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# On leap Zagreb indices of some nanostructures

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**Abstract**

In recent years, higher order topological indices are gaining much importance because of their greater correlation with many chemical properties. One among them is leap Zagreb index which is based on both distance and degree. For a graph $G$, the first, second and third leap Zagreb indices are the sum of squares of 2-distance degree of vertices of $G$; the sum of product of 2-distance degree of end vertices of edges in $G$ and the sum of product of 1-distance degree and 2-distance degrees of vertices of $G$, respectively. In this paper, we compute the expressions for these three leap Zagreb indices of some nanostructures.

**Keywords**

Degree, distance, leap Zagreb index, nanostructure.

**AMS Subject Classification**

05C07, 05C12, 05C90.

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## Contents



## 1. Introduction

Let $G$ be a simple graph with a vertex set $V(G)$ and an edge set $E(G)$. The *k-neighbourhood* [21] of a vertex $v \in V(G)$ is denoted and defined as $N_k(v/G) = \{u \in V(G) : d(u,v) = k\}$ where $d(u,v)$ is the distance between the two vertices $u$ and $v$ in $G$. The *k-distance degree of a vertex* $v \in V(G)$ is denoted by $d_k(v/G)$ and $d_k(v/G) = |N_k(v/G)|$. Also, we denote $N_G(v)$ by $N_1(v/G)$ and $d_G(v)$ by $d_1(v/G)$. The *degree of an edge* $e = uv$ in $G$ is given by $d_1(e/G) = d_1(u/G) + d_1(v/G) - 2$. If all the vertices of $G$ have same degree and is equal to $r \in Z^+$, then $G$ is called an *r-regular graph*. For undefined graph terminology and notations, a reader can refer [10] or [16].

In chemical graph theory and in mathematical chemistry, a molecular graph or chemical graph is a representation of the structural formula of a chemical compound in terms of graph theory. A *molecular graph* is a graph whose vertices correspond to the atoms of the chemical compound and edges to the chemical bonds. Chemical graph theory is a branch of mathematical chemistry which has an important effect on the development of the chemical sciences. A single number that can be used to characterize some property of a molecule is called a *topological index* of that graph. There are numerous molecular descriptors, which are also referred to as topological indices, see [9], that have found some applications in theoretical chemistry, especially in QSPR/QSAR research. There are plenty of topological indices defined in the literature. Wiener index [22], Zagreb indices [9], F-index [8], connectivity index ( or Randić index ) [5], are few of them. Recently, indices like Sanskruti index [11], second order first Zagreb index [3] and $(\beta,\alpha)$-connectivity index [4] were introduced. Higher order topological indices have advanced chemical applications in QSPR/QSAR study. The authors in the papers [3, 4, 8, 12, 13, 15, 19, 20] calculated various topological indices for some of the nanostructures. Many topological indices for nanostructures such as armchair polyhex nanotube, armchair polyhex nanotorus, V-phenylenic nanotube, V-phenylenic nanotorus, H-tetracenic nanotube, V-tetracenic nanotube and tetracenic nanotorus can be found in [1, 2, 6, 7, 14, 18].

Recently in [17], Naji et al. has introduced three topological indices called first leap Zagreb index, second leap Zagreb index and third leap Zagreb index which are denoted and defined as:

$$LM_1(G) = \sum_{v \in V(G)} d_2(v/G)^2,$$
$$LM_2(G) = \sum_{uv \in E(G)} d_2(u/G)d_2(v/G),$$
$$LM_3(G) = \sum_{v \in V(G)} d_1(v/G)d_2(v/G).$$

In this paper, we compute the expressions for first, second, third leap Zagreb indices of some nanostructures.

