \\
&+ m_{4,4}\sqrt{\frac{(4+4-2)}{4 \cdot 4}} + m_{1,4}\sqrt{\frac{(1+4-2)}{1 \cdot 4}} \\
&= 2(s+t+1)\sqrt{\frac{2}{3}} + (t+4)\sqrt{\frac{4}{9}} + (4s+2t-4)\sqrt{\frac{5}{12}} + (3st-2s-t-1)\sqrt{\frac{6}{16}} \\
&+ 2(st-1)\sqrt{\frac{3}{4}} \\
&= 5.4397s + 2.9783t + 3.5692st - 0.62675.
\end{aligned}
$$

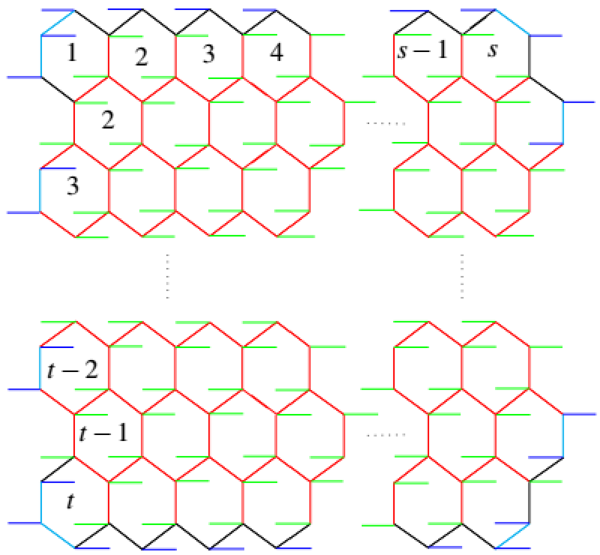

Figure 1. 2-dimensional structure of fluorographene.

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

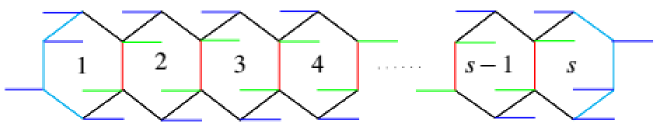

Figure 2. Edges of Case 2.

Row	$m_{1,3}$	$m_{3,3}$	$m_{3,4}$	$m_{4,4}$	$m_{1,4}$
1	$s+3$	3	$2s$	$3s-2$	$2s$ -1
2	2	1	2	$3s-1$	$2s$
3	2	1	2	$3s-1$	$2s$
4	2	1	2	$3s-1$	$2s$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
$(t-2)$	2	1	2	$3s-1$	$2s$
$(t-1)$	2	1	2	$3s-1$	$2s$
t	$s+3$	3	$2s$	$s-1$	$2s-1$
Total	$2(s+t+1)$	$t+4$	$4s+2t-4$	$3st-2s-t-1$	$2(st-1)$

Table 1. The number of edges in each row.

$$\begin{aligned}
ABC(G) &= \sum_{uv\in E(G)} \sqrt{\frac{(d_u+d_v-2)}{d_u d_v}} \\
&= m_{1,3}\sqrt{\frac{(1+3-2)}{1\cdot 3}} + m_{3,3}\sqrt{\frac{(3+3-2)}{3\cdot 3}} + m_{3,4}\sqrt{\frac{(3+4-2)}{3\cdot 4}} \\
&+ m_{4,4}\sqrt{\frac{(4+4-2)}{4\cdot 4}} + m_{1,4}\sqrt{\frac{(1+4-2)}{1\cdot 4}} \\
&= (2s+4)\sqrt{\frac{2}{3}} + 6\sqrt{\frac{4}{9}} + 4(s-1)\sqrt{\frac{5}{12}} + (s-1)\sqrt{\frac{6}{16}} + 2(s-1)\sqrt{\frac{3}{4}} \\
&= \frac{1}{12}((11\sqrt{6}+8\sqrt{15}+3\sqrt{3})s + (13\sqrt{6}-8\sqrt{15}-12\sqrt{3}+12)).
\end{aligned}$$

