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Research Article

Computation of New Degree-Based Topological Indices of Graphene

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Graphene 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. Inspired by recent work on Graphene of computing topological indices, here we propose new topological indices, namely, Arithmetic-Geometric index (AG_1 index), SK index, SK_1 index, and SK_2 index of a molecular graph G and obtain the explicit formulae of these indices for Graphene.

1. Introduction

A topological index of a chemical compound is an integer, derived following a certain rule, which can be used to characterize the chemical compound and predict certain physiochemical properties like boiling point, molecular weight, density, refractive index, and so forth [1, 2].

A molecular graph $G = (V, E)$ is a simple graph having $n = |V|$ vertices and $m = |E|$ edges. The vertices $v_i \in V$ represent nonhydrogen atoms and the edges $(v_i, v_j) \in E$ represent covalent bonds between the corresponding atoms. In particular, hydrocarbons are formed only by carbon and hydrogen atom and their molecular graphs represent the carbon skeleton of the molecule [1, 2].

Molecular graphs are a special type of chemical graphs, which represent the constitution of molecules. They are also called constitutional graphs. When the constitutional graph of a molecule is represented in a two-dimensional basis, it is called structural graph [1, 2].

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 du and is the number of vertices that are adjacent to u. The edge connecting the vertices u and v is denoted by uv [3].

2. Computing the Topological Indices of Graphene

Graphene is an atomic scale honeycomb lattice made of carbon atoms. 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 industrialists 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. Now we focus on computation of topological indices of Graphene [4–6].

Motivated by previous research on Graphene, here we introduce four new topological indices and computed their corresponding topological index value of Graphene [7–13].

In Figure 1, the molecular graph of Graphene is shown.

2.1. Motivation. By looking at the earlier results for computing the topological indices for Graphene, here we introduce new degree-based topological indices to compute their values for Graphene.

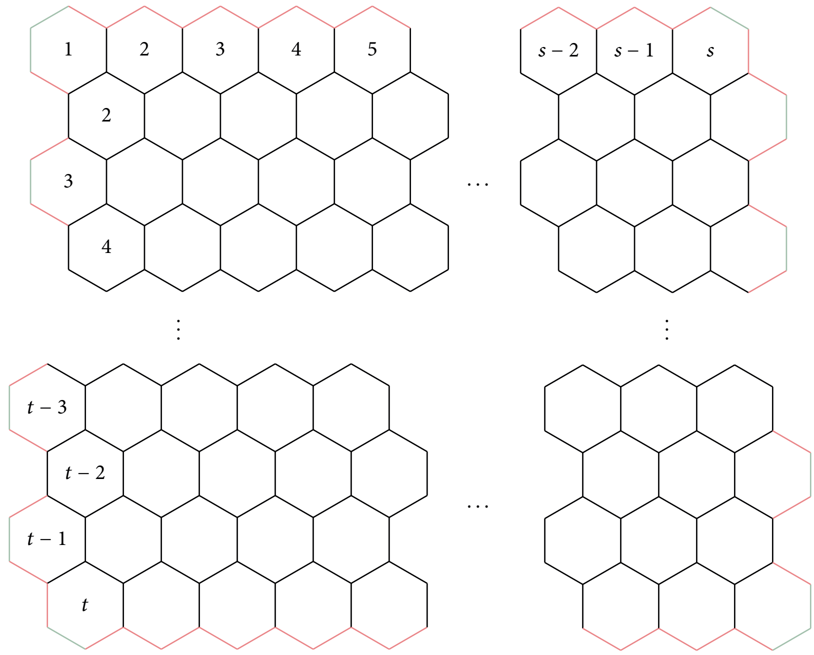

Figure 1

In the upcoming sections, topological indices and their computation of topological indices for Graphene are discussed.

