

## Second and third leap Zagreb indices of some nanostructures

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### Abstract

Higher order topological indices have gained a lot of traction in recent years due to their stronger association with a variety of chemical characteristics. The leap Zagreb index is one of them, and it is based on both degree and distance. The second and third leap Zagreb indices of some nanostructures are computed in this research.

**Mathematics Subject Classification:** 05C07, 05C12, 05C90.

**Keywords and Phrases:** Leap zagreb index, degree, nanostructures.

### INTRODUCTION

Let  $G$  be a connected, finite, simple, undirected graph. The length of the “shortest path between any two vertices  $u$  and  $v$  of a graph  $G$ ” is denoted by  $d_G(u, v)$ . The open  $k$ -neighborhood of  $v$  in a graph  $G$  represented by  $N_k(v/G)$  and is stated as  $N_k(v/G) = \{u \in V(G) : d(u, v) = k\}$  for a vertex  $v \in V(G)$  and a positive integer  $k$ .

The number of  $k$ -neighbors of a vertex  $v$  in  $G$  is indicated by  $d_k(v/G)$  and is stated as  $d_k(v/G) = |N_k(v/G)|$ . For every  $v \in V(G)$ ,  $d_1(v/G) = d_G(v)$ .

A chemical graph or molecular graph is a representation of a chemical compound's structural formula in terms of graph theory used in chemical graph theory and mathematical chemistry. Chemical graph theory is an area of mathematical chemistry that has a significant impact on the advancement of chemical science. The edges and vertices corresponds to the chemical bonds and atoms respectively.

A topological index of that graph is a single number that can be used to characterise a molecule's attributes. Numerous molecular descriptors, sometimes known as topological indices [2], have found use in theoretical chemistry, particularly in QSPR/QSAR research. Different topological indices were calculated by the authors in the studies [3, 4, 5]. Harold Wiener [9] a chemist, was the first to use a topological index in 1947. In terms of carbon-carbon bonds, Wiener defined path number as the total of distances between any two carbon atoms in a molecule. Wiener based his index (W) on trees and investigated how it may be used to correlate physico-chemical properties of alkanes, alcohols, amines, and their similar compounds. Biochemistry, nanotechnology, and pharmacology are just a few of the fields where it can be used.

A chemical compound's bond energy is a measurement of its bond strength. The bond length is the distance between two atoms. The lower the bond length between those atoms, the higher the bond energy. The oldest vertex-degree-based graph invariants are the Zagreb indices. They debuted in the 1970s [7, 8]. The newly discovered 2-degree based topological invariants, known as leap Zagreb indices, are analogous to innovative graph invariants (Zagreb indices) and can be used to examine binding energy between atoms in a molecular graph of a chemical molecule.

Naji et al. [1] developed a new distance-degree-based topological indices based on the second degrees of vertices, known as leap Zagreb indices of a graph  $G$  in 2017. The second and third Zagreb leap indices are as follows

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

$$LM_2(G) = \sum_{uv \in E} [(d_2 u/G) d_2(v/G)].$$

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

Several chemical applications exist for the leap Zagreb indices. Surprisingly, physical properties of chemical compounds such as accentric factor, accentric factor, boiling point, HVAP and DHVAP have a very good correlation with the "first leap Zagreb index" [6]. We discuss 2D-Lattice, nanotorus and nanotube of  $TUC_4C_8(p, q)$  in this paper. Here  $q$  and  $p$  signify the number of rows of squares and the number of squares in a row, respectively. The examples of 2D-lattice, nanotube, and nanotorus of  $TUC_4C_8[4, 3]$ , are shown in Figure 1 (a), (b) and (c) respectively.

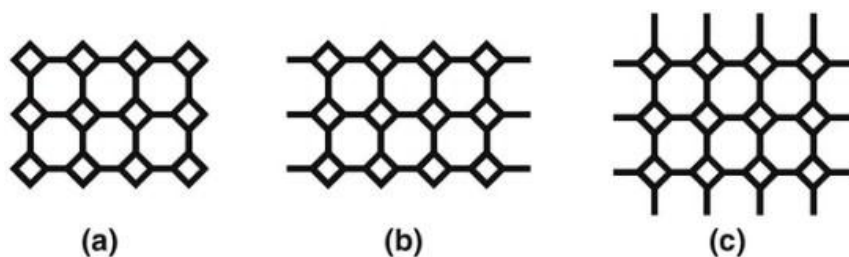


Fig-1

## 2. MAIN RESULTS

A  $TUC_4C_8(p, q)$  nanotube is a “mathematically beautiful object” constructed from squares and octagons. The nanotube is made by wrapping the lattice in such a way that each hanging edge from the left side connects to the row’s rightmost vertex. In one layer of the nanotube, the number of squares and octagons is equal to  $p + 1$ . Here  $(p + 1)$  and  $(q + 1)$  denotes total cardinality of squares in rows and columns respectively in the 2D lattice of  $TUC_4C_8(p, q)$  nanotorus.