□

Theorem 2.2. *The fourth atom-bond connectivity index of fluorographene is*

$$ABC_4(G) = \begin{cases} \frac{4}{7}(\sqrt{42}+3\sqrt{3}), & \text{if } t=1, s=1; \\ 4.4164s - 2.2542, & \text{if } t=1,\ s>1; \\ 2.2128s + 2.2159t + 2.2047st - 1.6037, & \text{if } t \neq 1. \end{cases}$$

Proof. Let $e_{i,j}$ denote the number of edges of fluorographene with $i = S_u$ and $j = S_v$. Two-dimensional structure of fluorographene contains only $e_{3,7}$, $e_{3,8}$, $e_{3,9}$, $e_{4,11}$, $e_{4,12}$, $e_{4,13}$, $e_{7,8}$, $e_{8,8}$, $e_{8,11}$, $e_{8,12}$, $e_{9,11}$, $e_{11,13}$, $e_{12,12}$, $e_{12,13}$ and $e_{13,13}$ edges which are colored in apricot, brown, magenta, green, blue, orange, violet, gray, cyan, peach, black, yellow, maroon, sepia and red respectively as shown in Figure 3. The numbers of $e_{3,7}$,$e_{3,8}$,$e_{3,9}$,$e_{4,11}$,$e_{4,12}$, $e_{4,13}$, $e_{7,8}$, $e_{8,8}$, $e_{8,11}$, $e_{8,12}$, $e_{9,11}$, $e_{11,13}$, $e_{12,12}$, $e_{12,13}$ and $e_{13,13}$ edges in each row is mentioned in Table 2.

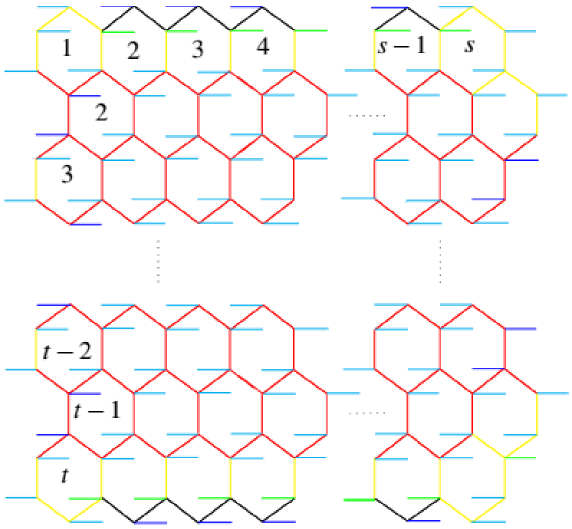

Figure 3. The color of edges in Theorem 2.2.

