

Computing Some Degree-Based Topological Indices of Graphene

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Abstract

Graphene is one of the most promising nanomaterial 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 bio devices. Inspired by recent work on Graphene of computing topological indices, here we compute new topological indices viz. Arithmetic-Geometric index (AG2 index), SK3 index and Sanskruti index of a molecular graph G and obtain the explicit formulae of these indices for Graphene.

Keywords: Arithmetic-Geometric index (AG2 index), SK3 index, sanskruti index, graphene.

1. Introduction

A molecular graph is a representation of a chemical compound having atoms as vertices and the bonds between atoms correspond to the edge of the graph. The collection of vertices of a graph, says G , is denoted by $V(G)$ and the set of edges is denoted by $E(G)$. The degree of a vertex v of a graph is the number of vertices of G adjacent to v , denoted by $d_G(v)$ or simply as dv [3].

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 graphs [7, 8].

Topological invariant of a graph is a single number descriptor which is correlated to certain chemical, thermodynamical and biological behavior of the chemical compounds. Several topological indices have been defined over past decades which depend on degree of vertices.

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 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. Now we focus on computation of topological indices of Graphene [1, 4].

Motivated by previous research on Graphene [4,6,11-14], here we compute three new topological indices viz. Arithmetic-Geometric index (AG2 index), SK3 index and Sanskruti index of a molecular graph G and obtain the explicit formulae of these indices for Graphene.

2.1. Arithmetic-Geometric (AG₂) Index

Let $G = (V, E)$ be a molecular graph, and $S_G(u)$ is the degree of the vertex u , then AG2 index of G is defined as

$$AG_2(G) = \sum_{u,v \in E(G)} \frac{S_G(u) + S_G(v)}{2\sqrt{S_G(u) \cdot S_G(v)}}$$

where, AG2 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 $SG(u)$ (or $SG(v)$) is the summation of degrees of all neighbours of vertex u (or v) in G .

$$SG(u) = \sum_{u,v \in E(G)} d_G(u) \quad \text{and } NG(u) = \{v \in V(G) / uv \in E(G)\}$$

2.2. SK₃ Index

The SK3 index of a graph $G = (V, E)$ is defined as

$$SK3(G) = \sum_{u,v \in E(G)} \frac{S_G(u) + S_G(v)}{2}$$

where $SG(u)$ (or $SG(v)$) is the summation of degrees of all neighbours of vertex u (or v) in G .

$$SG(u) = \sum_{u,v \in E(G)} d_G(u) \quad \text{and } NG(u) = \{v \in V(G) / uv \in E(G)\}$$

2.3. Sanskruti Index

Recently, Hosamani [9], studied a novel topological index, namely the Sanskruti index $S(G)$ of a molecular graph G , which is denoted as

$$S(G) = \sum_{uv \in E(G)} \left(\frac{S_G(u) \cdot S_G(v)}{S_G(u) + S_G(v) - 2} \right)^3$$

where $SG(u)$ (or $SG(v)$) is the summation of degrees of all neighbours of vertex u (or v) in G .

$$SG(u) = \sum_{u,v \in E(G)} d_G(u) \quad \text{and } NG(u) = \{v \in V(G) / uv \in E(G)\}$$

3. Main Results

3.1. The AG₂ index of Graphene is

$$AG_2(G) = \begin{cases} 6.0588t + 2.0277s + 3ts - 1.0032 & \text{if } t \neq 1 \\ 5.0119s + 1.0578 & \text{if } t = 1 \\ 6 & \text{if } t = 1, s > 1 \end{cases}$$

Let $e_{i,j}$ denote the number of edges with $i=Su$ and $j=Sv$. 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 Table 1. For convenience these edge type are colored by grey, yellow, red, purple, blue, green, light blue, brown, and black, respectively, as shown in Figure 1.

