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Multiplicative 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. Motivated by this Raad Sehen and his co-authors defined multiplicative leap Zagreb indices of Graphs. In this article, we have computed first, second and third multiplicative leap Zagreb indices of Graphene.

Keywords: Topological index, first multiplicative leap Zagreb index, second multiplicative leap Zagreb index, third multiplicative leap Zagreb index.

Contents

1. Introduction

In the article [1], Sridhara and his co-authors stated that "Graphene is an atomic-scale honeycomb lattice composed of carbon atoms. It is the world's first two-dimensional material, which was isolated from graphite in 2004 by Professors Andre Geim and Kostya Novoselov. Graphene is 200 times stronger than steel, one million times thinner than a human hair, and the most conductive material known. Owing to these exceptional properties, it has attracted the attention of scientists, researchers, and industries worldwide. It is considered one of the most promising nanomaterials because of its unique combination of superior properties, enabling its use in a wide range of applications, from electronics to optics, sensors, and biodevices. Furthermore, it is regarded as the most effective material for electromagnetic interference (EMI) shielding." They have also computed several topological indices of graphene in [1,2].

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 correspond 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 vaporisation, stability, boiling point, etc.

In the paper cite 1, Sridhara 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 the 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.

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$$M_1(G) = \sum_{v \in V(G)} d^2(v)$$
$$M_2(G) = \sum_{uv \in E(G)} d(u)d(v)$$

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:

$$LM_1(G) = \sum_{v \in V(G)} d_2^2(v/G).$$
$$LM_2(G) = \sum_{uv \in E(G)} d_2(u/G)d_2(v/G).$$
$$LM_3(G) = \sum_{uv \in E(G)} (d_2(u/G) + d_2(v/G)).$$

The leap Zagreb indices have several chemical applications. Surprisingly, the first leap Zagreb index has very good correlation with physical properties of chemical compounds, like boiling point, entropy, DHVAP, HVAP and eccentric factor [5].
In the year 2020, Raad Sehen et al. [6] introduced multiplicative leap Zagreb indices as follows.

$$L\prod_1(G) = \prod_{v \in V(G)} d_2^2(v/G).$$
$$L\prod_2(G) = \prod_{uv \in E(G)} d_2(u/G)d_2(v/G).$$
$$L\prod_3(G) = \prod_{uv \in E(G)} (d_2(u/G) + d_2(v/G)).$$

In this paper the first, second and third multiplicative leap Zagreb indices of Graphene are calculated without using a computer.

2. Main Results

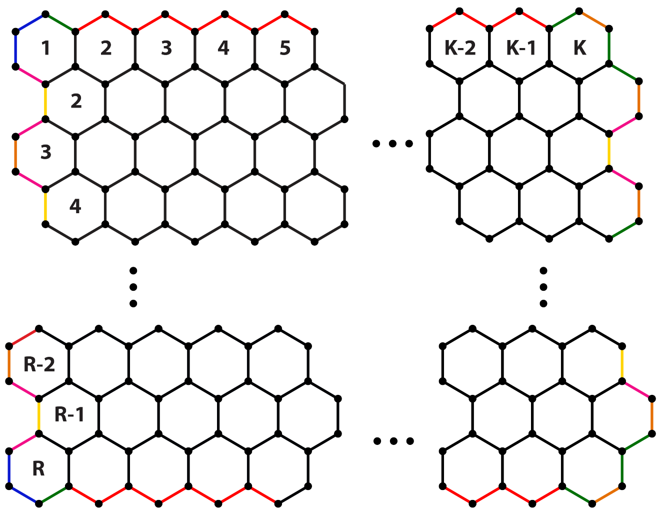
2.1. First multiplicative leap Zagreb index of Graphene

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

$$L\prod_1(G) = \begin{cases} 4096 & \text{if } R = K = 1 \\ 2^{8K} \times 3^{4K} & \text{if } R = 1 \text{ and } K \geq 2 \\ 2^{16} \times 3^{4R} \times 5^{4R-4} & \text{if } R \geq 2 \text{ and } K = 1 \\ 2^{4(-2+3k+RK-R)} \times 3^{4(3+RK-K)} \times 5^{4(R-2)} & \text{if } R \neq 1 \text{ and } K \neq 1. \end{cases}$$

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

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



In this case, Graphene contains vertices of 2-degrees 2, 3, 4, 5 and 6. Therefore, 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 vertices of 2-degree i. The number of vertices of 2-degree 2, 3, 4, 5 and 6 are given in the following 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).