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

$$
\begin{aligned}
ABC_4(G) &= \sum_{uv\in E(G)} \sqrt{\frac{(S_u+S_v-2)}{S_uS_v}} \\
&= e_{3,7}\sqrt{\frac{(3+7-2)}{3\cdot 7}} + e_{3,8}\sqrt{\frac{(3+8-2)}{3\cdot 8}} + e_{3,9}\sqrt{\frac{(3+9-2)}{3\cdot 9}} \\
&+ e_{4,11}\sqrt{\frac{(4+11-2)}{4\cdot 11}} + e_{4,12}\sqrt{\frac{(4+12-2)}{4\cdot 12}} + e_{4,13}\sqrt{\frac{(4+13-2)}{4\cdot 13}} \\
&+ e_{7,8}\sqrt{\frac{(7+8-2)}{7\cdot 8}} + e_{8,8}\sqrt{\frac{(8+8-2)}{8\cdot 8}} + e_{8,11}\sqrt{\frac{(8+11-2)}{8\cdot 11}} \\
&+ e_{8,12}\sqrt{\frac{(8+12-2)}{8\cdot 12}} + e_{9,11}\sqrt{\frac{(9+11-2)}{9\cdot 11}} + e_{11,13}\sqrt{\frac{(11+13-2)}{11\cdot 13}} \\
&+ e_{12,12}\sqrt{\frac{(12+12-2)}{12\cdot 12}} + e_{12,13}\sqrt{\frac{(12+13-2)}{12\cdot 13}} + e_{13,13}\sqrt{\frac{(13+13-2)}{13\cdot 13}} \\
&= 2\sqrt{\frac{8}{21}} + 2(t+2)\sqrt{\frac{9}{24}} + 2(s-2)\sqrt{\frac{10}{27}} + 2s\sqrt{\frac{13}{22}} + 2(t-2)\sqrt{\frac{14}{48}} \\
&+ 2(t-1)(s-1)\sqrt{\frac{15}{52}} + 4\sqrt{\frac{13}{56}} + t\frac{\sqrt{14}}{8} + 8\sqrt{\frac{17}{88}} + 2(t-3)\sqrt{\frac{18}{96}} \\
&+ 4(s-2)\frac{\sqrt{18}}{3\sqrt{11}} + 2s\sqrt{\frac{22}{143}} + (t-2)\frac{\sqrt{22}}{12} + 2(t-3)\sqrt{\frac{23}{156}} \\
&+ (3st-4s-4t+5)\frac{\sqrt{24}}{13} \\
&= 2.2128s + 2.2159t + 2.2047st - 1.6037.
\end{aligned}
$$

Case 2: $t = 1$ and $s > 1$. Fluorographene contains only $e_{3,7} = 4$, $e_{3,8} = 4$, $e_{3,9} = 2(s-2)$, $e_{4,11} = 2(s-1)$, $e_{7,7} = 2$, $e_{7,8} = 4$, $e_{8,11} = 4$, $e_{9,11} = 4(s-2)$, and $e_{11,11} = s-1$, edges are colored

Row	$e_{3,7}$	$e_{3,8}$	$e_{3,9}$	$e_{4,11}$	$e_{4,12}$	$e_{4,13}$	$e_{7,8}$	$e_{8,8}$	$e_{8,11}$
1	1	4	$s-2$	s	-	$(s-1)$	2	1	4
2	-	2	-	-	2	$2(s-1)$	-	1	-
3	-	2	-	-	2	$2(s-1)$	-	1	-
4	-	2	-	-	2	$2(s-1)$	-	1	-
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
$(t-2)$	-	2	-	-	2	$2(s-1)$	-	1	-
$(t-1)$	-	2	-	-	2	$2(s-1)$	-	1	-
t	1	4	$s-2$	s	-	$s-1$	2	1	4
Total	2	$2(t+2)$	$2(s-2)$	$2s$	$2(t-2)$	$2(t-1)(s-1)$	4	t	8

Row	$e_{8,12}$	$e_{9,11}$	$e_{11,13}$	$e_{12,12}$	$e_{12,13}$	$e_{13,13}$
1	1	$2(s-2)$	s	-	1	$2s-3$
2	2	-	-	1	2	$3s-4$
3	2	-	-	1	2	$3s-4$
4	2	-	-	1	2	$3s-4$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
$(t-2)$	2	-	-	1	2	$3s-4$
$(t-1)$	2	-	-	1	2	$3s-4$
t	1	$2(s-2)$	s	-	1	-
Total	$2(t-3)$	$4(s-2)$	$2s$	$t-2$	$2(t-3)$	$3st-4s-4t+5$

Table 2. The number of edges in each row.

in blue, brown, magenta, green, gray, violet, cyan, black and red, respectively as shown in Figure 4.

