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FIRST NEIGHBOURHOOD ZAGREB INDEX OF SOME NANOSTRUCTURES

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Abstract: Motivated by chemical applications of topological indices in the QSPR/QSAR analysis, we introduce here a new topological index that we call, First Neighbourhood Zagreb Index (FNZI) and denote it by NM_1(G). In this paper, FNZI is tested with physico-chemical properties of octane isomers such as entropy, acentric factor, enthalpy of vaporization (HVAP) and DHVAP using the linear models. The FNZI shows excellent correlation with these chemical properties. Specially, high correlation with acentric factor (coefficient of correlation 0.994557). Later, we obtain bounds for NM_1(G) in terms of order and size of original graph and determine the extremal graphs which achieve the bounds. Finally, as an application we compute the FNZI of line graphs of subdivision graphs of 2D-lattice, nanotube and nanotorus of $TUC_4C_8[p,q]$.

Keywords: first Zagreb index, first neighbourhood Zagreb index, line graph, subdivision graph.

AMS Subject Classification: 05C07, 05C35, 05C76, 05C90.

1. Introduction

Let $G=(V,E)$ be a simple graph with V as vertex set and E as edge set. Let $|V|=n$ and $|E|=m$. The set of neighbourhood of a vertex $v\in G$ is defined as the number of vertices adjacent to v and denoted by $N_G(v)$. The degree of a vertex $v\in V(G)$, denoted by $d_G(v)$ and is defined as $|N_G(v)|$. A graph G is said to be r-regular if degree of each vertex in G is equal to $r(\in Z^+)$. The subdivision graph $S(G)$ is the graph obtained from G by replacing each of its edge by a path of length two [9]. The line graph $L(G)$ of G is the graph whose vertex set is $E(G)$ in which two vertices are adjacent if and only if they are adjacent in G [9]. For unexplained graph terminology and notation refer [9, 13].

In the recent days chemical graph theory is growing big because of its application in QSAR/QSPR study. A graph associated to a chemical molecule is easier to study in terms of graph invariants. Topological indices are such graph invariants. Due to this special property, topological indices are extensively used in chemistry. There are numerous indices defined so far. Among them, first Zagreb index is the first degree based topological index conceived in 1972 [8].

Later, second Zagreb index [7], F-index [6], connectivity index (or Randic' index) [21] are defined and extensively studied. Very recently, indices like Sanskruti index [10], second order first Zagreb index [3] and (β,α)-connectivity index [2] were introduced. The higher-order connectivity indices have found numerous applications in chemistry. For details see [12, 17, 20, 21].

Let $S_G(v)=\sum_{u\in N_G(v)} d_G(u)$ be the degree sum of neighbour vertices and $N_G(v)=\{u: uv\in E(G)\}$. We denote First Neighbourhood Zagreb index (FNZI) as $NM_1(G)$ and define as $NM_1(G)=\sum_{v\in V(G)} S_G(v)^2$.

Let p and q be the number of squares in a row and the number of rows of squares respectively in $2D$-lattice, nanotube and nanotorus of $TUC_4C_8[p,q]$. The $2D$-lattice, nanotube and nanotorus of $TUC_4C_8[4,3]$ is shown in Fig. 1. (a), (b) and (c) respectively. Much of the research work has been done on $TUC_4C_8[p,q]$ nanostructures. For example, authors in [1], computed Weiner index of $TUC_4C_8[p,q]$ nanotorus, and in [1, 2, 3, 10, 15], authors have obtained the expressions for some topological indices of line graph of subdivision graphs of 2D-lattice, nanotube and nanotorus of $TUC_4C_8[p,q]$. For more on topological indices of line graphs of subdivision graphs refer [14, 22].

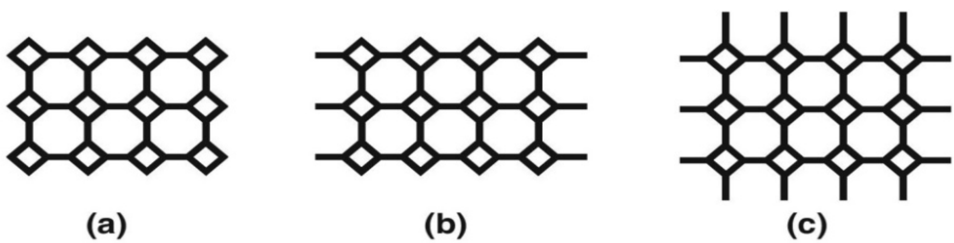

Figure 1: (a) 2D-lattice of $TUC_4C_8[4,3]$; (b) $TUC_4C_8[4,3]$ nanotube; (c) $TUC_4C_8[4,3]$ nanotorus.

