Int. J. Math. And Appl., 6(2–B)(2018), 141–150
ISSN: 2347-1557
Available Online: http://ijmaa.in/

International Journal of *Mathematics And its Applications*

Computing First Leap Zagreb Index of Some Nano Structures

B. Basavanagoud[1,*] and Praveen Jakkannavar[1]

1 Department of Mathematics, Karnatak University, Dharwad, Karnataka, India.

Abstract: Topological indices have several chemical applications in the quantitative structure-property relationships (QSPR) and quantitative structure-activity relationships (QSAR) analysis of chemical compounds. In this paper, we study the linear regression analysis of the first leap Zagreb index with respect to entropy, acentric factor, enthalpy of vaporization (HVAP), standard enthalpy of vaporization (DHVAP) and boiling point of octane isomers. Finally, we present the expressions for first leap Zagreb index of certain nano structures.

MSC: 05C90, 05C35, 05C12.

Keywords: First Zagreb index, leap Zagreb index, line graph, subdivision graph, line graph.

Accepted on: 19.04.2018

1. Introduction

Let $G = (n, m)$ be a simple graph with vertex set V and edge set E. The *k-neighborhood* [13] of a vertex $v \in V(G)$, denoted by $N_k(v/G)$, and $N_k(v/G) = \{u \in V(G) : d(u, v) = k\}$ in which $d(u, v)$ is the distance between the vertices u and v in G, i.e., the length of the shortest path joining u and v in G. The *k-distance degree of a vertex* $v \in V(G)$, denoted by $d_k(v/G)$, and $d_k(v/G) = |N_k(v/G)|$. Also, we denote $N_1(v/G)$ by $N_G(v)$ and $d_1(v/G)$ by $d_G(v)$. The *degree of an edge* $e = uv$ in G, denoted by $d_1(e/G)$ (or $d_G(e)$), is defined by $d_1(e/G) = d_1(u/G) + d_1(v/G) - 2$. If all the vertices of G have same degree equal to $r \in Z^+$, then G is called a r-regular graph. The subdivision graph of a graph G, denoted by $S(G)$, is the graph obtained from G by inserting a new vertex of degree two on each of its edge [8]. The line graph of a graph G, denoted by $L(G)$, is the graph with vertex set $E(G)$ and two vertices in $L(G)$ are adjacent if and only if they correspond to two adjacent edges in G [8]. For unexplained graph terminology and notation refer [8].

The physico-chemical properties of a molecule can be easily studied by graph invariants associated with the graphs corresponding to the chemical molecule. One of such graph invariants is topological index. Recently in [12], Naji et al. has introduced a novel topological index called first leap Zagreb index which is defined as the sum of squares of *2-distance degree* of vertices of a graph G, denoted by $LM_1(G)$, i.e., $LM_1(G) = \sum_{v \in V(G)} (d_2(v/G))^2$. There are plenty of topological indices defined in the literature. Zagreb indices[7], F-index[6], connectivity index (or Randić index) [5] are few of them. Very recently indices like Sanskruti index[9], second order first Zagreb index [2] and (β, α)-connectivity index [3] are introduced. Since it is higher order topological index and it has advanced chemical applications in quantitative structure-property relationships (QSPR) and quantitative structure-activity relationships (QSAR) study.

* E-mail: b.basavanagoud@gmail.com

In [12], Naji et al. have left to identify the chemical applications of first leap Zagreb index. Surprisingly, this index has very good correlation with physical properties of chemical compounds like boiling point, entropy, DHVAP, HVAP and accentric factor. Therefore, we present here a linear regression model of these physical properties with first leap Zagreb index.

