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Computation of Leap Zagreb Indices of Graphene

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ABSTRACT

Based on second distance degrees of the vertices, A.M. Naji et al. defined Leap Zagreb indices of Graphs. In this article, we have computed first, second and third Leap Zagreb indices of Graphene.

Mathematics Subject Classification: Primary 05C50, 05C69.

Key words: Topological index, Zagreb index, First Leap Zagreb Index, Second Leap Zagreb Index, Third Leap Zagreb Index, Graphene.

INTRODUCTION

In the article [1] Sridhara and his co-authors mentioned “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”.

In this article we considered only finite, connected, undirected graphs without multiple edges and loops. Let G be a graph with a vertex set V (G) and an edge set E(G). A molecular graph is a connected graph whose vertices and edges corresponds to the atoms and chemical bonds. The structures of chemical compounds are described by molecular descriptors which are nothing but topological indices. They help us to forecast certain physical and chemical properties like enthalpy of vaporization, stability, boiling point, etc.

In the paper [1] Sridhar and his co-authors determined some basic topological indices of Graphene. One of the most used topological indices with high correlation with many physical and chemical indices of molecular compounds is the Wiener index which was studied in [2]. The Zagreb indices were first introduced in [3] where the authors examined the dependence of total pi-electron energy of molecular structures. For a molecular graph, the first Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$ are defined, respectively, as follows.

$$M_1(G) = \sum_{v \in V(G)} d^2(v)$$

$$M_2(G) = \sum_{uv \in E(G)} d(u)d(v)$$

Motivated by this, in 2017, Naji et al., [4] have introduced a new distance-degree-based topological indices conceived depending on the second degrees of vertices, and are so-called leap Zagreb indices of a graph G and are defined as:

$$LM_1(G) = \sum_{v \in V(G)} d_2^2(v/G)$$

$$LM_2(G) = \sum_{uv \in E(G)} d_2(u/G)\, \boldsymbol{d_2(v/G)}$$

$$LM_3(G) = \sum_{uv \in E(G)} (d_2(u/G) + \boldsymbol{d_2(v/G)})$$

The leap Zagreb indices have several chemical applications. Surprisingly, the first leap Zagreb index has very good correlation with physical properties of chemical compound, like boiling point, entropy, DHVAP, HVAP and eccentric factor [5].

MAIN RESULTS AND DISCUSSION

Theorem 2.1: First Leap Zagreb index of Graphene with 'R' rows and 'K' benzene rings in each row is given by

$$LM_1(G) = \begin{cases} 24 & \text{If } R = K = 1 \\ 50K - 16 & \text{If } R = 1 \text{ and } K \geq 2 \\ 68R - 52 & \text{If } R \geq 2 \text{ and } K = 1 \\ 14(18K - R - 2K - 12) & \text{If } R \neq 1 \text{ and } K \neq 1. \end{cases}$$

Proof: Consider a graphene with R rows and K benzene rings in each rows. We can show that Graphene contains $2R + 2K + 2RK$ vertices and $2R + 2K + 3RK - 1$ edges.

Case1: If $R \neq 1$ and $K \neq 1$.

