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On first closed neighborhood Zagreb index of graph

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Abstract

Topological indices are widely employed in the determination of the correlation between the physico-chemical properties of nanostructures. The development of novel nanostructures has important implications for the food science, electronics, pharmaceutical, medical, communication, and information sectors among others. In this paper, we introduce a new topological index called the first closed neighborhood Zagreb index and it exhibits good correlation with acentric factor of an octane isomers. We compute the formula for first closed neighborhood Zagreb index for some standard classes of graphs and investigate their mathematical properties. Further, we derive the expression for first closed neighborhood Zagreb index of $TUC_4C_8(R)[p,q]$ nanostructures as well as subdivision graph and the line graph of the subdivision graph of $TUC_4C_8(R)[p,q]$ nanostructures.

Keywords: First closed neighborhood Zagreb index, Nanostructures, Subdivision graph, Line graph.

2020 MSC: Primary 05C07, Secondary 05C76, 05C35, 05C90.

1. Introduction

Now a days chemical graph theory gaining attention due to its applications in QSAR / QSPR study. The quantitative structure property relationship (QSPR) and quantitative structure activity relationship (QSAR) reflects the applications of topological indices [10, 15]. Topological descriptors defined on chemical structures plays a key role in examining the properties and activities of the chemical molecules. According to the IUPAC definition, a topological index (or molecular structure descriptor) is a numerical value associated with chemical constitution for correlation of chemical structure with various physical properties, chemical reactivity or biological activity [7]. These indices are widely utilized in the study of chemical graph theory, where graphs represent molecular structures, but they also have applications in various fields, such as network analysis, biology, and computer science, engineering etc. A molecular graph is a simple graph whose vertices corresponds to the atoms and whose edges corresponds to the bonds. There are various topological indices defined till today among them, first Zagreb index is the first degree based topological index proposed in 1972 [5].

In this article, we considered simple, finite, undirected and connected graphs. Let G be a graph with vertex set $V(G)$ and edge set $E(G)$ having order n and size m respectively. The degree of a vertex u in G

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is the number of vertices adjacent to u and denoted by $d_G(u)$ and the degree of an edge $e{=}uv$ is defined as $d_G(e) = d_G(u) + d_G(v) - 2$. The neighborhood of a vertex u is defined as the set of vertices adjacent to u. We refer [4, 9] for undefined graph terminologies and notations. The degree sum of neighbor of a vertex u is $S_G(u) = \sum_{u\in N_G(u)} d_G(u)$. Let $N_G[u]$ be the closed neighborhood of a vertex u, that includes u and its neighbors. The degree sum of closed neighbor of a vertex u is $S_G[u] = \sum_{u\in N_G[u]} S_G(u) + d_G(u)$. Let G be a graph, then subdivision graph $S(G)$ is a graph obtained from G by inserting a vertex of degree two into every edge of G [9]. The line graph $L(G)$ is a graph derived from G in such a way that the edges in G are replaced by vertices in $L(G)$ and two vertices in $L(G)$ are connected whenever the corresponding edges in G are adjacent [9].

In 1972, Gutman and Trinajstić defined the first and second Zagreb indices [8].

The first Zagreb index is defined as

$$M_1(G) = \sum_{u\in V(G)} (d_G(u))^2 = \sum_{uv\in E(G)} (d_G(u) + d_G(v)). \tag{1.1}$$

The second Zagreb index is defined as

$$M_2(G) = \sum_{uv\in E(G)} d_G(u)d_G(v). \tag{1.2}$$

The first neighborhood Zagreb index is defined in [2] as

$$NM_1(G) = \sum_{u\in V(G)} S_G(u)^2. \tag{1.3}$$

Inspired by the first neighborhood Zagreb index, we defined the new molecular descriptor called first closed neighborhood Zagreb index(FCNZI). The first closed neighborhood Zagreb index is defined as the sum of square of closed neighborhood degree sum of vertices of a graph G and is denoted by $CM_1(G)$. Then

$$CM_1(G) = \sum_{u\in V(G)} S_G[u]^2. \tag{1.4}$$

The following discussion is organized into four sections that covers various features of the first closed neighborhood Zagreb index. In first section, we study its chemical applications to octane isomers. The FCNZI for some standard classes of graphs is examined in the second section. The mathematical properties of FCNZI are explored in the third section and the fourth section delves with the FCNZI of some nanostructures.

2. Chemical applicability of first closed neighborhood Zagreb index to octane isomers

The correlation coefficient is determined to evaluate the efficiency of a topological index in predicting the physicochemical behavior of the chemical substances. The topological index with significant correlation coefficient value greater than 0.8 are highly recommendable in QSAR/QSPR analysis. The first closed neighborhood Zagreb index exhibits strong correlation factors, making it highly valuable in quantitative structure-property relationships (QSPR) and quantitative structure-activity relationships (QSAR) analysis. This section explores the linear regression analysis between FCNZI and various properties, including entropy (S), acentric factor (AcentFac), and standard enthalpy of vaporization (DHVAP) to octane isomers. We have observed that FCNZI is highly correlated with acentric factor. The physico-chemical properties of octane isomers (column 1-4) were sourced from the International Academy of Mathematical Chemistry website (http://www.iamc-online.org/) [11], and the last column is obtained by the definition of FCNZI as detailed in Table 1.