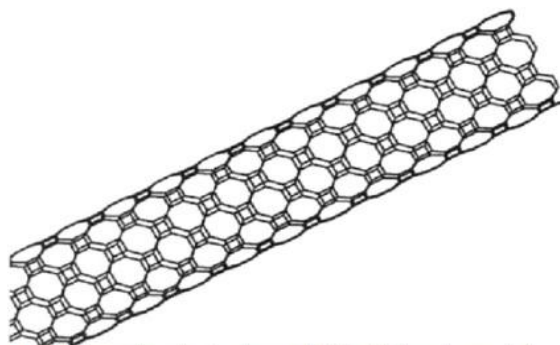
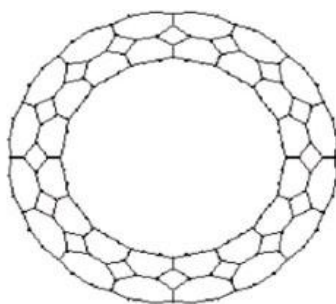


Fig-2 : 3-Dimensional structure of  $TUC_4C_8(p, q)$  nanotube



3-D Structure of  $TUC_4C_8(p, q)$  nanotorus

Fig-3

| Graph                          | Number of vertices | Number of edges |
|--------------------------------|--------------------|-----------------|
| 2D lattice of $TUC_4C_8(p, q)$ | $4pq$              | $6pq - p - q$   |
| $TUC_4C_8(p, q)$ nanotube      | $4pq$              | $6pq - p$       |
| $TUC_4C_8(p, q)$ nanotorus     | $4pq$              | $6pq$           |

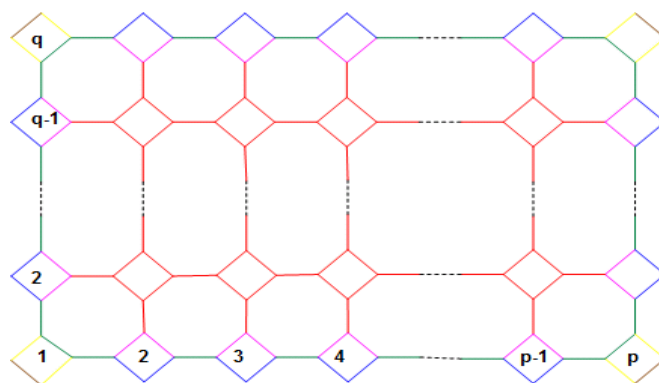
**Theorem 2.1.** The second leap zagreb index of 2D-lattice  $TUC_4C_8(p, q)$  is given by,

$$LM_2(G) = \begin{cases} -115p - 115q + 150pq + 68 & \text{if } p > 1, \quad q > 1 \\ 45p - 49 & \text{if } p > 1, q = 1 \text{ and } p = 1, q > 1 \\ 4 & \text{if } p = 1, q = 1 \end{cases}$$

**Proof.** Consider a 2D-lattice  $TUC_4C_8(p, q)$  with ‘q’ rows and ‘p’ squares in each row. “Let  $E_{ij}$  denotes the number of edges connecting the vertices of 2 degree i and 2 degree j”.

**CASE 1:**

If  $q > 1, p > 1$ , It has 6 type of edges  $\{E_{(2,2)}, E_{(2,4)}, E_{(3,4)}, E_{(4,4)}, E_{(4,5)}, E_{(5,5)}\}$  that are enumerated in following table. For convenience these edge types are colored by yellow, black, blue, green, pink and red respectively as shown in the following figure-4.

**Fig-4**

| $d_2(u/G), d_2(v/G)$ | (2, 2) | (2, 4) | (3, 4)     | (4, 4)  | (4, 5)     | (5, 5)           |
|----------------------|--------|--------|------------|---------|------------|------------------|
| Number of edges      | 4      | 8      | $4p+4q-16$ | $2p+2q$ | $4p+4q-16$ | $6pq-11p-11q+20$ |