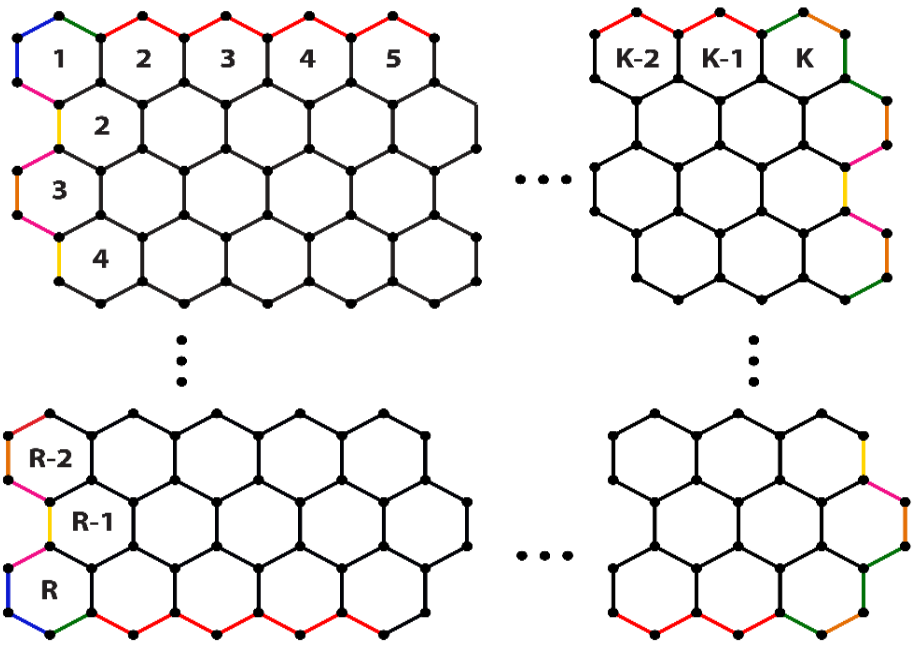

Fig-1

In this case Graphene contains vertices of 2-degrees 2, 3, 4, 5 and 6 only and we can partition the vertices of Graphene into five sets, viz. V_2, V_3, V_4, V_5 and V_6, where each set V_i represents the collection of all vertices with 2-degree i. The number of vertices of 2-degree 2, 3, 4, 5 and 6 are given in the following table-1.

TABLE – 1

Vertices of 2-degree i	$V_2(G)$	$V_3(G)$	$V_4(G)$	$V_5(G)$	$V_6(G)$
Frequency	2	2R+4	4(K-1)	2R-4	(2R-2)(K-1)

Consider,

$$LM_1(G) = \sum_{v\in V(G)} d_2^2(v/G)$$

$$= \sum_{v\in V_2(G)} d_2^2(v/G) + \sum_{v\in V_3(G)} d_2^2(v/G) + \sum_{v\in V_4(G)} d_2^2(v/G) + \sum_{v\in V_5(G)} d_2^2(v/G) + \sum_{v\in V_6(G)} d_2^2(v/G)$$

$$= 2(2)^2 + (2R+4)3^2 + 4(K-1)4^2 + (2R-4)5^2 + (2R-2)(K-1)6^2$$

= 8 + 9(2R+4) + 64(K-1) + 25(2R-4) + 36(2R-2)(K-1)

= 8 + 18R + 36 + 64K -64 + 50R – 100 + 36[2RK-2R-2K+2]

= -4R – 8K + 72RK – 48

= 4(18RK- R – 2K- 12).

Case2: If R=1 and K ≥ 2.

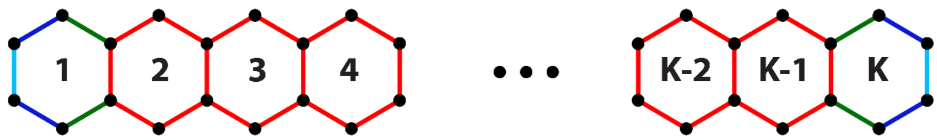

Fig-2

In this case Graphene contains vertices of 2-degrees 2, 3 and 4 only and we can partition the vertex set in to three sets as V_2, V_3 and V_4 , where each set is the collection of vertices with 2-degree i. i.e., $V_i = \{ v\in V(G)/\ d_i(v) = i\}$ for i=2, 3, 4. The frequency of such vertices are shown in the following table-2.

TABLE -2

Vertices of 2-degree i	$V_2(G)$	$V_3(G)$	$V_4(G)$
Frequency	4	2K	2K-2

Consider,

$$\mathrm{LM_1(G)} = \sum_{\mathrm{v \in V(G)}} \mathrm{d_2^2(v/G)}$$

$$= \sum\nolimits_{\mathrm{v \in V_2(G)}} \mathrm{d_2^2(v/G)} + \sum\nolimits_{\mathrm{v \in V_3(G)}} \mathrm{d_2^2(v/G)} + \sum\nolimits_{\mathrm{v \in V_4(G)}} \mathrm{d_2^2(v/G)}$$

$$= 4(2)^2 + 2\mathrm{K}(3)^2 + (2\mathrm{K}-2)4^2$$

= 4(4) +2K(9) + 16(2K-2)

= 16 + 18K+ 32K – 32

= 50K-16.

