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On the Second Order First Zagreb Index

B. BASAVANAGOUD[1], S. PATIL[1] AND H. DENG[2,•]

[1]Department of Mathematics, Karnatak University, Dharwad − 580 003, Karnataka, India

[2]Key Laboratoryof High Performance Computing and Stochastic Information Processing, College of Mathematics and Computer Science, Hunan Normal University, Changsha, Hunan, 410081, P. R. China

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ABSTRACT

Inspired by the chemical applications of higher-order connectivity index (or Randic′ index), we consider here the higher-order first Zagreb index of a molecular graph. In this paper, we study the linear regression analysis of the second order first Zagreb index with the entropy and acentric factor of an octane isomers. The linear model, based on the second order first Zagreb index, is better than models corresponding to the first Zagreb index and F-index. Further, we compute the second order first Zagreb index of line graphs of subdivision graphs of 2D-lattice, nanotube and nanotorus of $TUC_4C_8[p,q]$, tadpole graphs, wheel graphs and ladder graphs.

1. INTRODUCTION

Let $G = (V, E)$ be a simple (molecular) graph. The number of vertices and edges of G are denoted by n and m, respectively. As usual n is said to be the order and m the size of G. The degree of a vertex $v \in V(G)$, denoted by $d_G(v)$, is the number of vertices adjacent to v in G, and $s_G(v) = \sum_{u \in N_G(v)} d_G(u)$, where $N_G(v) = \{u | uv \in E(G)\}$ is the set of neighbor vertices of v in G. Let $E_\alpha(G)$ be the set of all paths of length α in G and clearly $E_1(G) = E(G)$. If all the vertices of G have same degree equal to r, then G is called a r-regular graph. The tadpole graph $T_{n,k}$ is a graph of order $n + k$ obtained by joining an end of a path of length k to a vertex of a cycle graph C_n [34].

•Corresponding Author (Email address: hydeng@hunnu.edu.cn)
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The join $G + H$ of graphs G and H is a graph with the vertex set $V(G) \cup V(H)$ and edge set $E(G) \cup E(H) \cup \{uv | u \in V(G)$ and $v \in V(H)\}$. The join $C_n + K_1$ of a cycle C_n and a single vertex is referred to as a wheel graph W_{n+1} of order $n + 1$. The Cartesian product $G \times H$ of graphs G and H has the vertex set $V(G \times H) = V(G) \times V(H)$ and $(a, x)(b, y)$ is an edge of $G \times H$ if and only if $[a = b$ and $xy \in E(H)]$ or $[x = y$ and $ab \in E(G)]$. The ladder graph L_n is given by $L_n = K_2 \times P_n$, where P_n is a path of order n. The subdivision graph $S(G)$ [14] of a graph G is the graph obtained from G by replacing each of its edges by a path of length 2. The line graph $L(G)$ of a graph G [14] is the graph whose vertex set is $E(G)$ in which two vertices are adjacent if and only if they share a common vertex in G. We refer to [14] for unexplained graph theoretic terminology and notation.

Chemical graph theory is a branch of mathematics which combines graph theory and chemistry. Graph theory is used to mathematically model molecules in order to gain insight into the physical properties of these chemical compounds. The basic idea of chemical graph theory is that physico-chemical properties of molecules can be studied by using the information encoded in their corresponding chemical graphs. A graph invariant is any function on a graph that does not depend on a labeling of its vertices. Such quantities are called topological indices. The Zagreb indices have been introduced in 1972 in the report of Gutman and Trinajstić on the topological basis of the π-electron energy-two terms appeared in the topological formula for the total π-energy of alternate hydrocarbons, which were in 1975 used by Gutman et al. as branching indices, and later employed as molecular descriptors in QSAR and QSPR. The first Zagreb index M_1 and second Zagreb index M_2 of a graph G are defined as

$$M_1(G) = \sum_{v \in V(G)} d_G(v)^2 \text{ and } M_2(G) = \sum_{uv \in E_1(G)} d_G(u) d_G(v).$$

The first Zagreb index can be written also as

$$M_1(G) = \sum_{uv \in E_1(G)} [d_G(u) + d_G(v)]. \quad (1.1)$$

Another vertex-degree-based graph invariant

$$F(G) = \sum_{v \in V(G)} d_G(v)^3$$

was encountered in [13] and also called F-index [12].