## 2. Order and size of some nanostructures

**Table 1.** Order and Size of nanostructures

| Sl. No. | Graph | Order | Size |
|---|---|---|---|
| 1 | Armchair polyhex nanotube $TUAC_6[2p,q]$ | $2pq$ | $3pq-2p$ |
| 2 | Armchair polyhex nanotorus $TUAC_6[p,q]$ | $2pq$ | $3pq$ |
| 3 | V-Phenylenic nanotube $VPHX[p,q]$ | $6pq$ | $9pq-p$ |
| 4 | V-Phenylenic nanotorus $VPHY[p,q]$ | $6pq$ | $9pq$ |
| 5 | V-Tetracenic nanotube G[p,q] | $18pq$ | $27pq-4p$ |
| 6 | H-Tetracenic nanotube G[p,q] | $18pq$ | $27pq-2q$ |
| 7 | Tetracenic nanotorus G[p,q] | $18pq$ | $27pq$ |

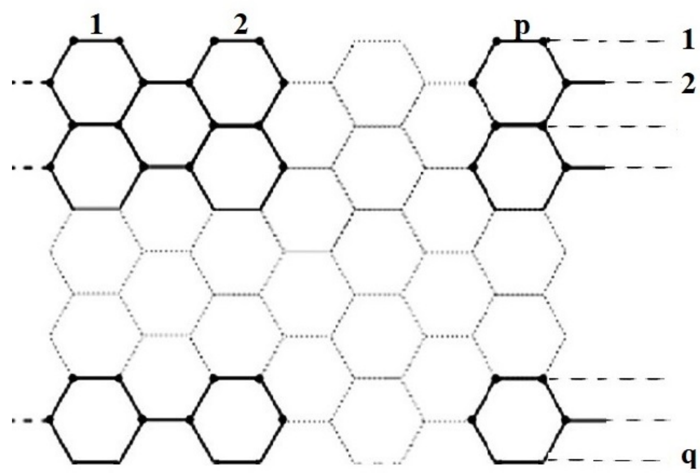
## 3. Main results

In this section, we compute the expressions for leap Zagreb indices of some nanostructures.

For the sake of convenience we use the names $A$, $B$, $C$, $D$, $E$, $F$, $H$ for the molecular graphs of armchair polyhex nanotube, armchair polyhex nanotorus, V-phenylenic nanotube, V-phenylenic nanotorus, V-tetracenic nanotube, H-tetracenic nanotube, tetracenic nanotorus respectively.

**Theorem 3.1.** *If $A$ is an armchair polyhex nanotube $TUAC_6[2p,q]$, where $p > 1$ and $q > 1$, then*

*(i)* $LM_1(A) = 72pq - 152p$,




(A)

**Figure 1.** (A) armchair polyhex nanotube

**Table 2.** Vertex set partition of graph $A$

| $d_2(v/A)$ | No. of vertices |
|---|---|
| 3 | $4p$ |
| 5 | $4p$ |
| 6 | $2pq-8p$ |

**Table 3.** Edge set partition of graph $A$. Here $uv \in E(A)$

| No. of edges | $d_2(u/A)$ | $d_2(v/A)$ |
|---|---|---|
| $2p$ | 3 | 3 |
| $4p$ | 3 | 5 |
| $2p$ | 5 | 5 |
| $4p$ | 5 | 6 |
| $3pq-14p$ | 6 | 6 |

*(ii)* $LM_2(A) = 108pq - 256p$,

*(iii)* $LM_3(A) = 36pq - 60p$.

*Proof.* The graph $A = TUAC_6[2p,q]$ has $2pq$ vertices and $3pq - 2p$ edges.
Using the definition of first leap Zagreb index and vertex set partition of the graph $A$ given in Table 2 we get,

$$\begin{aligned} LM_1(A) &= \sum_{v \in V(A)} d_2(v/A)^2 \\ &= 3^2(4p) + 5^2(4p) + 6^2(2pq - 8p) \\ &= 72pq - 152p. \end{aligned}$$