The present paper is organized as follows: In section 2, we study the chemical applicability of the FNZI. In section 3, we obtain the upper and lower bounds for FNZI. In Section 4, we derive explicit formula for computing the FNZI of line graphs of subdivision graphs of 2D-lattice, nanotube and nanotorus of $TUC_4C_8[p,q]$.

2. On the chemical applicability of First neighbourhood Zagreb index

The topological indices with the high 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 FNZI with entropy (S), acentric factor (AcentFac), enthalpy of vaporization (HVAP) and DHVAP of octane isomers. The FNZI was tested using a dataset of octane isomers found at http://www.moleculardiscriptors.eu/dataset.htm. Interestingly, we have noticed that this index is highly correlated with acentric factor ($|r|$=0.994557). The dataset of octane isomers (columns 1-5 of Table 1) are taken from above web link whereas last column of Table 1 is calculated by definition of FNZI.

Table 1: Experimental values of the entropy, AcentFac, HVAP, DHVAP and corresponding value of FNZI of octane isomers.

Alkane	**S**	**AcentFac**	**DHVAP**	**HVAP**	**NM_1**
n-octane	111.67	0.397898	9.915	73.19	90
2-methyl-heptane	109.84	0.377916	9.484	70.3	104
3-methyl-heptane	111.26	0.371002	9.521	71.3	108
4-methyl-heptane	109.32	0.371504	9.483	70.91	110
3-ethyl-hexane	109.43	0.362472	9.476	71.7	114
2,2-dimethyl-hexane	103.42	0.339426	8.915	67.7	138
2,3-dimethyl-hexane	108.02	0.348247	9.272	70.2	126
2,4-dimethyl-hexane	106.98	0.344223	9.029	68.5	124
2,5-dimethyl-hexane	105.72	0.35683	9.051	68.6	118
3,3-dimethyl-hexane	104.74	0.322596	8.973	68.5	146
3,4-dimethyl-hexane	106.59	0.340345	9.316	70.2	130
2-methyl-3-ethyl-pentane	106.06	0.332433	9.209	69.7	132
3-methyl-3-ethyl-pentane	101.48	0.306899	9.081	69.3	152
2,2,3-trimethyl-pentane	101.31	0.300816	8.826	67.3	162
2,2,4-trimethyl-pentane	104.09	0.30537	8.402	64.87	156
2,3,3-trimethyl-pentane	102.06	0.293177	8.897	68.1	164
2,3,4-trimethyl-pentane	102.39	0.317422	9.014	68.37	144
2,2,3,3-tetramethylbutane	93.06	0.255294	8.41	66.2	194

The linear regression models for the entropy, acentric factor, DHVAP and HVAP using the data of Table 1 are obtained using the least squares fitting procedure as implemented in R software [19]. The fitted models are:

$$S = 127.80036(\pm 1.81803) - 0.16707(\pm 0.01334) NM_1 \quad (1)$$

$$AcentFac = 0.5192(\pm 0.004887) - 0.001369(\pm 0.00003585) NM_1 \quad (2)$$

$$DHVAP = 10.90808(\pm 0.22768) - 0.01330(\pm 0.00167) NM_1 \quad (3)$$

$$HVAP = 77.870488(\pm 1.51089) - 0.06498(\pm 0.01108) NM_1 \quad (4)$$

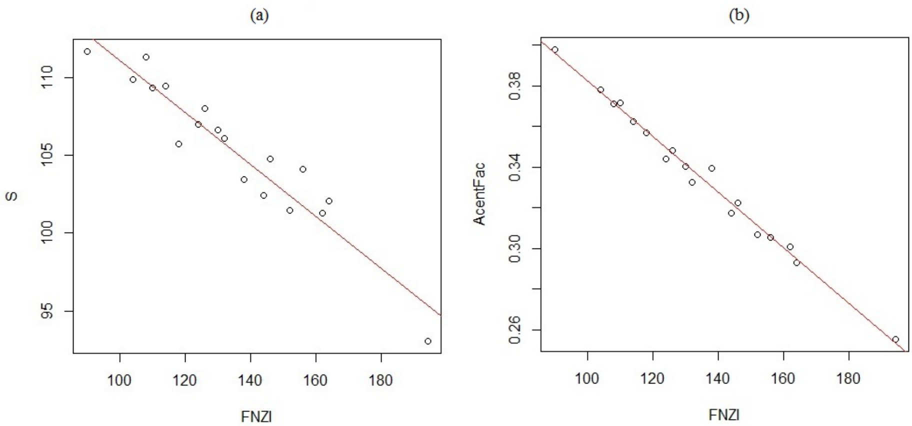

Figure 2: Scatter diagram of (a) S on $FNZI$, (b) $AcentFac$ on $FNZI$ superimposed by the fitted regression line.

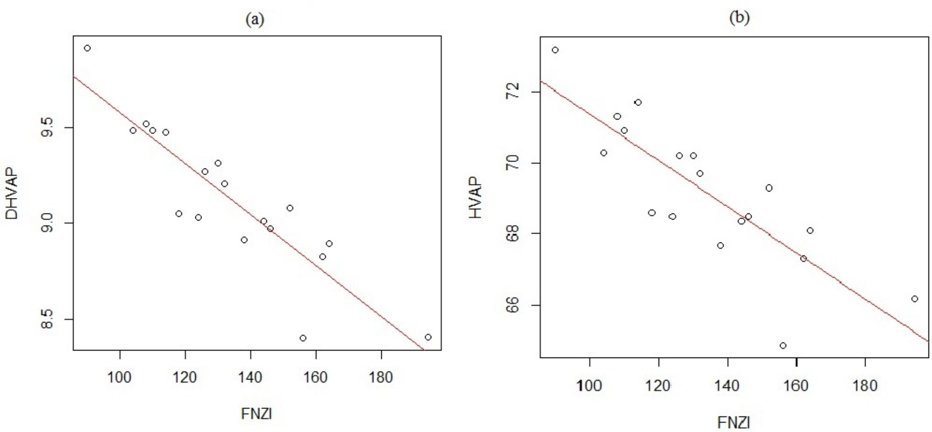

Figure 3: Scatter diagram of (a) $DHVAP$ on $FNZI$ (b) $HVAP$ on $FNZI$, superimposed by the fitted regression line.

Note: The values in the brackets of Eq. (1) to (4) are the corresponding standard errors of the regression coefficients.

Table 2: Correlation coefficient and residual standard error of regression models

Physical Property	**Absolute value of the correlation coefficient ($\|r\|$)**	**Residual standard error**
Enthalpy	0.9526144	1.416
Acentric Factor	**0.9945570**	**0.003807**
DHVAP	0.8935526	0.1774
HVAP	0.8260472	0.8260472

From Table 2, we can observe that FNZI highly correlates with acentric factor which is better than first Zagreb index ($|r|$=0.973087869 and residual standard error is 0.008424), second order first Zagreb index ($|r|$=0.99020 and residual standard error is 0.005101) [3] and $(\beta,\alpha)-$connectivity index ($|r|$ =0.95802 and residual standard error is 0.01047) [2]. Closer the $|r|$ to 1, better is the index.

3. Mathematical Properties of the First neighbourhood Zagreb index

Firstly, we mention below some results which are important for our result.

Lemma 1.1 [11] *Let G be connected graph with n, $n \geq 2$ vertices and m edges. Then*

$$M_1(G) \quad \geq \quad \frac{4m^2}{n}. \qquad (4)$$

Equality holds if and only if G is isomorphic with a regular graph.

Theorem 3.1 [18] *Suppose a_i and b_i, $1 \leq i \leq n$ are positive real numbers, then*

$$\sum_{i=1}^{n} a_i^2 \sum_{i=1}^{n} b_i^2 \quad \leq \quad \frac{1}{4}\left(\sqrt{\frac{M_1 M_2}{m_1 m_2}} + \sqrt{\frac{m_1 m_2}{M_1 M_2}}\right)^2 \left(\sum_{i=1}^{n} a_i b_i\right)^2 \qquad (5)$$

where $M_1 = \max\limits_{1 \leq i \leq n}(a_i)$; $M_2 = \max\limits_{1 \leq i \leq n}(b_i)$; $m_1 = \min\limits_{1 \leq i \leq n}(a_i)$ and $m_2 = \min\limits_{1 \leq i \leq n}(b_i)$

Theorem 3.2 [16] *Let a_i and b_i, $1 \leq i \leq n$ are non-negative real numbers, then*

$$\sum_{i=1}^{n} a_i^2 \sum_{i=1}^{n} b_i^2 - \left(\sum_{i=1}^{n} a_i b_i\right)^2 \quad \leq \quad \frac{n^2}{4}\left(M_1 M_2 - m_1 m_2\right)^2 \qquad (6)$$

where M_i and m_i are defined similarly to Theorem 3.1.