The connectivity index (or Randić index) of a graph G, denoted by $\chi(G)$, was introduced by Randić [31] in the study of branching properties of alkanes. It is defined as

$$\chi(G) = \sum_{uv \in E_1(G)} \frac{1}{\sqrt{d_G(u) d_G(v)}} \quad (1.2)$$

In [16, 17], with the intention of extending the applicability of the connectivity index, Kier, Hall, Murray and Randic′ considered the higher-order connectivity index of a graph G as

$${}^{\alpha}\chi(G) = \sum_{u_1 u_2 \cdots u_{\alpha+1} \in E_\alpha(G)} \frac{1}{\sqrt{d_G(u_1) d_G(u_2) \cdots d_G(u_{\alpha+1})}} \quad (1.3)$$

It has found numerous applications [6, 18, 19, 22, 23, 24, 25, 26, 35, 36]. Results related to the mathematical properties of this index have been reported in [27, 28].

Bearing in mind Eqs. (1.2) and (1.3), we can consider the higher-order first Zagreb index of Eq. (1.1) as

$$ {}^{\alpha}M_1(G) = \sum_{u_1u_2\cdots u_{\alpha+1}\in E_\alpha(G)} [d_G(u_1) + d_G(u_2) + \cdots + d_G(u_{\alpha+1})] \quad (1.4)$$

By Eq. (1.4), it is consistent to define the second order first Zagreb index as

$$ {}^{2}M_1(G) = \sum_{u_1u_2u_3\in E_2(G)} [d_G(u_1) + d_G(u_2) + d_G(u_3)]. \quad (1.5)$$

The present paper is organized as follows: In Section 2, we study the chemical applicability of the second order first Zagreb index. In Section 3, we establish some basic results on ${}^{2}M_1$ which are useful in later sections. In Sections 4, we obtain explicit formula for computing the second order first Zagreb index of line graphs of subdivision graphs of 2D-lattice, nanotube and nanotorus of $TUC_4C_8[p,q]$, tadpole graphs, wheel graphs and ladder graphs.

2. On the Chemical Applicability of the Second Order First Zagreb Index

In this section, we will discuss the regression analysis of entropy (S) and acentric factor (AcentFac) of an octane isomers on the degree based topological indices of the corresponding molecular graph. The productivity of the second order first Zagreb index was tested by using a data set of octane isomers, that can be found at http://www.moleculardiscriptors.eu/dataset.htm, it is shown that the second order first Zagreb index is highly correlated with the entropy (R = 0.961093128) and also with acentric factor (R = 0.990202) of octane isomers. The data set of octane isomers (columns 1-3 and 5 of Table 1) are taken from above web link whereas last column taken form [5], and the fourth column of Table 1 is computed by Eq. (1.5).

The linear regression models for the entropy and acentric factor of Table 1 are obtained by using the least squares fitting procedure as implemented in R software [2]. More details about the linear regression can be found in [33]. The fitted models are:

$$S = 123.14880(\pm 1.30984) - 0.31608(\pm 0.02271)^2M_1 \quad (2.1)$$

$$S = 150.8878(\pm 3.5756) - 1.4722(\pm 0.1153)M_1 \quad (2.2)$$

$$S = 122.31091(\pm 1.38791) - 0.20607(\pm 0.01643)F \quad (2.3)$$

$$AcentFac = 0.4792(\pm 0.005195) - 0.002555(\pm 0.00009006)^2M_1 \quad (2.4)$$

$$AcentFac = 0.6996325(\pm 0.0216422) - 0.0117797(\pm 0.0006977)M_1 \quad (2.5)$$

$$AcentFac = 0.4700828(\pm 0.0093940) - 0.0016380(\pm 0.0001112)F \quad (2.6)$$

where the values in the brackets of Eqs. (2.1) to (2.6) are the corresponding standard errors of the regression coefficients (intercept and slope).

Tables 2 and 3 show that, the correlation coefficient (R = 0.961093128 and R = 0.990202) of the experimental entropy and acentric factor of an octane isomers with

second order first Zagreb index in the models (2.1) and (2.4) are better than in the models (2.2), (2.3) and (2.5), (2.6), respectively, also the model (2.1) is better than the model related to entropy of octane isomers on Sanskruti index ($R = 0.829$ and residual standard error is 17.837) [15].