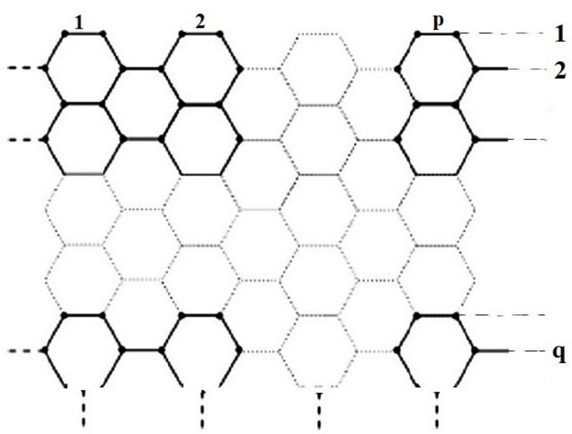
Using the definition of second leap Zagreb index and edge set partition of the graph $A$ given in Table 3 we get,

$$\begin{aligned} LM_2(A) &= \sum_{uv\in E(A)} d_2(u/A)d_2(v/A) \\ &= 3\cdot 3(2p)+3\cdot 5(4p)+5\cdot 5(2p)+5\cdot 6(4p) \\ &\quad +6\cdot 6(3pq-14p) \\ &= 108pq-256p. \end{aligned}$$

Using the definition of third leap Zagreb index, degree sequence of vertices and vertex set partition of the graph $A$ given in Table 2 we get,

$$\begin{aligned} LM_3(A) &= \sum_{v\in V(A)} d_1(v/A)d_2(v/A) \\ &= 2\cdot 3(4p)+3\cdot 5(4p)+3\cdot 6(2pq-8p) \\ &= 36pq-60p. \end{aligned}$$

□




(B)

**Figure 2.** (B) armchair polyhex nanotorus

**Table 4.** Vertex set partition of graph $B$

| $d_2(v/B)$ | 6 |
|---|---|
| No. of vertices | $2pq$ |

**Table 5.** Edge set partition of graph $B$. Here $uv\in E(B)$

| No. of edges | $d_2(u/B)$ | $d_2(v/B)$ |
|---|---|---|
| $3pq$ | 6 | 6 |

**Theorem 3.2.** *If $B$ is an armchair polyhex nanotorus $TUAC_6[p,q]$, where $p>1$ and $q>1$, then*

*(i) $LM_1(B)=72pq$,*

*(ii) $LM_2(B)=108pq$,*

*(iii) $LM_3(B)=36pq$.*

*Proof.* The graph $B=TUAC_6[p,q]$ has $2pq$ vertices and $3pq$ edges.
Using the definition of first leap Zagreb index and vertex set partition of the graph $B$ given in Table 4 we get,

$$\begin{aligned} LM_1(B) &= \sum_{v\in V(B)} d_2(v/B)^2 \\ &= 6^2(2pq) \\ &= 72pq. \end{aligned}$$

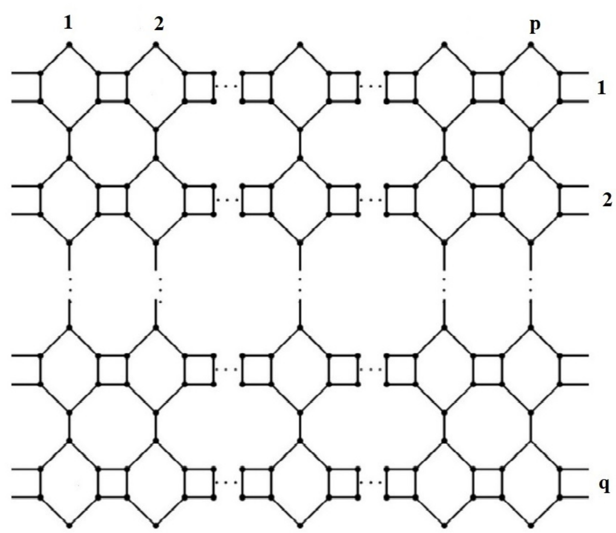
Using the definition of second leap Zagreb index and edge set partition of the graph $B$ given in Table 5 we get,

$$\begin{aligned} LM_2(B) &= \sum_{uv\in E(B)} d_2(u/B)d_2(v/B) \\ &= 6\cdot 6(3pq) \\ &= 108pq. \end{aligned}$$