Case3: If K=1 $and\ R \geq 2$

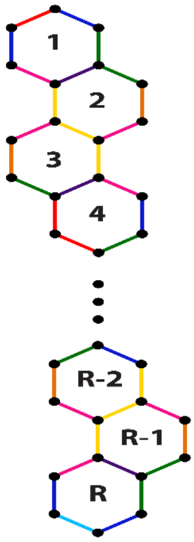

Fig-3

In this case Graphene contains vertices of 2-degrees 2, 3, 4 and 5 only and we can partition the vertex set in to four sets, V_2, V_3, V_4 and V_5 respectively, where each set is the collection of vertices with 2-degree i. The frequency of such vertices are shown in the following table-3.

TABLE -3

Vertices of 2-degree i	$V_2(G)$	$V_3(G)$	$V_4(G)$	$V_5(G)$
Frequency	4	2R	2	2R-4

$\mathrm{L}M_1(G) = 4(2)^2 + 2R(3)^2 + 2(4)^2 + (2R-4)5^2$

= 4(4) + 2R(9) + 2(16) +25(2R-4)

= 16 + 18R + 32 + 50R – 100

= 68R – 52.

Case 4: If R =1 and K = 1

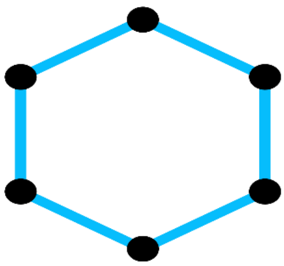

Fig-4

In this case Graphene contains vertices of 2-degree 2 only.

TABLE -4

Vertices of 2-degree i	$V_2(G)$
Frequency	6

Consider, $\mathrm{L}M_1(G) = 6(2)^2$

=24

$$\text{Therefore, } \mathrm{L}M_1(G) = \begin{cases} 24 & \text{If R} = \text{K} = 1 \\ 50\text{K} - 16 & \text{If R} = 1 \text{ and K} \geq 2 \\ 68\text{R} - 52 & \text{If R} \geq 2 \text{ and K} = 1 \\ 4(18\text{K} - \text{R} - 2\text{K} - 12) & \text{If R} \neq 1 \text{ and K} \neq 1 \end{cases}$$

Theorem 2.2: Second Leap Zagreb index of Graphene with 'R' rows and 'K' benzene rings in each row is given by,

$$LM_2(G) = \begin{cases} 24 & \text{If R} = \text{K} = 1 \\ 96 & If\ R = 2\ and\ K = 1 \\ 89R - 83 & If\ R \geq 3\ and\ K = 1 \\ 64K - 32 & If\ R = 1\ and\ K \geq 2 \\ 108RK - 20R - 32K - 58 & If\ R \neq 1\ and\ K \neq 1 \end{cases}$$

Proof:

Case1: If R$\neq$ 1 and K$\neq$ 1

In this case Graphene contains vertices of 2-degrees 2, 3, 4, 5 and 6 and edges of the type $e_{2,3}, e_{3,3}, e_{3,4}, e_{3,5}, e_{4,4}, e_{4,6}, e_{5,5}, e_{5,6}$ $and\ e_{6,6}\ respectively$. The frequency of such edges are shown in the following table-5, $where\ E_{i,j}$ is the collection of all edges joining the vertices of 2-degrees i and j in G.

