Proceedings of the Jangjeon Mathematical Society
23 (2020), No. 2, pp. 253 – 270

www.jangjeon.or.kr
http://dx.doi.org/10.17777/pjms2020.23.2.253

Some edge degree based topological indices of Graphene

Dedicated to Prof. Chandrashekar Adiga on his 62nd birthday

K. B. Sudhakara[1], P. S. Guruprasad[2] and M. A. Sriraj[3]

[1]Research Scholar, Department of Mathematics, Vidyavardhaka College of Engineering, Mysuru-570 002, Karnataka, India
[1]Department of Mathematics, Government Science College, Hassan-573 201, Karnataka, India
[2]Department of Mathematics, Government First Grade College, Chamarajanagar-571 313, Karnataka, India
[3]Department of Mathematics, Vidyavardhaka College of Engineering, Mysuru-570 002, Karnataka, India
E-mail: sudhakarkb.maths@gmail.com, guruprasad18881@gmail.com, masriraj@gmail.com

Abstract

Graphene is a two dimensional material consisting of a single layer of carbon atom arranged in a honeycomb structure. Its properties include high strength and good conductivity of heat and electricity. In this paper, we compute some edge degree based topological indices namely, Generalized Zagreb index, Atom Bond Connectivity index, Augmented Zagreb Index, Geometric Arithmetic index, Harmonic index, ,Symmetric division degree index, Modified first multiple Zagreb index, second multiple Zagreb index, first, second and third Zagreb polynomial of Graphene.

Mathematics Subject Classification (2000): 05C10

Keywords: Topological Indices.

1. **Introduction**

Graph theory provides simple rules by which chemists may obtain qualitative predictions about the structure and reactivity of various compounds. It may be used as a foundation for the representation, classification and categorization of a very large number of chemical systems. Chemical graph theory is a branch of mathematical chemistry that is concerned with all aspects of the application of graph theory to chemistry. A molecular graph is a connected graph whose vertices correspond to the atoms of the compound and edges correspond to chemical bonds. A topological index is a real number related to a graph G which is invariant under graph isomorphism i.e., it does not depend on the labeling or the pictorial representation of a graph [16]. The molecular graphs considered in this paper are simple connected undirected graph. Graphene is an exciting material that is getting a lot of attention. It is the thinnest material known to man at one atom thick and also incredibly stronger than steel. Also it is an excellent conductor of heat and electricity and has interesting light absorption abilities. Researchers all over the world continue to constantly investigate to learn its various properties and possible applications. Motivated by the earlier research work on graphene [15, 10], in this paper we compute some edge degree based topological indices namely, Generalized Zagreb index, Atom Bond Connectivity index, Augmented Zagreb Index, Geometric Arithmetic index, Harmonic index, Symmetric division degree index, Modified first multiple Zagreb index, second multiple Zagreb index, first, second and third Zagreb polynomial of Graphene. Since the edge degree of a graph is the vertex degree of its line graph, we compute the above mentioned topological indices for line graph of graphene.

2. Preliminaries

Let $G = (V, E)$ be a simple graph, where $V = V(G)$ is a non-empty set of elements called vertices or points and $E = E(G)$ is a set of unordered pairs of distinct elements of $V(G)$ called edges or lines. The sets $V(G)$ and $E(G)$ are called vertex set and edge set of G respectively. The degree of a vertex $v \in V(G)$ denoted by d_v is the number of edges incident with v. Two vertices u and v of G are adjacent if there is an edge $e = uv$ between them.The line graph L(G) of a graph G is the graph each of whose vertex represents an edge of G and two of its vertices are adjacent if their corresponding edges are adjacent in G.

The generalized Zagreb index [8] is defined as

$$M_{\alpha,\beta} = M_{\alpha,\beta}(G) = \sum_{e=uv\in E(G)} \frac{(d_u \cdot d_v)^{\alpha}}{(d_u + d_v)^{\beta}}$$

Where α and β are arbitrary real numbers.

Remark:

(1) If $\alpha = 0$ and $\beta = -1$, we have the first Zagreb index [7]

$$M_{0,-1}(G) = M_1(G) = \sum_{e=uv\in E(G)} (d_u + d_v).$$

(2) If $\alpha = 1$ and $\beta = 0$, we have the second Zagreb index [7]

$$M_{1,0}(G) = M_2(G) = \sum_{e=uv\in E(G)} (d_u \cdot d_v).$$

(3) If $\alpha = -\frac{1}{2}$ and $\beta = 0$, we have the Randic connectivity index [11]

$$M_{-\frac{1}{2},0}(G) = \chi(G) = \sum_{e=uv\in E(G)} \frac{1}{\sqrt{(d_u \cdot d_v)}}.$$

(4) If $\alpha = 0$ and $\beta = \frac{1}{2}$, we have the Sum connectivity index [20]

$$M_{0,\frac{1}{2}}(G) = SCI(G) = \sum_{e=uv\in E(G)} \frac{1}{\sqrt{(d_u + d_v)}}.$$

(5) If $\alpha = 0$ and $\beta = -2$, we have the hyper Zagreb index [14]

$$M_{0,-2}(G) = HM(G) = \sum_{e=uv\in E(G)} (d_u + d_v)^2.$$

(6) If $\alpha = 1$ and $\beta = 1$, we have the second refined Zagreb index [12]

$$M_{1,1}(G) = ReZG_2(G) = \sum_{e=uv\in E(G)} \left(\frac{d_u \cdot d_v}{d_u + d_v} \right).$$

(7) If $\alpha = 1$ and $\beta = -1$, we have the third refined Zagreb index or Inverse sum index [12]

$$M_{1,-1}(G) = ReZG_3(G) = \sum_{e=uv\in E(G)} (d_u \cdot d_v)\,(d_u + d_v).$$

The third Zagreb index [4] is defined as

$$M_3 = M_3(G) = \sum_{e=uv\in E(G)} |d_u - d_v| \ .$$

The fourth Zagreb index [13] is defined as

$$M_4 = M_4(G) = \sum_{e=uv\in E(G)} |d_u^2 - d_v^2| \ .$$

The modified first multiple Zagreb index [2] is defined as

$$\Pi_1^*(G) = \prod_{e=uv\in E(G)} (d_u + d_v) \ .$$

The second multiple Zagreb index [9] is defined as

$$\Pi_2(G) = \prod_{e=uv\in E(G)} (d_u \cdot d_v) \ .$$

The first, second [5] and third [1] Zagreb polynomials are respectively defined as

$$ZG_1(G,x) = \sum_{e=uv\in E(G)} x^{d_u+d_v} \ ,$$

$$ZG_2(G,x) = \sum_{e=uv\in E(G)} x^{d_u \cdot d_v} \text{ and}$$

$$ZG_3(G,x) = \sum_{e=uv\in E(G)} x^{|d_u-d_v|} \ .$$

The Atom-Bond connectivity index [3] is defined as

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

The Augmented Zagreb index [6] is defined as

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

The Geometric-Arithmetic index [17] is defined as

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

The Symmetric Division Degree index [18] is defined as

$$SDD(G) = \sum_{e=uv \in E(G)} \left(\frac{d_u^2 + d_v^2}{d_u \cdot d_v} \right).$$

