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ON THE M-POLYNOMIAL AND SOME TOPOLOGICAL INDICES OF THE PARA-LINE GRAPHS OF THE NANOSTRUCTURE $TUC_4C_8(R)$

Narahari N. Swamy, Chandan K. G. and B. Sooryanarayana*

Department of Mathematics,
University College of Science,
Tumkur University, Tumakuru - 572103, Karnataka, INDIA

E-mail : narahari_nittur@yahoo.com

*Department of Mathematical and Computational Studies,
Dr. Ambedkar Institute of Technology, Bengaluru - 560056, Karnataka, INDIA

E-mail : dr_bsnrao@yahoo.co.in

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Abstract: The study of topological indices associated with molecular graphs is very helpful in understanding many of their physico-chemical properties. Various degree based topological indices such as generalized Randić index, Zagreb index, Arithmetic-Geometric index and harmonic index are found to be particularly useful in the study of many molecular nanostructures. In this paper, we obtain the M-polynomial of the para-line graphs of the $2D$-lattice, nanotube and nanotorus of $TUC_4C_8(R)\,[p, q]$, by means of which, we compute some of their topological indices.

Keywords and Phrases: Topological indices, subdivision, para-line graph, M-polynomial, $2D$-lattice, nanotube, nanotorus.

2020 Mathematics Subject Classification: 05C09, 05C31, 92E10.

1. Introduction

The graphs discussed in this article are simple, undirected, finite and connected. The degree $deg_G(v)$ of a vertex $v \in V$ in a graph $G = (V,\ E)$ is the number of vertices adjacent with v in G and is closely related to the valence of an atom in chemistry. The distance between any two vertices u and v in G is the length of the shortest path between u and v and is denoted $d_G(u, v)$. The subdivision $S(G)$ of a graph G is a graph that is obtained by replacing each of the edges $e = uv$ of G with a vertex of degree two which is adjacent with u and v. The line graph $L(G)$ of a graph G is obtained by replacing each of its edges by a vertex and adding edges to it in such a way that two vertices in $L(G)$ are adjacent if and only if their corresponding edges in G are adjacent. The para-line graph $L(S(G))$ of a graph G is the line graph of the subdivision graph of G. For standard graph terminologies used in the paper, we refer [4, 14, 15].

A topological index is a number associated with a molecular graph that is significant in understanding many of its physico-chemical properties. It is particularly found to be useful in analysing the quantitative structure property relationship (QSPR) and quantitative structure activity relationship (QSAR) [3, 7] of such graphs. The first topological index, called the Wiener index, was introduced by H. Wiener [25] to study the correlation of the measured properties of molecules in a compound with their structural properties. Hosoya [16] defined the Wiener index, in an alternate manner, in terms of the vertex distances in a graph. Over the years, various topological indices have been introduced and obtained for different chemical graphs [20, 13, 11, 12, 9, 10, 5, 23, 24]. In particular, these topological indices have been obtained for the line graph of subdivision graphs of some nanostructures such as those in [19, 1].

The M-polynomial of a graph, introduced by Deutsch and Klavžar [8], is helpful in determining the closed form of certain degree based topological indices of families of graphs for which the number of edges adjacent to a pair of vertices u, v is known. Several authors have used the M-polynomial to find topological indices such as the first and second Zagreb index, general Ŕandic index and symmetric division index of nanostructures [18, 17].

The study of materials in the size of nano units, i. e., 10^{-9} units, comprises the field of nanoscience. Materials and structures, that take nanosize range, often called nanomaterials/structures, are found to exhibit exceptional intrinsic properties in terms of many aspects such as strength, stability, conductivity and absorption. This has enabled scientists and researchers from various domains such as physical science, material science, electronics, medical science and biological science to study nanomaterials and adopt them as substructures in the construction of larger structures [21, 2, 6, 22]. In particular, a $TUC_4C_8\,[p, q]$ nanotube is an elegant nanostructure that can be constructed mathematically from alternating squares and octagons, consisting of p squares and their q rows. The $2D$-lattice, nanotube and nanotorus of $TUC_4C_8(R)\,[p, q]$ are illustrated in Fig. 1.