Theorem 3.3. [4] *Suppose* a_i *and* b_i, $1 \le i \le n$ *are positive real numbers, then*

$$\left| n\sum_{i=1}^{n} a_i b_i - \sum_{i=1}^{n} a_i \sum_{i=1}^{n} b_i \right| \le \alpha(n)(A-a)(B-b) \tag{7}$$

where a, b, A and B are real constants, that for each i, $1 \le i \le n$, $a \le a_i \le A$ and $b \le b_i \le B$. Further, $\alpha(n) = n\left\lfloor \frac{n}{2} \right\rfloor \left(1 - \frac{1}{n}\left\lfloor \frac{n}{2} \right\rfloor\right)$.

Theorem 3.4. [5] *Let* a_i *and* b_i, $1 \le i \le n$ *are nonnegative real numbers, then*

$$\sum_{i=1}^{n} b_i^2 + rR\sum_{i=1}^{n} a_i^2 \le (r+R)\left(\sum_{i=1}^{n} a_i b_i\right) \tag{8}$$

where r and R are real constants, so that for each i, $1 \le i \le n$, holds, $ra_i \le b_i \le Ra_i$.

We have the following observations.

Observation 3.5. *Let* $G = (V, E)$ *be a graph with* $|V| = n$ *and* $|E| = m$. *Then*

$$\sum_{v_i \in V(G)} S_G(v_i) \le 2m(n-1). \tag{9}$$

The Observation 3.5 holds, from the fact that maximum degree of a vertex in any graph G of order n is $n-1$ and the remaining vertices may have degree $\le n-1$. If all the vertices have degree $n-1$ then their degree sum of neighbourhood vertices is equal to $(n-1)^2$. For $m = \binom{n}{2}$ we get, $\sum_{v_i \in V(G)} S_G(v_i) = 2m(n-1)$.

This is possible only if G is a complete graph. This leads to the following observation:

Observation 3.6. *If* $G = K_n$ *be a complete graph of order* $n \ge 2$ *and size* m, *then*

$$\sum_{v_i \in V(G)} S_G(v_i) = 2m(n-1). \tag{10}$$

The following theorem gives an upper bound for $NM_1(G)$ in terms of order and size of G. We use Observations 3.5 and 3.6 to prove the following theorem.

Theorem 3.7. *Let* $G = (V, E)$ *be a graph with* $|V| = n$ *and* $|E| = m$. *Then*

$$NM_1(G) \le \frac{4m^2(n-1)^2}{n}. \tag{11}$$

Further, equality holds if and only if $G = K_n$, $n \ge 2$.

Proof. Let $a_1, a_2, \ldots, a_n$ and $b_1, b_2, \ldots, b_n$ be any two sequence of real numbers. Then by Cauchy-Schwartz inequality, we have

$$\left(\sum_{i=1}^{n} a_i b_i\right)^2 \leq \sum_{i=1}^{n} a_i^2 \cdot \sum_{i=1}^{n} b_i^2. \tag{12}$$

By setting $a_i = 1$ and $b_i = S_G(v_i)$ in Eq. (12), we get

$$\left(\sum_{i=1}^{n} S_G(v_i)\right)^2 \leq n \cdot \sum_{i=1}^{n} S_G(v_i)^2 \tag{13}$$

$$\left(\sum_{i=1}^{n} S_G(v_i)\right)^2 \leq nNM_1(G) \tag{14}$$

$$\sum_{i=1}^{n} S_G(v_i) \leq \sqrt{nNM_1(G)} \tag{15}$$

From Eq. (9) and Eq. (15), we have the following inequality

$$1 \leq \frac{2m(n-1)}{\sqrt{nNM_1(G)}}$$

$$\sqrt{nNM_1(G)} \leq 2m(n-1)$$

which implies,

$$NM_1(G) \leq \frac{4m^2(n-1)^2}{n} \tag{16}$$

For equality, suppose $G = K_n,\ n \geq 2$, then the result follows from Observation 3.6 Conversely, if the equality of Eq. (11) holds then $\sum_{i=1}^{n} S_G(v_i)^2 = \frac{4m^2(n-1)^2}{n}$. Then we conclude that the neighbourhood degree sum of every vertex is $S_G(v_i) = 2m(n-1)$. This is possible only for complete graphs $K_n,\ n \geq 2$. Hence the theorem follows.