$$\begin{aligned}
 LM_2(G) &= \sum_{uv \in E} [d_2(u/G) d_2(v/G)] \\
 &= \sum_{uv \in E_{2,2}(G)} [d_2(u/G) d_2(v/G)] + \sum_{uv \in E_{2,4}(G)} [d_2(u/G) d_2(v/G)] + \sum_{uv \in E_{3,4}(G)} [d_2(u/G) d_2(v/G)] \\
 &\quad + \sum_{uv \in E_{4,4}(G)} [d_2(u/G) d_2(v/G)] + \sum_{uv \in E_{4,5}(G)} [d_2(u/G) d_2(v/G)] \\
 &\quad + \sum_{uv \in E_{5,5}(G)} [d_2(u/G) d_2(v/G)] \\
 &= |E_{2,2}|(2 \times 2) + |E_{2,4}|(2 \times 4) + |E_{3,4}|(3 \times 4) + |E_{4,4}|(4 \times 4) + |E_{4,5}|(4 \times 5) + |E_{5,5}|(5 \times 5) \\
 &= 4(4) + 8(8) + (4p + 4q - 16)(12) + (2p + 2q)(16) + (4p + 4q - 16)(20) \\
 &\quad + (6pq - 11p - 11q + 20)(25). \\
 &= -115p - 115q + 150pq + 68. \\
 \therefore LM_2(G) &= -115p - 115q + 150pq + 68 \quad p > 1, \quad q > 1.
 \end{aligned}$$

**CASE 2:**

If  $q = 1, p > 1$ , It has 3 type of edges  $\{E_{1,2}, E_{2,3}, E_{3,3}\}$  these edges are colored in orange, brown and blue respectively as shown in the following figure-5 and also the number of edges are represented in the table given below.



Fig-5

|                      |        |        |        |
|----------------------|--------|--------|--------|
| $d_2(u/G), d_2(v/G)$ | (1, 2) | (2, 3) | (3, 3) |
| Number of edges      | 4      | 4      | $5p-9$ |

$$\begin{aligned}
 LM_2(G) &= \sum_{uv \in E} [d_2(u/G) d_2(v/G)] \\
 &= \sum_{uv \in E_{1,2}(G)} [d_2(u/G) d_2(v/G)] \\
 &\quad + \sum_{uv \in E_{2,3}(G)} [d_2(u/G) d_2(v/G)] + \sum_{uv \in E_{3,3}(G)} [d_2(u/G) d_2(v/G)] \\
 &= |E_{1,2}|(1 \times 2) + |E_{2,3}|(2 \times 3) + |E_{3,3}|(3 \times 3). \\
 &= 4(2) + 4(6) + (5p - 9)(9). \\
 &= 45p - 49.
 \end{aligned}$$

$$\therefore LM_2(G) = 45p - 49 \quad p > 1, \quad q = 1.$$

**CASE 3:**

If  $q = 1, p = 1$ , we have only 4 edges of the type  $E_{1,1}$  as shown in the below figure-6:

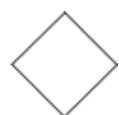


Fig 6

|                      |        |
|----------------------|--------|
| $d_2(u/G), d_2(v/G)$ | (1, 1) |
| Number of edges      | 4      |

$$\begin{aligned}
LM_2(G) &= \sum_{uv \in E} [d_2(u/G) d_2(v/G)] \\
&= \sum_{uv \in E_{1,1}(G)} [d_2(u/G), d_2(v/G)] \\
&= |E_{1,1}|(1 \times 1) \\
&= 4(1). \\
&= 4.
\end{aligned}$$

$$\therefore LM_2(G) = 4 \quad p = 1, \quad q = 1.$$

**Theorem 2. 2.** The third leap zagreb index of 2D-lattice  $TUC_4C_8(p, q)$  is given by,

$$LM_3(G) = \begin{cases} -30p - 30q + 60pq + 8 & \text{if } p > 1, \quad q > 1 \\ 30p - 22 & \text{if } p > 1, q = 1 \\ 8 & \text{if } p = 1, \quad q = 1 \end{cases}$$

**Proof.** Consider a 2D-lattice  $TUC_4C_8(p, q)$  with 'q' rows and 'p' squares in each row. Let  $E_{i,j}$  denotes the number of edges connecting the vertices of 2 degree i and 2 degree j.