The Harmonic index [19] is defined as

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

3. Main Results

Consider the line graph L(G) of graphene with t rows and s benzene rings in each row. Let E_{d_i,d_j} denote the number of edges connecting the vertices of degree d_i and d_j. The line graph of 2-D graphene (Figure 1) has only $E_{2,2}$, $E_{2,3}$, $E_{3,3}$, $E_{3,4}$, $E_{4,4}$ edges. The number of these edges in each row is mentioned in Table 1.
For $t \neq 1$ and $s \neq 1$ the line graph L(G) of graphene contains

$$E_{2,2}[L(G)]=\{e = uv \in E[L(G)] \mid d_u = 2, d_v = 2\}$$
$$E_{2,3}[L(G)]=\{e = uv \in E[L(G)] \mid d_u = 2, d_v = 3\}$$
$$E_{3,3}[L(G)]=\{e = uv \in E[L(G)] \mid d_u = 3, d_v = 3\}$$
$$E_{3,4}[L(G)]=\{e = uv \in E[L(G)] \mid d_u = 3, d_v = 4\}$$
$$E_{4,4}[L(G)]=\{e = uv \in E[L(G)] \mid d_u = 4, d_v = 4\}$$

From the Figure 1, we have
$\mid E_{2,2}[L(G)] \mid= 2$, $\mid E_{2,3}[L(G)] \mid= 2t + 4$, $\mid E_{3,3}[L(G)] \mid= 4s - 4$,
$\mid E_{3,4}[L(G)] \mid= 4t + 4s - 8$, $\mid E_{4,4}[L(G)] \mid= 6ts - 6s - 4t + 2$.

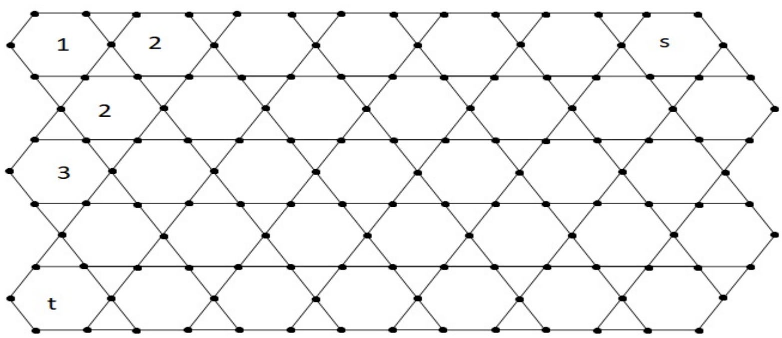

Figure 1 - Line Graph of Graphene

Row	$\mid E_{2,2} \mid$	$\mid E_{2,3} \mid$	$\mid E_{3,3} \mid$	$\mid E_{3,4} \mid$	$\mid E_{4,4} \mid$
1	1	4	2s-2	2s+1	4s-4
2	0	2	0	4	6s-4
3	0	2	0	4	6s-4
4	0	2	0	4	6s-4
⋮	⋮	⋮	⋮	⋮	⋮
t	1	4	2s-2	2s-1	2s-2
total	2	2t+4	4s-4	4t+4s-8	6ts-6s-4t+2

Table - 1

For $t = 1$ and $s \neq 1$, we have the following edges as shown in Figure 2
$\mid E_{2,2}[L(G)] \mid = 4$, $\mid E_{2,3}[L(G)] \mid = 4$, $\mid E_{3,3}[L(G)] \mid = 4s - 6$,
$\mid E_{3,4}[L(G)] \mid = 4s - 4$.

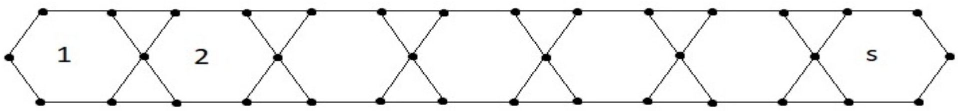

Figure 2

For $t \neq 1$ and $s = 1$, we have the following edges as shown in Figure 3
$\mid E_{2,2}[L(G)] \mid = 4$, $\mid E_{2,3}[L(G)] \mid = 2t$, $\mid E_{3,3}[L(G)] \mid = 2$,
$\mid E_{3,4}[L(G)] \mid = 4t - 4$, $\mid E_{4,4}[L(G)] \mid = 2t - 4$.

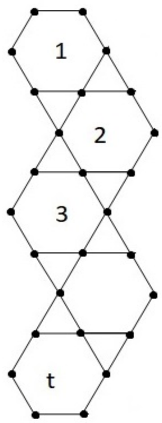

Figure 3

Row	$\mid E_{2,2} \mid$	$\mid E_{2,3} \mid$	$\mid E_{3,3} \mid$	$\mid E_{3,4} \mid$	$\mid E_{4,4} \mid$
1	2	2	1	3	0
2	0	2	0	4	2
3	0	2	0	4	2
4	0	2	0	4	2
⋮	⋮	⋮	⋮	⋮	⋮
t	2	2	1	1	0
total	4	2t	2	4t-4	2t-4

Table - 2

Theorem 3.1. *The Generalized Zagreb index of the line graph L(G) of graphene is*

$$M_{\alpha,\beta}[L(G)] = \begin{cases} 4^{1+\alpha-\beta} + 4\frac{6^\alpha}{5^\beta} + (4s-6)\frac{9^\alpha}{6^\beta} + (4s-4)\frac{12^\alpha}{7^\beta}, & \text{for } t=1,\ s\neq 1 \\ 2^{1+2\alpha-2\beta} + (2t+4)\frac{6^\alpha}{5^\beta} + (4s-4)\frac{9^\alpha}{6^\beta} + (4t+4s-8)\frac{12^\alpha}{7^\beta} + (6ts-6s-4t+2)\frac{16^\alpha}{8^\beta}, & \text{for } t\neq 1,\ s\neq 1 \\ 4^{1+\alpha-\beta} + 2t\frac{6^\alpha}{5^\beta} + 2\frac{9^\alpha}{6^\beta} + (4t-4)\frac{12^\alpha}{7^\beta} + (2t-4)\frac{16^\alpha}{8^\beta}, & \text{for } t\neq 1,\ s=1 \\ 6\cdot 4^{\alpha-\beta}, & \text{for } t=1,\ s=1 \end{cases}$$

where α and β are arbitrary real numbers.

Proof. **Case 1**: for $t=1$, $s\neq 1$

The Generalized Zagreb index of the line graph L(G) of graphene is

$$M_{\alpha,\beta}[L(G)] = \sum_{e=uv\in E[L(G)]} \frac{(d_u\cdot d_v)^\alpha}{(d_u+d_v)^\beta}$$

$$= |E_{2,2}[L(G)]|\frac{(2\cdot 2)^\alpha}{(2+2)^\beta} + |E_{2,3}[L(G)]|\frac{(2\cdot 3)^\alpha}{(2+3)^\beta} + |E_{3,3}[L(G)]|\frac{(3\cdot 3)^\alpha}{(3+3)^\beta}$$

$$+ |E_{3,4}[L(G)]|\frac{(3\cdot 4)^\alpha}{(3+4)^\beta} + |E_{4,4}[L(G)]|\frac{(4\cdot 4)^\alpha}{(4+4)^\beta}$$

$$= 4^{1+\alpha-\beta} + 4\frac{6^\alpha}{5^\beta} + (4s-6)\frac{9^\alpha}{6^\beta} + (4s-4)\frac{12^\alpha}{7^\beta}.$$