Using the definition of third leap Zagreb index, degree sequence of vertices and vertex set partition of the graph $B$ given in Table 4 we get,

$$\begin{aligned} LM_3(B) &= \sum_{v\in V(B)} d_1(v/B)d_2(v/B) \\ &= 3\cdot 6(2pq) \\ &= 36pq. \end{aligned}$$

□




(C)

**Figure 3.** (C) V-phenylenic nanotube

**Table 6.** Vertex set partition of graph $C$

| $d_2(v/C)$ | 4 | 5 | 6 |
|---|---|---|---|
| No. of vertices | $6p$ | $4p(q-1)$ | $2p(q-1)$ |

**Table 7.** Edge set partition of graph $C$. Here $uv \in E(C)$

| No. of edges | $d_2(u/C)$ | $d_2(v/C)$ |
|---|---|---|
| $6p$ | 4 | 4 |
| $4p$ | 4 | 5 |
| $2p(2q-3)$ | 5 | 5 |
| $4p(q-1)$ | 5 | 6 |
| $p(q-1)$ | 6 | 6 |

**Theorem 3.3.** *If $C$ is a V-phenylenic nanotube $VPHX[p,q]$, where $p > 1$ and $q > 1$, then*

*(i)* $LM_1(C) = 172pq - 76p$,

*(ii)* $LM_2(C) = 256pq - 130p$,

*(iii)* $LM_3(C) = 96pq - 32p$.

*Proof.* The graph $C = VPHX[p,q]$ has $6pq$ vertices and $9pq - p$ edges.
Using the definition of first leap Zagreb index and vertex set partition of the graph $C$ given in Table 6 we get,

$$\begin{aligned} LM_1(C) &= \sum_{v\in V(C)} d_2(v/C)^2 \\ &= 4^2(6p) + 5^2[4p(q-1)] + 6^2[2p(q-1)] \\ &= 172pq - 76p. \end{aligned}$$

Using the definition of second leap Zagreb index and edge set partition of the graph $C$ given in Table 7 we get,

$$\begin{aligned} LM_2(C) &= \sum_{uv\in E(C)} d_2(u/C)d_2(v/C) \\ &= 4\cdot 4(6p) + 4\cdot 5(4p) + 5\cdot 5[2p(2q-3)] \\ &\quad +5\cdot 6[4p(q-1)] + 6\cdot 6[p(q-1)] \\ &= 256pq - 130p. \end{aligned}$$

Using the definition of third leap Zagreb index, degree sequence of vertices and vertex set partition of the graph $C$ given in Table 6 we get,

$$\begin{aligned} LM_3(C) &= \sum_{v\in V(C)} d_1(v/C)d_2(v/C) \\ &= 2\cdot 4(2p) + 3\cdot 4(4p) + 3\cdot 5[4p(q-1)] \\ &\quad +3\cdot 6[2p(q-1)] \\ &= 96pq - 32p. \end{aligned}$$

□

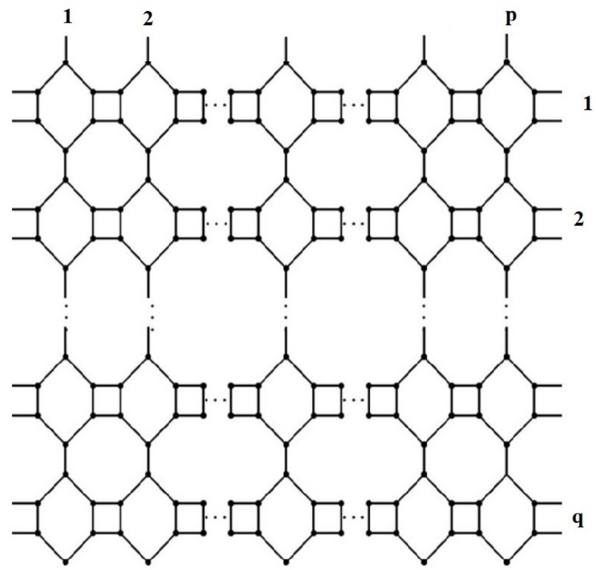
**Table 8.** Vertex set partition of graph $D$