As an immediate consequence of Theorem 3.7 , we have the following result.

Corollary 3.8. *Let $G = (V, E)$ be a graph with $|V| = n$ and $|E| = m$. Then*

$$NM_1(G) \leq (n-1)^2 M_1(G). \tag{17}$$

Equality holds if and only if $G = K_n,\ n \geq 2$.

Proof. Follows from Lemma 1 and Theorem 3.7.

Before going for our next results, we define the following notions:

Definition 1. *Let $\Delta'(G)$ and $\delta'(G)$ denote the maximum and minimum neighbourhood degree sum of a graph G, where*

$$\Delta'(G) = max|S_G(v_i)|, \tag{18}$$

$$\delta'(G) = min|S_G(v_i)|. \tag{19}$$

The following theorem gives the upper bound for $NM_1(G)$ in terms of order, size, maximum and minimum neighbourhood degree sum of G.

Theorem 3.9. *Let G be a graph of order n and size m with maximum(minimum) neighbourhood degree $\Delta'(G)\,(\delta'(G))$ respectively. Then*

$$NM_1(G) \;\le\; \frac{m^2(n-1)^2}{n}\left(\frac{\Delta'(G)}{\delta'(G)}+\frac{\delta'(G)}{\Delta'(G)}\right)^2. \tag{20}$$

Proof. Let G be a graph with vertex set $V=\{v_1,v_2,\ldots,v_n\}$ and let $S_G(v_1),S_G(v_2),\ldots,S_G(v_n)$ are the corresponding neighbourhood degrees of vertices of G. We assume that $a_i=1$, $b_i=S_G(v_i)$, $M_1=M_2=\Delta'(G)$ and $m_1=m_2=\delta'(G)$ in Eq. (5) and by Eq. (16) we get

$$\begin{aligned}
nNM_1(G) &\le \frac{1}{4}\left(\sqrt{\frac{\Delta'(G)^2}{\delta'(G)^2}}+\sqrt{\frac{\delta'(G)^2}{\Delta'(G)^2}}\right)^2\cdot\left(\sum_{i=1}^{n}S_G(v_i)\right)^2\\
NM_1(G) &\le \frac{1}{4n}\left(\frac{\Delta'(G)}{\delta'(G)}+\frac{\delta'(G)}{\Delta'(G)}\right)^2\cdot 4m^2(n-1)^2\\
&\le \frac{m^2(n-1)^2}{n}\left(\frac{\Delta'(G)}{\delta'(G)}+\frac{\delta'(G)}{\Delta'(G)}\right)^2
\end{aligned}$$

as desired.

Theorem 3.10. *Let G be a graph of order n and size m. Then*

$$NM_1(G) \;\le\; \frac{1}{n}\left[\frac{n^2}{4}(\Delta'^2(G)-\delta'^2(G))+4m^2(n-1)^2\right]. \tag{21}$$

Proof. The required inequality follows by setting $a_1=1$, $b_i=S_G(v_i)$, $M_1=M_2=\Delta'(G)$ and $m_1=m_2=\delta'(G)$ in Eq. (6).

Theorem 3.11. *Let G be a nontrivial graph of order n and size m. Then*

$$NM_1(G)\le\frac{\alpha(n)(\Delta'(G)-\delta'(G))^2+4m^2(n-1)^2}{n},$$

where, $\alpha(n)=n\left\lfloor\frac{n}{2}\right\rfloor\left(1-\frac{1}{n}\left\lfloor\frac{n}{2}\right\rfloor\right)$. Further, equality holds if and only if $G=K_n$, $n\ge 2$.