Case 2: for $t\neq 1$, $s\neq 1$

$$M_{\alpha,\beta}[L(G)] = \sum_{e=uv\in E[L(G)]} \frac{(d_u\cdot d_v)^\alpha}{(d_u+d_v)^\beta}$$

$$= |E_{2,2}[L(G)]|\frac{(2\cdot 2)^\alpha}{(2+2)^\beta} + |E_{2,3}[L(G)]|\frac{(2\cdot 3)^\alpha}{(2+3)^\beta} + |E_{3,3}[L(G)]|\frac{(3\cdot 3)^\alpha}{(3+3)^\beta}$$

$$+ |E_{3,4}[L(G)]|\frac{(3\cdot 4)^\alpha}{(3+4)^\beta} + |E_{4,4}[L(G)]|\frac{(4\cdot 4)^\alpha}{(4+4)^\beta}$$

$$= 2^{1+2\alpha-2\beta} + (2t+4)\frac{6^\alpha}{5^\beta} + (4s-4)\frac{9^\alpha}{6^\beta} + (4t+4s-8)\frac{12^\alpha}{7^\beta} + (6ts-6s-4t+2)\frac{16^\alpha}{8^\beta}.$$

Case 3: for $t\neq 1$, $s=1$

$$M_{\alpha,\beta}[L(G)] = \sum_{e=uv\in E[L(G)]} \frac{(d_u\cdot d_v)^\alpha}{(d_u+d_v)^\beta}$$

$$= |E_{2,2}[L(G)]|\frac{(2\cdot 2)^\alpha}{(2+2)^\beta} + |E_{2,3}[L(G)]|\frac{(2\cdot 3)^\alpha}{(2+3)^\beta} + |E_{3,3}[L(G)]|\frac{(3\cdot 3)^\alpha}{(3+3)^\beta}$$

$$+ |E_{3,4}[L(G)]|\frac{(3\cdot 4)^\alpha}{(3+4)^\beta} + |E_{4,4}[L(G)]|\frac{(4\cdot 4)^\alpha}{(4+4)^\beta}$$

$$= 4^{1+\alpha-\beta} + 2t\frac{6^\alpha}{5^\beta} + 2\frac{9^\alpha}{6^\beta} + (4t-4)\frac{12^\alpha}{7^\beta} + (2t-4)\frac{16^\alpha}{8^\beta}.$$

Case 4: for $t = 1,\ s = 1$

$$M_{\alpha,\beta}[L(G)] = \sum_{e=uv\in E[L(G)]} \frac{(d_u \cdot d_v)^{\alpha}}{(d_u + d_v)^{\beta}}$$
$$= \mid E_{2,2}[L(G)] \mid \frac{(2\cdot 2)^{\alpha}}{(2+2)^{\beta}}$$
$$= 6 \cdot 4^{\alpha-\beta}.$$

□

Remark:

(1) If $\alpha = 0$ and $\beta = -1$, we get the first Zagreb index $M_1[L(G)]$ of the line graph L(G) of Graphene.
(2) If $\alpha = 1$ and $\beta = 0$, we get the second Zagreb index $M_2[L(G)]$ of the line graph L(G) of Graphene.
(3) If $\alpha = -\frac{1}{2}$ and $\beta = 0$, we get the Randic connectivity index $\chi[L(G)]$ of the line graph L(G) of Graphene.
(4) If $\alpha = 0$ and $\beta = \frac{1}{2}$, we get the Sum connectivity index $SCI[L(G)]$ of the line graph L(G) of Graphene.
(5) If $\alpha = 0$ and $\beta = -2$, we get the hyper Zagreb index of $HM_1[L(G)]$ of the line graph L(G)of Graphene.
(6) If $\alpha = 1$ and $\beta = 1$, we get the second refined Zagreb index of $ReZG_2[L(G)]$ of the line graph L(G) of Graphene.
(7) If $\alpha = 1$ and $\beta = -1$, we get the third refined Zagreb index $ReZG_3[L(G)]$ or Inverse sum index of the line graph L(G) of Graphene.

Theorem 3.2. *The Atom-Bond connectivity index of the line graph L(G) of graphene is*

$$ABC[L(G)] = \begin{cases} \frac{(6\sqrt{3}+6\sqrt{10}-18)t+(8\sqrt{6}+6\sqrt{10}-27)s+(18\sqrt{3}-4\sqrt{6}-12\sqrt{10}+9)}{3\sqrt{6}}, & \text{for } t \neq 1,\ s \neq 1 \\ \frac{(8\sqrt{3}+6\sqrt{5})s+(12\sqrt{6}-12\sqrt{3}-6\sqrt{5})}{3\sqrt{3}}, & \text{for } t = 1,\ s \neq 1 \\ \frac{(6\sqrt{3}+30\sqrt{2}+9)t+(6\sqrt{3}+4\sqrt{6}-30\sqrt{2}-18)}{3\sqrt{6}}, & \text{for } t \neq 1,\ s = 1 \\ 3\sqrt{2}, & \text{for } t = 1,\ s = 1 \end{cases}$$

Proof. **Case 1**: for $t \neq 1,\ s \neq 1$

The Atom-Bond connectivity index of the line graph L(G) of graphene $= ABC[L(G)]$

$$= \sum_{e=uv\in E[L(G)]} \sqrt{\frac{d_u + d_v - 2}{d_u \cdot d_v}}$$
$$= \mid E_{2,2}[L(G)] \mid \sqrt{\frac{2+2-2}{2\cdot 2}} + \mid E_{2,3}[L(G)] \mid \sqrt{\frac{2+3-2}{2\cdot 3}} + \mid E_{3,3}[L(G)] \mid \sqrt{\frac{3+3-2}{3\cdot 3}}$$
$$+ \mid E_{3,4}[L(G)] \mid \sqrt{\frac{3+4-2}{3\cdot 4}} + \mid E_{4,4}[L(G)] \mid \sqrt{\frac{4+4-2}{4\cdot 4}}$$
$$= \frac{2}{\sqrt{2}} + \frac{(2t+4)}{\sqrt{2}} + (4s-4)\frac{2}{3} + (4t+4s-8)\frac{\sqrt{5}}{2\sqrt{3}} + (6ts-6s-4t+2)\frac{\sqrt{3}}{2\sqrt{2}}$$
$$= \frac{(6\sqrt{3}+6\sqrt{10}-18)t + (8\sqrt{6}+6\sqrt{10}-27)s + (18\sqrt{3}-4\sqrt{6}-12\sqrt{10}+9)}{3\sqrt{6}}.$$

Case 2: for $t = 1,\ s \neq 1$
$ABC[L(G)]$

$$= \sum_{e=uv\in E[L(G)]} \sqrt{\frac{d_u + d_v - 2}{d_u \cdot d_v}}$$

$$= \mid E_{2,2}[L(G)] \mid \sqrt{\frac{2+2-2}{2\cdot 2}} + \mid E_{2,3}[L(G)] \mid \sqrt{\frac{2+3-2}{2\cdot 3}} + \mid E_{3,3}[L(G)] \mid \sqrt{\frac{3+3-2}{3\cdot 3}}$$

$$+ \mid E_{3,4}[L(G)] \mid \sqrt{\frac{3+4-2}{3\cdot 4}}$$

$$= \frac{4}{\sqrt{2}} + \frac{4}{\sqrt{2}} + (4s-6)\frac{2}{3} + (4s-4)\frac{\sqrt{5}}{2\sqrt{3}}$$

$$= \frac{(8\sqrt{3}+6\sqrt{5})s + (12\sqrt{6} - 12\sqrt{3} - 6\sqrt{5})}{3\sqrt{3}}.$$