Table 1: Experimental values of the entropy, acentric factor and the corresponding values of degree based topological indices of octane isomers.

Alkane	S	AcentFac	$^2M_1$	M_1	F
n-octane	111.67	0.397898	34	26	50
2-methyl-heptane	109.84	0.377916	41	28	62
3-methyl-heptane	111.26	0.371002	43	28	62
4-methyl-heptane	109.32	0.371504	43	28	62
3-ethyl-hexane	109.43	0.362472	45	28	62
2,2-dimethyl-hexane	103.42	0.339426	58	32	92
2,3-dimethyl-hexane	108.02	0.348247	52	30	74
2,4-dimethyl-hexane	106.98	0.344223	50	30	74
2,5-dimethyl-hexane	105.72	0.35683	48	30	74
3,3-dimethyl-hexane	104.74	0.322596	62	32	92
3,4-dimethyl-hexane	106.59	0.340345	54	30	74
2-methyl-3-ethyl-pentane	106.06	0.332433	54	30	74
3-methyl-3-ethyl-pentane	101.48	0.306899	66	32	92
2,2,3-trimethyl-pentane	101.31	0.300816	71	34	104
2,2,4-trimethyl-pentane	104.09	0.30537	65	34	104
2,3,3-trimethyl-pentane	102.06	0.293177	73	34	104
2,3,4-trimethyl-pentane	102.39	0.317422	61	32	86
2,2,3,3-tetramethylbutane	93.06	0.255294	90	38	134

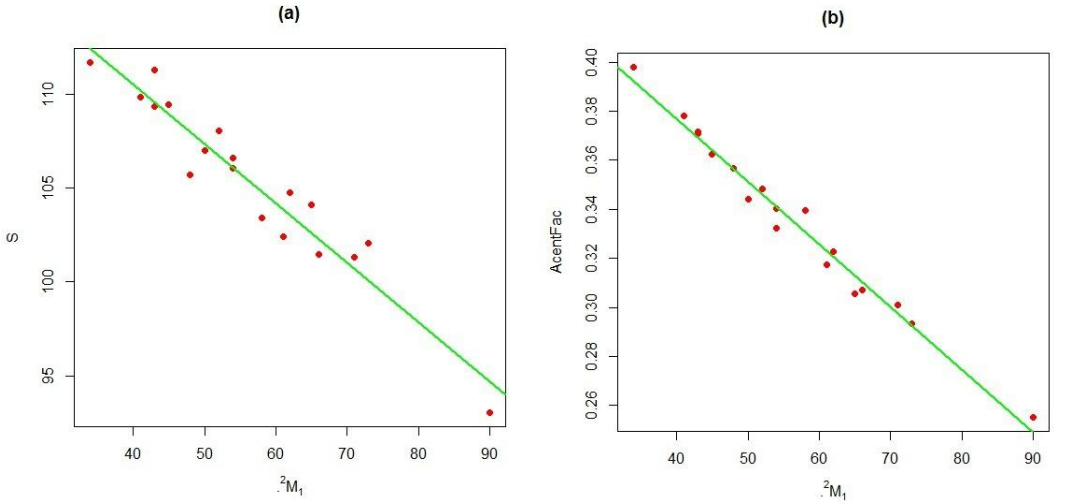

Figure 1: Scatter diagram of (a) S on $^2M_1$; (b) $AcentFac$ on $^2M_1$, superimposed by the fitted regression line.