### CASE 1:

If  $q > 1, p > 1$ , It has 6 type of edges  $\{E_{2,2}, E_{2,4}, E_{3,4}, E_{4,4}, E_{4,5}, E_{5,5}\}$  that are enumerated in following table. For convenience these edge types are colored by yellow, black, blue, green, pink and red respectively as shown in the following figure-4.

| $d_2(u/G), d_2(v/G)$ | (2, 2) | (2, 4) | (3, 4)     | (4, 4)  | (4, 5)     | (5, 5)           |
|----------------------|--------|--------|------------|---------|------------|------------------|
| Number of edges      | 4      | 8      | $4p+4q-16$ | $2p+2q$ | $4p+4q-16$ | $6pq-11p-11q+20$ |

$$\begin{aligned}
LM_3(G) &= \sum_{uv \in E} [d_2(u/G) + d_2(v/G)] \\
&= \sum_{uv \in E_{2,2}(G)} [d_2(u/G) + d_2(v/G)] \\
&\quad + \sum_{uv \in E_{2,4}(G)} [d_2(u/G) + d_2(v/G)] + \sum_{uv \in E_{3,4}(G)} [d_2(u/G) + d_2(v/G)] \\
&\quad + \sum_{uv \in E_{4,4}(G)} [d_2(u/G) + d_2(v/G)] + \sum_{uv \in E_{4,5}(G)} [d_2(u/G) + d_2(v/G)] \\
&\quad + \sum_{uv \in E_{5,5}(G)} [d_2(u/G) + d_2(v/G)] \\
&= |E_{2,2}|(2+2) + |E_{2,4}|(2+4) + |E_{3,4}|(3+4) + |E_{4,4}|(4+4) + |E_{4,5}|(4+5) + |E_{5,5}|(5+5) \\
&= 4(4) + 8(6) + (4p+4q-16)(7) + (2p+2q)(8) + (4p+4q-16)(9) \\
&\quad + (6pq-11p-11q+20)(10). \\
&= -115p - 115q + 150pq + 68. \\
\therefore LM_3(G) &= -30p - 30q + 60pq + 8 \quad p > 1, \quad q > 1.
\end{aligned}$$

**CASE 2:**

If  $q = 1, p > 1$ , It has 3 type of edges  $\{E_{1,2}, E_{2,3}, E_{3,3}\}$  these edges are colored in orange, brown and blue respectively as shown in the following figure-5 and also the number of edges are represented in the table given below.

| $d_2(u/G), d_2(v/G)$ | (1, 2) | (2, 3) | (3, 3) |
|----------------------|--------|--------|--------|
| Number of edges      | 4      | 4      | 5p-9   |

$$\begin{aligned}
LM_3(G) &= \sum_{uv \in E} [d_2(u/G) + d_2(v/G)] \\
&= \sum_{uv \in E_{1,2}(G)} [d_2(u/G) + d_2(v/G)] \\
&\quad + \sum_{uv \in E_{2,3}(G)} [d_2(u/G) + d_2(v/G)] + \sum_{uv \in E_{3,3}(G)} [d_2(u/G) + d_2(v/G)] \\
&= |E_{1,2}|(1+2) + |E_{2,3}|(2+3) + |E_{3,3}|(3+3). \\
&= 4(3) + 4(5) + (5p-9)(6). \\
&= 30p - 22. \\
\therefore LM_2(G) &= 30p - 22. \quad p > 1, \quad q = 1.
\end{aligned}$$

**CASE 3:**

If  $q = 1, p = 1$ , we have only 4 edges of the type  $E_{1,1}$  as shown in the below figure-6:

|                      |        |
|----------------------|--------|
| $d_2(u/G), d_2(v/G)$ | (1, 1) |
| Number of edges      | 4      |

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

$$= \sum_{uv \in E_{1,1}(G)} [d_2(u/G) + d_2(v/G)]$$

$$= |E_{1,1}|(1 + 1)$$

$$= 4(2).$$

$$= 8.$$

$$\therefore LM_2(G) = 8 \quad p = 1, \quad q = 1.$$

**Theorem 2.3.** The second leap zagreb index of  $TUC_4C_8(p, q)$  nanotube is given by,

$$LM_2(G) = \begin{cases} -115p + 150pq + 68 & \text{if } p > 1, \quad q > 1 \\ 45p & \text{if } p > 1, q = 1 \\ 37q - 47 & \text{if } p = 1, q > 1 \\ 0 & \text{if } p = 1, q = 1 \end{cases}$$

**Proof. CASE 1:**

If  $q > 1, p > 1$ , It has 4 type of edges  $E_{3,4}, E_{4,5}, E_{4,4}, E_{5,5}$  that are enumerated in following table. For convenience these edge types are colored by green, blue, red and black respectively as shown in the following figure-7.