Table-1

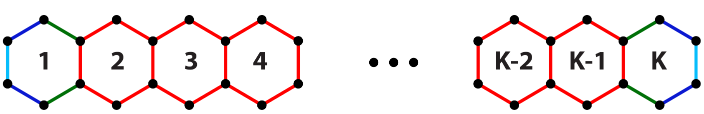
$$L\prod_1(G) = \prod_{v\in V(G)} d_2^2(v/G)$$

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

$$= (2^2)^2 \times (3^2)^{(2R+4)} \times (4^2)^{4(K-1)} \times (5^2)^{(2R-4)} \times (6^2)^{(2R-2)(K-1)}$$

$$= 2^{4(-2+3k+RK-R)} \times 3^{4(3+RK-K)} \times 5^{4(R-2)}.$$

Case2: If R=1 and $K\ \geq 2$.



In this case, Graphene contains vertices of 2-degrees 2, 3 and 4 only. Therefore, we can partition the vertex set into three sets V_2, V_3 and V_4, where each set V_i is the collection of vertices with 2-degree i. i.e., $V_i = \{v \in V(G)/d_2(v) = i\}$ for i=2, 3, 4. The frequency of such vertices is shown in the following Table 2

Types of vertex set	$V_2(G)$	$V_3(G)$	$V_4(G)$
. Frequency	4	2K	2K-2

Table-2

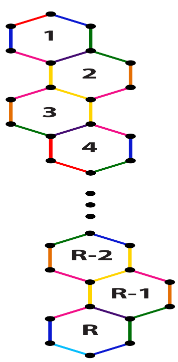
Consider, $L\prod_1(G) = \prod_{v\in V(G)} d_2^2(v/G)$

$= \prod_{v\in V_2(G)} d_2^2(v/G) \times \prod_{v\in V_3(G)} d_2^2(v/G) \times \prod_{v\in V_4(G)} d_2^2(v/G)$

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

$= 2^{8K} \times 3^{4K}$.

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



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

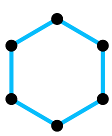
Type of vertex set	V_2	V_3	V_4	V_5
frequency	4	2R	2	2R-4

Table-3

Consider, $L\prod_1(G) = (2^2)^4 \times (3^2)^{2R} \times (4^2)^2 \times (5^2)^{(2R-4)}$

$= 2^{16} \times 3^{4R} \times 5^{4R-4}$.

Case4: If R =1 and K = 1



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

Vertices of 2-degree i	V_2
Frequency	6

Table-4

Consider, $L\prod_1(G) = (2^2)^6 = 2^{12} = 4096$.

$$\therefore L\prod_1(G) = \begin{cases} 4096 & \text{if } R = K = 1 \\ 2^{8K} \times 3^{4K} & \text{if } R = 1 \text{ and } K \geq 2 \\ 2^{16} \times 3^{4R} \times 5^{4R-4} & \text{if } R \geq 2 \text{ and } K = 1 \\ 2^{4(-2+3k+RK-R)} \times 3^{4(3+RK-K)} \times 5^{4(R-2)} & \text{if } R \neq 1 \text{ and } K \neq 1. \end{cases}$$

□

2.2. Second multiplicative leap Zagreb index of Graphene

Theorem 2.2 *Second multiplicative leap Zagreb index of Graphene with 'R' rows and 'K' benzene rings in each row is given by*

$$L\prod_2(G) = \begin{cases} 2^{12} & \textit{if } R = K = 1 \\ 2^{20} \times 3^8 & \textit{if } R = 2 \textit{ and } K = 1 \\ 2^{20} \times 3^{4R} \times 5^{6(R-2)} & \textit{if } R \geq 3 \textit{ and } K = 1 \\ 2^{4(3k-1)} \times 3^{4K} & \textit{if } R = 1 \textit{ and } K \geq 2 \\ 2^{2(-3+7K-3R+3RK)} \times 3^{2(7-R-3K+3RK)} \times 5^{6(R-2)} & \textit{if } R \neq 1 \textit{ and } K \neq 1. \end{cases}$$

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.

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

Table-5

Consider, $L\prod_2(G) = \prod_{uv\in E(G)} d_2(u/G)d_2(v/G)$.

$= \prod_{uv\in E_{2,3}(G)} d_2(u/G)d_2(v/G) \times \prod_{uv\in E_{3,3}(G)} d_2(u/G)d_2(v/G) \times \prod_{uv\in E_{3,4}(G)} d_2(u/G)d_2(v/G)\times$
$\prod_{uv\in E_{3,5}(G)} d_2(u/G)d_2(v/G) \times \prod_{uv\in E_{4,4}(G)} d_2(u/G)d_2(v/G) \times \prod_{uv\in E_{4,6}(G)} d_2(u/G)d_2(v/G) \times$
$\prod_{uv\in E_{5,5}(G)} d_2(u/G)d_2(v/G) \times \prod_{uv\in E_{5,6}(G)} d_2(u/G)d_2(v/G) \times \prod_{uv\in E_{6,6}(G)} d_2(u/G)d_2(v/G)$.