Definition 1 (Arithmetic-Geometric (AG_1) index). Let $G = (V, E)$ be a molecular graph and du be the degree of the vertex u; then AG_1 index of G is defined as

$$AG_1(G) = \sum_{u,v \in E(G)} \frac{d_G(u) + d_G(v)}{2\sqrt{d_G(u) \cdot d_G(v)}}, \tag{1}$$

where AG_1 index is considered for distinct vertices.

The above equation is the sum of the ratio of the Arithmetic mean and Geometric mean of u and v, where $d_G(u)$ (or $d_G(v)$) denote the degree of the vertex u (or v).

Definition 2 (SK index). The SK index of a graph $G = (V, E)$ is defined as $SK(G) = \sum_{u,v \in E(G)}((d_G(u) + d_G(v))/2)$, where $d_G(u)$ and $d_G(v)$ are the degrees of the vertices u and v in G, respectively.

Definition 3 (SK_1 index). The SK_1 index of a graph $G = (V, E)$ is defined as $SK_1(G) = \sum_{u,v \in E(G)}((d_G(u) \cdot d_G(v))/2)$, where $d_G(u)$ and $d_G(v)$ are the product of the degrees of the vertices u and v in G, respectively.

Definition 4 (SK_2 index). The SK_2 index of a graph $G = (V, E)$ is defined as $SK_2(G) = \sum_{u,v \in E(G)}((d_G(u) + d_G(v))/2)^2$, where $d_G(u)$ and $d_G(v)$ are the degrees of the vertices u and v in G, respectively.

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	$3s$	$s - 1$
Total	$t + 4$	$4s + 2t - 4$	$3ts - 2s - t - 1$

3. Main Results

Theorem 5. *The AG_1 index of Graphene having "t" rows of Benzene rings with "s" Benzene rings in each row is given by*

$$AG_1(G) = \begin{cases} \dfrac{6\sqrt{6}st + (20 - 4\sqrt{6})s + 10t - (20 - 6\sqrt{6})}{2\sqrt{6}}, & \text{if } t \neq 1 \\ \dfrac{(2\sqrt{6} + 20)s + 6\sqrt{6} - 10}{2\sqrt{6}}, & \text{if } t = 1. \end{cases} \tag{2}$$

Proof. Consider a Graphene having "t" rows with "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 (Figure 1) contains only $m_{2,2}$, $m_{2,3}$, and $m_{3,3}$ edges. The number of $m_{2,2}$, $m_{2,3}$, and $m_{3,3}$ edge in each row is mentioned in Table 1.

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

$$\begin{aligned}
\mathrm{AG}_1(G) &= \sum_{u,v\in E(G)} \frac{d_G(u)+d_G(v)}{2\sqrt{d_G(u)\cdot d_G(v)}}, \\
\mathrm{AG}_1(G) &= m_{2,2}\left(\frac{2+2}{2\sqrt{2.2}}\right) + m_{2,3}\left(\frac{2+3}{2\sqrt{2.3}}\right) + m_{3,3}\left(\frac{3+3}{2\sqrt{3.3}}\right) \\
&= (t+4)\left(\frac{4}{4}\right) + (4s+2t-4)\left(\frac{5}{2\sqrt{6}}\right) + (3ts-2s-t-1)\left(\frac{6}{6}\right) \\
&= (t+4) + (4s+2t-4)\left(\frac{5}{2\sqrt{6}}\right) + 3ts - 2s - t - 1 \\
&= (3ts-2s+3) + (4s+2t-4)\left(\frac{5}{2\sqrt{6}}\right) \\
&= \frac{2\sqrt{6}(3ts-2s+3) + 5(4s+2t-4)}{2\sqrt{6}} \\
&= \frac{6\sqrt{6}ts - 4\sqrt{6}s + 6\sqrt{6} + 20s + 10t - 20}{2\sqrt{6}} \\
&= \frac{6\sqrt{6} + \left(20-4\sqrt{6}\right)s + 10t - \left(20-6\sqrt{6}\right)}{2\sqrt{6}}.
\end{aligned} \tag{3}$$

Now consider the following cases.