In the present work, we consider 2D-Lattice, nanotube, nanotorus of $TUC_4C_8[p,q]$. Let p and q denote the number of squares in a row and the number of rows of squares, respectively in $2D$-lattice, nanotube and nanotorus of $TUC_4C_8[p,q]$. An example of $2D$-lattice, nanotube and nanotorus of $TUC_4C_8[4,3]$ is given in Fig. 1 (a), (b) and (c) respectively. Recently in [1, 2, 9–11], authors obtained the expressions for certain topological indices of line graph of subdivision graphs of 2D-lattice, nanotube and nanotorus of $TUC_4C_8[p,q]$.

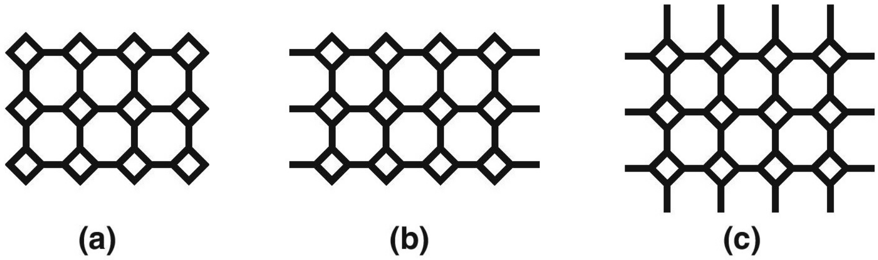

Figure 1. **(a) 2D-lattice of $TUC_4C_8[4,3]$; (b) $TUC_4C_8[4,3]$ nanotube; (c) $TUC_4C_8[4,3]$ nanotorus.**

The present work is organized as follows; In Section 2, we study the chemical applicability of the first leap Zagreb index. In Sections 3 and 4, we obtain explicit formulae for computing the first leap Zagreb index of 2D-lattice, nanotube and nanotorus of $TUC_4C_8[p,q]$ together with those of line graphs of subdivision graphs of 2D-lattice, nanotube and nanotorus of $TUC_4C_8[p,q]$ respectively.

2. On chemical applicability of the first leap Zagreb index

The topological indices with the higher correlation factor are of foremost important in quantitative structure-property relationships (QSPR) and quantitative structure-activity relationships (QSAR) analysis. In this section we discuss the linear regression analysis of first leap Zagreb index with entropy(S), acentric factor(AcentFac), enthalpy of vaporization (HVAP), standard enthalpy of vaporization (DHVAP) and boiling point(BP) of octane isomers on the degree based topological indices of the corresponding molecular graph. The first leap Zagreb index was tested using a dataset of octane isomers found at http://www.moleculardiscriptors.eu/dataset.htm. The dataset of octane isomers(columns 1-6 of Table 1) are taken from above web link whereas last column of Table 1 is computed by definition of first leap Zagreb index.

Alkane	BP	S	AcentFac	DHVAP	HVAP	LM_1
n-octane	125.665	111.67	0.397898	9.915	73.19	20
2-methyl-heptane	117.647	109.84	0.377916	9.484	70.3	28
3-methyl-heptane	118.925	111.26	0.371002	9.521	71.3	28
4-methyl-heptane	117.709	109.32	0.371504	9.483	70.91	30
3-ethyl-hexane	118.534	109.43	0.362472	9.476	71.7	30
2,2-dimethyl-hexane	106.84	103.42	0.339426	8.915	67.7	50
2,3-dimethyl-hexane	115.607	108.02	0.348247	9.272	70.2	36
2,4-dimethyl-hexane	109.429	106.98	0.344223	9.029	68.5	48
2,5-dimethyl-hexane	109.103	105.72	0.35683	9.051	68.6	36
3,3-dimethyl-hexane	111.969	104.74	0.322596	8.973	68.5	50
3,4-dimethyl-hexane	117.725	106.59	0.340345	9.316	70.2	36
2-methyl-3-ethyl-pentane	115.45	106.06	0.332433	9.209	69.7	38