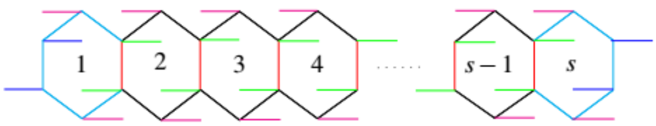

Figure 4. The color of edges in Theorem 2.2.

$$\begin{aligned}
ABC_4(G) &= \sum_{uv\in E(G)} \sqrt{\frac{(S_u+S_v-2)}{S_uS_v}} \\
&= e_{3,7}\sqrt{\frac{(3+7-2)}{3\cdot 7}} + e_{7,7}\sqrt{\frac{(7+7-2)}{7\cdot 7}} \\
&= 6\sqrt{\frac{8}{21}} + 6\sqrt{\frac{12}{49}} \\
&= \frac{4}{7}(\sqrt{42}+3\sqrt{3}).
\end{aligned}$$

□

Theorem 2.3. *The Randić connectivity index of fluorographene is*

$$\chi(G) = \begin{cases} \frac{1}{4\sqrt{3}}((16+5\sqrt{3})s + (8+3\sqrt{3})), & \text{if } t = 1; \\ \\ \frac{1}{12}((16\sqrt{3}-6)s + (12\sqrt{3}+1)t + 21st + 1), & \text{if } t \neq 1. \end{cases}$$

Proof. We consider the following cases:

Case 1: $t \neq 1$,

$$\begin{aligned} \chi(G) &= \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}} \\ &= m_{1,3}\frac{1}{\sqrt{1\cdot 3}} + m_{3,3}\frac{1}{\sqrt{3\cdot 3}} + m_{3,4}\frac{1}{\sqrt{3\cdot 4}} + m_{4,4}\frac{1}{\sqrt{4\cdot 4}} + m_{1,4}\frac{1}{\sqrt{1\cdot 4}} \\ &= 2(s+t+1)\frac{1}{\sqrt{3}} + (t+4)\frac{1}{3} + (4s+2t-4)\frac{1}{2\sqrt{3}} + (3st-2s-t-1)\frac{1}{4} + 2(st-1)\frac{1}{2} \\ &= \frac{1}{12}((16\sqrt{3}-6)s + (12\sqrt{3}+1)t + 21st + 1). \end{aligned}$$

Case 2: $t = 1$,

$$\begin{aligned} \chi(G) &= \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}} \\ &= m_{1,3}\frac{1}{\sqrt{1\cdot 3}} + m_{3,3}\frac{1}{\sqrt{3\cdot 3}} + m_{3,4}\frac{1}{\sqrt{3\cdot 4}} + m_{4,4}\frac{1}{\sqrt{4\cdot 4}} + m_{1,4}\frac{1}{\sqrt{1\cdot 4}} \\ &= (2s+4)\frac{1}{\sqrt{3}} + 6\frac{1}{3} + 4(s-1)\frac{1}{2\sqrt{3}} + (s-1)\frac{1}{4} + 2(s-1)\frac{1}{2} \\ &= \frac{1}{4\sqrt{3}}((16+5\sqrt{3})s + (8+3\sqrt{3})). \end{aligned}$$

□

Theorem 2.4. *The sum connectivity index of fluorographene is*

$$S(G) = \begin{cases} 3.7598s + 1.6897, & \text{if } t = 1; \\ \\ 1.8048s + 1.8106t + 1.9551st - 0.12685, & \text{if } t \neq 1. \end{cases}$$

Proof. We consider the following cases:

Case 1: $t \neq 1$,

$$
\begin{aligned}
S(G) &= \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u + d_v}} \\
&= m_{1,3}\frac{1}{\sqrt{1+3}} + m_{3,3}\frac{1}{\sqrt{3+3}} + m_{3,4}\frac{1}{\sqrt{3+4}} + m_{4,4}\frac{1}{\sqrt{4+4}} + m_{1,4}\frac{1}{\sqrt{1+4}} \\
&= 2(s+t+1)\frac{1}{2} + (t+4)\frac{1}{\sqrt{6}} + 2(2s+t-2)\frac{1}{\sqrt{7}} \\
&+ (3st-2s-t-1)\frac{1}{\sqrt{8}} + 2(st-1)\frac{1}{\sqrt{5}} \\
&= 1.8048s + 1.8106t + 1.9551st - 0.12685.
\end{aligned}
$$

Case 2: $t = 1$,

$$
\begin{aligned}
S(G) &= \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u + d_v}} \\
&= m_{1,3}\frac{1}{\sqrt{1+3}} + m_{3,3}\frac{1}{\sqrt{3+3}} + m_{3,4}\frac{1}{\sqrt{3+4}} + m_{4,4}\frac{1}{\sqrt{4+4}} + m_{1,4}\frac{1}{\sqrt{1+4}} \\
&= 2(s+2)\frac{1}{2} + 6\frac{1}{\sqrt{6}} + 4(s-1)\frac{1}{\sqrt{7}} + (s-1)\frac{1}{\sqrt{8}} + 2(s-1)\frac{1}{\sqrt{5}} \\
&= 3.7598s + 1.6897.
\end{aligned}
$$

□

Theorem 2.5. *The geometric-arithmetic index of fluorographene is*

$$
GA(G) = \begin{cases} \frac{1}{35}((115\sqrt{3}+91)s + (119 - 10\sqrt{3})), & \text{if } t = 1; \\ \frac{1}{35}((105\sqrt{3}+70)s + (75\sqrt{3}+70)t + 161st + (105\sqrt{3}+49)), & \text{if } t \neq 1. \end{cases}
$$

Proof. We consider the following cases:
Case 1: $t \neq 1$,

$$
\begin{aligned}
GA(G) &= \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v} \\
&= m_{1,3}\frac{2\sqrt{1\cdot 3}}{1+3} + m_{3,3}\frac{2\sqrt{3\cdot 3}}{3+3} + m_{3,4}\frac{2\sqrt{3\cdot 4}}{3+4} + m_{4,4}\frac{2\sqrt{4\cdot 4}}{4+4} + m_{1,4}\frac{2\sqrt{1\cdot 4}}{1+4} \\
&= 2(s+t+1)\frac{2\sqrt{3}}{4} + (t+4)\frac{6}{6} + 2(2s+t-2)\frac{4\sqrt{3}}{7} \\
&+ (3st-2s-t-1)\frac{8}{8} + 2(st-1)\frac{4}{5} \\
&= \frac{1}{35}((105\sqrt{3}+70)s + (75\sqrt{3}+70)t + 161st + (105\sqrt{3}+49)).
\end{aligned}
$$

Case 2: $t = 1$,

$$\begin{aligned} GA(G) &= \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v} \\ &= m_{1,3}\frac{2\sqrt{1\cdot 3}}{1+3} + m_{3,3}\frac{2\sqrt{3\cdot 3}}{3+3} + m_{3,4}\frac{2\sqrt{3\cdot 4}}{3+4} + m_{4,4}\frac{2\sqrt{4\cdot 4}}{4+4} + m_{1,4}\frac{2\sqrt{1\cdot 4}}{1+4} \\ &= 2(s+2)\frac{2\sqrt{3}}{4} + 6\frac{6}{6} + 4(S-1)\frac{4\sqrt{3}}{7} + (S-1)\frac{8}{8} + 2(s-1)\frac{4}{5} \\ &= \frac{1}{35}((115\sqrt{3}+91)s + (119 - 10\sqrt{3})). \end{aligned}$$

□

Theorem 2.6. *The fifth geometric-arithmetic index of fluorographene is*

$$GA_5(G) = \begin{cases} 6(1+\frac{\sqrt{21}}{5}), & \text{if } t = 1, s = 1; \\ 8.4809s + 2.977, & \text{if } t = 1,\ s > 1; \\ 73.534s + 3.7748t + 4.6967st - 4.7787, & \text{if } t \neq 1. \end{cases}$$