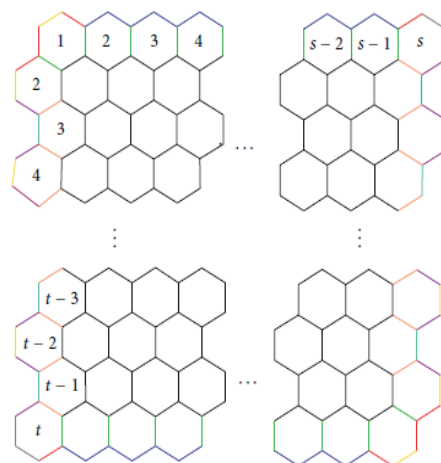


Figure 1. Colors of Graphene Edge (1)

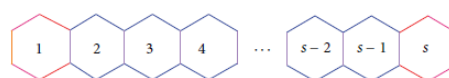


Figure 2. Colors of Graphene Edge (2)

Case 1. The AG_2 index of Graphene for $t \neq 1$ is

$$AG_2(G) = \sum_{u,v \in E(G)} \frac{S_G(u) + S_G(v)}{2\sqrt{S_G(u) \cdot S_G(v)}}$$

Table 1. Nine edge types of Graphene

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
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮
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

$$\begin{aligned}
 AG_2(G) &= (e_{4,5}) \left(\frac{4+5}{2\sqrt{20}} \right) + (e_{5,5}) \left(\frac{5+5}{2\sqrt{25}} \right) + (e_{5,7}) \left(\frac{5+7}{2\sqrt{35}} \right) + (e_{5,8}) \left(\frac{5+8}{2\sqrt{40}} \right) + (e_{6,7}) \\
 &\quad \left(\frac{6+7}{2\sqrt{42}} \right) + (e_{7,9}) \left(\frac{7+9}{2\sqrt{63}} \right) + (e_{8,8}) \left(\frac{8+8}{2\sqrt{64}} \right) + (e_{9,8}) \left(\frac{9+8}{2\sqrt{72}} \right) + (e_{9,9}) \left(\frac{9+9}{2\sqrt{81}} \right) \\
 &= (4) \left(\frac{9}{2\sqrt{20}} \right) + (t) \left(\frac{10}{2\sqrt{25}} \right) + (8) \left(\frac{12}{2\sqrt{35}} \right) + (2t-4) \left(\frac{13}{2\sqrt{40}} \right) + (4s-8) \left(\frac{13}{2\sqrt{42}} \right)
 \end{aligned}$$

$$\begin{aligned}
& + (2s) \left(\frac{16}{2\sqrt{63}} \right) + (t-2) \left(\frac{16}{2\sqrt{64}} \right) + (2t-4) \left(\frac{17}{2\sqrt{72}} \right) + (3ts-4s-4t+5) \left(\frac{18}{2\sqrt{81}} \right) \\
& = \left(5 + \frac{13}{\sqrt{40}} + 1 + \frac{17}{\sqrt{72}} - 4 \right) t + \left(\frac{26}{\sqrt{42}} + \frac{16}{\sqrt{63}} - 4 \right) s + 3ts + \\
& \quad \left(\frac{18}{\sqrt{20}} + \frac{48}{\sqrt{35}} - \frac{26}{\sqrt{40}} - \frac{52}{\sqrt{42}} - 2 - \frac{34}{\sqrt{72}} + 5 \right) \\
& = 6.0588t + 2.0277s + 3ts - 1.0032
\end{aligned}$$

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 $e_{7,7}$. These edges are colored in orange, pink, red, blue, and lavender, respectively, as shown in Figure 2. The number of edges of these types is shown in Table 2

Table 2. The Number of Edges

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

$$\begin{aligned}
AG_2(G) &= (e_{4,4}) \left(\frac{4+4}{2\sqrt{16}} \right) + (e_{4,5}) \left(\frac{4+5}{2\sqrt{20}} \right) + (e_{5,7}) \left(\frac{5+7}{2\sqrt{35}} \right) + (e_{6,7}) \left(\frac{6+7}{2\sqrt{42}} \right) + (e_{7,7}) \left(\frac{7+7}{2\sqrt{49}} \right) \\
&= (2) \left(\frac{8}{2\sqrt{16}} \right) + (4) \left(\frac{9}{2\sqrt{20}} \right) + (4) \left(\frac{12}{2\sqrt{35}} \right) + (4s-8) \left(\frac{13}{2\sqrt{42}} \right) + (s-1) \left(\frac{14}{2\sqrt{49}} \right) \\
&= \left(2 + \frac{18}{\sqrt{20}} + \frac{24}{\sqrt{35}} - \frac{52}{\sqrt{42}} - 1 \right) t + \left(\frac{26}{\sqrt{42}} + 1 \right) s \\
&= 5.0119s + 1.0578
\end{aligned}$$