Alkane	BP	S	AcentFac	DHVAP	HVAP	LM_1
3-methyl-3-ethyl-pentane	118.259	101.48	0.306899	9.081	69.3	48
2,2,3-trimethyl-pentane	109.841	101.31	0.300816	8.826	67.3	56
2,2,4-trimethyl-pentane	99.238	104.09	0.30537	8.402	64.87	62
2,3,3-trimethyl-pentane	114.76	102.06	0.293177	8.897	68.1	54
2,3,4-trimethyl-pentane	113.467	102.39	0.317422	9.014	68.37	44
2,2,3,3-tetramethylbutane	106.47	93.06	0.255294	8.41	66.2	72

Table 1. Experimental values of the entropy, acentric factor, HVAP, DHVAP, boiling point and the corresponding value of first leap Zagreb index of octane isomers.

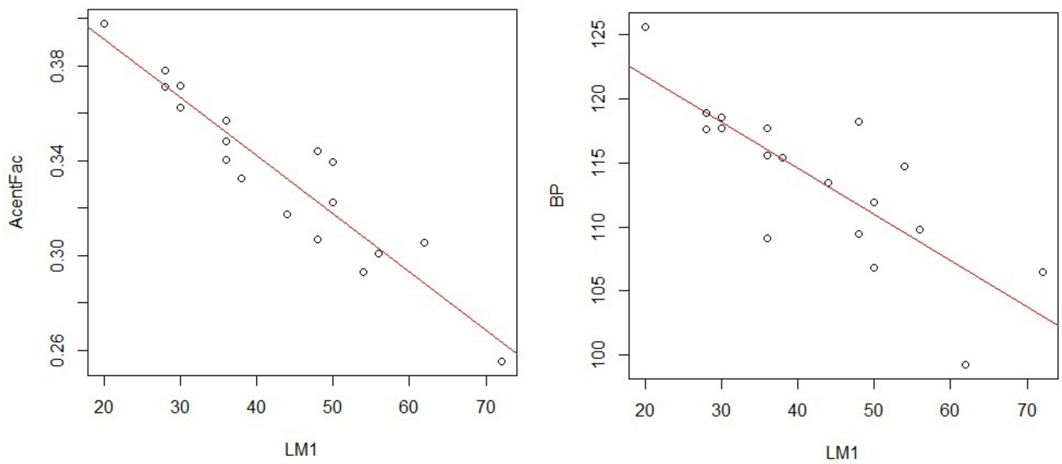

Figure 2. **Scatter diagram of (a)** $AcentFac$ **on** LM_1**, (b)** BP **on** LM_1 **superimposed by the fitted regression line.**

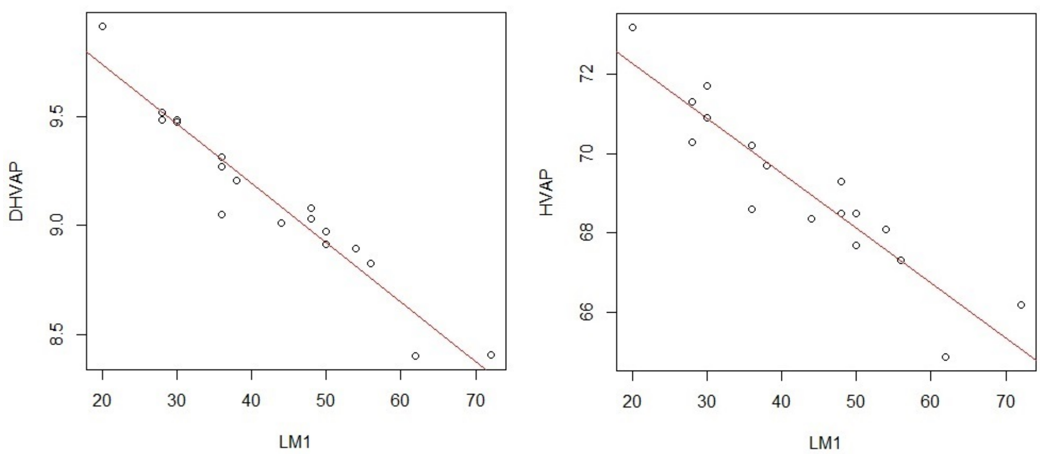

Figure 3. **Scatter diagram of (a)** $DHVAP$ **on** LM_1 **(b)** $HVAP$ **on** LM_1**, super imposed by the fitted regression line.**