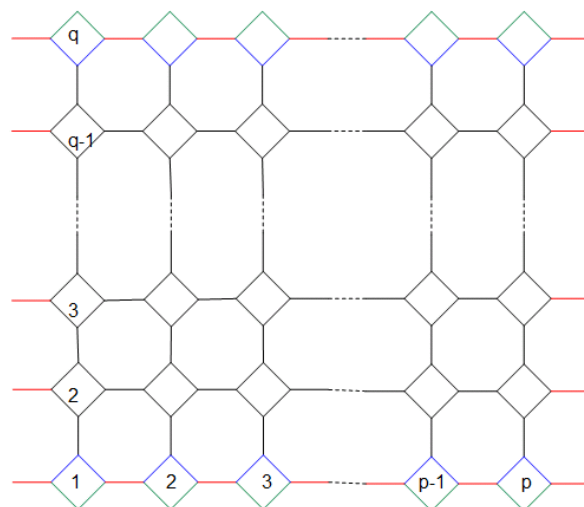


Fig-7

|                      |        |        |        |         |
|----------------------|--------|--------|--------|---------|
| $d_2(u/G), d_2(v/G)$ | (3, 4) | (4, 5) | (4, 4) | (5, 5)  |
| Number of edges      | 4p     | 4p     | 2p     | 6pq-11p |

$$\begin{aligned}
 LM_2(G) &= \sum_{uv \in E} [d_2(u/G) d_2(v/G)] \\
 &= \sum_{uv \in E_{3,4}(G)} [d_2(u/G) d_2(v/G)] + \sum_{uv \in E_{4,5}(G)} [d_2(u/G) d_2(v/G)] \\
 &\quad + \sum_{uv \in E_{4,4}(G)} [d_2(u/G) d_2(v/G)] + \sum_{uv \in E_{5,5}(G)} [d_2(u/G) d_2(v/G)] \\
 &= |E_{3,4}|(3 \times 4) + |E_{4,5}|(4 \times 5) + |E_{4,4}|(4 \times 4) + |E_{5,5}|(5 \times 5) \\
 &= 4p(12) + 4p(20) + (2p)(16) + (6pq - 11p)(25). \\
 &= -115p + 150pq. \\
 \therefore LM_2(G) &= -115p + 150pq \quad p > 1, \quad q > 1.
 \end{aligned}$$

**CASE 2:**

If  $q = 1, p > 1$ , we have  $E_{3,3} = 5p$  as shown in figure- 8.

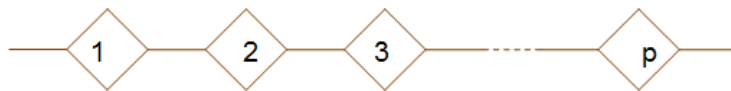


Fig-8

$$\begin{aligned}
 LM_2(G) &= \sum_{uv \in E} [d_2(u/G) d_2(v/G)] \\
 &= \sum_{uv \in E_{3,3}(G)} [d_2(u/G) d_2(v/G)] \\
 &= |E_{3,3}|(3 \times 3). \\
 &= 5p(9). \\
 &= 45p.
 \end{aligned}$$

$$\therefore LM_2(G) = 45p \quad p > 1, \quad q = 1.$$

**CASE 3:**

If  $q > 1, p = 1$ , It has 3 type of edges  $E_{1,1}, E_{1,3}, E_{2,3}, E_{2,2}$  and  $E_{3,3}$  these edges are colored in green, red, black, orange and pink respectively as shown in the following figure-9 and also the number of edges are represented in the table given below

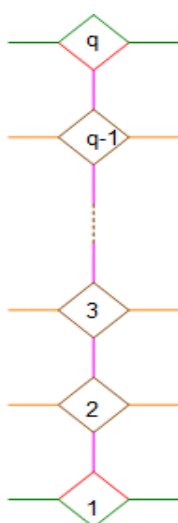


Fig-9

| $d_2(u/G), d_2(v/G)$ | (1, 1) | (1, 3) | (2, 3) | (2, 2) | (3, 3) |
|----------------------|--------|--------|--------|--------|--------|
| Number of edges      | 6      | 4      | $4q-8$ | $q-2$  | $q-1$  |

$$\begin{aligned}
LM_2(G) &= \sum_{uv \in E} [d_2(u/G) d_2(v/G)] \\
&= \sum_{uv \in E_{1,1}(G)} [d_2(u/G) d_2(v/G)] + \sum_{uv \in E_{1,3}(G)} [d_2(u/G) d_2(v/G)] \\
&\quad + \sum_{uv \in E_{2,3}(G)} [d_2(u/G) d_2(v/G)] \\
&\quad + \sum_{uv \in E_{2,2}(G)} [d_2(u/G) d_2(v/G)] + \sum_{uv \in E_{3,3}(G)} [d_2(u/G) d_2(v/G)] \\
&= |E_{1,1}|(1 \times 1) + |E_{1,3}|(1 \times 3) + |E_{2,3}|(2 \times 3) + |E_{2,2}|(2 \times 2) + |E_{3,3}|(3 \times 3) \\
&= 6(1) + 4(3) + (4q - 8)(6) + (q - 2)(4) + (q - 1)(9). \\
&= 37q - 47.
\end{aligned}$$

$$\therefore LM_2(G) = 37q - 47 \quad p = 1, \quad q > 1.$$

**CASE 4:**

If  $q = 1, p = 1$  we have the edges of the type  $E_{1,0}$  and  $E_{0,0}$  as shown in the figure 10 and the number of edges are represented in the following table