Table 1: Physico-chemical properties of Octane isomers

Octane Isomer	Entropy	AccentFac	DHVAP	$\mathbf{CM_1(G)}$
octane	111.67	0.397898	9.915	212
2-methyl-heptane	109.84	0.377916	9.484	236
3-methyl-heptane	111.26	0.371002	9.521	280
4-methyl-heptane	109.32	0.371504	9.483	246
3-ethyl-hexane	109.43	0.362472	9.476	254
2,2-dimethyl-hexane	103.42	0.339426	8.915	290
2,3-dimethyl-hexane	108.02	0.348247	9.272	276
2,4-dimethyl-hexane	106.98	0.344223	9.029	278
2,5-dimethyl-hexane	105.72	0.356883	9.051	260
3,3-dimethyl-hexane	104.74	0.322596	8.973	306
3,4-dimethyl-hexane	106.59	0.340345	9.316	324
2-methyl-3-ethyl pentane	106.06	0.332433	9.209	286
3-methyl-3-ethyl pentane	101.48	0.306899	9.081	320
2,2,3-trimethyl-pentane	101.61	0.300816	8.826	336
2,2,4-trimethyl-pentane	104.03	0.30537	8.402	318
2,3,3-trimethyl-pentane	102.02	0.293177	8.897	342
2,3,4-trimethyl-pentane	102.3	0.317422	9.014	308
2,2,3,3-tetramethylbutane	93.06	0.25294	8.41	392

Using the information in Table 1, we generate the linear regression models for each physical parameter such as (entropy (S), acentric factor (AcentFac), and standard enthalpy of vaporization (DHVAP)) with FCNZI are obtained by utilizing the least squares fitting method as implemented in R software [13]. The fitted models are

$$S = -0.09253(\pm 0.01183)CM_1(G) + 132.47(\pm 0.7928) \tag{2.1}$$

$$AcentFac = -0.00077(\pm 1.773e - 02)CM_1(G) + 0.5636(\pm 0.004466) \tag{2.2}$$

$$DHVAP = -0.007174(\pm 0.001282)CM_1(G) + 11.2244(\pm 0.2297) \tag{2.3}$$

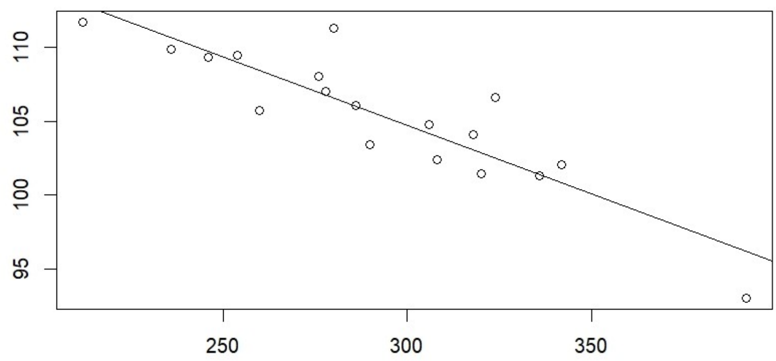

Figure 1: Linear regression of the entropy v/s FCNZI

3. The first closed neighborhood Zagreb index of some standard classes of graphs

Definition 3.1. [9] A complete bipartite graph $K_{m,n}$ is a graph whose vertex set V can be partitioned into