Case 1. The Arithmetic-Geometric index of Graphene for $t \neq 1$ is

$$\mathrm{AG}_1(G) = \frac{6\sqrt{6} + \left(20-4\sqrt{6}\right)s + 10t - \left(20-6\sqrt{6}\right)}{2\sqrt{6}}. \tag{4}$$

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

$$\begin{aligned}
\mathrm{AG}_1(G) &= \sum_{u,v\in E(G)} \frac{d_G(u)+d_G(v)}{2\sqrt{d_G(u)\cdot d_G(v)}}, \\
\mathrm{AG}_1(G) &= m_{2,2}\left(\frac{2+2}{2\sqrt{2.2}}\right) + m_{2,3}\left(\frac{2+3}{2\sqrt{2.3}}\right) + m_{3,3}\left(\frac{3+3}{2\sqrt{3.3}}\right) \\
&= (t+4)\left(\frac{4}{4}\right) + (4s+2t-4)\left(\frac{5}{2\sqrt{6}}\right) + (3ts-2s-t-1)\left(\frac{6}{6}\right) \\
&= 5(1) + (4s-2)\left(\frac{5}{2\sqrt{6}}\right) + (s-2)(1) \\
&= s + 3 + (4s-2)\left(\frac{5}{2\sqrt{6}}\right) \\
&= \frac{2\sqrt{6}(s) + 6\sqrt{6} + 20s - 10}{2\sqrt{6}} \\
&= \frac{\left(2\sqrt{6}+20\right)s + 6\sqrt{6} - 10}{2\sqrt{6}}.
\end{aligned} \tag{5}$$

□

Theorem 6. *The SK index of Graphene having "t" rows of Benzene rings with "s" Benzene rings in each row is given by*

$$SK(G) = \begin{cases} \dfrac{18ts + 8s + 8t - 10}{2}, & if\ t \neq 1 \\ \dfrac{26s-2}{2}, & if\ t = 1. \end{cases} \tag{6}$$

Proof. Consider Graphene having "t" rows with "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 (Figure 1) contains only $m_{2,2}$, $m_{2,3}$, and $m_{3,3}$ edges. The number of $m_{2,2}$, $m_{2,3}$, and $m_{3,3}$ edge in each row is mentioned in Table 1.

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

$$\begin{aligned}
SK(G) &= \sum_{u,v\in E(G)} \frac{d_G(u)+d_G(v)}{2}, \\
SK(G) &= m_{2,2}\left(\frac{2+2}{2}\right) + m_{2,3}\left(\frac{2+3}{2}\right) + m_{3,3}\left(\frac{3+3}{2}\right) \\
&= (t+4)\left(\frac{4}{2}\right) + (4s+2t-4)\left(\frac{5}{2}\right) + (3ts-2s-1)\left(\frac{6}{2}\right) \\
&= 2(t+4) + (4s+2t-4)\left(\frac{5}{2}\right) + 3(3ts-2s-t-1) \\
&= 2t + 8 + (4s+2t-4)\left(\frac{5}{2}\right) + 9ts - 6s - 3t - 3 \\
&= \frac{4t + 16 + 20s + 10t - 20 + 18ts - 12s - 6t - 6}{2} \\
&= \frac{18ts + 8s + 8t - 10}{2}.
\end{aligned} \tag{7}$$

Now consider the following cases.