Case 3: for $t \neq 1,\ s = 1$
$ABC[L(G)]$

$$= \sum_{e=uv\in E[L(G)]} \sqrt{\frac{d_u + d_v - 2}{d_u \cdot d_v}}$$

$$= \mid E_{2,2}[L(G)] \mid \sqrt{\frac{2+2-2}{2\cdot 2}} + \mid E_{2,3}[L(G)] \mid \sqrt{\frac{2+3-2}{2\cdot 3}} + \mid E_{3,3}[L(G)] \mid \sqrt{\frac{3+3-2}{3\cdot 3}}$$

$$+ \mid E_{3,4}[L(G)] \mid \sqrt{\frac{3+4-2}{3\cdot 4}} + \mid E_{4,4}[L(G)] \mid \sqrt{\frac{4+4-2}{4\cdot 4}}$$

$$= \frac{4}{\sqrt{2}} + \frac{(2t)}{\sqrt{2}} + \frac{4}{3} + (2t-2)\frac{5}{\sqrt{3}} + (t-2)\frac{\sqrt{3}}{\sqrt{2}}$$

$$= \frac{(6\sqrt{3}+30\sqrt{2}+9)t + (12\sqrt{3} + 4\sqrt{6} - 30\sqrt{2} - 18)}{3\sqrt{6}}.$$

Case 4: for $t = 1,\ s = 1$
$ABC[L(G)]$

$$= \sum_{e=uv\in E[L(G)]} \sqrt{\frac{d_u + d_v - 2}{d_u \cdot d_v}}$$

$$= \mid E_{2,2}[L(G)] \mid \sqrt{\frac{2+2-2}{2\cdot 2}}$$

$$= \frac{6}{\sqrt{2}} = 3\sqrt{2}.$$

□

Theorem 3.3. *The Augmented Zagreb index of the line graph $L(G)$ of graphene is*

$$AZI[L(G)] = \begin{cases} \frac{(6144000s-246016)t-697641s-3792343}{54000}, & \text{for } t \neq 1,\ s \neq 1 \\ \frac{(403434s-238559)}{4000}, & \text{for } t = 1,\ s \neq 1 \\ \frac{(11795968t-8247593)}{108000}, & \text{for } t \neq 1,\ s = 1 \\ 48, & \text{for } t = 1,\ s = 1 \end{cases}$$

Proof. **Case 1**: for $t \neq 1,\ s \neq 1$
The Augmented Zagreb index of the line graph L(G) of graphene $= AZI[L(G)]$

$$= \sum_{e=uv\in E[L(G)]} \left(\frac{d_u \cdot d_v}{d_u + d_v - 2}\right)^3$$

$$= \mid E_{2,2}[L(G)] \mid \left(\frac{2\cdot 2}{2+2-2}\right)^3 + \mid E_{2,3}[L(G)] \mid \left(\frac{2\cdot 3}{2+3-2}\right)^3 + \mid E_{3,3}[L(G)] \mid \left(\frac{3\cdot 3}{3+3-2}\right)^3$$

$$+ \mid E_{3,4}[L(G)] \mid \left(\frac{3\cdot 4}{3+4-2}\right)^3 + \mid E_{4,4}[L(G)] \mid \left(\frac{4\cdot 4}{4+4-2}\right)^3$$

$$= 16 + (2t+4)8 + (4s-4)\frac{729}{64} + (4t+4s-8)\frac{1728}{125} + (6ts-6s-4t+2)\frac{512}{27} = \frac{(6144000s - 246016)t - 697}{54000}$$

Case 2: for $t = 1,\ s \neq 1$
$AZI[L(G)]$

$$= \sum_{e=uv\in E[L(G)]} \left(\frac{d_u \cdot d_v}{d_u + d_v - 2}\right)^3$$

$$= \mid E_{2,2}[L(G)] \mid \left(\frac{2\cdot 2}{2+2-2}\right)^3 + \mid E_{2,3}[L(G)] \mid \left(\frac{2\cdot 3}{2+3-2}\right)^3 + \mid E_{3,3}[L(G)] \mid \left(\frac{3\cdot 3}{3+3-2}\right)^3$$

$$+ \mid E_{3,4}[L(G)] \mid \left(\frac{3\cdot 4}{3+4-2}\right)^3$$

$$= 64 + (2s-3)\frac{729}{32} + (4s-4)\frac{1728}{125}$$

$$= \frac{(403434s - 238559)}{4000}.$$

Case 3: for $t \neq 1,\ s = 1$
$AZI[L(G)]$

$$= \sum_{e=uv\in E[L(G)]} \left(\frac{d_u \cdot d_v}{d_u + d_v - 2}\right)^3$$

$$= \mid E_{2,2}[L(G)] \mid \left(\frac{2\cdot 2}{2+2-2}\right)^3 + \mid E_{2,3}[L(G)] \mid \left(\frac{2\cdot 3}{2+3-2}\right)^3 + \mid E_{3,3}[L(G)] \mid \left(\frac{3\cdot 3}{3+3-2}\right)^3$$

$$+ \mid E_{3,4}[L(G)] \mid \left(\frac{3\cdot 4}{3+4-2}\right)^3 + \mid E_{4,4}[L(G)] \mid \left(\frac{4\cdot 4}{4+4-2}\right)^3$$

$$= 32 + 16t + \frac{729}{32} + (4t-4)\frac{1728}{125} + (2t-4)\frac{512}{27}$$

$$= \frac{(11795968t - 8247593)}{108000}.$$

Case 4: for $t = 1,\ s = 1$
$AZI[L(G)]$

$$= \sum_{e=uv\in E[L(G)]} \left(\frac{d_u \cdot d_v}{d_u + d_v - 2}\right)^3$$

$$= \mid E_{2,2}[L(G)] \mid \left(\frac{2\cdot 2}{2+2-2}\right)^3$$

$$= 48.$$

Theorem 3.4. *The Geometric-Arithmetic index of the line graph L(G) of graphene is*

$$GA[L(G)] = \begin{cases} \frac{(80\sqrt{3}-70)s+(210s+80\sqrt{3}+28\sqrt{6}-140)t+(56\sqrt{6}-160\sqrt{3})}{35}, & \text{for } t \neq 1,\ s \neq 1 \\ \frac{(80\sqrt{3}+140)s+(56\sqrt{6}-80\sqrt{3}-70)}{35}, & \text{for } t = 1,\ s \neq 1 \\ \frac{(28\sqrt{6}+80\sqrt{3}+70)t-80\sqrt{3}+70}{35}, & \text{for } t \neq 1,\ s = 1 \\ 6, & \text{for } t = 1,\ s = 1 \end{cases}$$

Proof. **Case 1**: for $t \neq 1,\ s \neq 1$
The Geometric-Arithmetic index of the line graph L(G) of graphene

$$= GA[L(G)]$$
$$= \sum_{e=uv\in E[L(G)]} \frac{2\sqrt{d_u \cdot d_v}}{d_u + d_v}$$
$$= |E_{2,2}[L(G)]| \frac{2\sqrt{2\cdot 2}}{2+2} + |E_{2,3}[L(G)]| \frac{2\sqrt{2\cdot 3}}{2+3} + |E_{3,3}[L(G)]| \frac{2\sqrt{3\cdot 3}}{3+3}$$
$$+ |E_{3,4}[L(G)]| \frac{2\sqrt{3\cdot 4}}{3+4} + |E_{4,4}[L(G)]| \frac{2\sqrt{4\cdot 4}}{4+4}$$
$$= 2 + (4t+8)\frac{\sqrt{6}}{5} + (4s-4) + (16t+16s-32)\frac{\sqrt{3}}{7} + (6ts-6s-4t+2)$$
$$= \frac{(80\sqrt{3}-70)s + (210s+80\sqrt{3}+28\sqrt{6}-140)t + (56\sqrt{6}-160\sqrt{3})}{35}.$$