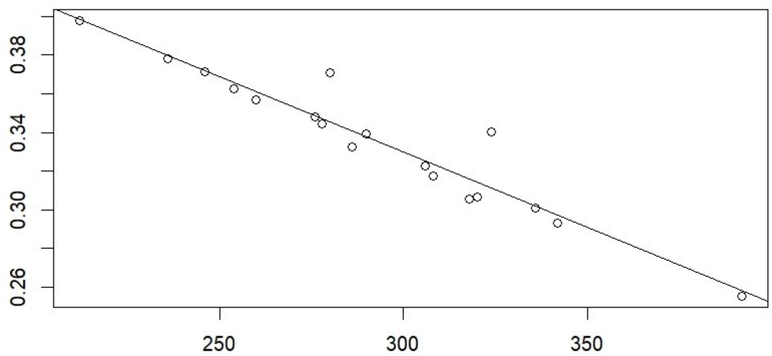

Figure 2: Linear regression of the acentFac v/s FCNZI

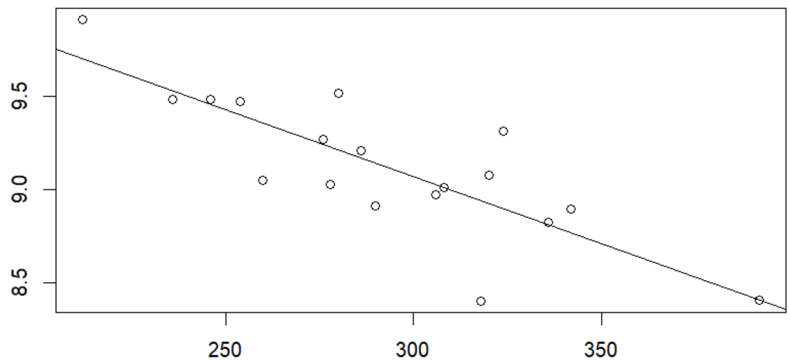

Figure 3: Linear regression of the DHVAP v/s FCNZI

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

Physical property	Absolute value of the correlation coefficient	Residual standard error
Entropy	0.8903812	2.119758
Acentric Factor	0.9556892	0.0107568
DHVAP	0.8136345	0.2297067

two subsets V_1 and V_2 with m and n vertices respectively, such that every vertex of V_1 joins to every other vertices of V_2.

Definition 3.2. [9] A complete bipartite graph $K_{1,n}$ is called a $\mathtt{star\ graph}$.

Definition 3.3. [1] The crown graph S_n^0 for an integer $n \geqslant 3$ is the graph with vertex set $\{u_1, u_2, ..., u_n, v_1, v_2, ..., v_n\}$ and edge set $\left\{u_i v_j; 1 \leqslant i, j \leqslant n, i \neq j\right\}$. Therefore S_n^0 coincides with the complete bipartite graph $k_{n,n}$ with the horizontal edges removed.

Definition 3.4. [6] The ladder graph L_n $(n \geqslant 2)$ is the Cartesian product graph $P_2 \times P_n$, and contains $2n$ vertices and $3n-2$ edges.

Definition 3.5. [6] The wheel graph W_n is constructed by adding an edge from the single vertex of K_1(central vertex) to each of the vertices in the cycle C_n. Therefore, W_n is essentially the join graph $C_n + K_1$, where K_1 is connected to all vertices of C_n.

Definition 3.6. [3] The gear graph G_n is obtained from the wheel graph W_n by adding a vertex between every pair of adjacent vertices of the cycle C_n.

Definition 3.7. [6] A friendship graph F_n is a graph in which every two distinct vertices have exactly one common adjacent vertex.

Definition 3.8. [6] The cocktail party graph $CP_{n,n}$ is the graph consisting of two rows of paired vertex in which all vertex but the paired ones are connected with a graph edge.

Definition 3.9. [6] The helm graph H_n is the graph obtained from the wheel graph W_n by adjoining a pendant edge at each vertex of the cycle C_n.

In this section, we obtain the expressions of FCNZI for path, cycle, complete graph, complete bipartite graph, star graph, crown graph, ladder graph, wheel graph, gear graph, friendship graph, cocktail party graph and helm graph.

Theorem 3.10. For path P_n, where n $\geqslant 5$, $CM_1(P_n) = 36n - 76$.

Proof. Let P_n be the path having order n and size $n-1$. For $n \geqslant 5$, the closed neighborhood degree of two pendant vertex is 3, the closed neighborhood degree of two vertices which is adjacent to pendant vertex is 5 and the closed neighborhood degree of remaining vertices is $n-4$, then we have following Table 3.

Table 3: Vertex partition of the path based on closed neighborhood degree.

$S_{P_n}[u]$, where $u \in V(P_n)$	3	5	6
Number of vertices	2	2	$n-4$

Using the values from Table 3 in equation 1.4, we obtain

$$CM_1(P_n) = 2 \times 3^2 + 2 \times 5^2 + (n-4) \times 6^2 = 36n - 76.$$

□

Theorem 3.11. For cycle C_n, where n $\geqslant 3$, $CM_1(C_n) = 36$n.

Proof. Let C_n be the cycle having order n and size m. For $n \geqslant 3$, the closed neighborhood degree of each vertex is 6. Then

$$CM_1(C_n) = n \times 6^2 = 36n.$$

□

Theorem 3.12. For complete graph K_n, where n $\geqslant 3$, $CM_1(K_n) = n[n^2 - n]^2$.

Proof. Let K_n be the complete graph having order n and size $n(n-1)/2$. For $n \geqslant 3$, the closed neighborhood degree of each vertex is $[(n-1)^2 + (n-1)]$. Then

$$\begin{aligned} CM_1(K_n) &= n[(n-1)^2 + (n-1)]^2 \\ &= n[n^2 - n]^2. \end{aligned}$$

□

Theorem 3.13. For complete bipartite graph $K_{m,n}$, where m,n $\geqslant$2,

$$CM_1(K_{m,n}) = m^2n^2(m+n) + mn(m+n) + 4m^2n^2.$$

Proof. Let $K_{m,n}$ be the complete bipartite graph having order $m+n$ and size mn. Here the vertex set $V(K_{m,n})$ can be partitioned into two sets V_1 and V_2 such that $|V_1| = m$ and $|V_2| = n$. For $m, n \geqslant 2$, the closed neighborhood degree of each vertex in V_1 is $n(m+1)$ and the closed neighborhood degree of each vertex in V_2 is $m(n+1)$. Then

$$\begin{aligned} CM_1(K_{m,n}) &= m \times [n(m+1)]^2 + n \times [m(n+1)]^2 \\ &= m[nm+n]^2 + n[mn+m]^2 \\ &= m^2n^2(m+n) + mn(m+n) + 4m^2n^2. \end{aligned}$$

□

Theorem 3.14. For star graph $K_{1,n}$, where $n \geqslant 3$, $CM_1(K_{1,n}) = n[n^2 + 6n + 1]$.