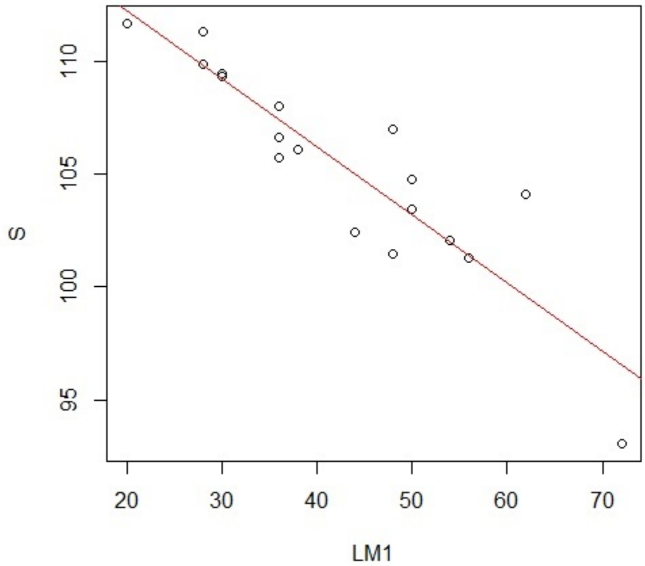

Figure 4. **Scatter diagram of (a) S on LM_1, super imposed by the fitted regression line.**

The linear regression models for the entropy, acentric factor, DHVAP, HVAP and boiling point using the data of Table 1 are obtained using the least squares fitting procedure as implemented in R software [4]. The fitted models are:

$$\hat{S} = 118.20831(\pm 1.59739) - 0.30067(\pm 0.03586)LM_1 \quad (1)$$

$$Acen\hat{t}Fac = 0.4402084(\pm 0.0100259) - 0.0024542(\pm 0.0002251)LM_1 \quad (2)$$

$$DH\hat{V}AP = 10.285778(\pm 0.083792) - 0.027245(\pm 0.001881)LM_1 \quad (3)$$

$$H\hat{V}AP = 75.04885(\pm 0.62979) - 0.13830(\pm 0.01414)LM_1 \quad (4)$$

$$\hat{B}P = 129.05174(\pm 3.01640) - 0.36070(\pm 0.06771)LM_1 \quad (5)$$

Note: The values in the brackets of Equations (1) to (5) are the corresponding standard errors of the regression coefficients. The index is better as $|r|$ approaches 1.

Physical Property	Absolute value of the correlation coefficient ($\|r\|$)	Residual standard error
Entropy	0.9025673	2.005
Acentric Factor	0.9388335	0.01258
DHVAP	0.9639245	0.1052
HVAP	0.9256201	0.7904
BP	0.7996668	3.786

Table 2. **Correlation coefficient and residual standard error of regression models**

From Table 2, we can observe that LM_1 correlates highly with DHVAP with the correlation coefficient $|r| = 0.9639245$. The most interesting observation is that it has more correlation with boiling point as compared to that of Wiener index. Also LM_1 has good correlation ($|r| > 0.9$) with entropy, accentric factor, DHVAP and HVAP.