TABLE-5

Edge type	$E_{2,3}$	$E_{3,3}$	$E_{3,4}$	$E_{3,5}$	$E_{4,4}$	$E_{4,6}$	$E_{5,5}$	$E_{5,6}$	$E_{6,6}$
Frequency	4	R	8	2R-4	4K-8	2K	R-2	2R-4	3RK-4R-4K+5

$$LM_2(G) = \sum_{uv\in E(G)} d_2(u/G)\, \boldsymbol{d_2(v/G)}$$

$$= \sum_{uv\in E_{2,3}(G)} d_2(u/G)\, \boldsymbol{d_2(v/G)} \sum_{uv\in E_{3,3}(G)} d_2(u/G)\, \boldsymbol{d_2(G)} + \sum_{uv\in E_{3,4}(G)} d_2(u/G)\, \boldsymbol{d_2(G)} +$$

$$\sum_{\mathrm{uv\in E_{3,5}(G)}} \mathrm{d_2(u/G)\, d_2(v/G)} + \sum_{uv\in E_{4,4}(G)} d_2(u/G)\, \boldsymbol{d_2(v/G)} + \sum_{uv\in E_{4,6}(G)} d_2(u/G)\, \boldsymbol{d_2(v/G)}$$
$$+ \sum_{uv\in E_{5,5}(G)} d_2(u/G)\, \boldsymbol{d_2(v/G)}$$
$$+ \sum_{uv\in E_{5,6}(G)} d_2(u/G)\, \boldsymbol{d_2(v/G)} \sum_{uv\in E_{6,6}(G)} d_2(u/G)\, \boldsymbol{d_2(v/G)}$$

= 4(2×3)+R(3×3)+8(3× 4)+(2R-4)(3× 5)+(4K-8)(4× 4)+2K(4× 6)+(R-2)(5× 5)+(2R-4)(5× 6)+(3RK-4R-4K+5)(6× 6)

= 4× 6+R× 9+8× 12+(2R-4)(15)+(4K-8)(16)+2K(24)+(R-2)(25)+(2R-4)30+(3RK-4R-4K+5)36

= -58-20R-32K+108RK.

Case 2: If R=1 and K$\geq$2.

In this case Graphene contains vertices of 2-defrees 2, 3 and 4 and edges of the type $e_{2,2}, e_{2,3}, e_{3,4}$ $and\ \ e_{4,4}\ respectively$. We can partition the edge set of Graphene into sets $E_{2,2},\ E_{2,3}, E_{3,4}$ $and\ E_{4,4}. Here\ the\ set\ E_{i,j}$ denotes the collection of all edges joining the vertices of 2-degrees i and j. The number of elements in each such set is given in the following table-6

TABLE-6

Edge type sets	$E_{2,2}$	$E_{2,3}$	$E_{3,4}$	$E_{4,4}$
frequency	2	4	4(K-1)	K-1

$$LM_2(G) = \sum_{uv\in E(G)} d_2(u/G)\, \boldsymbol{d_2(v/G)}$$

$$\sum_{uv\in E_{2,2}(G)} d_2(u/G)\, \boldsymbol{d_2(v/G)}$$

$$+ \sum_{uv\in E_{2,3}(G)} d_2(u/G)\, \boldsymbol{d_2(v\big/G)} + \sum_{uv\in E_{3,4}(G)} d_2(u/G)\, \boldsymbol{d_2(v\big/G)} + \sum_{uv\in E_{4,4}(G)} d_2(u/G)\, \boldsymbol{d_2(v/G)}$$

= 2×(2× 2)+ 4× (2 × 3)+4(K-1)(3× 4)+(K-1)(4× 4)

= 2× 4+4× 6+(4K-4)12+(K-1)16

= 32(2K-1).

Case 3: If K=1 and $R \geq 3$

In this case Graphene contains edges of the types $e_{2,2}, e_{2,3}, e_{3,3}, e_{3,4}, e_{3,5}, e_{4,5}$ *and* $e_{5,5}$ *respectively*. We can partition the edge set of Graphene into sets $E_{2,2}, E_{2,3}, E_{3,3}, E_{3,4}, E_{3,5}, E_{4,5}$ *and* $E_{5,5}$. *Here the set* $E_{i,j}$ denotes the collection of all edges joining the vertices of 2-degrees i and j. The number of elements in each such set is given in the following table-7.