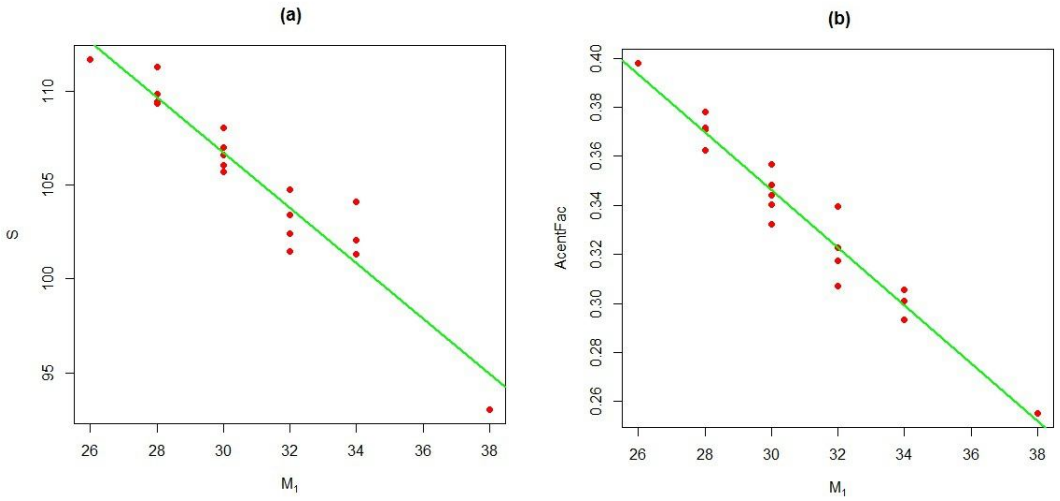

Figure 2: Scatter diagram of (a) S on M_1; (b) $AcentFac$ on M_1, superimposed by the fitted regression line.

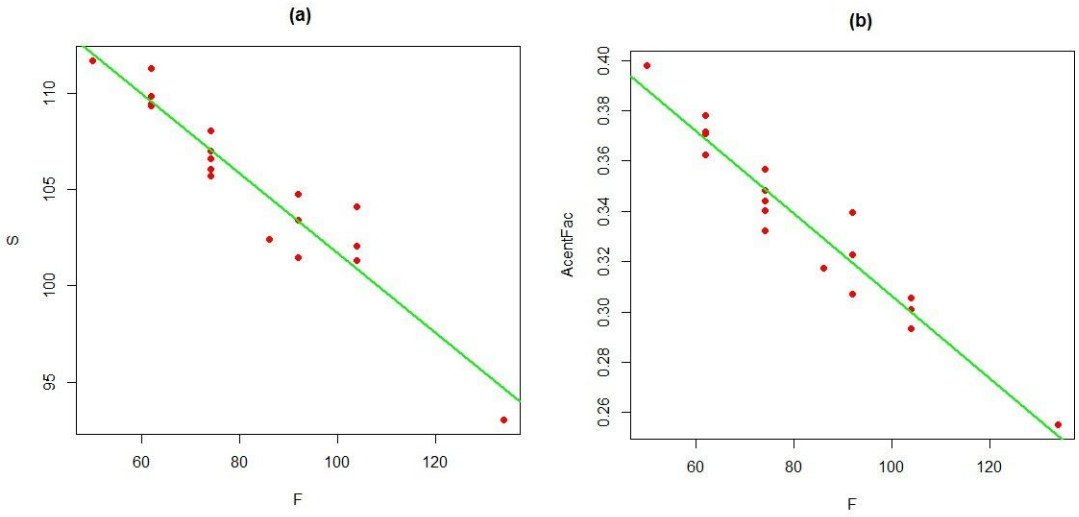

Figure 3: Scatter diagram of (a) S on F; (b) $AcentFac$ on F, superimposed by the fitted regression line.

Table 2: Correlation coefficient and residual standard error of regression model.

Index	Correlation coefficient (R) with entropy	Residual standard error
${}^2M_1$	0.961093128	1.286
M_1	0.954306031	1.392
F	0.952732911	1.415

Table 3: Correlation coefficient and residual standard error of regression model

Index	Correlation coefficient (R) with acentric fac	Residual standard error
${}^2M_1$	0.990202	0.005101
M_1	0.973087869	0.008424
F	0.965038859	0.009577

3. MATHEMATICAL PROPERTIES FOR THE SECOND ORDER FIRST ZAGREB INDEX OF A GRAPH

In this section, we will establish some basic results on ${}^2M_1$ which are useful in later sections.