Fig-10

|                      |        |        |
|----------------------|--------|--------|
| $d_2(u/G), d_2(v/G)$ | (1, 0) | (0, 0) |
| Number of edges      | 4      | 1      |

$$\begin{aligned}
LM_2(G) &= \sum_{uv \in E} [d_2(u/G) d_2(v/G)] \\
&= \sum_{uv \in E_{1,0}(G)} [d_2(u/G) d_2(v/G)] + \sum_{uv \in E_{0,0}(G)} [d_2(u/G) d_2(v/G)] \\
&= |E_{1,0}|(1 \times 0) + |E_{0,0}|(0 \times 0) \\
&= 4(0) + 1(0). \\
&= 0.
\end{aligned}$$

$$\therefore LM_2(G) = 0 \quad p = 1, \quad q = 1.$$

**Theorem 2. 4.** The third leap zagreb index of  $TUC_4C_8(p, q)$  nanotube is given by,

$$LM_2(G) = \begin{cases} -30p + 60pq & \text{if } p > 1, q > 1 \\ 30p & \text{if } p > 1, q = 1 \\ 30q - 26 & \text{if } p = 1, q > 1 \\ 4 & \text{if } p = 1, q = 1 \end{cases}$$

**Proof. CASE 1:**

If  $q > 1, p > 1$ , It has 4 type of edges  $E_{3,4}, E_{4,5}, E_{4,4}, E_{5,5}$  that are enumerated in following table. For convenience these edge types are colored by green, blue, red and black respectively as shown in the following figure-7.

|                      |        |        |        |         |
|----------------------|--------|--------|--------|---------|
| $d_2(u/G), d_2(v/G)$ | (3, 4) | (4, 5) | (4, 4) | (5, 5)  |
| Number of edges      | 4p     | 4p     | 2p     | 6pq-11p |

$$\begin{aligned}
 LM_3(G) &= \sum_{uv \in E} d_2(u/G) + d_2(v/G) \\
 &= \sum_{uv \in E_{3,4}(G)} [d_2(u/G) + d_2(v/G)] + \sum_{uv \in E_{4,5}(G)} [d_2(u/G) + d_2(v/G)] \\
 &\quad + \sum_{uv \in E_{4,4}(G)} [d_2(u/G) + d_2(v/G)] + \sum_{uv \in E_{5,5}(G)} \left[ d_2\left(\frac{u}{G}\right) + d_2\left(\frac{v}{G}\right) \right] \\
 &= |E_{3,4}|(3 + 4) + |E_{4,5}|(4 + 5) + |E_{4,4}|(4 + 4) + |E_{5,5}|(5 + 5) \\
 &= 4p(7) + 4p(9) + (2p)(8) + (6pq - 11p)(10). \\
 &= -30p + 60pq.
 \end{aligned}$$

$$\therefore LM_3(G) = -30p + 60pq. \quad p > 1, \quad q > 1.$$

**CASE 2:**

If  $q = 1, p > 1$ , we have  $E_{1,1} = 5p$  as shown in figure- 8 .

$$\begin{aligned}
 LM_3(G) &= \sum_{uv \in E} d_2(u/G) + d_2(v/G) \\
 &= \sum_{uv \in E_{3,3}(G)} [d_2(u/G) + d_2(v/G)] \\
 &= |E_{3,3}|(3 + 3). \\
 &= 5p(6). \\
 &= 30p.
 \end{aligned}$$

$$\therefore LM_3(G) = 30p \quad p > 1, \quad q = 1.$$

**CASE 3:**

If  $q > 1, p = 1$ , It has 3 type of edges  $E_{1,1}, E_{1,3}, E_{2,3}, E_{2,2}$  and  $E_{3,3}$  these edges are colored in green, red, black, orange and pink respectively as shown in the following figure-9 and also the number of edges are represented in the table given below

| $d_2(u/G), d_2(v/G)$ | (1, 1) | (1, 3) | (2, 3) | (2, 2) | (3, 3) |
|----------------------|--------|--------|--------|--------|--------|
| Number of edges      | 6      | 4      | $4q-8$ | $q-2$  | $q-1$  |