3. First Leap Zagreb Index of 2D-lattice, Nanotube and Nanotorus of $TUC_4C_8[p,q]$

Graph	Order	Size
2D-Lattice of $TUC_4C_8[p,q]$	$4pq$	$6pq-p-q$
$TUC_4C_8[p,q]$ Nanotube	$4pq$	$6pq-p$
$TUC_4C_8[p,q]$ Nonotorus	$4pq$	$6pq$

Table 3. **Order and Size of graphs**

$d_2(v/A)$	2	3	4	5
Number of Vertices	8	$2(p+q-4)$	4(p+q-2)	$2(2pq-3p-3q+4)$

Table 4. **Vertex partition of the Graph A when $p>1, q>1$**

$d_2(v/A)$	1	2	3
Number of Vertices	2	4	$2(2p-3)$

Table 5. **Vertex partition of the Graph A when $p>1, q=1$**

Theorem 3.1. *Let A be a 2D-lattice of $TUC_4C_8[p,q]$. Then*

$$LM_1(A)=\begin{cases} 4(25pq-17p-17q+8) & if\ p>1, q>1 \\ 36(p-1) & if\ p>1, q=1. \end{cases}$$

Proof. The 2D-lattice of $TUC_4C_8[p,q]$ has $4pq$ vertices and $6pq-p-q$ edges. Therefore, we can partition the vertex set of A into the following cases:

Case 1: when $p>1$ and $q>1$. From the Table 4, we can see that the vertex partition is obtained based on the *2-distance degree* of each vertex. Now,

$$\begin{aligned} LM_1(A) &= \sum_{v\in V(A)} (d_2(v/A))^2 \\ &= 8\times(2)^2+2(p+q-4)\times 3^2+4(p+q-2)\times 4^2+2(2pq-3p-3q+4)\times 5^2 \\ &= 4(25pq-17p-17q+8). \end{aligned}$$

Case 2: when $p>1$ and $q=1$. The vertex partition is obtained on the base of the *2-distance degree* of each vertex which is shown in Table 5. Now,

$$\begin{aligned} LM_1(A) &= \sum_{v\in V(A)} (d_2(v/A))^2 \\ &= 2\times(1)^2+4\times 2^2+2(2p-3)\times 3^2 = 36(p-1). \end{aligned}$$

□

$d_2(v/B)$	3	4	5
Number of Vertices	$2p$	$4p$	$2p(2q-3)$

Table 6. **Vertex partition of the Graph B when $p>1, q>1$**

$d_2(v/B)$	3
Number of Vertices	$4p$

Table 7. **Vertex partition of the Graph B when $p > 1, q = 1$**

Theorem 3.2. *Let B be a $TUC_4C_8[p, q]$ nanotube. Then*

$$LM_1(B) = \begin{cases} 4p(25q - 17) & if\ p > 1, q > 1 \\ 36p & if\ p > 1, q = 1. \end{cases}$$

Proof. The $TUC_4C_8[p, q]$ nanotube has $4pq$ vertices and $6pq - p$ edges. Therefore, we can partition the vertex set of B into the following cases:

Case 1: when $p > 1$ and $q > 1$. From the Table 6, we can see that the vertex partition is obtained based on the *2-distance degree* of each vertex. Now,

$$\begin{aligned} LM_1(B) &= \sum_{v \in V(B)} (d_2(v/B))^2 \\ &= 2p \times 3^2 + 4p \times 4^2 + 2p(2q - 3) \times 5^2 \\ &= 4p(25q - 17). \end{aligned}$$

Case 2: when $p > 1$ and $q = 1$, the vertex partition is obtained on the base of the *2-distance degree* of each vertex which is shown in Table 7. Now,

$$\begin{aligned} LM_1(B) &= \sum_{v \in V(B)} (d_2(v/B))^2 \\ &= 4p \times 3^2 \\ &= 36p. \end{aligned}$$

□

Table 8. **Vertex partition of the Graph C**

$d_2(v/C)$	5
Number of Vertices	$4pq$

Theorem 3.3. *Let C be a $TUC_4C_8[p, q]$ nanotorus. Then $LM_1(C) = 100pq$.*

Proof. The $TUC_4C_8[p, q]$ nanotorus is shown in Fig. 1. The graph C is 3-regular with $4pq$ vertices and has *2-distance degree* of each vertex as 5. Therefore,

$$\begin{aligned} LM_1(C) &= \sum_{v \in V(C)} (d_2(v/C))^2 \\ &= 4pq \times 5^2 \\ &= 100pq. \end{aligned}$$