$= (2\times 3)^4 + (3\times 3)^R + (3\times 4)^8 + (3\times 5)^{2R-4} + (4\times 4)^{4K-8} + (4\times 6)^{2K} + (5\times 5)^{R-2} +$
$(5\times 6)^{2R-4} + (6\times 6)^{3RK-4R-4K+5}$

$= 2^{2(-3+7K-3R+3RK)} \times 3^{2(7-R-3K+3RK)} \times 5^{6(R-2)}$.

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

In this case Graphene contains vertices of 2-degrees $2, 3$ 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

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

Table-6

Consider, $L\prod_2(G) = \prod_{uv\in E(G)} d_2(u/G)d_2(v/G)$.

$$= \prod_{uv\in E_{2,2}(G)} d_2(u/G)d_2(v/G) \times \prod_{uv\in E_{2,3}(G)} d_2(u/G)d_2(v/G) \times \prod_{uv\in E_{3,4}(G)} d_2(u/G)d_2(v/G) \times \prod_{uv\in E_{4,4}(G)} d_2(u/G)d_2(v/G)$$

$$= (2 \times 2)^2 + (2 \times 3)^4 + (3 \times 4)^{4(k-1)} + (4 \times 4)^{(K-1)}$$

$$= 2^{4(3k-1)} \times 3^{4K}$$

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.

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	$2R-5$

Table-7

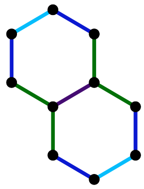
$$L\prod_2(G) = \prod_{uv\in E(G)} d_2(u/G)d_2(v/G)$$

$$= \prod_{uv\in E_{2,2}(G)} d_2(u/G)d_2(v/G) \times \prod_{uv\in E_{2,3}(G)} d_2(u/G)d_2(v/G) \times \prod_{uv\in E_{3,3}(G)} d_2(u/G)d_2(v/G) \times \prod_{uv\in E_{3,4}(G)} d_2(u/G)d_2(v/G) \times \prod_{uv\in E_{3,5}(G)} d_2(u/G)d_2(v/G) \times \prod_{uv\in E_{4,5}(G)} d_2(u/G)d_2(v/G) \times \prod_{uv\in E_{5,5}(G)} d_2(u/G)d_2(v/G).$$

$$= (2 \times 2)^2 + (2 \times 3)^4 + (3 \times 3)^{(R-2)} + (3 \times 4)^4 + (3 \times 5)^{(2R-4)} + (4 \times 5)^2 + (5 \times 5)^{(2R-5)}$$

$$= 2^{20} \times 3^{4R} \times 5^{6(R-2)}.$$

Case 4: If $K = 1$ and $R = 2$



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.

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

Table-8

$$L\prod_2(G) = \prod_{uv\in E(G)} d_2(u/G)d_2(v/G)$$

$$= \prod_{uv\in E_{2,2}(G)} d_2(u/G)d_2(v/G) \times \prod_{uv\in E_{2,3}(G)} d_2(u/G)d_2(v/G) \times \prod_{uv\in E_{3,4}(G)} d_2(u/G)d_2(v/G) \times \prod_{uv\in E_{4,4}(G)} d_2(u/G)d_2(v/G)$$

$$= (2\times 2)^2 \times (2\times 3)^4 \times (3\times 4)^4 \times (4\times 4)^1$$

$$=2^{20} \times 3^8.$$

Case 5: If $R = 1$ and $K = 1$

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

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

Table-9

$$L\prod_2(G) = \prod_{uv\in E(G)} d_2(u/G)d_2(v/G)$$

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

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

$$=2^{12}.$$

$\therefore$

$$L\prod_2(G) = \begin{cases} 2^{12} & \text{if } R = K = 1 \\ 2^{20} \times 3^8 & \text{if } R = 2 \text{ and } K = 1 \\ 2^{20} \times 3^{4R} \times 5^{6(R-2)} & \text{if } R \geq 3 \text{ and K=1} \\ 2^{4(3k-1)} \times 3^{4K} & \text{if } R = 1 \text{ and } K \geq 2 \\ 2^{2(-3+7K-3R+3RK)} \times 3^{2(7-R-3K+3RK)} \times 5^{6(R-2)} & \text{if } R \neq 1 \text{ and } K \neq 1 \end{cases}$$