$$\begin{aligned}
 LM_3(G) &= \sum_{uv \in E} d_2(u/G) + d_2(v/G) \\
 &= \sum_{uv \in E_{1,1}(G)} [d_2(u/G) + d_2(v/G)] + \sum_{uv \in E_{1,3}(G)} [d_2(u/G) + d_2(v/G)] \\
 &\quad + \sum_{uv \in E_{2,3}(G)} [d_2(u/G) + d_2(v/G)] \\
 &\quad + \sum_{uv \in E_{2,2}(G)} [d_2(u/G) + d_2(v/G)] + \sum_{uv \in E_{3,3}(G)} [d_2(u/G) + d_2(v/G)] \\
 &= |E_{1,1}|(1 + 1) + |E_{1,3}|(1 + 3) + |E_{2,3}|(2 + 3) + |E_{2,2}|(2 + 2) + |E_{3,3}|(3 + 3) \\
 &= 6(2) + 4(4) + (4q - 8)(5) + (q - 2)(4) + (q - 1)(6). \\
 &= 30q - 26.
 \end{aligned}$$

$$\therefore LM_3(G) = 30q - 26. \quad p = 1, \quad q > 1.$$

**CASE 4:**

If  $q = 1, p = 1$  we have the edges of the type  $E_{1,0}$  and  $E_{0,0}$  as shown in the figure 10 and the number of edges are represented in the following table

|                      |        |        |
|----------------------|--------|--------|
| $d_2(u/G), d_2(v/G)$ | (1, 0) | (0, 0) |
| Number of edges      | 4      | 1      |

$$\begin{aligned}
 LM_3(G) &= \sum_{uv \in E} d_2(u/G) + d_2(v/G) \\
 &= \sum_{uv \in E_{1,0}(G)} [d_2(u/G) + d_2(v/G)] + \sum_{uv \in E_{0,0}(G)} [d_2(u/G) + d_2(v/G)] \\
 &= |E_{1,0}|(1 + 0) + |E_{0,0}|(0 + 0) \\
 &= 4(1) + 1(0). \\
 &= 4.
 \end{aligned}$$

$$\therefore LM_3(G) = 4 \quad p = 1, \quad q = 1.$$

**Theorem 2.5.** The second leap zagreb index of  $TUC_4C_8(p, q)$  nanotorus is given by,

$$LM_2(G) = \begin{cases} 150pq & \text{if } p > 1, \quad q > 1 \\ 37p & \text{if } p > 1, q = 1 \\ 0 & \text{if } p = 1, q = 1 \end{cases}$$

**Proof. CASE 1:**

If  $q > 1, p > 1$ , we have  $E_{5,5} = 6pq$  as shown in the figure-11

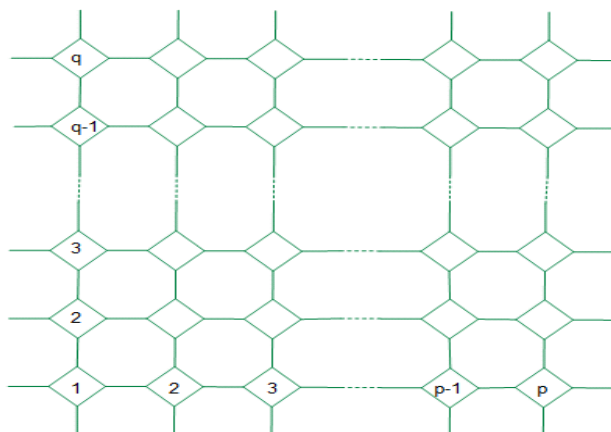


Fig-11

$$\begin{aligned}
LM_2(G) &= \sum_{uv \in E} d_2(u/G) d_2(v/G) \\
&= \sum_{uv \in E_{5,5}(G)} [d_2(u/G) d_2(v/G)] \\
&= |E_{5,5}|(5 \times 5) \\
&= 6pq(25) \\
&= 150pq.
\end{aligned}$$

$$\therefore LM_2(G) = 150pq \quad p > 1, \quad q > 1.$$

**CASE 2:**

If  $q = 1, p > 1$ , it has 3 type of edges  $E_{2,3}, E_{2,2}, E_{3,3}$  that are enumerated in following table. For convenience these edge type are colored by green, red and black respectively as shown in figure 12

|                      |        |        |        |
|----------------------|--------|--------|--------|
| $d_2(u/G), d_2(v/G)$ | (2, 3) | (2, 2) | (3, 3) |
| Number of edges      | 4p     | p      | p      |