Theorem 3.1 *For a graph* $G = (V, E)$,

$$ {}^2M_1(G) = 2M_2(G) + \frac{1}{2}F(G) - \frac{3}{2}M_1(G). \tag{3.1}$$

Proof. By Eq. (1.5), we have

$$\begin{aligned} {}^2M_1(G) &= \sum_{uvw \in E_2(G)} (d_G(u) + d_G(v) + d_G(w)) \\ &= \sum_{v \in V(G)} \sum_{u \neq w \in N_G(v)} (d_G(u) + d_G(v) + d_G(w)). \end{aligned}$$

In $\sum_{u \neq w \in N_G(v)} (d_G(u) + d_G(v) + d_G(w))$, the quantity $d_G(v)$ appears $\binom{d_G(v)}{2} = \frac{d_G(v)(d_G(v)-1)}{2}$ times, and each quantity $d_G(u)$ of $\{d_G(u) | u \in N_G(v)\}$ appears $(d_G(v) - 1)$ times, i.e., the quantity $s_G(v) = \sum_{u \in N_G(v)} d_G(u)$ appears $(d_G(v) - 1)$ times. So,

$$\begin{aligned} {}^2M_1(G) &= \sum_{v \in V(G)} \sum_{u \neq w \in N_G(v)} (d_G(u) + d_G(v) + d_G(w)) \\ &= \sum_{v \in V(G)} \left[\frac{d_G(v)(d_G(v)-1)}{2} d_G(v) + (d_G(v) - 1)s_G(v)\right] \\ &= \frac{1}{2}\left[\sum_{v \in V(G)} d_G^3(v) - \sum_v d_G^2(v)\right] + \sum_v d_G(v)s_G(v) - \sum_v s_G(v) \\ &= \frac{1}{2}[F(G) - M_1(G)] + 2\sum_{uv \in E(G)} d(u)d(v) - \sum_{v \in V(G)} d^2(v) \\ &= \frac{1}{2}F(G) - \frac{1}{2}M_1(G) + 2M_2(G) - M_1(G) \\ &= 2M_2(G) + \frac{1}{2}F(G) - \frac{3}{2}M_1(G). \end{aligned}$$

Theorem 3.1 shows that the second order first Zagreb index ${}^2M_1$ is a linear combination of the first Zagreb index M_1, the second Zagreb index M_2 and the F-index F. For the path P_n, the wheel W_{n+1} $(n \geq 3)$ and the complete bipartite graph $K_{r,s}$, we have

$$\begin{gathered} F(P_n) = 8n - 14, M_1(P_n) = 4n - 6, M_2(P_n) = 4n - 8; \\ F(W_{n+1}) = n^3 + 27n, M_1(W_{n+1}) = n^2 + 9n, M_2(W_{n+1}) = 3n^2 + 9n; \\ F(K_{r,s}) = rs(r^2 + s^2), M_1(K_{r,s}) = rs(r + s), M_2(K_{r,s}) = r^2s^2. \end{gathered}$$

By Eq. (3.1) in Theorem 3.1, we can get the following result.

Corollary 3.2 *For* $n \geq 3$, $^2M_1(P_n) = 6n - 14$.

Corollary 3.3 *For* $n \geq 3$, $^2M_1(W_{n+1}) = \frac{1}{2}[n^3 + 9n^2 + 36n]$.

Corollary 3.4 $^2M_1(K_{r,s}) = \frac{rs}{2}[r^2 + s^2 + 4rs - 3r - 3s]$.

Theorem 3.5 *Let* G *be a* r*-regular graph on* n *vertices. Then* $^2M_1(G) = \frac{3n}{2}[r^3 - r^2]$.

Proof. Since G is a r-regular graph, $M_1(G) = nr^2$, $F(G) = nr^3$ and $M_2(G) = \frac{r^3n}{2}$. Hence, by Theorem 3.1, we get the desired result.

Corollary 3.6 *For the cycle* C_n *on* $n \geq 3$ *vertices,* $^2M_1(C_n) = 6n$.

Corollary 3.7 *For the complete graph* K_n *on* $n \geq 3$ *vertices,* $^2M_1(K_n) = \frac{3n(n-2)(n-1)^2}{2}$.

Lemma 3.8 [3] *Let* G *be a graph with* n *vertices and* m *edges. Then*

$$M_1(G) \leq m(\frac{2m}{n-1} + n - 2). \tag{3.2}$$

Lemma 3.9 [4] *Let* G *be a graph with* n *vertices and* m *edges,* $m > 0$. *Then the equality*

$$M_1(G) = m\left(\frac{2m}{n-1} + n - 2\right)$$

holds if and only if G is isomorphic to the star graph S_n or K_n or $K_{n-1} \cup K_1$.