Proof. Let $K_{1,n}$ be the star graph having order $n+1$ and size n. For $n \geqslant 3$, the closed neighborhood degree of n pendant vertices is $n+1$ and the closed neighborhood degree of center vertex is $2n$. Then

$$\begin{aligned} CM_1(K_{1,n}) &= n(n+1)^2 + 1(2n)^2 \\ &= n^3 + n + 2n^2 + 4n^2 \\ &= n[n^2 + 6n + 1]. \end{aligned}$$

□

Theorem 3.15. For crown graph S_n^0, where n $\geqslant 3$, $CM_1(S_n^0) = 2n(n^2 - n)^2$.

Proof. The crown graph S_n^0 have $2n$ vertices and $n(n-1)$ edges. For $n \geqslant 3$, the closed neighborhood degree of each vertex is $[(n-1)^2 + (n-1)]$. Then

$$\begin{aligned} CM_1(S_n^0) &= 2n[(n-1)^2 + (n-1)]^2 \\ &= 2n(n^2 - n)^2. \end{aligned}$$

□

Theorem 3.16. For ladder graph L_n, where n $\geqslant 5$, $CM_1(L_n) = 288n - 472$.

Proof. Let L_n be the ladder graph having order $2n$ and size $n + 2(n-1)$. For $n \geqslant 5$, the closed neighborhood degree of both end vertices is 7, the closed neighborhood degree of vertices which is adjacent to end vertex is 11 and the closed neighborhood degree of remaining vertices is $2(n-4)$. By definition of L_n, we have following Table 4.
Using the values from Table 4 in equation 1.4, we obtain

Table 4: Vertex partition of the ladder graph based on closed neighborhood degree.

$S_{L_n}[u]$, where $u \in V(L_n)$	7	11	12
Number of vertices	4	4	$2(n-4)$

$$\begin{aligned} CM_1(L_n) &= 4(7)^2 + 4(11)^2 + 2(n-4)(12)^2 \\ &= 196 + 484 + 288(n-4) \\ &= 288n - 472. \end{aligned}$$

□

Theorem 3.17. For wheel graph W_n, where n $\geqslant$ 4, $CM_1(W_n) = n(n^2 + 34n + 81)$.

Proof. The order and size of the wheel graph W_n is $n+1$ and $2n$ respectively. The closed neighborhood degree of each corner vertex is $9+n$ and the closed neighborhood degree of the center vertex is $4n$. Then

$$\begin{aligned} CM_1(W_n) &= 1(4n)^2 + n(9+n)^2 \\ &= 16n^2 + 81n + n^3 + 18n^2 \\ &= n(n^2 + 34n + 81). \end{aligned}$$

□

Theorem 3.18. For gear graph G_n, where n $\geqslant$ 3, $CM_1(G_n) = n(n^2 + 30n + 113)$.

Proof. The order and size of the gear graph G_n is $2n+1$ and $3n$ respectively. By definition of G_n, the center vertex is of degree n and outer layer vertex is of degree alternative 3 and 2. The closed neighborhood degree of the center vertex is $4n$, the closed neighborhood degree of each corner vertex adjacent to the center vertex is $n+7$ and the closed neighborhood degree of remaining vertices is 8. Then

$$\begin{aligned} CM_1(G_n) &= 1(4n)^2 + n(n+7)^2 + n(8)^2 \\ &= 16n^2 + n^3 + 49n + 14n^2 + 64n \\ &= n(n^2 + 30n + 113). \end{aligned}$$

□

Theorem 3.19. For friendship graph F_n, where n $\geqslant$ 2, $CM_1(F_n) = 4n(2n^2 + 17n + 8)$.

Proof. The order and size of the friendship graph F_n is $2n+1$ and $3n$ respectively. By definition of F_n, $2n$ vertices are of degree 2 and the center vertex is of degree $2n$. The closed neighborhood degree of the center vertex is $6n$ and the closed neighborhood degree of the remaining vertices is $2n+4$. Then

$$\begin{aligned} CM_1(F_n) &= 1(6n)^2 + 2n(2n+4)^2 \\ &= 36n^2 + (8n^3 + 32n + 32n^2) \\ &= 4n(2n^2 + 17n + 8). \end{aligned}$$

□

Theorem 3.20. For cocktail party graph $CP_{n,n}$, where n $\geqslant$ 2, $CM_1(CP_{n,n}) = 2n(4n^2 - 6n + 2)^2$.