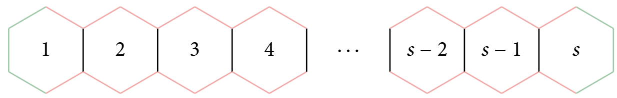

Figure 2

Case 1. The SK index of Graphene for $t \neq 1$ is

$$\mathrm{SK}(G) = \frac{18ts + 8s + 8t - 10}{2}. \quad (8)$$

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

$$\begin{aligned}
\mathrm{SK}(G) &= \sum_{u,v \in E(G)} \frac{d_G(u) + d_G(v)}{2}, \\
\mathrm{SK}(G) &= m_{2,2}\left(\frac{2+2}{2}\right) + m_{2,3}\left(\frac{2+3}{2}\right) \\
&\quad + m_{3,3}\left(\frac{3+3}{2}\right) \\
&= (t+4)\left(\frac{4}{2}\right) + (4s + 2t - 4)\left(\frac{5}{2}\right) \\
&\quad + (3ts - 2s - t - 1)\left(\frac{6}{2}\right).
\end{aligned} \quad (9)$$

For $t = 1$,

$$\begin{aligned}
&= 5(2) + (4s - 2)\left(\frac{5}{2}\right) + (s - 2)(3) \\
&= 10 + (4s - 2)\left(\frac{5}{2}\right) + 3s - 6 \\
&= \frac{20 + 20s - 10 + 6s - 12}{2} = \frac{26s - 2}{2}.
\end{aligned} \quad (10)$$

□

Theorem 7. *The SK_1 index of Graphene having "t" rows of Benzene rings with "s" Benzene rings in each row is given by*

$$SK_1(G) = \begin{cases} \dfrac{27ts + 7t + 6s - 17}{2}, & \text{if } t \neq 1 \\ \dfrac{33s - 10}{2}, & \text{if } t = 1. \end{cases} \quad (11)$$

Proof. Consider Graphene having "t" rows with "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 (Figure 1) contains only $m_{2,2}$, $m_{2,3}$, and $m_{3,3}$ edges. The number of $m_{2,2}$, $m_{2,3}$, and $m_{3,3}$ edge in each row is mentioned in Table 1.

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

$$\begin{aligned}
\mathrm{SK}_1(G) &= \sum_{u,v \in E(G)} \frac{d_G(u) \cdot d_G(v)}{2}, \\
\mathrm{SK}_1(G) & \\
&= m_{2,2}\left(\frac{2 \times 2}{2}\right) + m_{2,3}\left(\frac{2 \times 3}{2}\right) + m_{3,3}\left(\frac{3 \times 3}{2}\right) \\
&= (t+4)\left(\frac{4}{2}\right) + (4s + 2t - 4)\left(\frac{6}{2}\right) \\
&\quad + (3ts - 2s - 1)\left(\frac{9}{2}\right) \\
&= 2(t+4) + (4s + 2t - 4)(3) \\
&\quad + (3ts - 2s - t - 1)\left(\frac{9}{2}\right) \\
&= 2t + 8 + 12s + 6t - 12 + (3ts - 2s - t - 1)\left(\frac{9}{2}\right) \\
&= \frac{4t + 16 + 24s + 12t - 24 + 27ts - 18s - 9t - 9}{2} \\
&= \frac{27ts + 7t + 6s - 17}{2}.
\end{aligned} \quad (12)$$

Now consider the following cases.

Case 1. The SK_1 index of Graphene for $t \neq 1$ is

$$\mathrm{SK}_1(G) = \frac{27ts + 7t + 6s - 17}{2}. \quad (13)$$

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

$$\begin{aligned}
\mathrm{SK}_1(G) &= \sum_{u,v \in E(G)} \frac{d_G(u) \cdot d_G(v)}{2}, \\
\mathrm{SK}_1(G) &= m_{2,2}\left(\frac{2 \times 2}{2}\right) + m_{2,3}\left(\frac{2 \times 3}{2}\right) \\
&\quad + m_{3,3}\left(\frac{3 \times 3}{2}\right) \\
&= (t+4)\left(\frac{4}{2}\right) + (4s + 2t - 4)\left(\frac{6}{2}\right) \\
&\quad + (3ts - 2s - 1)\left(\frac{9}{2}\right) \\
&= 2(t+4) + (4s + 2t - 4)(3) \\
&\quad + (3ts - 2s - t - 1)\left(\frac{9}{2}\right).
\end{aligned} \quad (14)$$