| $d_2(v/D)$ | 5 | 6 |
|---|---|---|
| No. of vertices | $4pq$ | $2pq$ |

**Theorem 3.4.** *If $D$ is a V-phenylenic nanotorus $VPHY[p,q]$, where $p > 1$ and $q > 1$, then*

*(i)* $LM_1(D) = 172pq$,

*(ii)* $LM_2(D) = 256pq$,




**(D)**

**Figure 4.** (D) V-phenylenic nanotorus

**Table 9.** Edge set partition of graph $D$. Here $uv \in E(D)$

| No. of edges | $d_2(u)$ | $d_2(v)$ |
|---|---|---|
| $4pq$ | 5 | 5 |
| $4pq$ | 5 | 6 |
| $pq$ | 6 | 6 |

*(iii)* $LM_3(D) = 96pq$.

*Proof.* The graph $D = VPHY[p,q]$ has $6pq$ vertices and $9pq$ edges.
Using the definition of first leap Zagreb index and vertex set partition of the graph $D$ given in Table 8 we get,

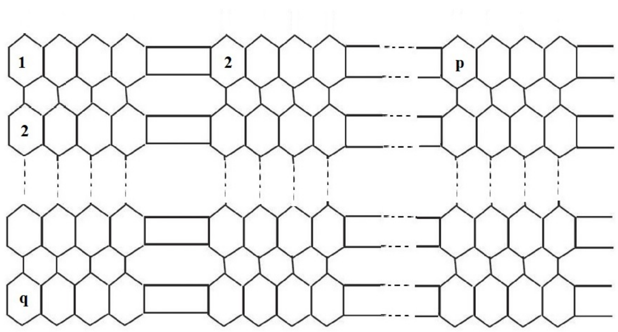
$$\begin{aligned} LM_1(D) &= \sum_{v\in V(D)} d_2(v/D)^2 \\ &= 5^2(4pq) + 6^2(2pq) \\ &= 172pq. \end{aligned}$$

Using the definition of second leap Zagreb index and edge set partition of the graph $D$ given in Table 9 we get,

$$\begin{aligned} LM_2(D) &= \sum_{uv\in E(D)} d_2(u/D)d_2(v/D) \\ &= 5\cdot 5(4pq) + 5\cdot 6(4pq) + 6\cdot 6(pq) \\ &= 256pq. \end{aligned}$$

Using the definition of third leap Zagreb index, vertex degree sequence and vertex set partition of the graph $D$ given in Table 8 we get,

$$\begin{aligned} LM_3(D) &= \sum_{v\in V(D)} d_1(v/D)d_2(v/D) \\ &= 3\cdot 5(4pq) + 3\cdot 6(2pq) \\ &= 96pq. \end{aligned}$$




**(E)**

**Figure 5.** (E) V-tetracenic nanotube G[p,q]

**Table 10.** Vertex set partition of graph $E$

| $d_2(v/E)$ | 4 | 5 | 6 |
|---|---|---|---|
| No. of vertices | $18p$ | $4p(q-1)$ | $14p(q-1)$ |

**Table 11.** Edge set partition of graph $E$. Here $uv \in E(E)$

| No. of edges | $d_2(u/E)$ | $d_2(v/E)$ |
|---|---|---|
| $18p$ | 4 | 4 |
| $4p$ | 4 | 5 |
| $6p$ | 4 | 6 |
| $4p$ | 5 | 6 |
| $9p(3q-4)$ | 6 | 6 |

**Theorem 3.5.** *If $E$ is a V-tetracenic nanotube $G[p,q]$, where $p > 1$ and $q > 1$, then*

*(i)* $LM_1(E) = 604pq - 316p$,

*(ii)* $LM_2(E) = 972pq - 664p$,

*(iii)* $LM_3(E) = 312pq - 128p$.