Proof. Let $a_1,a_2,\ldots,a_n$ and $b_1,b_2,\ldots,b_n$ be real numbers for which there exist real constants a,b,A and B, so that for each i, $i=1,2,\ldots,n, a\le a_i\le A$ and $b\le b_i\le B$. Then by Theorem 3.3, the following inequality is valid.

$$\left| n\sum_{i=1}^{n} a_i b_i - \sum_{i=1}^{n} a_i \sum_{i=1}^{n} b_i \right| \leq \alpha(n)(A-a)(B-b) \tag{22}$$

Where, $\alpha(n) = n\left\lfloor \frac{n}{2} \right\rfloor \left(1 - \frac{1}{n}\left\lfloor \frac{n}{2} \right\rfloor\right)$. Equality holds if and only if $a_1 = a_2 = \cdots = a_n$ and $b_1 = b_2 = \cdots = b_n$.

We choose $a_i = S_G(v_i) = b_i$, $A = \Delta'(G) = B$ and $a = \delta'(G) = b$, Eq. (22), becomes

$$n\sum_{i=1}^{n} S_G(v_i)^2 - \left(\sum_{i=1}^{n} S_G(v_i)\right)^2 \leq \alpha(n)(\Delta'(G) - \delta'(G))(\Delta'(G) - \delta'(G)) \tag{23}$$

$$nNM_1(G) \leq \alpha(n)(\Delta'(G) - \delta'(G))^2 + 4m^2(n-1)^2 \tag{24}$$

$$NM_1(G) \leq \frac{\alpha(n)(\Delta'(G) - \delta'(G))^2 + 4m^2(n-1)^2}{n} \tag{25}$$

The equality in above equation holds if and only if $a_1 = a_2 = \cdots = a_n$, $b_1 = b_2 = \cdots = b_n$ and $\sum_{v_i \in V(G)} S_G(v_i) = 2m(n-1)$. Therefore equality of the theorem holds if and only if $G = K_n,\ n \geq 2$.

Theorem 3.12. *Let G be a nontrivial graph of order n and size m. Then*

$$NM_1(G) \leq (\delta'(G) + \Delta'(G))\, 2m(n-1) - n\,\delta'(G)\Delta'(G). \tag{26}$$

Equality holds if and only if $G = K_n,\ n \geq 2$.

Proof. Let $a_1, a_2, \ldots, a_n$ and $b_1, b_2, \ldots, b_n$ be real numbers for which there exist real constants r and R so that for each i, $i = 1, 2, \ldots, n$ holds $ra_i \leq b_i \leq Ra_i$. Then the following inequality is valid.

$$\sum_{i=1}^{n} b_i^2 + rR\sum_{i=1}^{n} a_i^2 \leq (r+R)\sum_{i=1}^{n} a_i b_i. \tag{27}$$

Equality of (27) equation holds if and only if, for at least one i, $1 \leq i \leq n$ holds $ra_i = b_i = Ra_i$.

We choose $b_i = S_G(v_i)$, $a_i = 1$, $r = \delta'(G)$ and $R = \Delta'(G)$ in Eq. (27), then

$$\sum_{i=1}^{n} S_G(v_i)^2 + \delta'(G)\Delta'(G)\sum_{i=1}^{n} 1 \leq (\delta'(G) + \Delta'(G))\sum_{i=1}^{n} S_G(v_i)$$

$$NM_1(G) + \delta'(G)\Delta'(G)n \leq (\delta'(G) + \Delta'(G))\sum_{i=1}^{n} S_G(v_i)$$

$$NM_1(G) \leq (\delta'(G) + \Delta'(G))\, 2m(n-1) - n\,\delta'(G)\Delta'(G).$$

If for some i, $ra_i = b_i = Ra_i$ holds, then $b_i = r = R$ also holds. Therefore equality holds if and only if $\delta'(G) = \Delta'(G) = 2m(n-1)$. This implies that G is a complete graph $K_n,\ n \geq 2$.

4. First neighbourhood Zagreb index of some nanostructures

In this section, we obtain explicit formule for computing FNZI of line graph of subdivision graphs of 2D-lattice, nanotube and nanotorus of $TUC_4C_8[p,q]$. The proof technique used here is partitioning the edge set of nanostructures. Here, we denote p,q respectively to denote order and size of the underline molecular graph.