Proof. The order and size of the cocktail party graph $CP_{n,n}$ is $2n$ and $2n(n-1)$ respectively. The closed neighborhood degree of the each vertex is $4(n-1)^2 + 2(n-1)$. Then

$$\begin{aligned} CM_1(CP_{n,n}) &= 2n[4(n-1)^2 + 2(n-1)]^2 \\ &= 2n[4n^2 + 4 - 8n + 2n - 2]^2 \\ &= 2n(4n^2 - 6n + 2)^2. \end{aligned}$$

□

Theorem 3.21. For helm graph H_n, where $n \geqslant 3$, $CM_1(H_n) = n(n^2 + 51n + 194)$.

Proof. The order and size of the helm graph H_n is $2n+1$ and $3n$ respectively. By definition of H_n, the center vertex is of degree n and outer pendent vertex is of degree 1 and the rest is of degree 4. The closed neighborhood degree of center vertex is $5n$, the closed neighborhood degree of outer pendent vertex is 5 and the closed neighborhood degree of remaining vertices is $13+n$. Then

$$\begin{aligned} CM_1(H_n) &= 1(5n)^2 + n(13+n)^2 + 25n \\ &= 25n^2 + 169n + n^3 + 26n^2 + 25n \\ &= n(n^2 + 51n + 194). \end{aligned}$$

□

4. Mathematical properties of the first closed neighborhood Zagreb index

In this section, we obtain bounds for the first closed neighborhood Zagreb index of graphs.

Theorem 4.1. Let G be a graph. Then

$$CM_1(G) = NM_1(G) + M_1(G) + 4M_2(G).$$

Proof. By using equation 1.4, we have

$$\begin{aligned} CM_1(G) &= \sum_{u \in V(G)} S_G[u]^2 \\ &= \sum_{u \in V(G)} [S_G(u) + d_G(u)]^2 \\ &= \sum_{u \in V(G)} [S_G(u)^2 + 2d_G(u)^2 + 2S_G(u)d_G(u)] \\ &= NM_1(G) + M_1(G) + 4M_2(G). \end{aligned}$$

□

Theorem 4.2. Let G be a graph with n vertices and m edges, where $n \geqslant 3$. Then

$$CM_1(G) \leqslant n(n^4 + n^2 - 2n^3),$$

and equality holds if and only if G is isomorphic to K_n.

Proof. By Using equation 1.4, we have

$$\begin{aligned} CM_1(G) &= \sum_{u \in V(G)} S_G[u]^2 \\ &= \sum_{u \in V(G)} [S_G(u) + d_G(u)]^2 \\ &\leqslant \sum_{u \in V(G)} [(n-1)^2 + (n-1)]^2 \end{aligned}$$

$$\begin{aligned} &\leqslant n[n^2 + 1 - 2n + n - 1]^2 \\ &\leqslant n(n^2 - n)^2 \end{aligned}$$

$$\text{Therefore}, CM_1(G) \leqslant n(n^4 + n^2 - 2n^3).$$

□

Corollary 4.3. Let G be a graph with n vertices, where $n \geqslant 4$. Then

$$36n - 76 \leqslant CM_1(G) \leqslant n(n^4 + n^2 - 2n^3),$$

where equality for lower bound holds for path and equality for upper bound holds for complete graph.

5. First closed neighborhood Zagreb index of some nanostructures

Nanostructures generally refer to the material systems that are in the range of 1 to 100 nanometers. In a nanostructure, electrons are normally confined in one of the dimensions, whereas in the other dimensions, they are free to move in all directions. The term nanostructure describes a particular kind of nanotube that is specifically related to the investigation of topological characteristics in nanostructures. Because of their small size and large surface area, these structures have special physical and chemical characteristics.

2D-lattice nanostructures are defined by a regular, grid-like configuration of molecules or atoms in two dimensions, which resembles a flat, repeating pattern. Nanotubes are cylindrical nanostructures with a hollow centre, composed of carbon atoms arranged in a hexagonal lattice. Depending on the quantity of concentric tubes, these can be categorized as either single-walled or multi-walled. The toroidal (doughnut-shaped) nanostructures known as Nanotorus can be seen as a 2D lattice that has been wound around to create a torus. p and q stands for the number of squares in each row and the number of rows of squares, respectively, in the nanostructures of $TUC_4C_8(R)[p, q]$. In this section, we provide explicit formulas for calculating the FCNZI for various nanostructures by partitioning the vertex set of the $TUC_4C_8(R)[p, q]$ nanostructure based on closed neighborhood degree of subdivision graph and line graphs of subdivision graphs [12, 14].