Theorem 3.10 *Let* G *be a graph with* n *vertices and* m *edges. Then*

$$^2M_1(G) \leq 3m(n-1)(\frac{m}{n-1} + \frac{n-4}{2}) \tag{3.3}$$

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

Proof.

$$\begin{aligned} ^2M_1(G) &= \sum_{uvw \in E_2(G)} [d_G(u) + d_G(v) + d_G(w)] \\ &\leq \sum_{uvw \in E_2(G)} 3(n-1) \qquad (3.4) \\ &= 3(n-1)\sum_{v \in V(G)} \binom{d_G(v)}{2} = 3(n-1)(-m + \frac{1}{2}M_1(G)) \\ &\leq 3(n-1)(-m + \frac{1}{2}m(\frac{2m}{n-1} + n - 2)) \qquad (3.5) \\ &= 3m(n-1)\left(\frac{m}{n-1} + \frac{n-4}{2}\right). \end{aligned}$$

The relations (3.4) and (3.5) were obtained by taking into account $d_G(v) \leq n-1$ for each vertex $v \in V(G)$ and Eq. (3.2), respectively. The equality in (3.3) holds if and only if the equalities in (3.4) and (3.5) hold, if and only if $d_G(v) \leq n-1$ for each vertex $v \in V(G)$, i.e., G is a complete graph from Lemma 3.9.

Lemma 3.11 [4] *Let G be a graph with n vertices and m edges. Then*

$$M_1(G) \geq 2m(2p+1) - pn(1+p), \text{ where } p = \left\lfloor \frac{2m}{n} \right\rfloor,$$

and the equality holds if and only if the difference of the degrees of any two vertices of graph G is at most one.

Theorem 3.12 *Let G be a graph with n vertices, m edges and the minimum vertex degree δ. Then*

$$^2M_1(G) \geq \frac{3\delta}{2}(4mp - pn(p+1)), \text{ where} p = \left\lfloor \frac{2m}{n} \right\rfloor, \tag{3.6}$$

and the equality holds if and only if G is a regular graph.

Proof.

$$\begin{aligned} ^2M_1(G) &= \sum_{uvw \in E_2(G)} [d_G(u) + d_G(v) + d_G(w)] \\ &\geq \sum_{uvw \in E_2(G)} 3\delta \qquad (3.7) \\ &= 3\delta(-m + \tfrac{1}{2}M_1(G)) \\ &\geq 3\delta(-m + \tfrac{1}{2}(2m(2p+1) - pn(1+p))) \qquad (3.8) \\ &= \tfrac{3\delta}{2}(4mp - pn(p+1)). \end{aligned}$$

The relations (3.7) and (3.8) were obtained by taking into account $d_G(v) \geq \delta$ for each vertex $v \in V(G)$ and Lemma 3.11, respectively. The equality in (3.6) holds if and only if the equalities (3.7) and (3.8) hold, i.e., $d_G(v) \geq \delta$ for each vertex $v \in V(G)$ and G is a regular graph from Lemma 3.11.

4. THE SECOND ORDER FIRST ZAGREB INDICES OF SPECIAL FAMILIES OF GRAPH

Let p and q denote the number of squares in a row and the number of rows of squares, respectively in the $2D$-lattice, nanotube and nanotours of $TUC_4C_8[p,q]$, see Figure 3 (a), (b) and (c), where $p = 4$ and $q = 3$. In [29, 30], Ranjini et al. presented explicit formulas for computing the Shultz index and Zagreb indices of the subdivision graphs of the tadpole $T_{n,k}$, the wheel W_n and the ladder graph L_n. In 2015, Su and Xu [32] calculated the general sum-connectivity index and co-index of the $L(S(T_{n,k}))$, $L(S(W_n))$ and $L(S(L_n))$. In [20], Nadeem et al. derived some exact formulas for computing ABC_4 and GA_5 indices of the

line graphs of the tadpole $T_{n,k}$, the wheel W_n and the ladder graph L_n by using the notion of subdivision. Recently, authors in [1, 15, 21] obtained the expressions for certain topological indices of line graphs of subdivision graphs of $2D$-lattice, nanotube and nanotorus of $TUC_4C_8[p, q]$. For more information on nanostructures, we refer the articles [7, 8, 9, 10, 11].