Case 2: for $t = 1,\ s \neq 1$

$$GA[L(G)]$$
$$= \sum_{e=uv\in E[L(G)]} \frac{2\sqrt{d_u \cdot d_v}}{d_u + d_v}$$
$$= |E_{2,2}[L(G)]| \frac{2\sqrt{2\cdot 2}}{2+2} + |E_{2,3}[L(G)]| \frac{2\sqrt{2\cdot 3}}{2+3} + |E_{3,3}[L(G)]| \frac{2\sqrt{3\cdot 3}}{3+3}$$
$$+ |E_{3,4}[L(G)]| \frac{2\sqrt{3\cdot 4}}{3+4}$$
$$= 4 + 8\frac{\sqrt{6}}{5} + 4s - 6 + (16s-16)\frac{\sqrt{3}}{7}$$
$$= \frac{(80\sqrt{3}+140)s + (56\sqrt{6}-80\sqrt{3}-70)}{35}.$$

Case 3: for $t \neq 1,\ s = 1$

$$GA[L(G)]$$
$$= \sum_{e=uv\in E[L(G)]} \frac{2\sqrt{d_u \cdot d_v}}{d_u + d_v}$$
$$= |E_{2,2}[L(G)]| \frac{2\sqrt{2\cdot 2}}{2+2} + |E_{2,3}[L(G)]| \frac{2\sqrt{2\cdot 3}}{2+3} + |E_{3,3}[L(G)]| \frac{2\sqrt{3\cdot 3}}{3+3}$$
$$+ |E_{3,4}[L(G)]| \frac{2\sqrt{3\cdot 4}}{3+4} + |E_{4,4}[L(G)]| \frac{2\sqrt{4\cdot 4}}{4+4}$$

$= 4t\frac{\sqrt{6}}{5} + (4t-4)\frac{4\sqrt{3}}{7} + 2t + 2$
$= \frac{(28\sqrt{6} + 80\sqrt{3} + 70)t - 80\sqrt{3} + 70}{35}.$

Case 4: for $t = 1,\ s = 1$
$GA[L(G)]$
$= \sum_{e=uv \in E[L(G)]} \frac{2\sqrt{d_u \cdot d_v}}{d_u + d_v}$
$= \mid E_{2,2}[L(G)] \mid \frac{2\sqrt{2 \cdot 2}}{2+2}$
$= 6.$ □

Theorem 3.5. *The Harmonic index of L(G) is*

$$H[L(G)] = \begin{cases} \frac{(315s+198)t+205s-109}{210}, & for\ t \neq 1,\ s > 1 \\ \frac{260s+48}{105}, & for\ t = 1,\ s > 1 \\ \frac{513t+110}{210}, & for\ t \neq 1,\ s = 1 \\ 3, & for\ t = 1,\ s = 1 \end{cases}$$

Proof. **Case 1**: for $t \neq 1,\ s \neq 1$
The Harmonic index of the line graph L(G) of graphene $= H[L(G)]$
$= \sum_{e=uv \in E[L(G)]} \left(\frac{2}{d_u + d_v}\right)$
$= \mid E_{2,2}[L(G)] \mid \left(\frac{2}{2+2}\right) + \mid E_{2,3}[L(G)] \mid \left(\frac{2}{2+3}\right) + \mid E_{3,3}[L(G)] \mid \left(\frac{2}{3+3}\right)$
$+ \mid E_{3,4}[L(G)] \mid \left(\frac{2}{3+4}\right) + \mid E_{4,4}[L(G)] \mid \left(\frac{2}{4+4}\right)$
$= 1 + (2t+4)\frac{2}{5} + (4s-4)\frac{1}{3} + (4t+4s-8)\frac{2}{7} + (6ts - 6s - 4t + 2)\frac{1}{4}$
$= \frac{(315s + 198)t + 205s - 109}{210}.$

Case 2: for $t = 1,\ s \neq 1$
$H[L(G)]$
$= \sum_{e=uv \in E[L(G)]} \left(\frac{2}{d_u + d_v}\right)$
$= \mid E_{2,2}[L(G)] \mid \left(\frac{2}{2+2}\right) + \mid E_{2,3}[L(G)] \mid \left(\frac{2}{2+3}\right) + \mid E_{3,3}[L(G)] \mid \left(\frac{2}{3+3}\right)$
$+ \mid E_{3,4}[L(G)] \mid \left(\frac{2}{3+4}\right)$
$= 2 + \frac{8}{5} + (4s-6)\frac{1}{3} + (4s-4)\frac{2}{7}$
$= \frac{260s + 48}{105}.$

Case 3: for $t \neq 1,\ s = 1$
$H[L(G)]$
$= \sum_{e=uv \in E[L(G)]} \left(\frac{2}{d_u + d_v} \right)$
$= \mid E_{2,2}[L(G)] \mid \left(\frac{2}{2+2} \right) + \mid E_{2,3}[L(G)] \mid \left(\frac{2}{2+3} \right) + \mid E_{3,3}[L(G)] \mid \left(\frac{2}{3+3} \right)$
$+ \mid E_{3,4}[L(G)] \mid \left(\frac{2}{3+4} \right) + \mid E_{4,4}[L(G)] \mid \left(\frac{2}{4+4} \right)$
$= 2 + \frac{4t}{5} + \frac{2}{3} + \frac{8t-8}{7} + \frac{t-2}{2}$
$= \frac{513t + 110}{210}.$

Case 4: for $t = 1,\ s = 1$
$H[L(G)]$
$= \sum_{e=uv \in E[L(G)]} \left(\frac{2}{d_u + d_v} \right)$
$= \mid E_{2,2}[L(G)] \mid \left(\frac{2}{2+2} \right)$
$= 3.$

□

Theorem 3.6. *The Symmetric Division Degree index of the line graph L(G) of graphene is*

$$SDD[L(G)] = \begin{cases} \frac{14t+13s+36ts-24}{3}, & for\ t \neq 1,\ s \neq 1 \\ \frac{49s-11}{3}, & for\ t = 1,\ s \neq 1 \\ \frac{50t-13}{3}, & for\ t \neq 1,\ s = 1 \\ 12, & for\ t = 1,\ s = 1 \end{cases}$$

Proof. **Case 1**: for $t \neq 1,\ s \neq 1$
The Symmetric Division Degree index of the line graph L(G) of graphene $= SDD[L(G)]$
$= \sum_{e=uv \in E[L(G)]} \left(\frac{d_u^2 + d_v^2}{d_u \cdot d_v} \right)$
$= \mid E_{2,2}[L(G)] \mid \left(\frac{2^2+2^2}{2 \cdot 2} \right) + \mid E_{2,3}[L(G)] \mid \left(\frac{2^2+3^2}{2 \cdot 3} \right) + \mid E_{3,3}[L(G)] \mid \left(\frac{3^2+3^2}{3 \cdot 3} \right)$
$+ \mid E_{3,4}[L(G)] \mid \left(\frac{3^2+4^2}{3 \cdot 4} \right) + \mid E_{4,4}[L(G)] \mid \left(\frac{4^2+4^2}{4 \cdot 4} \right)$
$= 4 + (t+2)\frac{13}{3} + (8s-8) + (t+s-2)\frac{25}{3} + (12ts - 12s - 8t + 4)$
$= \frac{14t + 13s + 36ts - 24}{3}.$