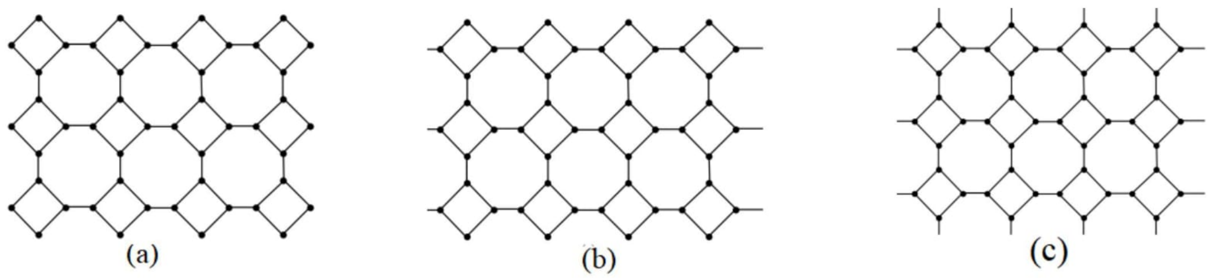

Figure 4: (a) 2D-lattice $TUC_4C_8(R)[4, 3]$ (b) Nanotube $TUC_4C_8(R)[4, 3]$ (c) Nanotorus $TUC_4C_8(R)[4, 3]$

Theorem 5.1. Let A be the 2D-lattice of $TUC_4C_8(R)[p, q]$. Then
(i)$CM_1(A) = 4[144pq - 63(p + q) + 64]$,
(ii)$CM_1(S(A)) = 810pq - 520p - 299q + 263$,
(iii)$CM_1(L(S(A))) = 4[432pq - 244p - 190q + 236]$.

Proof. (i) The 2D-lattice of $TUC_4C_8[p, q]$ has order $4pq$ and size $6pq - p - q$. The vertex partition of A is obtained based on degree sum of closed neighbour vertices of each vertex is as follows:

Table 5: Vertex partition of graph A, when $p > 1$, $q > 1$

$S_A[u]$ where $u \in V(A)$	7	11	8	12
Number of vertices	8	$4(p + q - 2)$	$2(p + q - 4)$	$2[2pq - 3(p + q) + 4]$

Using Table 5 in equation 1.4, we get

$$
\begin{aligned}
CM_1(A) &= \sum_{u\in V(A)} S_A[u]^2 \\
&= 8\times 7^2 + 4(p+q-2)\times 11^2 + 2(p+q-4)\times 8^2 + 2[2pq-3(p+q)+4]\times 12^2 \\
&= 392 + (4p+4q-8)121 + (2p+2q-8)64 + (4pq-6p-6q+8)144 \\
&= 4[144pq - 63(p+q) + 64].
\end{aligned}
$$

(ii) The subdivision graph of 2D-lattice $TUC_4C_8[p,q]$ has order $10pq-p-q$ and size $2(6pq-p-q)$. The vertex partition of S(A) is obtained based on degree sum of closed neighbour vertices of each vertex is as follows:

Table 6: Vertex partition of graph S(A), when $p > 1$, $q > 1$

$S_{S(A)}[u]$ where $u \in V(S(A))$	6	7	8	9
Number of vertices	$2(p+q+2)$	$4(p+q-2)$	$(13p-11)$	$(10pq-20p-7q+15)$

Using Table 6 in equation 1.4, we get

$$
\begin{aligned}
CM_1(S(A)) &= \sum_{u\in V(S(A))} S_{S(A)}[u]^2 \\
&= 2(p+q+2)\times 6^2 + 4(p+q-2)\times 7^2 + (13p-11)\times 8^2 + (10pq-20p-7q+15)\times 9^2 \\
&= (2p+2q+4)36 + (4p+4q-8)49 + (13p-11)64 + (10pq-20p-7q+15)81 \\
&= 810pq - 520p - 299q + 263.
\end{aligned}
$$

(iii) The line graph of subdivision graph of 2D-lattice $TUC_4C_8[p,q]$ has order $2(6pq-p-q)$ and size $(18pq-5p-5q)$. The vertex partition of $L(S(A))$, based on degree sum of closed neighbour vertices of each vertex is as follows:

Table 7: Vertex partition of graph L(S(A)), when $p > 1$, $q > 1$

$S_{L(S(A))}[u]$ where $u \in V(L(S(A)))$	6	7	11	12
Number of vertices	$2p$	$4[(p-1)+(q-1)]$	$4[(p-1)+(q-1)]$	$(12pq-12p-10q+16)$

Using Table 7 in equation 1.4, we get

$$
\begin{aligned}
CM_1(L(S(A))) &= \sum_{u\in V(L(S(A))} S_{L(S(A))}[u]^2 \\
&= 2p\times 6^2 + 4[(p-1)+(q-1)]\times 7^2 + 4[(p-1)+(q-1)]\times 11^2 \\
&+ (12pq-12p-10q+16)\times 12^2 \\
&= 2p\times 36 + 4[(p-1)+(q-1)]\times 49 + 4[(p-1)+(q-1)]\times 121 \\
&+ (12pq-12p-10q+16)\times 144 \\
&= 4[432pq - 244p - 190q + 236].
\end{aligned}
$$

□

Theorem 5.2. Let B be $TUC_4C_8(R)[p,q]$ nanotubes. Then
(i)$CM_1(B) = 576pq - 252p - 126q + 24$,
(ii)$CM_1(S(B)) = 776pq - 418p - 71q$,
(iii)$CM_1(L(S(B))) = 1728pq - 760p - 218q + 92$.