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



Figure 3. Type $e_{4,4}$ with 6 Edges

$$AG_2(G) = (e_{4,4}) \binom{4+4}{2\sqrt{16}} = 6$$

3.2. The SK_3 index of Graphene is

$$SK_3(G) = \begin{cases} 7t + 6s + 27ts - 17 & \text{if } t \neq 1 \\ 33s - 9 & \text{if } t = 1 \\ 24 & \text{if } t = 1, s > 1 \end{cases}$$

Proof: Let e_{ij} denote the number of edges with $i=Su$ and $j=Sv$. 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 Table1. For convenience these edge type are colored by grey, yellow, red, purple, blue, green, light blue, brown, and black, respectively, as shown in Figure1.

Case 1. The SK_3 index of Graphene for $t \neq 1$ is

$$\begin{aligned} SK_3(G) &= \sum_{u,v \in E(G)} \frac{S_G(u) + S_G(v)}{2} \\ SK_3(G) &= (e_{4,5}) \binom{4+5}{2} + (e_{5,5}) \binom{5+5}{2} + (e_{5,7}) \binom{5+7}{2} + (e_{5,8}) \binom{5+8}{2} + (e_{6,7}) \binom{6+7}{2} + \\ &\quad (e_{7,9}) \binom{7+9}{2} + (e_{8,8}) \binom{8+8}{2} + (e_{8,9}) \binom{9+8}{2} + (e_{9,9}) \binom{9+9}{2} \\ &= (4) \binom{9}{2} + (t) \binom{10}{2} + (8) \binom{12}{2} + (2t-4) \binom{13}{2} + (4s-8) \binom{13}{2} + (2s) \binom{16}{2} + (t-2) \\ &\quad \binom{16}{2} + (2t-4) \binom{17}{2} + (3ts-4s-4t+5) \binom{18}{2} \\ &= (5+13+8+17-36)t + (26+16-36)s + 27ts + (18+48-26-52-16-34+45) \\ &= 7t + 6s + 27ts - 17 \end{aligned}$$

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 $e_{7,7}$. These edges are colored in orange, pink, red, blue, and lavender, respectively, as shown in Figure 2. The number of edges of these types is shown in Table 2.

$$\begin{aligned} SK_3(G) &= (e_{4,4}) \binom{4+4}{2} + (e_{4,5}) \binom{4+5}{2} + (e_{5,7}) \binom{5+7}{2} + (e_{6,7}) \binom{6+7}{2} + (e_{7,7}) \binom{7+7}{2} \\ &= (2) \binom{8}{2} + (4) \binom{9}{2} + (4) \binom{12}{2} + (4s-8) \binom{13}{2} + (s-1) \binom{14}{2} \\ &= (8+18+24-52-7)t + (26+7)s \\ &= 33s - 9 \end{aligned}$$

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

$$SK_3(G) = \binom{e_{4,4}}{\left(\frac{4+4}{2}\right)} = 24$$

3.3. The Sanskruti index of Graphene is

$$S(G) = \begin{cases} 389.22ts - 75.58t - 114.06s - 186.08 & \text{if } t \neq 1 \\ 290.72s - 210.68 & \text{if } t = 1, s > 1 \\ 113.76 & \text{if } t = 1, s = 1 \end{cases}$$

Proof: Let $e_{i,j}$ denote the number of edges with $i=Su$ and $j=Sv$. 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 Table 1. For convenience these edge type are colored by grey, yellow, red, purple, blue, green, light blue, brown, and black, respectively, as shown in Figure 1.