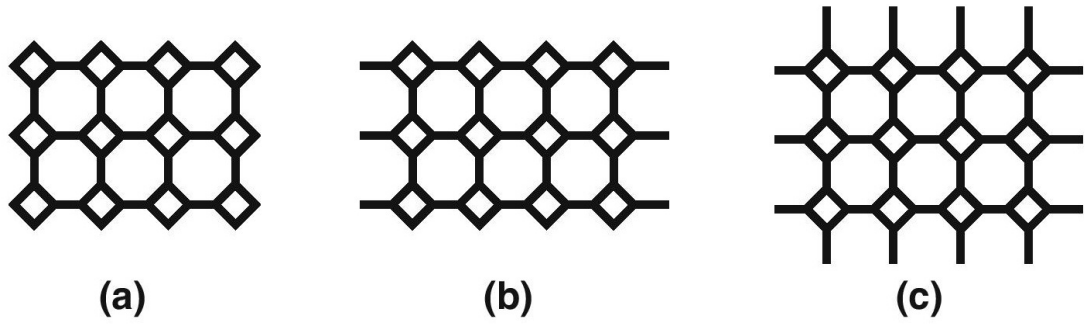

Figure 4: (a) 2D-lattice of $TUC_4C_8[4,3]$; (b) $TUC_4C_8[4,3]$ nanotube; (c) $TUC_4C_8[4,3]$ nanotorus.

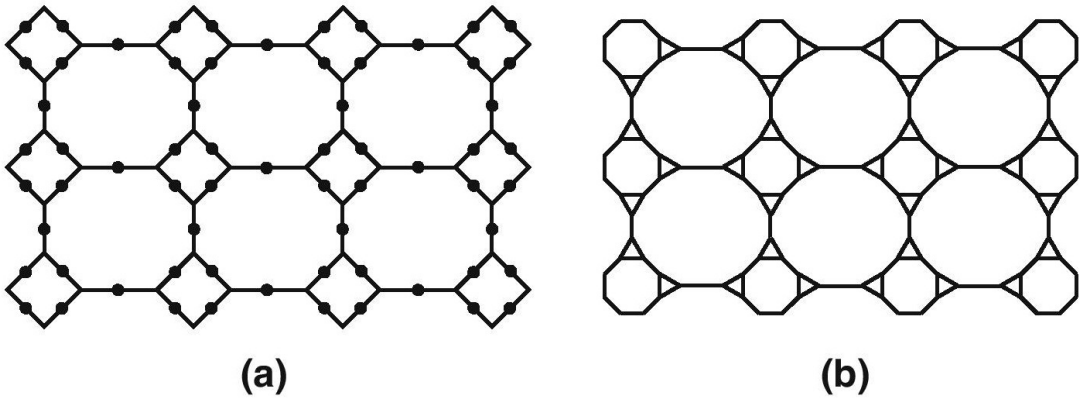

Figure 5: (a) Subdivision graph of 2D-lattice of $TUC_4C_8[4,3]$; (b) line graph of the subdivision graph of 2D-lattice of $TUC_4C_8[4,3]$.

Lemma 4.1 [21] *Let A be the line graph of the subdivision graph of $2D$-lattice of $TUC_4C_8[p, q]$. Then $M_1(A) = 108pq - 38p - 38q$, $F(A) = 324pq - 130p - 130q$ and $M_2(A) = 162pq - 67(p + q) + 4$.*

From Lemma 4.1 and Theorem 3.1, we can immediately get the following result.

Theorem 4.2 *Let A be the line graph of the subdivision graph of $2D$-lattice of $TUC_4C_8[p, q]$. Then* $^2M_1(A) = 324pq - 142p - 142q + 8$.

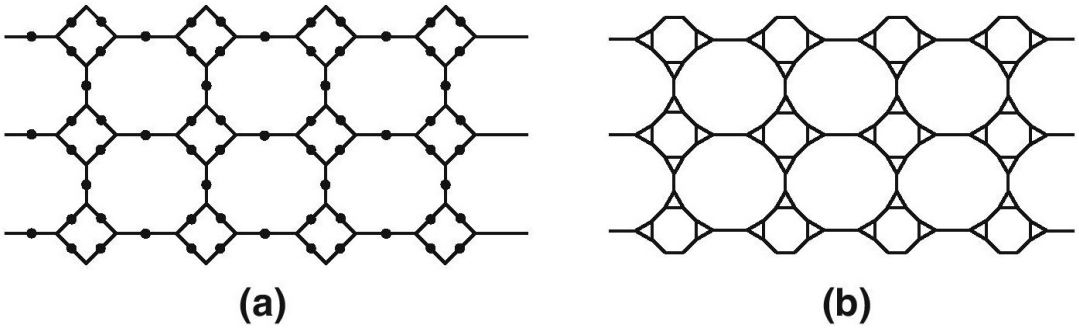

Figure 6: (a) Subdivision graph of $TUC_4C_8[4,3]$ of nanotube; (b) line graph of the subdivision graph of $TUC_4C_8[4,3]$ of nanotube.