Proof. We consider the following cases:

Case 1: $t \neq 1$,

$$\begin{aligned} GA_5(G) &= \sum_{uv \in E(G)} \frac{2\sqrt{S_u S_v}}{S_u + S_v} \\ &= e_{3,7}\frac{2\sqrt{3\cdot 7}}{3+7} + e_{3,8}\frac{2\sqrt{3\cdot 8}}{3+8} + e_{3,9}\frac{2\sqrt{3\cdot 9}}{3+9} + e_{4,11}\frac{2\sqrt{4\cdot 11}}{4+11} + e_{4,12}\frac{2\sqrt{4\cdot 12}}{4+12} \\ &+ e_{4,13}\frac{2\sqrt{4\cdot 13}}{4+13} + e_{7,8}\frac{2\sqrt{7\cdot 8}}{7+8} + e_{8,8}\frac{2\sqrt{8\cdot 8}}{8+8} + e_{8,11}\frac{2\sqrt{8\cdot 11}}{8+11} + e_{8,12}\frac{2\sqrt{8\cdot 12}}{8+12} \\ &+ e_{9,11}\frac{2\sqrt{9\cdot 11}}{9+11} + e_{11,13}\frac{2\sqrt{11\cdot 13}}{11+13} + e_{12,12}\frac{2\sqrt{12\cdot 12}}{12+12} \\ &+ e_{12,13}\frac{2\sqrt{12\cdot 13}}{12+13} + e_{13,13}\frac{2\sqrt{13\cdot 13}}{13+13} \\ &= 2\frac{2\sqrt{21}}{10} + 2(t+2)\frac{4\sqrt{6}}{11} + 2(s-2)\frac{6\sqrt{3}}{12} + 2s\frac{4\sqrt{11}}{15} + 2(t-2)\frac{8\sqrt{3}}{16} \\ &+ 2(t-1)(s-1)\frac{4\sqrt{13}}{17} + 4\frac{4\sqrt{14}}{15} + t\frac{16}{16} + 8\frac{4\sqrt{22}}{19} + 2(t-3)\frac{8\sqrt{6}}{20} \\ &+ 4(s-2)\frac{6\sqrt{11}}{20} + 2s\frac{2\sqrt{143}}{24} + (t-2)\frac{24}{24} + 2(t-3)\frac{4\sqrt{39}}{25} + (3st - 4s - 4t + 5)\frac{26}{26} \\ &= 73.534s + 3.7748t + 4.6967st - 4.7787. \end{aligned}$$

Case 2: $t = 1$ and $s > 1$. We have $e_{3,7} = 4$, $e_{3,8} = 4$, $e_{3,9} = 2(s-2)$, $e_{4,11} = 2(s-1)$, $e_{7,7} = 2$,

$e_{7,8} = 4$, $e_{8,11} = 4$, $e_{9,11} = 4(s-2)$, $e_{11,11} = s-1$, as shown in Figure 4.

$$\begin{aligned} GA_5(G) &= \sum_{uv\in E(G)} \frac{2\sqrt{S_uS_v}}{S_u+S_v} \\ &= e_{3,7}\frac{2\sqrt{3\cdot 7}}{3+7} + e_{3,8}\frac{2\sqrt{3\cdot 8}}{3+8} + e_{3,9}\frac{2\sqrt{3\cdot 9}}{3+9} + e_{4,11}\frac{2\sqrt{4\cdot 11}}{4+11} + e_{7,7}\frac{2\sqrt{7\cdot 7}}{7+7} + e_{7,8}\frac{2\sqrt{7\cdot 8}}{7+8} \\ &+ e_{8,11}\frac{2\sqrt{8\cdot 11}}{8+11} + e_{9,11}\frac{2\sqrt{9\cdot 11}}{9+11} + e_{11,11}\frac{2\sqrt{11\cdot 11}}{11+11} \\ &= 4\frac{2\sqrt{21}}{10} + 4\frac{4\sqrt{6}}{11} + 2(s-2)\frac{6\sqrt{3}}{12} + 2(s-1)\frac{4\sqrt{11}}{15} + 2\frac{14}{14} \\ &+ 4\frac{4\sqrt{14}}{15} + 4\frac{4\sqrt{22}}{19} + 4(s-2)\frac{6\sqrt{11}}{20} + (s-1)\frac{22}{22} \\ &= 8.4809s + 2.977. \end{aligned}$$