For $t = 1$,

$$\begin{aligned}
&= 2(1+4) + (4s - 2)3 + (s - 2)\left(\frac{9}{2}\right) \\
&= 10 + 12s - 6 + (s - 2)\left(\frac{9}{2}\right) \\
&= \frac{20 + 24s - 12 + 9s - 18}{2} = \frac{33s - 10}{2}.
\end{aligned} \quad (15)$$

□

Theorem 8. *The SK_2 index of Graphene having "t" rows of Benzene rings with "s" Benzene rings in each row is given by*

$$SK_2(G) = \begin{cases} \dfrac{108ts + 30t + 28s - 72}{4}, & \text{if } t \neq 1 \\ \dfrac{136s - 42}{4}, & \text{if } t = 1. \end{cases} \quad (16)$$

Proof. Consider Graphene having "t" rows with "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 (Figure 1) contains only $m_{2,2}$, $m_{2,3}$, and $m_{3,3}$ edges. The number of $m_{2,2}$, $m_{2,3}$, and $m_{3,3}$ edge in each row is mentioned in Table 1.

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

$$\mathrm{SK}_2(G) = \sum_{u,v\in E(G)} \left(\frac{d_G(u)+d_G(v)}{2}\right)^2,$$

$$\begin{aligned}
&\mathrm{SK}_2(G)\\
&= m_{2,2}\left(\frac{2+2}{2}\right)^2 + m_{2,3}\left(\frac{2+3}{2}\right)^2 + m_{3,3}\left(\frac{3+3}{2}\right)^2\\
&= (t+4)\left(\frac{4}{2}\right)^2 + (4s+2t-4)\left(\frac{5}{2}\right)^2\\
&\quad + (3ts-2s-1)\left(\frac{6}{2}\right)^2\\
&= 4(t+4) + (4s+2t-4)\left(\frac{25}{4}\right) + 9(3ts-2s-t-1)\\
&= 4t+16 + (4s+2t-4)\left(\frac{25}{4}\right) + 27ts-18s-9t-9\\
&= \frac{16t+64+100s+50t-100+108ts-72s-36t-36}{4}\\
&= \frac{108ts+30t+28s-72}{4}.
\end{aligned} \tag{17}$$

Now consider the following cases.

Case 1. The SK_2 index of Graphene for $t \neq 1$ is

$$\mathrm{SK}_2(G) = \frac{108ts+30t+28s-72}{4}. \tag{18}$$

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

$$\begin{aligned}
&\mathrm{SK}_2(G) = \sum_{u,v\in E(G)} \left(\frac{d_G(u)+d_G(v)}{2}\right)^2,\\
&\mathrm{SK}_2(G) = m_{2,2}\left(\frac{2+2}{2}\right)^2 + m_{2,3}\left(\frac{2+3}{2}\right)^2\\
&\quad + m_{3,3}\left(\frac{3+3}{2}\right)^2\\
&= (t+4)\left(\frac{4}{2}\right)^2 + (4s+2t-4)\left(\frac{5}{2}\right)^2\\
&\quad + (3ts-2s-1)\left(\frac{6}{2}\right)^2\\
&= 4(t+4) + (4s+2t-4)\left(\frac{25}{4}\right)\\
&\quad + 9(3ts-2s-t-1).
\end{aligned} \tag{19}$$

For $t = 1$,

$$\begin{aligned}
&= 4(1+4) + (4s-2)\left(\frac{25}{4}\right) + 9(s-2)\\
&= 20 + (4s-2)\left(\frac{25}{4}\right) + 9s - 18\\
&= \frac{80+100s-50+36s-72}{4} = \frac{136s-42}{4}.
\end{aligned} \tag{20}$$

□

3.1. Conclusion. A generalized formula for Arithmetic-Geometric index (AG_1 index), SK index, SK_1 index, and SK_2 index of Graphene has been obtained without using computer.

Competing Interests

The authors declare that there are no competing interests regarding the publication of this paper.

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