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

$$\begin{aligned} S(G) &= \sum_{w \in E(G)} \left(\frac{S_G(u) \cdot S_G(v)}{S_G(u) + S_G(v) - 2} \right)^3 \\ S(G) &= \binom{e_{4,5}}{\left(\frac{4 \times 5}{4+5-2}\right)^3} + \binom{e_{5,5}}{\left(\frac{5 \times 5}{5+5-2}\right)^3} + \binom{e_{5,7}}{\left(\frac{5 \times 7}{5+7-2}\right)^3} + \binom{e_{5,8}}{\left(\frac{5 \times 8}{5+8-2}\right)^3} + \\ &\binom{e_{6,7}}{\left(\frac{6 \times 7}{6+7-2}\right)^3} + \binom{e_{7,9}}{\left(\frac{7 \times 9}{7+9-2}\right)^3} + \binom{e_{8,8}}{\left(\frac{8 \times 8}{8+8-2}\right)^3} + \binom{e_{8,9}}{\left(\frac{8 \times 9}{8+9-2}\right)^3} + \binom{e_{9,9}}{\left(\frac{9 \times 9}{9+9-2}\right)^3} \\ &= \binom{4}{\left(\frac{20}{7}\right)^3} + \binom{t}{\left(\frac{25}{8}\right)^3} + \binom{8}{\left(\frac{35}{10}\right)^3} + \binom{2t-4}{\left(\frac{40}{11}\right)^3} + \binom{4s-8}{\left(\frac{42}{11}\right)^3} + \binom{2s}{\left(\frac{63}{14}\right)^3} + \\ &\binom{t-2}{\left(\frac{64}{14}\right)^3} + \binom{2t-4}{\left(\frac{72}{15}\right)^3} + \binom{3ts-4s-4t+5}{\left(\frac{81}{16}\right)^3} \\ &= \left(\left(\frac{25}{8}\right)^3 + 2\left(\frac{40}{11}\right)^3 + \left(\frac{64}{14}\right)^3 + 2\left(\frac{72}{15}\right)^3 - 4\left(\frac{81}{16}\right)^3 \right) t + \left(4\left(\frac{42}{11}\right)^3 + 2\left(\frac{63}{14}\right)^3 - 4\left(\frac{81}{16}\right)^3 \right) s + 3ts \left(\frac{81}{16}\right)^3 + \\ &\left(4\left(\frac{20}{7}\right)^3 + 8\left(\frac{35}{10}\right)^3 - 4\left(\frac{40}{11}\right)^3 - 8\left(\frac{42}{11}\right)^3 - 2\left(\frac{64}{14}\right)^3 - 4\left(\frac{72}{15}\right)^3 + 5\left(\frac{81}{16}\right)^3 \right) \\ &= 389.22ts - 75.58t - 114.06s - 186.08 \end{aligned}$$

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 $e_{7,7}$. These edges are colored in orange, pink, red, blue, and lavender, respectively, as shown in Figure 2. The number of edges of these types is shown in Table 2.

$$\begin{aligned}
S(G) &= (e_{4,4}) \left(\frac{4 \times 4}{4+4-2} \right)^3 + (e_{4,5}) \left(\frac{4 \times 5}{4+5-2} \right)^3 + (e_{5,7}) \left(\frac{5 \times 7}{5+7-2} \right)^3 + (e_{6,7}) \left(\frac{6 \times 7}{6+7-2} \right)^3 \\
&\quad + (e_{7,7}) \left(\frac{7 \times 7}{7+7-2} \right)^3 \\
&= (2) \left(\frac{16}{6} \right)^3 + (4) \left(\frac{20}{7} \right)^3 + (4) \left(\frac{35}{10} \right)^3 + (4s-8) \left(\frac{42}{11} \right)^3 + (s-1) \left(\frac{49}{12} \right)^3 \\
&= \left(4 \left(\frac{42}{11} \right)^3 + \left(\frac{49}{12} \right)^3 \right) s + \left(2 \left(\frac{16}{6} \right)^3 + 4 \left(\frac{20}{7} \right)^3 + 4 \left(\frac{35}{10} \right)^3 - 8 \left(\frac{42}{11} \right)^3 - 1 \left(\frac{49}{12} \right)^3 \right) \\
&= 290.72s - 210.68
\end{aligned}$$

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

$$S(G) = (e_{4,4}) \left(\frac{4 \times 4}{4+4-2} \right)^3 = 113.76$$

4. Conclusion

In this paper we have computed the Arithmetic-Geometric (AG_2) index, SK_3 index and Sanskruti index $S(G)$ of Graphene is obtained without using computer.

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