□

2.3. Third multiplicative leap Zagreb index of Graphene

Theorem 2.3 *Third multiplicative leap Zagreb index of Graphene with 'R' rows and 'K' benzene rings in each row is given by,* $L\prod_3(G)$

$$= \begin{cases} 4096 & \text{if } R=K=1 \\ 192080000 & \text{if } R=2 \text{ and } K=1 \\ 2^{(9R-15)} \times 3^{(R+2)} \times 5^{(2R-1)} \times 7^4 & \text{if } R\geq 3 \text{ and } K=1 \\ 2^{(3k+1)} \times 5^4 \times 7^{(4K-4)} & \text{if } R=1 \text{ and } K\geq 2 \\ 2^{2(-14+3K+3RK)} \times 3^{(-3R-4K+3RK+5)} \times 5^{(R+2K+2)} \times 7^8 \times 11^{2(R-2)} & \text{if } R\neq 1 \text{ and } K\neq 1 \end{cases}$$

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

$$L\prod_3(G)= \prod_{uv\in E(G)} (d_2(u/G)+d_2(v/G))$$

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

$$= (2+3)^2 \times (3+3)^R \times (3+4)^8 \times (3+5)^{(2R-4)} \times (4+4)^{(4K-8)} \times (4+6)^{(2K)} \times (5+5)^{(R-2)} \times (5+6)^{(2R-4)} \times (6+6)^{(3RK-4R-4K+5)}$$

$$= 2^{2(-14+3K+3RK)} \times 3^{(-3R-4K+3RK+5)} \times 5^{(R+2K+2)} \times 7^8 \times 11^{2(R-2)}.$$

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

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

$$L\prod_3(G)= \prod_{uv\in E(G)} (d_2(u/G)+d_2(v/G))$$

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

$$= (2+2)^2 + (2+3)^4 + (3+4)^{4(K-1)} + (4+4)^{(K-1)}$$
$$= 2^{(3k+1)} \times 5^4 \times 7^{(4K-4)}.$$

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

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

$$L\prod_3(G)= \prod_{uv\in E(G)} (d_2(u/G)+d_2(v/G))$$

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

$$= (2+2)^2 \times (2+3)^4 \times (3+3)^{(R-2)} \times (3+4)^4 \times (3+5)^{(2R-4)} \times (4+5)^2 \times (5+5)^{(2R-5)}$$

$= 2^{(9R-15)} \times 3^{(R+2)} \times 5^{(2R-1)} \times 7^4.$

Case 4: If $K = 1$ and $R = 2$

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

$$L\prod_3(G) = \prod_{uv\in E(G)} (d_2(u/G) + d_2(v/G))$$
$$= \prod_{uv\in E_{2,2}(G)} (d_2(u/G) + d_2(v/G)) \times \prod_{uv\in E_{2,3}(G)} (d_2(u/G) + d_2(v/G)) \times \prod_{uv\in E_{3,4}(G)} (d_2(u/G) + d_2(v/G))$$
$$\times \prod_{uv\in E_{4,4}(G)} (d_2(u/G) + d_2(v/G))$$
$$= (2+2)^2 \times (2+3)^4 \times (3+4)^4 \times (4+4)^1$$
$$= 192080000.$$

Case 5: If $R = 1$and $K = 1$

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

$$L\prod_3(G) = \prod_{uv\in E(G)} (d_2(u/G) + d_2(v/G))$$
$$= \prod_{uv\in E_{2,2}(G)} (d_2(u/G) + d_2(v/G))$$
$$= (2+2)^6$$
$$= 4^6$$
$$= 4096.$$

$$\therefore L\prod_3(G) = \begin{cases} 4096 & \text{if } R = K = 1 \\ 192080000 & \text{if } R = 2 \text{ and } K = 1 \\ 2^{(9R-15)} \times 3^{(R+2)} \times 5^{(2R-1)} \times 7^4 & \text{if } R \geq 3 \text{ and } K = 1 \\ 2^{(3k+1)} \times 5^4 \times 7^{(4K-4)} & \text{if } R = 1 \text{ and } K \geq 2 \\ 2^{2(-14+3K+3RK)} \times 3^{(-3R-4K+3RK+5)} \times 5^{(R+2K+2)} \times 7^8 \times 11^{2(R-2)} & \text{if } R \neq 1 \text{ and } K \neq 1. \end{cases}$$

□

3. Conclusions

The first, second, and third multiplicative leap Zagreb indices of Graphene are calculated without the use of a computer.

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