*Proof.* The graph $E = G[p,q]$ has $18pq$ vertices and $27pq - 4p$ edges.
Using the definition of first leap Zagreb index and vertex set partition of the graph $E$ given in Table 10 we get,

$$\begin{aligned} LM_1(E) &= \sum_{v\in V(E)} d_2(v/E)^2 \\ &= 4^2(18p) + 5^2[4p(q-1)]] + 6^2[14p(q-1)] \\ &= 604pq - 316p. \end{aligned}$$

Using the definition of second leap Zagreb index and edge set partition of the graph $E$ given in Table 11 we get,

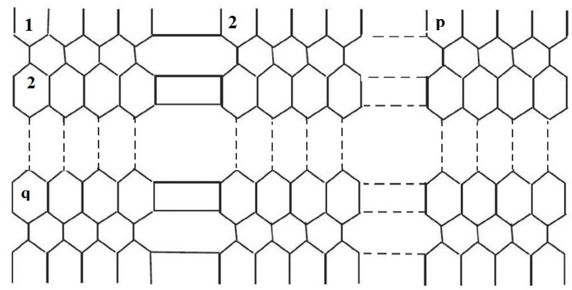
$$\begin{aligned} LM_2(E) &= \sum_{uv\in E(E)} d_2(u/E)d_2(v/E) \\ &= 4\cdot 4(18p) + 4\cdot 5(4p) + 4\cdot 6(6p) + 5\cdot 6(4p) \\ &\quad +6\cdot 6[9p(3q-4)] \\ &= 972pq - 664p. \end{aligned}$$

□

Using the definition of third leap Zagreb index, degree sequence of vertices and vertex set partition of the graph $E$ given in Table 10 we get,

$$\begin{aligned} LM_3(E) &= \sum_{v\in V(E)} d_1(v/E)d_2(v/E) \\ &= 2\cdot 4(8p) + 3\cdot 4(10p) + 3\cdot 5[4p(q-1)] \\ &\quad +3\cdot 6[14p(q-1)] \\ &= 312pq - 128p. \end{aligned}$$

□




**(F)**

**Figure 6.** (F) H-tetracenic nanotube G[p,q]

**Table 12.** Vertex set partition of graph $F$

| $d_2(v/F)$ | 3 | 5 | 6 |
|---|---|---|---|
| No. of vertices | $2pq$ | $4pq$ | $12pq$ |

**Table 13.** Edge set partition of graph $F$. Here $uv \in E(F)$

| No. of edges | $d_2(u/F)$ | $d_2(v/F)$ |
|---|---|---|
| $pq$ | 3 | 3 |
| $2pq$ | 3 | 5 |
| $3pq$ | 5 | 5 |
| $2pq$ | 5 | 6 |
| $19pq - 2q$ | 6 | 6 |

**Theorem 3.6.** *If $F$ is a H-tetracenic nanotube $G[p,q]$, where $p > 1$ and $q > 1$, then*

*(i)* $LM_1(F) = 550pq$,

*(ii)* $LM_2(F) = 858pq - 72q$,

*(iii)* $LM_3(F) = 288pq$.