□

4. First Leap Zagreb Index of Line Graph of Subdivision Graphs of 2D-lattice, Nanotube and Nanotorus of $TUC_4C_8[p,q]$

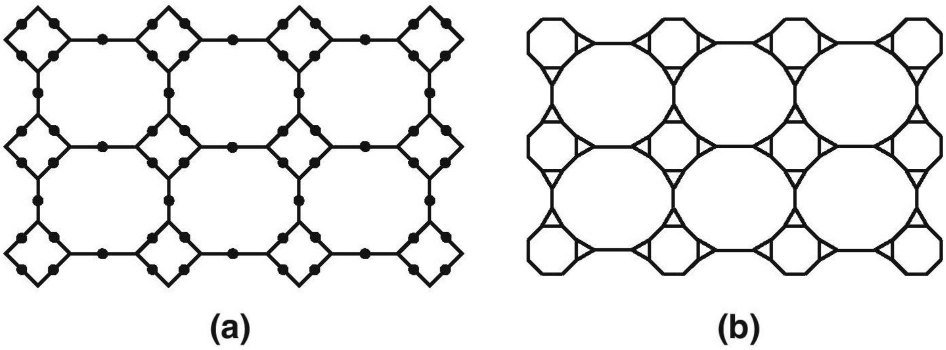

Figure 5. (a) Subdivision graph of 2D-lattice of $TUC_4C_8[4,3]$; (b) line graph of the subdivision graph of 2D-lattice of $TUC_4C_8[4,3]$.

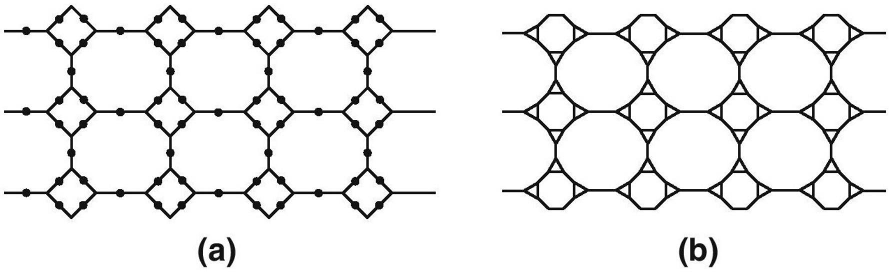

Figure 6. (a) Subdivision graph of $TUC_4C_8[4,3]$ of nanotube; (b) line graph of the subdivision graph of $TUC_4C_8[4,3]$ of nanotube.

$d_2(v/A_1)$	2	3	4
Number of Vertices	8	$4pq$	$2(4pq-p-q-4)$

Table 9. **Vertex partition of the Graph A_1 when $p>1, q>1$**

$d_2(v/A_1)$	2	3	4
Number of Vertices	8	$8(p-1)$	$2(p-1)$

Table 10. **Vertex partition of the Graph A_1 when $p>1, q=1$**

Theorem 4.1. *Let A_1 be a line graph of the subdivision graph of 2D-lattice of $TUC_4C_8[p,q]$. Then*

$$LM_1(A_1)=\begin{cases} 164pq-32p-32q-96 & if\ p>1, q>1 \\ 8(13p-9) & if\ p>1, q=1. \end{cases}$$

Proof. The $2D$-lattice of $TUC_4C_8[p,q]$ has $4pq$ vertices and $6pq-p-q$ edges. The subdivision graph of $2D$-lattice of $TUC_4C_8[p,q]$ has $10pq-p-q$ vertices and $2(6pq-p-q)$ edges. Thus, line graph of subdivision graph of $2D$-lattice of $TUC_4C_8[p,q]$ has vertices $2(6pq-6-q)$ and $18pq-5p-5q$ edges. Therefore, we can partition the vertex set of A_1 into the following cases:

Case 1: When $p>1$ and $q>1$. From the Table 9, we can see that the vertex partition is obtained based on the *2-distance* *degree* of each vertex. Now,

$$\begin{aligned} LM_1(A_1) &= \sum_{v\in V(A_1)} (d_2(v/A_1))^2 \\ &= 8\times(2)^2 + 4pq\times 3^2 + 2(4pq-p-q-4)\times 4^2 \\ &= 164pq - 32p - 32q - 96. \end{aligned}$$

Case 2: When $p>1$ and $q=1$. The vertex partition is obtained on the base of the *2-distance degree* of each vertex which is shown in Table 10. Now,

$$\begin{aligned} LM_1(A_1) &= \sum_{v\in V(A_1)} (d_2(v/A_1))^2 \\ &= 8\times(2)^2 + 8(p-1)\times 3^2 + 2(p-1)\times 4^2 \\ &= 8(13p-9). \end{aligned}$$

□

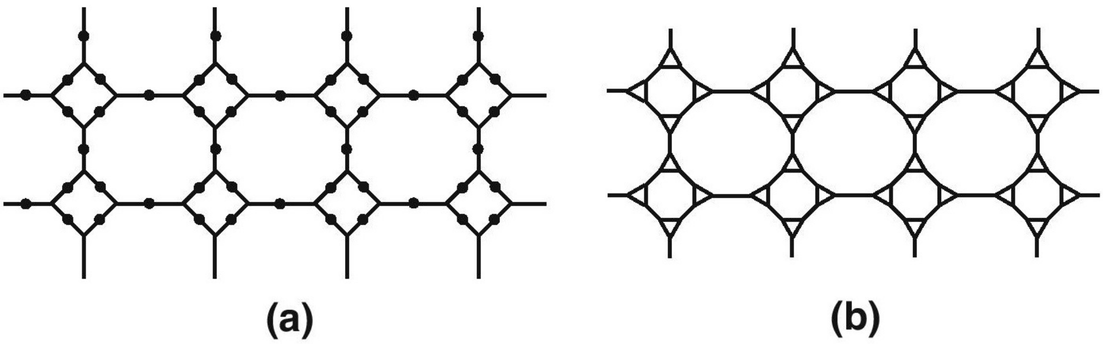

Figure 7. (a) Subdivision graph of $TUC_4C_8[4,3]$ of nanotorus; (b) line graph of the subdivision graph of $TUC_4C_8[4,3]$ of nanotorus.

$d_2(v/B_1)$	3	4
Number of Vertices	$8p$	$2p(6q-5)$

Table 11. **Vertex partition of the Graph B_1 when $p>1, q>1$**

$d_2(v/B_1)$	3	4
Number of Vertices	$8p$	$2p$

Table 12. **Vertex partition of the Graph B_1 when $p>1, q=1$**

Theorem 4.2. *Let B_1 be a line graph of the subdivision graph of $TUC_4C_8[p,q]$ nanotube. Then*

$$LM_1(B_1)=\begin{cases} 8p(24q-11) & if\ p>1, q>1 \\ 104p & if\ p>1, q=1. \end{cases}$$

Proof. The $TUC_4C_8[p,q]$ nanotube has $4pq$ vertices and $6pq-p$ edges. The subdivision graph of $TUC_4C_8[p,q]$ nanotube has $10pq-p$ vertices and $12pq-2p$ edges. Thus line graph of subdivision graph of $TUC_4C_8[p,q]$ nanotube has $12pq-2p$ vertices and $18pq-5p$ edges. Therefore, we can partition the vertex set of B_1 into the following cases:

Case 1: When $p > 1$ and $q > 1$. From the Table 11, we can see that the vertex partition is obtained based on the *2-distance degree* of each vertex. Now,

$$\begin{aligned} LM_1(B_1) &= \sum_{v \in V(B_1)} (d_2(v/B_1))^2 \\ &= 8p \times 3^2 + 2p(6q-5) \times 4^2 \\ &= 8p(24q-11). \end{aligned}$$