TABLE-7

Edge type sets	$E_{2,2}$	$E_{2,3}$	$E_{3,3}$	$E_{3,4}$	$E_{3,5}$	$E_{4,5}$	$E_{5,5}$
Frequency	2	4	R-2	4	2R-4	2	2R-5

$$LM_2(G) = \sum_{uv\in E(G)} d_2(u/G)\, \boldsymbol{d_2(v/G)}$$

$$= \sum_{uv\in E_{2,2}(G)} d_2(u/G)\, \boldsymbol{d_2(v/G)}$$

$$+ \sum_{uv\in E_{2,3}(G)} d_2(u/G)\, \boldsymbol{d_2(v/G)} + \sum_{uv\in E_{3,3}(G)} d_2(u/G)\, \boldsymbol{d_2(v/G)}$$

$$+ \sum_{uv\in E_{3,4}(G)} d_2(u/G)\, \boldsymbol{d_2(v/G)} + \sum_{uv\in E_{3,5}(G)} d_2(u/G)\, \boldsymbol{d_2(v/G)}$$

$$+ \sum_{uv\in E_{4,5}(G)} d_2(u/G)\, \boldsymbol{d_2(v/G)} + \sum_{uv\in E_{5,5}(G)} d_2(u/G)\, \boldsymbol{d_2(v/G)}$$

= 2(2×2)+4(2×3)+(R-2)(3× 3)+4(3× 4)+(2R-4)(3× 5)+2(4× 5)+(2R-5)(5× 5)

= 2× 4+4× 6+(R-2)9+4× 12+(2R-4)(15)+2(20)+(2R-5)(25)

= -83+89R

Case 4: If K=1 and R=2

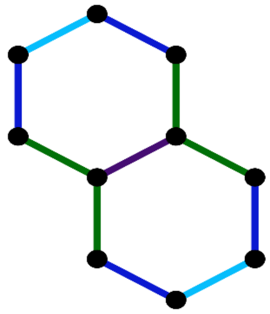

Fig-5

In this case Graphene contains edges of the types $e_{2,2},\ e_{2,3}, e_{3,4}$ *and* $e_{4,4}$ *respectively*. We can partition the edge set of Graphene into sets $E_{2,2},\ E_{2,3},\ E_{3,4},$ *and* $E_{4,4}$. *Here the set* $E_{i,j}$ denotes the collection of all edges joining the vertices of 2-degrees i and j. The number of elements in each such set is given in the following table-8.

TABLE-8

Edge type sets	$E_{2,2}$	$E_{2,3}$	$E_{3,4}$	$E_{4,4}$
Frequency	2	4	4	1

$$LM_2(G) = \sum_{uv\in E(G)} d_2(u/G)\, \boldsymbol{d_2(v/G)}$$

$$\sum_{uv\in E_{2,2}(G)} d_2(u/G)\, \boldsymbol{d_2(v/G)}$$

$$+ \sum_{uv\in E_{2,3}(G)} d_2(u/G)\, \boldsymbol{d_2(v/G)} + \sum_{uv\in E_{3,4}(G)} d_2(u/G)\, \boldsymbol{d_2(v/G)}$$

$$+ \sum_{uv\in E_{4,4}(G)} d_2(u/G)\, \boldsymbol{d_2(v/G)}$$

= 2×(2× 2)+ 4× (2 × 3)+4(3× 4)+1(4× 4)

= 2× 4+4× 6+4×12+1×16

= 8+24+48+16

=96.

Case 5: If R=1 and K=1

In this case Graphene contains edges of the types $e_{2,2}$ only.