Case 2: for $t = 1,\ s \neq 1$
$SDD[L(G)]$

$= \sum_{e=uv\in E[L(G)]} \left(\frac{d_u^2 + d_v^2}{d_u \cdot d_v}\right)$
$= \mid E_{2,2}[L(G)] \mid \left(\frac{2^2+2^2}{2\cdot 2}\right) + \mid E_{2,3}[L(G)] \mid \left(\frac{2^2+3^2}{2\cdot 3}\right) + \mid E_{3,3}[L(G)] \mid \left(\frac{3^2+3^2}{3\cdot 3}\right)$
$+ \mid E_{3,4}[L(G)] \mid \left(\frac{3^2+4^2}{3\cdot 4}\right)$
$= 8 + \frac{26}{3} + (8s-12) + (s-1)\frac{25}{3}$
$= \frac{49s-11}{3}.$

Case 3: for $t \neq 1,\ s = 1$
$SDD[L(G)]$
$= \sum_{e=uv\in E[L(G)]} \left(\frac{d_u^2 + d_v^2}{d_u \cdot d_v}\right)$
$= \mid E_{2,2}[L(G)] \mid \left(\frac{2^2+2^2}{2\cdot 2}\right) + \mid E_{2,3}[L(G)] \mid \left(\frac{2^2+3^2}{2\cdot 3}\right) + \mid E_{3,3}[L(G)] \mid \left(\frac{3^2+3^2}{3\cdot 3}\right)$
$+ \mid E_{3,4}[L(G)] \mid \left(\frac{3^2+4^2}{3\cdot 4}\right) + \mid E_{4,4}[L(G)] \mid \left(\frac{4^2+4^2}{4\cdot 4}\right)$
$= 8 + \frac{13t}{3} + 4 + (t-1)\frac{25}{3} + (4t-8)$
$= \frac{50t-13}{3}.$

Case 4: for $t = 1,\ s = 1$
$SDD[L(G)]$
$= \sum_{e=uv\in E[L(G)]} \left(\frac{d_u^2 + d_v^2}{d_u \cdot d_v}\right)$
$= \mid E_{2,2}[L(G)] \mid \left(\frac{2^2+2^2}{2\cdot 2}\right)$
$= 12.$

□

Theorem 3.7. *The modified first multiple Zagreb index of the line graph L(G) of graphene is*

$$\Pi_1^*[L(G)] = \begin{cases} 4^2 \cdot 5^{2t+4} \cdot 6^{4s-4} \cdot 7^{4t+4s-8} \cdot 8^{6ts-6s-4t+2}, & \text{for } t \neq 1,\ s \neq 1 \\ 4^4 \cdot 5^4 \cdot 6^{4s-6} \cdot 7^{4s-4}, & \text{for } t = 1,\ s \neq 1 \\ 4^4 \cdot 5^{2t} \cdot 6^2 \cdot 7^{4t-4} \cdot 8^{2t-4}, & \text{for } t \neq 1,\ s = 1 \\ 4096, & \text{for } t = 1,\ s = 1 \end{cases}$$

Proof. **Case 1**: for $t \neq 1,\ s \neq 1$
The modified first multiple Zagreb index of the line graph L(G) of graphene = $\Pi_1^*[L(G)]$
$= \prod_{e=uv\in E[L(G)]} (d_u + d_v)$

$= \prod_{e=uv\in E_{2,2}[L(G)]} (d_u + d_v) \cdot \prod_{e=uv\in E_{2,3}[L(G)]} (d_u + d_v) \cdot \prod_{e=uv\in E_{3,3}[L(G)]} (d_u + d_v)$
$\cdot \prod_{e=uv\in E_{3,4}[L(G)]} (d_u + d_v) \cdot \prod_{e=uv\in E_{4,4}[L(G)]} (d_u + d_v)$
$= 4^2 \cdot 5^{2t+4} \cdot 6^{4s-4} \cdot 7^{4t+4s-8} \cdot 8^{6ts-6s-4t+2}.$

Case 2: for $t = 1,\ s \neq 1$
$\Pi_1^*[L(G)]$
$= \prod_{e=uv\in E[L(G)]} (d_u + d_v)$
$= \prod_{e=uv\in E_{2,2}[L(G)]} (d_u + d_v) \cdot \prod_{e=uv\in E_{2,3}[L(G)]} (d_u + d_v) \cdot \prod_{e=uv\in E_{3,3}[L(G)]} (d_u + d_v)$
$\cdot \prod_{e=uv\in E_{3,4}[L(G)]} (d_u + d_v)$
$= 4^4 \cdot 5^4 \cdot 6^{4s-6} \cdot 7^{4s-4}.$

Case 3: for $t \neq 1,\ s = 1$
$\Pi_1^*[L(G)]$
$= \prod_{e=uv\in E[L(G)]} (d_u + d_v)$
$= \prod_{e=uv\in E_{2,2}[L(G)]} (d_u + d_v) \cdot \prod_{e=uv\in E_{2,3}[L(G)]} (d_u + d_v) \cdot \prod_{e=uv\in E_{3,3}[L(G)]} (d_u + d_v)$
$\cdot \prod_{e=uv\in E_{3,4}[L(G)]} (d_u + d_v) \cdot \prod_{e=uv\in E_{4,4}[L(G)]} (d_u + d_v)$
$= 4^4 \cdot 5^{2t} \cdot 6^2 \cdot 7^{4t-4} \cdot 8^{2t-4}.$

Case 4: for $t = 1,\ s = 1$
$\Pi_1^*[L(G)]$
$= \prod_{e=uv\in E[L(G)]} (d_u + d_v)$
$= \prod_{e=uv\in E_{2,2}[L(G)]} (d_u + d_v)$
$= 4096.$ □

Theorem 3.8. *The second multiple Zagreb index of the line graph L(G) of graphene is*

$$\Pi_2[L(G)] = \begin{cases} 4^2 \cdot 6^{2t+4} \cdot 9^{4s-4} \cdot 12^{4t+4s-8} \cdot 16^{6ts-6s-4t+2}, & \text{for } t \neq 1,\ s \neq 1 \\ 4^4 \cdot 6^4 \cdot 9^{4s-6} \cdot 16^{4s-4}, & \text{for } t = 1,\ s \neq 1 \\ 4^4 \cdot 6^{2t} \cdot 9^2 \cdot 12^{4t-4} \cdot 16^{2t-4}, & \text{for } t \neq 1,\ s = 1 \\ 4096, & \text{for } t = 1,\ s = 1 \end{cases}$$