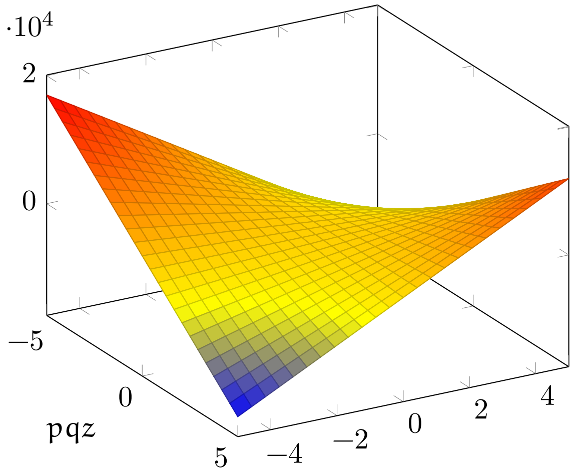

Figure 5: FCNZI of A

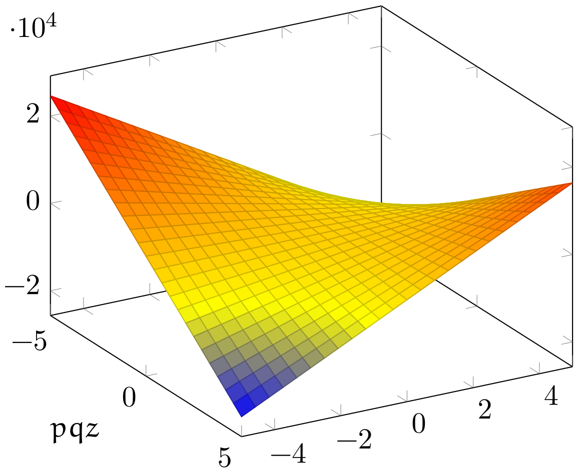

Figure 6: FCNZI of S(A)

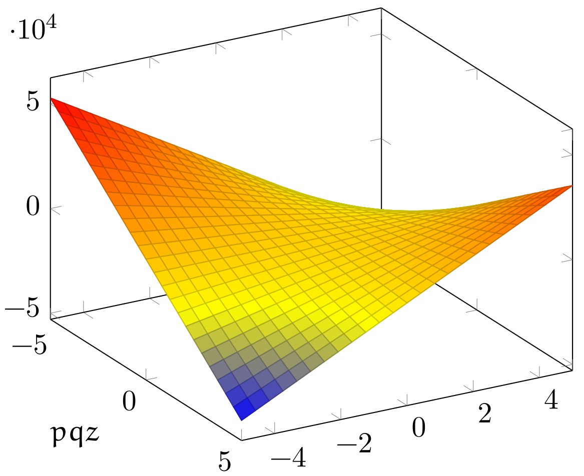

Figure 7: FCNZI of L(S(A))

Table 8: Vertex partition of graph B, when $p > 1$, $q > 1$

$S_B[u]$ where $u \in V(B)$	8	9	11	12
Number of vertices	$2(p+2)$	$2(q-2)$	$4(p-1)$	$2(2pq-3p-q+2)$

Proof. (i) The $TUC_4C_8[p,q]$ nanotube has order $4pq$ and size $6pq-p$. The Vertex partition of B, based on degree sum of closed neighbour vertices of each vertex is as follows:
Using Table 8 in equation 1.4, we get

$$\begin{aligned}
CM_1(B) &= \sum_{u\in V(B)} S_B[u]^2 \\
&= 2(p+2)\times 8^2 + 2(q-2)\times 9^2 + 4(p-1)\times 11^2 \\
&+ 2(2pq-3p-q+2)\times 12^2 \\
&= 2(p+2)\times 64 + 2(q-2)\times 81 + 4(p-1)\times 121 \\
&+ 2(2pq-3p-q+2)\times 144 \\
&= 576pq - 252p - 126q + 24.
\end{aligned}$$

(ii) The subdivision graph of $TUC_4C_8[p,q]$ nanotube has order $10pq-p$ and size $2(6pq-p)$. The vertex partition of $S(B)$, based on degree sum of closed neighbour vertices of each vertex is as follows:

Table 9: Vertex partition of graph S(B), when $p > 1$, $q > 1$

$S_{S(B)}[u]$ where $u \in V(S(B))$	5	6	7	8	9
Number of vertices	q	$2p$	$4p+q$	$8p+q(p-1)+p(q-1)$	$8pq-14p-q$

Using Table 9 in equation 1.4, we get

$$\begin{aligned}
CM_1(S(B)) &= \sum_{u\in V(S(B))} S_{S(B)}[u]^2 \\
&= q\times 5^2 + 2p\times 6^2 + (4p+q)\times 7^2 + [8p+q(p-1)+p(q-1)]\times 8^2 \\
&+ [8pq-14p-q]\times 9^2 \\
&= 25q + 72p + (4p+q)49 + [8p+q(p-1)+p(q-1)]64 + [8pq-14p-q]81 \\
&= 776pq - 418p - 71q.
\end{aligned}$$