TABLE -9

Edge type sets	$E_{2,2}$
Frequency	6

$$LM_2(G) = \sum_{uv\in E(G)} d_2(u/G)\, \boldsymbol{d_2(v/G)}$$

$$= \sum_{uv\in E_{2,2}(G)} d_2(u/G)\, \boldsymbol{d_2(v/G)}$$

$$= 6\times (2 \times 2)$$

$$= 6\times 4$$

$$= 24.$$

$$Hence, \quad LM_2(G) = \begin{cases} 24 & \text{If R} = \text{K} = 1 \\ 96 & If\ R = 2\ and\ K = 1 \\ 89R - 83 & If\ R \geq 3\ and\ K = 1 \\ 64K - 32 & If\ R = 1\ and\ K \geq 2 \\ 108RK - 20R - 32K - 58 & If\ R \neq 1\ and\ K \neq 1 \end{cases}$$

Theorem 2.3: Third Leap Zagreb index of Graphene with 'R' rows and 'K' benzene rings in each row is given by,

$$LM_3(G) = \begin{cases} 24 & \text{If R} = \text{K} = 1 \\ 64 & \text{If R} = 2 \text{ and K} = 1 \\ 42R - 20 & \text{If R} \geq 3 \text{ and K} = 1 \\ 36K - 8 & \text{If R} = 1 \text{ and K} \geq 2 \\ 36RK + 6R + 4K - 24 & \text{If R} \neq 1 \text{ and K} \neq 1 \end{cases}$$

Proof: Case 1: If R$\neq$ 1 and K$\neq$ 1

By definition of third Leap Zagreb index and by using table-5 we have

$$LM_3(G) = \sum_{uv\in E(G)} d_2(u/G) + \boldsymbol{d_2(v/G)}$$

$$= \sum_{uv\in E_{2,3}(G)} d_2(u/G) + \boldsymbol{d_2(v/G)} + \sum_{uv\in E_{3,3}(G)} d_2(u/G) + \boldsymbol{d_2(v/G)}$$
$$+ \sum_{uv\in E_{3,4}(G)} d_2(u/G) + \boldsymbol{d_2(v/G)}$$
$$+ \sum_{uv\in E_{3,5}(G)} d_2(u/G) + \boldsymbol{d_2(v/G)}$$
$$+ \sum_{uv\in E_{4,4}(G)} d_2(u/G) + \boldsymbol{d_2(v/G)}$$
$$+ \sum_{uv\in E_{4,6}(G)} d_2(u/G) + \boldsymbol{d_2(v/G)}$$
$$+ \sum_{uv\in E_{5,5}(G)} d_2(u/G) + \boldsymbol{d_2(v/G)}$$
$$+ \sum_{uv\in E_{5,6}(G)} d_2(u/G) + \boldsymbol{d_2(v/G)}$$
$$+ \sum_{uv\in E_{6,6}(G)} d_2(u/G) + \boldsymbol{d_2(v/G)}$$

= 4(2+3) + R(3+3) +8(3+4)+(2R-4)(3+5)+(4K-8)(4+4)+2K(4+6)+(R-2)(5+5)+(2R- 4)(5+6)+(3RK-4R-4K+5)(6+6)

= 4× 5+R(6) + 8(7) +(2R-4)(8)+(4K-8)(8)+2K(10)+(R-2)(10)+(2R-4)(11)+(3RK-4R-4K+5)12

= -24+6R+4K+36RK

= 36RK+6R+4K-24.

Case 2: If R=1 and K≥2.

By definition of third Leap Zagreb index and by using table-6 we have

$$LM_3(G) = \sum_{uv\in E(G)} d_2(u/G) + \boldsymbol{d_2(v/G)}$$

$$= \sum_{uv\in E_{2,2}(G)} d_2(u/G) + \boldsymbol{d_2(v/G)}$$
$$+ \sum_{uv\in E_{2,3}(G)} d_2(u/G) + \boldsymbol{d_2(v/G)} + \sum_{uv\in E_{3,4}(G)} d_2(u/G) + \boldsymbol{d_2(v/G)}$$
$$+ \sum_{uv\in E_{4,4}(G)} d_2(u/G) + \boldsymbol{d_2(v/G)}$$

= 2×(2+2)+ 4× (2 + 3)+4(K-1)(3+4)+(K-1)(4+4)

= 2× 4+4× 5+(4K-4)7+(K-1)8

= -8+36K

= 4(9K-2)