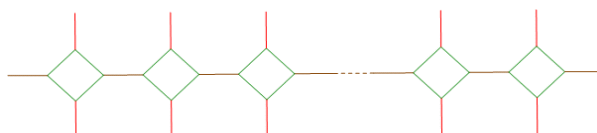


Fig-12

$$\begin{aligned}
LM_2(G) &= \sum_{uv \in E} d_2(u/G) d_2(v/G) \\
&= \sum_{uv \in E_{2,3}(G)} [d_2(u/G) d_2(v/G)] + \sum_{uv \in E_{2,2}(G)} [d_2(u/G) d_2(v/G)] \\
&\quad + \sum_{uv \in E_{3,3}(G)} [d_2(u/G) d_2(v/G)] \\
&= |E_{2,3}|(2 \times 3) + |E_{2,2}|(2 \times 2) + |E_{3,3}|(3 \times 3). \\
&= 4p(6) + p(4) + p(9). \\
&= 37p.
\end{aligned}$$

$$\therefore LM_2(G) = 37p \quad p > 1, \quad q = 1.$$

**CASE 3:**

when  $q = 1, p = 1$ , we have  $E_{0,0}=6$  as shown in the below figure-13



Fig-13

$$\begin{aligned}
 LM_2(G) &= \sum_{uv \in E} d_2(u/G) d_2(v/G) \\
 &= \sum_{uv \in E_{0,0}(G)} [d_2(u/G) d_2(v/G)] \\
 &= |E_{0,0}|(0 \times 0) \\
 &= 6(0). \\
 &= 0
 \end{aligned}$$

$$\therefore LM_2(G) = 0 \quad p = 1, \quad q = 1.$$

**Theorem 2.6.** The third leap zagreb index of  $TUC_4C_8(p, q)$  nanotorus is given by,

$$LM_2(G) = \begin{cases} 150pq & \text{if } p > 1, \quad q > 1 \\ 37p & \text{if } p > 1, q = 1 \\ 0 & \text{if } p = 1, q = 1 \end{cases}$$

**Proof. CASE 1:**

If  $q > 1, p > 1$ , we have  $E_{5,5} = 6pq$  as shown in the figure-11

$$\begin{aligned}
 LM_3(G) &= \sum_{uv \in E} d_2(u/G) + d_2(v/G) \\
 &= \sum_{uv \in E_{5,5}(G)} [d_2(u/G) + d_2(v/G)] \\
 &= |E_{5,5}|(5 + 5) \\
 &= 6pq(10) \\
 &= 60pq.
 \end{aligned}$$

$$\therefore LM_3(G) = 60pq \quad p > 1, \quad q > 1.$$

**CASE 2:**

If  $q = 1, p > 1$ , it has 3 type of edges  $E_{2,3}, E_{2,2}, E_{3,3}$  that are enumerated in following table. For convenience these edge type are colored by green, red and black respectively as shown in figure 12

|                      |        |        |        |
|----------------------|--------|--------|--------|
| $d_2(u/G), d_2(v/G)$ | (2, 3) | (2, 2) | (3, 3) |
| Number of edges      | 4p     | p      | p      |

$$\begin{aligned}
 LM_3(G) &= \sum_{uv \in E} d_2(u/G) + d_2(v/G) \\
 &= \sum_{uv \in E_{2,3}(G)} [d_2(u/G) + d_2(v/G)] + \sum_{uv \in E_{2,2}(G)} [d_2(u/G) + d_2(v/G)] \\
 &\quad + \sum_{uv \in E_{3,3}(G)} [d_2(u/G) + d_2(v/G)] \\
 &= |E_{2,3}|(2 + 3) + |E_{2,2}|(2 + 2) + |E_{3,3}|(3 + 3). \\
 &= 4p(5) + p(4) + p(6). \\
 &= 30p.
 \end{aligned}$$

$$\therefore LM_3(G) = 30p \quad p > 1, \quad q = 1.$$

**CASE 3:**

when  $q = 1, p = 1$ , we have  $E_{0,0}=6$  as shown in the below figure-13



Fig-13

$$\begin{aligned}
 LM_3(G) &= \sum_{uv \in E} d_2(u/G) + d_2(v/G) \\
 &= \sum_{uv \in E_{0,0}(G)} [d_2(u/G) + d_2(v/G)] \\
 &= |E_{0,0}|(0 + 0) \\
 &= 6(0). \\
 &= 0
 \end{aligned}$$

$$\therefore LM_3(G) = 0 \quad p = 1, \quad q = 1.$$

**CONCLUSIONS**

In this article we have calculated leap Zagreb indices of  $TUC_4C_8(p, q)$  without using computer.

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