Case 3: $t = 1$ and $s = 1$. We have $e_{3,7} = 6$, $e_{7,7} = 6$, as shown in Figure 5.

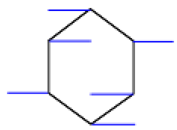

Figure 5. Case 3 in the proof of Theorem 2.6.

$$GA_5(G) = \sum_{uv\in E(G)} \frac{2\sqrt{S_uS_v}}{S_u+S_v} = e_{3,7}\frac{2\sqrt{3\cdot 7}}{3+7} + e_{7,7}\frac{2\sqrt{7\cdot 7}}{7+7} = 6\frac{2\sqrt{21}}{10} + 6\frac{14}{14} = 6(1+\frac{\sqrt{21}}{5}).$$

□

Theorem 2.7. *The harmonic index of fluorographene is*

$$H(G) = \begin{cases} \frac{1}{140}(447s+253), & \text{if } t=1; \\ 1.6429s + 1.6548t + 1.55st + 0.14048, & \text{if } t \neq 1. \end{cases}$$

Proof. We consider the following cases:

Case 1: $t \neq 1$,

$$\begin{aligned} H(G) &= \sum_{uv\in E(G)} \frac{2}{d_u+d_v} \\ &= m_{1,3}\frac{2}{1+3} + m_{3,3}\frac{2}{3+3} + m_{3,4}\frac{2}{3+4} + m_{4,4}\frac{2}{4+4} + m_{1,4}\frac{2}{1+4} \\ &= 2(s+t+1)\frac{2}{4} + (t+4)\frac{2}{6} + 2(2s+t-2)\frac{2}{7} + (3st-2s-t-1)\frac{2}{8} + 2(st-1)\frac{2}{5} \\ &= 1.6429s + 1.6548t + 1.55st + 0.14048. \end{aligned}$$

Case 2: $t = 1$,

$$\begin{aligned}
H(G) &= \sum_{uv \in E(G)} \frac{2}{d_u + d_v} \\
&= m_{1,3}\frac{2}{1+3} + m_{3,3}\frac{2}{3+3} + m_{3,4}\frac{2}{3+4} + m_{4,4}\frac{2}{4+4} + m_{1,4}\frac{2}{1+4} \\
&= 2(s+2)\frac{2}{4} + 6\frac{2}{6} + 4(s-1)\frac{2}{7} + (s-1)\frac{2}{8} + 2(s-1)\frac{2}{5} \\
&= \frac{1}{140}(447s + 253).
\end{aligned}$$

□

Theorem 2.8. *The second Zagreb index of fluorographene is*

$$M_2(G) = \begin{cases} 6(13s-1), & \text{if } t = 1; \\ 22s + 23t + 52st - 30, & \text{if } t \neq 1. \end{cases}$$

Proof. We consider the following cases:

Case 1: $t \neq 1$,

$$\begin{aligned}
M_2(G) &= \sum_{uv \in E(G)} d_u d_v \\
&= m_{1,3}(1 \cdot 3) + m_{3,3}(3 \cdot 3) + m_{3,4}(3 \cdot 4) + m_{4,4}(4 \cdot 4) + m_{1,4}(1 \cdot 4) \\
&= 2(s+t+1)3 + (t+4)9 + 2(2s+t-2)12 + (3st - 2s - t - 1)16 + 2(st-1)4 \\
&= 22s + 23t + 52st - 30.
\end{aligned}$$