Case 3: If K=1 and $R \geq 3$

By definition of third Leap Zagreb index and by using table-7 we have

$$LM_3(G) = \sum_{uv\in E(G)} d_2(u/G) + \boldsymbol{d_2}(\boldsymbol{v}/\boldsymbol{G})$$

$$= \sum_{uv\in E_{2,2}(G)} d_2(u/G) + \boldsymbol{d_2}(\boldsymbol{v}/\boldsymbol{G})$$

$$+ \sum_{uv\in E_{2,3}(G)} d_2(u/G) + \boldsymbol{d_2}(\boldsymbol{v}/\boldsymbol{G}) + \sum_{uv\in E_{3,3}(G)} d_2(u/G) + \boldsymbol{d_2}(\boldsymbol{v}/\boldsymbol{G})$$

$$+ \sum_{uv\in E_{3,4}(G)} d_2(u/G) + \boldsymbol{d_2}(\boldsymbol{v}/\boldsymbol{G}) + \sum_{uv\in E_{3,5}(G)} d_2(u/G) + \boldsymbol{d_2}(\boldsymbol{v}/\boldsymbol{G})$$

$$+ \sum_{uv\in E_{4,5}(G)} d_2(u/G) + \boldsymbol{d_2}(\boldsymbol{v}/\boldsymbol{G}) + \sum_{uv\in E_{5,5}(G)} d_2(u/G) + \boldsymbol{d_2}(\boldsymbol{v}/\boldsymbol{G})$$

= 2(2+2) + 4(2+3) + (R-2)(3+3) + 4(3+4) + (2R-4)(3+5) +2 (4+5) + (2R-5)(5+5)

= 2× 4+4× 5+(R-2)6+4(7)+(2R-4)(8)+2(9)+(2R-5)(10)

= -20+42R

= 42R-20.

Case 4: If K=1 and R=2

By definition of third Leap Zagreb index and by using table-8 we have

$$LM_3(G) = \sum_{uv\in E(G)} d_2(u/G) + \boldsymbol{d_2}(\boldsymbol{v}/\boldsymbol{G})$$

$$= \sum_{uv\in E_{2,2}(G)} d_2(u/G) + \boldsymbol{d_2}(\boldsymbol{v}/\boldsymbol{G}) + \sum_{uv\in E_{2,3}(G)} d_2(u/G) + \boldsymbol{d_2}(\boldsymbol{v}/\boldsymbol{G}) +$$

$$+ \sum_{uv\in E_{3,4}(G)} d_2(u/G) + \boldsymbol{d_2}(\boldsymbol{v}/\boldsymbol{G}) + \sum_{uv\in E_{4,4}(G)} d_2(u/G) + \boldsymbol{d_2}(\boldsymbol{v}/\boldsymbol{G})$$

= 2×(2+2)+ 4× (2 + 3)+4(3+4)+1(4+4)

$= 2\times 4+4\times 5+4\times 7+1(8)$

$= 8+20+28+8$

$= 64$

Case 5: If R=1and K=1

By definition of third Leap Zagreb index and by using table-9 we have

$$LM_3(G) = \sum_{uv\in E(G)} d_2(u/G) + \boldsymbol{d_2(v/G)}$$

$$= \sum_{uv\in E_{2,2}(G)} d_2(u/G) + \boldsymbol{d_2(v/G)}$$

$$= 6\times (2+2)$$

$$= 6\times 4$$

$$= 24$$

Hence, $$LM_3(G) = \begin{cases} 24 & \text{If } R = K = 1 \\ 64 & If\ R = 2\ and\ K = 1 \\ 42R - 20 & If\ R \geq 3\ and\ K = 1 \\ 36K - 8 & If\ R = 1\ and\ K \geq 2 \\ 36RK + 6R + 4K - 24 & If\ R \neq 1\ and\ K \neq 1 \end{cases}$$

CONCLUSIONS:

The first, second and third Leap Zagreb indices of Graphene are calculated without using computer.

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