Lemma 4.3 [21] *Let B be the line graph of the subdivision graph of $TUC_4C_8[p,q]$ nanotube. Then $M_1(B) = 108pq - 38p$, $F(B) = 324pq - 130p$ and $M_2(B) = 162pq - 67p$.*

The following result is immediate from Lemma 4.3 and Theorem 3.1.

Theorem 4.4 *Let B be the line graph of the subdivision graph of $TUC_4C_8[p,q]$ nanotube. Then $^2M_1(B) = 324pq - 142p$.*

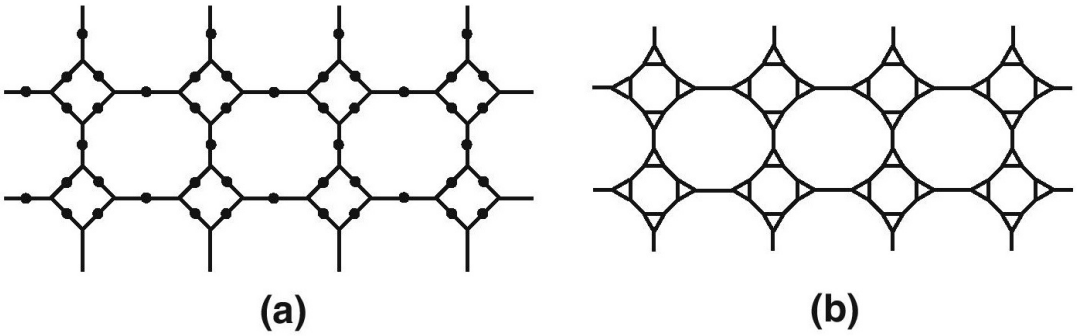

Figure 7: (a) Subdivision graph of $TUC_4C_8[4,3]$ of nanotorus; (b) line graph of the subdivision graph of $TUC_4C_8[4,3]$ of nanotorus.

Theorem 4.5 *Let C be the line graph of the subdivision graph of $TUC_4C_8[p,q]$ nanotorus. Then $^2M_1(C) = 324pq$.*

Proof. The subdivision graph of $TUC_4C_8[p,q]$ nanotorus and the graph C are shown in Figure 6 (a) and (b). The graph C is 3-regular with $12pq$ vertices. By Theorem 3.5, we get required result.

Lemma 4.6 [30, 32] (*i*) *Let X be the line graph of the subdivision graph of the tadpole graph $T_{n,k}$. Then $M_1(X) = 8n + 8k + 12$, $F(X) = 16n + 16k + 50$ and $M_2(X) = 8n + 8k + 23$.*

(*ii*) *Let Y be the line graph of the subdivision graph of the wheel graph with order $n + 1$. Then $M_1(Y) = n^3 + 27n$, $F(Y) = n^4 + 81n$ and $M_2(Y) = n(\frac{n^3-n^2+6n+72}{2})$.*

(*iii*) *Let Z be the line graph of subdivision graph of a ladder graph with order n. Then $M_1(Z) = 54n - 76$, $F(Z) = 162n - 260$ and $M_2(Z) = 81n - 132$.*

From Lemma 4.6 and Theorem 3.1, we can immediately get the following result.

Theorem 4.7 (*i*) *Let X be the line graph of the subdivision graph of the tadpole graph $T_{n,k}$. Then* $^2M_1(X) = 12n + 12k + 53$.

(*ii*) *Let Y be the line graph of the subdivision graph of the wheel graph with order $n + 1$. Then* $^2M_1(Y) = \frac{n}{2}(3n^3 - 5n^2 + 12n + 144)$.

(*iii*) *Let Z be the line graph of subdivision graph of a ladder graph with order n. Then* $^2M_1(Z) = 162n - 280$.

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