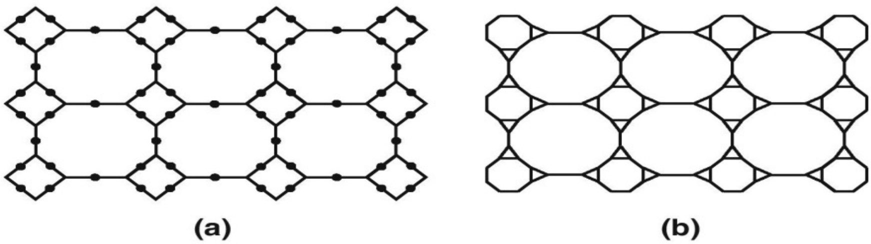

Figure 4: (a) Subdivision graph of 2D-lattice of $TUC_4C_8[4,3]$; (b) line graph of the subdivision graph of 2D-lattice of $TUC_4C_8[4,3]$.

Table 3:Order and Size of graphs

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 4:Vertex partition Graph A when $p>1, q>1$

$(d_A(v), S_A(v))$	(2, 4)	(2, 5)	(3, 8)	(3, 9)
Number of Vertices	8	$4(p+q-2)$	$4(p+q-2)$	$2(6pq-5p-5q+4)$

Table 5: Vertex partition Graph A when $p>1, q=1$

$(d_A(v), S_A(v))$	(2, 4)	(2, 5)	(3, 8)	(3, 9)
Number of Vertices	8	$4(p-1)$	$4(p-1)$	$2(p-1)$

The following theorem gives the FNZI of line graph of the subdivision graph of $2D$-lattice of $TUC_4C_8[p,q]$.

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

$$NM_1(A)=\begin{cases}128+356(p+q-2)+162(6pq-5p-5q+4) & if\ \ p>1, q>1,\\ 128+518(p-1) & if\ \ p>1, q=1.\end{cases}$$

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

Case 1: when $p>1$ and $q>1$.

From the Table 4, we see that the vertex partition is obtained based on the degree sum of neighbour vertices of each vertex.

Now,

$$\begin{aligned} NM_1(A) &= \sum_{v\in V(G)}\left(S_A(v)\right)^2\\ &= 8\times(4)^2+4(p+q-2)\times5^2+4(p+q-2)\times8^2+2(6pq-5p-5q+4)\times9^2\\ &= 162(6pq-5p-5q+4)+356(p+q-2)+128.\end{aligned}$$

Case 2: when $p>1$ and $q=1$.

The vertex partition is obtained on the base of the degree sum of neighbour vertices is shown in Table 5.

Now,

$$\begin{aligned} NM_1(A) &= \sum_{v\in V(G)}\left(S_A(v)\right)^2\\ &= 8\times(4)^2+4(p-1)\times5^2+4(p-1)\times8^2+2(p-1)\times9^2\\ &= 128+518(p-1).\end{aligned}$$

Table 6:Vertex partition of Graph B when $p>1, q>1$

$(d_B(v), S_B(v))$	**(2, 5)**	**(3, 8)**	**(3, 9)**
Number of Vertices	$4p$	$4p$	$12pq-10p$

Table 7:Vertex partition Graph B when $p>1, q=1$

$(d_B(v), S_B(v))$	**(2, 5)**	**(3, 8)**	**(3, 9)**
Number of Vertices	$4p$	$4p$	$2p$

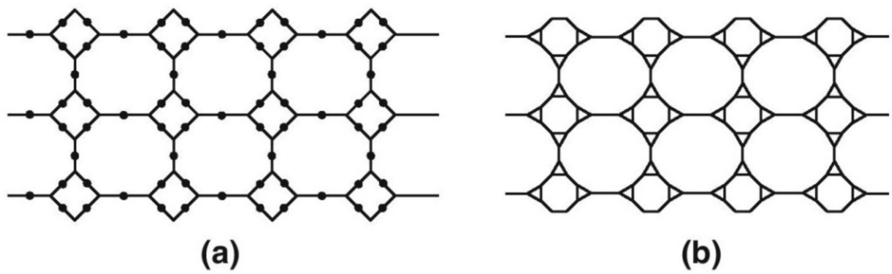

Figure 5: (a) Subdivision graph of $TUC_4C_8[4,3]$ of nanotube; (b) line graph of the subdivision graph of $TUC_4C_8[4,3]$ of nanotube.

The next theorem gives FNZI of line graph of the subdivision graph of $TUC_4C_8[p,q]$ nanotube.

Theorem 4.2. *If B be a line graph of the subdivision graph of $TUC_4C_8[p,q]$ nanotube, then*

$$NM_1(B) = \begin{cases} 972pq - 454p & if \ \ p > 1, q > 1, \\ 518p & if \ \ p > 1, q = 1. \end{cases}$$

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 G into the following cases:

Case 1: when $p > 1$ and $q > 1$.