Proof. **Case 1**: for $t \neq 1,\ s \neq 1$
The second multiple Zagreb index of the line graph L(G) of graphene $= \Pi_2[L(G)]$

$$= \prod_{e=uv\in E[L(G)]} (d_u \cdot d_v)$$
$$= \prod_{e=uv\in E_{2,2}[L(G)]} (d_u \cdot d_v) \cdot \prod_{e=uv\in E_{2,3}[L(G)]} (d_u \cdot d_v) \cdot \prod_{e=uv\in E_{3,3}[L(G)]} (d_u \cdot d_v)$$
$$\cdot \prod_{e=uv\in E_{3,4}[L(G)]} (d_u \cdot d_v) \cdot \prod_{e=uv\in E_{4,4}[L(G)]} (d_u \cdot d_v)$$
$$= 4^2 \cdot 6^{2t+4} \cdot 9^{4s-4} \cdot 12^{4t+4s-8} \cdot 16^{6ts-6s-4t+2}.$$

Case 2: for $t = 1,\ s \neq 1$
$\Pi_2[L(G)]$
$$= \prod_{e=uv\in E[L(G)]} (d_u \cdot d_v)$$
$$= \prod_{e=uv\in E_{2,2}[L(G)]} (d_u \cdot d_v) \cdot \prod_{e=uv\in E_{2,3}[L(G)]} (d_u \cdot d_v) \cdot \prod_{e=uv\in E_{3,3}[L(G)]} (d_u \cdot d_v)$$
$$\cdot \prod_{e=uv\in E_{3,4}[L(G)]} (d_u \cdot d_v)$$
$$= 4^4 \cdot 6^4 \cdot 9^{4s-6} \cdot 16^{4s-4}.$$

Case 3: for $t \neq 1,\ s = 1$
$\Pi_2[L(G)]$
$$= \prod_{e=uv\in E[L(G)]} (d_u \cdot d_v)$$
$$= \prod_{e=uv\in E_{2,2}[L(G)]} (d_u \cdot d_v) \cdot \prod_{e=uv\in E_{2,3}[L(G)]} (d_u \cdot d_v) \cdot \prod_{e=uv\in E_{3,3}[L(G)]} (d_u \cdot d_v)$$
$$\cdot \prod_{e=uv\in E_{3,4}[L(G)]} (d_u \cdot d_v) \cdot \prod_{e=uv\in E_{4,4}[L(G)]} (d_u \cdot d_v)$$
$$= 4^4 \cdot 6^{2t} \cdot 9^2 \cdot 12^{4t-4} \cdot 16^{2t-4}.$$

Case 4: for $t = 1,\ s = 1$
$\Pi_2[L(G)]$
$$= \prod_{e=uv\in E[L(G)]} (d_u \cdot d_v)$$
$$= \prod_{e=uv\in E_{2,2}[L(G)]} (d_u \cdot d_v)$$
$$= 4096.$$ □

Theorem 3.9. *The first Zagreb polynomial of the line graph $L(G)$ of graphene is*
$$ZG_1(L(G),x) = \begin{cases} 2x^4 + (2t+4)x^5 + (4s-4)x^6 + (4t+4s-8)x^7 + (6ts-6s-4t+2)x^8, \\ \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \textit{for } t \neq 1,\ s \neq 1 \\ 4x^4 + 4x^5 + (4s-6)x^6 + (4s-4)x^7, \ \ \textit{for } t = 1,\ s \neq 1 \\ 4x^4 + 2tx^5 + 2x^6 + (4t-4)x^7 + (2t-4)x^8, \ \ \textit{for } t \neq 1,\ s = 1 \\ 6x^4, \ \ \textit{for } t = 1,\ s = 1 \end{cases}$$

Proof. **Case 1**: for $t \neq 1,\ s \neq 1$

The first Zagreb polynomial of the line graph L(G) of graphene = $ZG_1(L(G), x)$

$= \sum_{e=uv \in E[L(G)]} x^{d_u + d_v}$

$= |\ E_{2,2}[L(G)]\ |\ x^{2+2} + |\ E_{2,3}[L(G)]\ |\ x^{2+3} + |\ E_{3,3}[L(G)]\ |\ x^{3+3} + |\ E_{3,4}[L(G)]\ |\ x^{3+4} + |\ E_{4,4}[L(G)]\ |\ x^{4+4}$

$= 2x^4 + (2t+4)x^5 + (4s-4)x^6 + (4t+4s-8)x^7 + (6ts-6s-4t+2)x^8.$

Case 2: for $t = 1,\ s \neq 1$

$ZG_1(L(G), x)$

$= \sum_{e=uv \in E[L(G)]} x^{d_u + d_v}$

$= |\ E_{2,2}[L(G)]\ |\ x^{2+2} + |\ E_{2,3}[L(G)]\ |\ x^{2+3} + |\ E_{3,3}[L(G)]\ |\ x^{3+3} + |\ E_{3,4}[L(G)]\ |\ x^{3+4}$

$= 4x^4 + 4x^5 + (4s-6)x^6 + (4s-4)x^7.$

Case 3: for $t \neq 1,\ s = 1$

$ZG_1(L(G), x)$

$= |\ E_{2,2}[L(G)]\ |\ x^{2+2} + |\ E_{2,3}[L(G)]\ |\ x^{2+3} + |\ E_{3,3}[L(G)]\ |\ x^{3+3}$

$+ |\ E_{3,4}[L(G)]\ |\ x^{3+4} + |\ E_{4,4}[L(G)]\ |\ x^{4+4}$

$= 4x^4 + 2tx^5 + 2x^6 + (4t-4)x^7 + (2t-4)x^8.$

Case 4: for $t = 1,\ s = 1$

$ZG_1(L(G), x)$

$= |\ E_{2,2}[L(G)]\ |\ x^{2+2}$

$= 6x^4.$ □

Theorem 3.10. *The second Zagreb polynomial of the line graph L(G) of graphene is*

$$ZG_2(L(G), x) = \begin{cases} 2x^4 + (2t+4)x^6 + (4s-4)x^9 + (4t+4s-8)x^{12} + (6ts-6s-4t+2)x^{16}, \\ \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \textit{for } t \neq 1,\ s \neq 1 \\ 4x^4 + 4x^6 + (4s-6)x^9 + (4s-4)x^{12}, \ \textit{for } t = 1,\ s \neq 1 \\ 4x^4 + 2tx^6 + 2x^9 + (4t-4)x^{12} + (2t-4)x^{16}, \ \textit{for } t \neq 1,\ s = 1 \\ 6x^4, \ \textit{for } t = 1,\ s = 1 \end{cases}$$

Proof. **Case 1**: for $t \neq 1,\ s \neq 1$

The second Zagreb polynomial of the line graph L(G) of graphene = $ZG_2(L(G), x)$

$= \sum_{e=uv \in E[L(G)]} x^{d_u \cdot d_v}$

$= |\ E_{2,2}[L(G)]\ |\ x^{2 \cdot 2} + |\ E_{2,3}[L(G)]\ |\ x^{2 \cdot 3} + |\ E_{3,3}[L(G)]\ |\ x^{3 \cdot 3}$

$+ |\ E_{3,4}[L(G)]\ |\ x^{3 \cdot 4} + |\ E_{4,4}[L(G)]\ |\ x^{4 \cdot 4}$

$= 2x^4 + (2t+4)x^6 + (4s-4)x^9 + (4t+4s-8)x^{12} + (6ts-6s-4t+2)x^{16}.$

Case 2: for $t = 1,\ s \neq 1$

$ZG_2(L(G), x)$

$= \sum_{e=uv \in E[L(G)]} x^{d_u \cdot d_v}$

$= \mid E_{2,2}[L(G)] \mid x^{2\cdot 2} + \mid E_{2,3}[L(G)] \mid x^{2\cdot 3} + \mid E_{3,3}[L(G)] \mid x^{3\cdot 3}$
$+ \mid E_{3,4}[L(G)] \mid x^{3\cdot 4}$
$= 4x^4 + 4x^6 + (4s-6)x^9 + (4s-4)x^{12}.$