(iii) The line graph of subdivision graph of $TUC_4C_8[p,q]$ nanotube has order $2(6pq-p)$ and size $(18pq-5p)$. The vertex partition of $L(S(B))$, based on degree sum of closed neighbour vertices of each vertex is as follows:

Table 10: Vertex partition of graph L(S(B)), when $p > 1$, $q > 1$

$S_{L(S(B))}[u]$ where $u \in V(L(S(B)))$	7	9	11	12
Number of vertices	$4p$	$2q$	$4p+4(q-1)$	$12pq-10p-6q+4$

Using Table 10 in equation 1.4, we get

$$\begin{aligned}CM_1(L(S(B))) &= \sum_{u \in V(L(S(B)))} S_{L(S(B))}[u]^2\\ &= 4p \times 7^2 + 2q \times 9^2 + [4p + 4(q-1)] \times 11^2 + [12pq - 10p - 6q + 4] \times 12^2\\ &= 196p + 162q + 484p + 484q - 484 + 1728pq - 1440p - 864q + 576\\ &= 1728pq - 760p - 218q + 92.\end{aligned}$$

□

Theorem 5.3. Let C be $TUC_4C_8(R)[p, q]$ nanotorus. Then
(i)$CM_1(C) = 576pq - 126(p + q)$,
(ii)$CM_1(S(C)) = 776pq - 275p - 71q$,
(iii)$CM_1(L(S(C))) = 1728pq - 126(p + q)$.

Proof. (i) The $TUC_4C_8[p, q]$ nanotorus has order $4pq$ and size $6pq$. The vertex partition of C, based on degree sum of closed neighbour vertices of each vertex is as follows:

Table 11: Vertex partition of graph C, when $p > 1$, $q > 1$

$S_C[u]$ where $u \in V(C)$	9	12
Number of vertices	$2(p + q)$	$4pq - 2(p + q)$

Using Table 11 in equation 1.4, we get

$$\begin{aligned}CM_1(C) &= \sum_{u \in V(C)} S_C[u]^2\\ &= 2(p + q) \times 9^2 + [4pq - 2(p + q)] \times 12^2\\ &= 2(p + q) \times 81 + [4pq - 2(p + q)] \times 144\\ &= 576pq - 126(p + q).\end{aligned}$$

(ii) The subdivision graph of $TUC_4C_8[p, q]$ nanotorus has order $10pq$ and size $12pq$. The Vertex partition of $S(C)$, based on degree sum of closed neighbour vertices of each vertex is as follows:

Table 12: Vertex partition of graph S(C), when $p > 1$, $q > 1$

$S_{S(C)}[u]$ where $u \in V(S(C))$	5	7	8	9
Number of vertices	$p + q$	$p + q$	$[2pq + 12p - (p + q)]$	$8pq - 13p - q$

Using Table 12 in equation 1.4, we get

$$\begin{aligned}CM_1(S(C)) &= \sum_{u \in V(S(C))} S_{S(C)}[u]^2\\ &= (p + q) \times 5^2 + (p + q) \times 7^2 + [2pq + 12p - (p + q)] \times 8^2 + [8pq - 13p - q] \times 9^2\\ &= (p + q)25 + (p + q)49 + [2pq + 12p - (p + q)]64 + [8pq - 13p - q]81\\ &= 776pq - 275p - 71q.\end{aligned}$$

(iii) The line graph of subdivision graph of $TUC_4C_8[p, q]$ nanotorus has order $12pq$ and size $18pq$. The vertex partition of $L(S(C))$, based on degree sum of closed neighbour vertices of each vertex is as follows:

Using Table 13 in equation 1.4, we get

Table 13: vertex partition of graph L(S(C)), when $p > 1$, $q > 1$

$S_{L(S(C))}[u]$ where $u \in V(L(S(C)))$	9	12
Number of vertices	$2(p+q)$	$12pq - 2(p+q)$

$$\begin{aligned} CM_1(L(S(C))) &= \sum_{u \in V(S(C))} S_{L(S(C))}[u]^2 \\ &= 2(p+q) \times 9^2 + [12pq - 2(p+q)] \times 12^2 \\ &= 2(p+q) \times 81 + [4pq - 2(p+q)] \times 144 \\ &= 1728pq - 126(p+q). \end{aligned}$$

□

6. Conclusion

In the field of chemical graph theory, the research conducted in the framework of the line graph operator is a novel approach to structural chemistry. In this paper, we introduced new degree based topological index called first closed neighborhood Zagreb index. These topological indices are help us to understand the physico-chemical properties such as Entropy, Enthalpy, Acentric factor and DHVAP etc. FCNZI is highly correlate with acentric factor. Finally we have obtained explicit formulae of first closed neighborhood Zagreb index for some nanostructures such as 2D-Lattice, Nanotube and Nanotorus.

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