From the Table 6, we observe that the vertex partition is obtained based on the degree sum of neighbour vertices of each vertex.

Now,

$$\begin{aligned} NM_1(B) &= \sum_{v \in V(G)} (S_B(v))^2 \\ &= 4p \times 5^2 + 4p \times 8^2 + (12pq - 10p) \times 9^2 \\ &= 972pq - 454p. \end{aligned}$$

Case 2: when $p > 1$ and $q = 1$, the vertex partition is obtained on the base of the degree sum of neighbour vertices is shown in Table 7.

Now,

$$
\begin{aligned}
NM_1(B) &= \sum_{v\in V(G)} (S_B(v))^2 \\
&= 4p\times 5^2 + 4p\times 8^2 + 2p\times 9^2 \\
&= 518p.
\end{aligned}
$$

The following theorem gives FNZI of line graph of the subdivision graph of $TUC_4C_8[p,q]$ nanotorus.

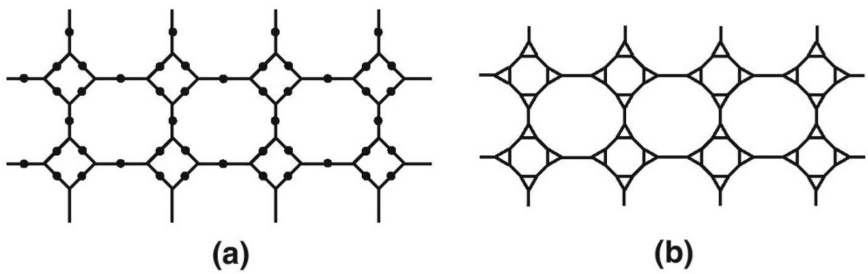

Figure 6: (a) Subdivision graph of $TUC_4C_8[4,3]$ of nanotorus; (b) line graph of the subdivision graph of $TUC_4C_8[4,3]$ of nanotorus.

Table 8:Vertex partition of Graph C

$(d_C(v), S_C(v))$	**(3, 9)**
Number of Vertices	$12pq$

Theorem 4.3. *Let* C *be a line graph of the subdivision graph of* $TUC_4C_8[p,q]$ *of nanotorus. Then* $NM_1(C) = 972pq$.

Proof. The subdivision graph of $TUC_4C_8[p,q]$ of nanotorus and the graph C are shown in Fig. 6 (a) and (b). The graph C is 3-regular with $12pq$ vertices. Therefore, degree sum of each neighbour vertices is 9.
Now,

$$
\begin{aligned}
NM_1(C) &= \sum_{v\in V(G)} (S_C(v))^2 \\
&= 12pq\times 9^2 \\
&= 972pq.
\end{aligned}
$$

3. Conclusion

In this paper, we have introduced a novel topological index namely the first neighbourhood Zagreb index (FNZI) in the field of mathematical chemistry, it has chemical applicability in determining several physico-chemical properties of octane isomers as it has coefficient of correlation close to 1, which is far better than other indices. Next, we have studied mathematical properties of FNZI by obtaining several bounds (both lower and upper). Finally, we have obtained explicit formulae for FNZI of certain nanostructures.

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ПЕРВАЯ ОКРЕСТНОСТЬ ЗАГРЕБСКОГО ИНДЕКСА НЕКОТОРЫХ НАНОСТРУКТУР

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РЕЗЮМЕ

Основываясь на химических применениях топологических индексов в анализе QSPR / QSAR, мы вводим новый топологический индекс, который называем Загребский индекс первой окрестности (FNZI), и обозначаем его как NM_1(G). В этой статье FNZI тестируется с физико-химическими свойствами изомеров октана, такими как энтропия, ацентрический фактор, энтальпия испарения (HVAP) и DHVAP с использованием линейных моделей. FNZI показывает отличную корреляцию с этими химическими свойствами. Особенно высокая корреляция с ацентрическим фактором (коэффициент корреляции 0,994557). Позже мы получаем оценки для NM_1(G) в терминах порядка и размера исходного графа и определяем экстремальные графы, которые достигают границ. Наконец, в качестве приложения мы вычисляем FNZI линейных графов подразделов графов 2D-решетки, нанотрубок и нанотора $TUC_4C_8[p,q]$.

Ключевые слова: первый загребский индекс, первая окрестность загребского индекса, линейный граф, граф подразделений.