*Proof.* The graph $F = G[p,q]$ has $18pq$ vertices and $27pq - 2q$ edges.
Using the definition of first leap Zagreb index and vertex set partition of the graph $F$ given in Table 12 we get,

$$\begin{aligned} LM_1(F) &= \sum_{v\in V(F)} d_2(v/F)^2 \\ &= 3^2(2pq) + 5^2(4pq) + 6^2(12pq) \\ &= 550pq. \end{aligned}$$

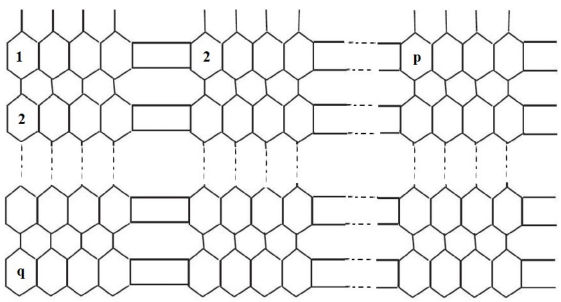
Using the definition of second leap Zagreb index and edge set partition of the graph $F$ given in Table 13 we get,

$$\begin{aligned} LM_2(F) &= \sum_{uv\in E(F)} d_2(u/F)d_2(v/F) \\ &= 3\cdot 3(pq)+3\cdot 5(2pq)+5\cdot 5(3pq) \\ &\quad +5\cdot 6(2pq)+6\cdot 6[(19pq-2q)] \\ &= 858pq-72q. \end{aligned}$$

Using the definition of third leap Zagreb index, vertex degree sequence and vertex set partition of the graph $F$ given in Table 12 we get,

$$\begin{aligned} LM_3(F) &= \sum_{v\in V(F)} d_1(v/F)d_2(v/F) \\ &= 2\cdot 3(2pq)+3\cdot 5(4pq)+3\cdot 6(12pq) \\ &= 288pq. \end{aligned}$$

□



**(H)**

**Figure 7.** (H) tetracenic nanotorus G[p,q]

**Table 14.** Vertex set partition of graph $H$

| $d_2(v/H)$ | 5 | 6 |
|---|---|---|
| No. of vertices | $4pq$ | $14pq$ |

**Table 15.** Edge set partition of graph $H$. Here $uv \in E(H)$

| No. of edges | $d_2(u/H)$ | $d_2(v/H)$ |
|---|---|---|
| $4pq$ | 5 | 5 |
| $4pq$ | 5 | 6 |
| $19pq$ | 6 | 6 |

**Theorem 3.7.** *If $H$ is a tetracenic nanotorus $G[p,q]$, where $p>1$ and $q>1$, then*

*(i) $LM_1(H) = 604pq$,*

*(ii) $LM_2(H) = 904pq$,*

*(iii) $LM_3(H) = 312pq$.*

*Proof.* The graph $H = G[p,q]$ has $18pq$ vertices and $27pq$ edges.

Using the definition of first leap Zagreb index and vertex set partition of the graph $H$ given in Table 14 we get,

$$\begin{aligned} LM_1(H) &= \sum_{v\in V(H)} d_2(v/H)^2 \\ &= 5^2(4pq)+6^2(14pq) \\ &= 604pq. \end{aligned}$$

Using the definition of second leap Zagreb index and edge set partition of the graph $H$ given in Table 15 we get,

$$\begin{aligned} LM_2(H) &= \sum_{uv\in E(H)} d_2(u/H)d_2(v/H) \\ &= 5\cdot 5(4pq)+5\cdot 6(4pq)+6\cdot 6(19pq) \\ &= 904pq. \end{aligned}$$

Using the definition of third leap Zagreb index, degree sequence of vertices and vertex set partition of the graph $H$ given in Table 14 we get,

$$\begin{aligned} LM_3(H) &= \sum_{v\in V(H)} d_1(v/H)d_2(v/H) \\ &= 3\cdot 5(4pq)+3\cdot 6(14pq) \\ &= 312pq. \end{aligned}$$

□

## 4. Conclusion

In this paper, we have computed the expressions for first, second and third leap Zagreb indices of some nanostructures. It is interesting to find these three leap Zagreb indices of some other nanotubes and networks for future studies.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