Case 3: for $t \neq 1,\ s = 1$
$ZG_2(L(G), x)$
$= \sum_{e=uv \in E[L(G)]} x^{d_u \cdot d_v}$
$= \mid E_{2,2}[L(G)] \mid x^{2\cdot 2} + \mid E_{2,3}[L(G)] \mid x^{2\cdot 3} + \mid E_{3,3}[L(G)] \mid x^{3\cdot 3}$
$+ \mid E_{3,4}[L(G)] \mid x^{3\cdot 4} + \mid E_{4,4}[L(G)] \mid x^{4\cdot 4}$
$= 4x^4 + 2tx^6 + 2x^9 + (4t-4)x^{12} + (2t-4)x^{16}.$

Case 4: for $t = 1,\ s = 1$
$ZG_2(L(G), x)$
$= \sum_{e=uv \in E[L(G)]} x^{d_u \cdot d_v}$
$= \mid E_{2,2}[L(G)] \mid x^{2\cdot 2}$
$= 6x^4.$

□

Theorem 3.11. *The third Zagreb polynomial of the line graph $L(G)$ of graphene is*

$$ZG_3(L(G), x) = \begin{cases} (6t+4s-4)x + 6ts - 2s - 4t, & \text{for } t \neq 1,\ s \neq 1 \\ 4sx + 4s - 2, & \text{for } t = 1,\ s \neq 1 \\ (6t-4)x + 2t + 2, & \text{for } t \neq 1,\ s = 1 \\ 6, & \text{for } t = 1,\ s = 1 \end{cases}$$

Proof. **Case 1**: for $t \neq 1,\ s \neq 1$
The third Zagreb polynomial of the line graph L(G) of graphene $= ZG_3(L(G), x)$
$= \sum_{e=uv \in E[L(G)]} x^{|d_u - d_v|}$
$= \mid E_{2,2}[L(G)] \mid x^{|2-2|} + \mid E_{2,3}[L(G)] \mid x^{|2-3|} + \mid E_{3,3}[L(G)] \mid x^{|3-3|}$
$+ \mid E_{3,4}[L(G)] \mid x^{|3-4|} + \mid E_{4,4}[L(G)] \mid x^{|4-4|}$
$= (6t+4s-4)x + 6ts - 2s - 4t.$

Case 2: for $t = 1,\ s \neq 1$
$ZG_3(L(G), x)$
$= \sum_{e=uv \in E[L(G)]} x^{|d_u - d_v|}$
$= \mid E_{2,2}[L(G)] \mid x^{|2-2|} + \mid E_{2,3}[L(G)] \mid x^{|2-3|} + \mid E_{3,3}[L(G)] \mid x^{|3-3|}$
$+ \mid E_{3,4}[L(G)] \mid x^{|3-4|}$
$= 4sx + 4s - 2.$

Case 3: for $t \neq 1,\ s = 1$
$ZG_3(L(G), x)$

$= \sum_{e=uv \in E[L(G)]} x^{|d_u - d_v|}$
$= | E_{2,2}[L(G)] | x^{|2-2|} + | E_{2,3}[L(G)] | x^{|2-3|} + | E_{3,3}[L(G)] | x^{|3-3|}$
$+ | E_{3,4}[L(G)] | x^{|3-4|} + | E_{4,4}[L(G)] | x^{|4-4|}$
$= (6t - 4)x + 2t + 2.$

Case 4: for $t = 1$, $s = 1$
$ZG_3(L(G), x)$
$= \sum_{e=uv \in E[L(G)]} x^{|d_u - d_v|}$
$= | E_{2,2}[L(G)] | x^{|2-2|}$
$= 6.$ □

References

[1] Ali Astanesh-Asl and G. H. Fath-Taber, Computing the first and third Zagreb polynomials of certain products of graphs, Irainan J. Math. Chem., 2(2) (2011), 73-78.

[2] M. Eliasi, A. Iranmanesh and I. Gutman, Multiplicative versions of first Zagreb index, MATCH Commun. Math. Comput. Chem., 68 (2012) 217-230.

[3] E. Estrada, L. Torres, L. Rodr?guez and I. Gutman, An atom-bond connectivity index: modelling the enthalpy of formation of alkanes, Indian J. Chem., 37A (1998) 849-855.

[4] G. H. Fath-Tabar, Old and New Zagreb indices of Graphs, MATCH Commun. Math. Comput. Chem., 65 (2011) 79-84.

[5] G. H. Fath-Tabar, Zagreb polynomial and pi indices of some Nano structure, Dig. J. Nanomaterials & Biostructures, 4(1) (2009), 189-191.

[6] B. Furtula, A. Graovac and D. Vukicevic, Augmented Zagreb index, J. Math. Chem., 48 (2010) 370-380.

[7] I. Gutman and N. Trinajstic, Graph theory and molecular orbitals. Total π-electron energy of alternant hydrocarbons, Chem. Phys. Lett., 17 (1972) 535-538.

[8] I. Gutman, E. Milovanovic and I. Milovanovic, Beyond the Zagreb indicies, AKCE International Journal of Graphs and Combinatorics, (2018), (Aricle in press).

[9] I. Gutman, Multiplicative Zagreb Indices of Trees, Bull. Soc. Math. Banja Luka., 1 (2011) 13-19.

[10] Gul E Mehak and Akhlaq Ahmad Bhatti, Forgotten Topological index of line graphs of some chemical structures in drugs, ACTA CHEMICA IASI, 26_2 (2018), 181 - 206.

[11] M. Randic, On characterization of molecular branching, J. Amer. Chem. Soc., 97 (1975) 6609-6615.

[12] P. S. Ranjini, V. Lokesha and A. Usha, Relation between phenylene and hexagonal squeeze using harmonic index, International Journal of Graph Theory, 1 (2013), 116-121.

[13] K. V. S. Sarma and I. H. Nagaraja Rao, On the fourth Zagreb index of a graph, International Journal of Mathematical archive, 5(12) (2014), 136-141.

[14] G. H. Shirdel, H. Rezapour and A. M. Sayadi, The Hyper-Zagreb index of graph operations, Irainan J. Math. Chem., 4(2) (2013) 213-220.

[15] G. Sridhara, M. R. Rajesh kanna and R. S. Indumathi, Computation of Topological Indices of Graphene, Article in Journal of Naomaterials, Volume 2015.

[16] N. Trinajstic, Chemical Graph Theory, Mathematical Chemistry Series, CRC Press, Boca Raton, Fla, USA, 2nd edition, 1992.

[17] D. Vukicevic and B. Furtula, Toplological index based on the ratios of geometrical and arithmetical means of end-vertex degrees of edges, J. Math. Chem., 46 (2009), 1369-1376.

[18] D. Vukicevic and M. Gasperov, Bond additive modeling 1. Adriatic indices, Croat. Chem. Acta, 83(3) (2010), 243-260.

[19] L. Zhong, The harmonic index on graphs, Appl. Math. Lett., 25 (2012) 561-566.

[20] B. Zhou and N. Trinajstic, On a novel connectivity index, J. Math. Chem., 46 (2009) 1252-1270.