Case 2: When $p > 1$ and $q = 1$, the vertex partition is obtained on the base of the *2-distance degree* of each vertex which is shown in Table 12. Now,

$$\begin{aligned} LM_1(B_1) &= \sum_{v \in V(B_1)} (d_2(v/B_1))^2 \\ &= 8p \times 3^2 + 2p \times 4^2 \\ &= 104p. \end{aligned}$$

□

Table 13. **Vertex partition of Graph C_1**

$d_2(v/C_1)$	4
Number of Vertices	$12pq$

Theorem 4.3. *Let C_1 be a line graph of the subdivision graph of $TUC_4C_8[p, q]$ of nanotorus. Then $LM_1(C_1) = 192pq$.*

Proof. The subdivision graph of $TUC_4C_8[p, q]$ of nanotorus and the graph C_1 are shown in Fig. 7 (a) and (b). The graph C_1 is 3-regular with $12pq$ vertices and has *2-distance degree* of each vertex as 4. Therefore,

$$\begin{aligned} LM_1(C_1) &= \sum_{v \in V(C_1)} (d_2(v/C_1))^2 \\ &= 12pq \times 4^2 \\ &= 192pq. \end{aligned}$$

□

Acknowledgement

* This work is partially supported by the University Grants Commission (UGC), New Delhi, through UGC-SAP DRS-III for 2016-2021: F.510/3/DRS-III/2016(SAP-I).

[1] This work is supported by Directorate of Minorities Fellowship: Ph. D/M. Phil - 2017-18, No. DOM/FELLOWSHIP/CR-29/2017-18.

References

[1] A. R. Ashrafi and S. Yousefi, *Computing Wiener index of a $TUC_4C_8(S)$ nanotorus*, MATCH Commun. Math. Comput. Chem., 57(2007), 403-410.

[2] B. Basavanagoud, S. Patil and H. Deng, *On the second order first Zagreb index*, Iranian J. Math. Chem., 8(3)(2017), 299-311.

[3] B. Basavanagoud, V. R. Desai and S. Patil, $(\beta, \alpha)-$ *connectivity index of graphs*, Appl. Math. and Nonlinear Sciences, 2(1)(2017), 21-30.

[4] R Core Team, *A language and environment for statistical computing*, R Foundation for Statistical Computing, Vienna, Austria, (2016).

[5] H. Deng, *Catacondensed Benzenoids and Phenylenes with the extremal third-order Randić Index*, MATCH Commun. Math. Comput. Chem., 64(2010), 471-496.

[6] B. Furtula and I. Gutman, *A forgotten topological index*, J. Math. Chem., 53(2015), 1184-1190.

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

[8] F. Harary, *Graph Theory*, Addison-Wesely, Reading, Mass, (1969).

[9] S. M. Hosamani, *Computing Sanskruti index of certain nanostructures*, J. Appl. Math. Comput., (2016), DOI. 10.1007/s12190-016-1016-9.

[10] M. F. Nadeem, S. Zafar and Z. Zahid, *On certain topological indices of the line graph of subdivision graphs*, Appl. Math. Comput., 271(2015), 790794.

[11] M. F. Nadeem, S. Zafar and Z. Zahid, *On topological properties of the line graphs of subdivision graphs of certain nanostructures*, Appl. Math. Comput., 273(2016), 125130.

[12] A. M. Naji, N. D. Soner and Ivan Gutman, *On Leap Zagreb indices of graphs*, Commun. Comb. Optim., 2(2)(2017), 113-124.

[13] N. D. Soner and A. M. Naji, *The k-distance neighbourhood polynomial of a graph*, Int. J. Math. Comput. Sci. WASET Conference Proceedings, San Francico, USA, 3(9-XV)(2016), 2359-2364.