Case 2: $t = 1$,

$$\begin{aligned}
M_2(G) &= \sum_{uv \in E(G)} d_u d_v \\
&= m_{1,3}(1 \cdot 3) + m_{3,3}(3 \cdot 3) + m_{3,4}(3 \cdot 4) + m_{4,4}(4 \cdot 4) + m_{1,4}(1 \cdot 4) \\
&= 2(s+2)3 + 6.9 + 4(s-1)12 + (s-1)16 + 2(s-1)4 \\
&= 6(13s - 1).
\end{aligned}$$

□

Theorem 2.9. *The augmented Zagreb index of fluorographene is*

$$AZI(G) = \begin{cases} 85.750s + 2.844, & \text{if } t = 1; \\ 24.12s + 26.826t + 61.630st - 26.687, & \text{if } t \neq 1. \end{cases}$$

Proof. We consider the following cases:

Case 1: $t \neq 1$,

$$\begin{aligned}
AZI(G) &= \sum_{uv \in E(G)} \left(\frac{d_u d_v}{d_u + d_v - 2} \right)^3 \\
&= m_{1,3} \left(\frac{1 \cdot 3}{1+3-2} \right)^3 + m_{3,3} \left(\frac{3 \cdot 3}{3+3-2} \right)^3 + m_{3,4} \left(\frac{3 \cdot 4}{3+4-2} \right)^3 \\
&+ m_{4,4} \left(\frac{4 \cdot 4}{4+4-2} \right)^3 + m_{1,4} \left(\frac{1 \cdot 4}{1+4-2} \right)^3 \\
&= 2(s+t+1) \left(\frac{3}{2} \right)^3 + (t+4) \left(\frac{9}{4} \right)^3 + (4s+2t-4) \left(\frac{12}{5} \right)^3 \\
&+ (3st - 2s - t - 1) \left(\frac{16}{6} \right)^3 + 2(st-1) \left(\frac{4}{3} \right)^3 \\
&= 24.12s + 26.826t + 61.630st - 26.687.
\end{aligned}$$

Case 2: $t = 1$,

$$\begin{aligned}
AZI(G) &= \sum_{uv \in E(G)} \left(\frac{d_u d_v}{d_u + d_v - 2} \right)^3 \\
&= m_{1,3} \left(\frac{1 \cdot 3}{1+3-2} \right)^3 + m_{3,3} \left(\frac{3 \cdot 3}{3+3-2} \right)^3 + m_{3,4} \left(\frac{3 \cdot 4}{3+4-2} \right)^3 \\
&+ m_{4,4} \left(\frac{4 \cdot 4}{4+4-2} \right)^3 + m_{1,4} \left(\frac{1 \cdot 4}{1+4-2} \right)^3 \\
&= (2s+4) \left(\frac{3}{2} \right)^3 + 6 \left(\frac{9}{4} \right)^3 + 4(s-1) \left(\frac{12}{5} \right)^3 + (s-1) \left(\frac{16}{6} \right)^3 + 2(s-1) \left(\frac{4}{3} \right)^3 \\
&= 85.750s + 2.844.
\end{aligned}$$

□

Concluding Remarks: The problem of finding the general formula for ABC index, ABC_4 index, Randić connectivity index, sum connectivity index, GA index, GA_5 index, harmonic index, second zagreb index and AZI of fluorographene is solved analytically without using a computer. The obtained values of indices of fluorographene are greater than those of the graphen. This confirms that the fluorographene is more stable than the graphene and this correlates with chemical analysis. Further, analysis of molecules using graph theory will give an idea to study and compare the chemical nature and stability of the molecules.

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