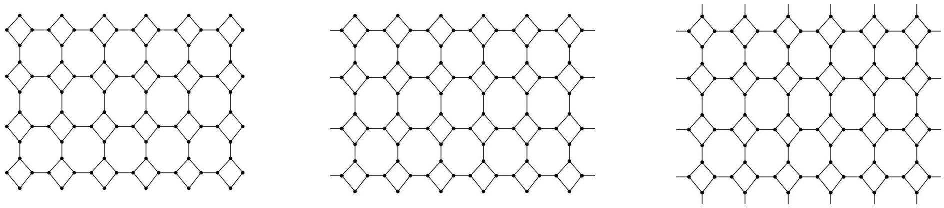

Figure 1: The graphs of the $TUC_4C_8(R)[6,4]$ $2D$-lattice, nanotube and nanotorus

In this paper, we construct the M-polynomial of the para-line graphs of the $TUC_4C_8(R)\,[p,q]$ $2D$-lattice, nanotube and nanotorus, by means of which, we compute some of their topological indices.

2. Preliminary Definitions and Known Results

We begin the section with some standard definitions and notation, found in literature, that we commonly use in the paper.

Definition 2.1. [8] *For a graph G, the M-polynomial is defined as*

$$M(G;x,y) = \sum_{\delta(G)\le i\le j\le\Delta(G)} m_{ij}(G)x^iy^j \tag{1}$$

where $\delta(G)$ and $\Delta(G)$ are the minimum and maximum degrees of any vertex, respectively, in G and $m_{ij}(G)$ is the number of edges $e = uv \in E(G)$ such that $\{deg_G(u), deg_G(v)\} = \{i,j\}$.

Definition 2.2. *Given any real number α, the general Randić index of a graph G is defined as*

$$R_\alpha(G) = \sum_{uv\in E(G)} (deg_G(u)deg_G(v))^\alpha. \tag{2}$$

and the general inverse Randić index of G is defined as

$$RR_\alpha(G) = \sum_{uv\in E(G)} \frac{1}{(deg_G(u)deg_G(v))^\alpha} \tag{3}$$

The Randić index of G is obtained by choosing $\alpha = -\frac{1}{2}$ in the expression for the general Randić index of G.

Definition 2.3. *The first and second Zagreb indices of a graph G are defined as*

$$M_1(G) = \sum_{uv\in E(G)} (deg_G(u) + deg_G(v)) \tag{4}$$

and

$$M_2(G) = \sum_{uv \in E(G)} (deg_G(u)deg_G(v)). \tag{5}$$

Definition 2.4. *The second modified Zagreb index of a graph G is defined as*

$$^mM_2(G) = \sum_{uv \in E(G)} \frac{1}{deg_G(u)deg_G(v)}. \tag{6}$$

Definition 2.5. *The symmetric division index of a graph G is defined as*

$$SDD(G) = \sum_{uv \in E(G)} \left[\frac{min(deg_G(u), deg_G(v))}{max(deg_G(u), deg_G(v))} + \frac{max(deg_G(u), deg_G(v))}{min(deg_G(u), deg_G(v))} \right]. \tag{7}$$

Definition 2.6. *The harmonic index of a graph G is defined as*

$$H(G) = \sum_{uv \in E(G)} \frac{2}{deg_G(u) + deg_G(v)}. \tag{8}$$

Definition 2.7. *The inverse sum index of a graph G is defined as*

$$I(G) = \sum_{uv \in E(G)} \frac{deg_G(u)deg_G(v)}{deg_G(u) + deg_G(v)}. \tag{9}$$

Definition 2.8. *The augmented Zagreb index of a graph G is defined as*

$$A(G) = \sum_{uv \in E(G)} \left[\frac{deg_G(u)deg_G(v)}{deg_G(u) + deg_G(v) - 2} \right]^3. \tag{10}$$

Topological Index	**Expression in terms of $M(G; x, y)$**
$M_1(G)$	$(D_x + D_y)(M(G; x, y))\|_{x=y=1}$
$M_2(G)$	$(D_x D_y)(M(G; x, y))\|_{x=y=1}$
$^mM_2(G)$	$(S_x S_y)(M(G; x, y))\|_{x=y=1}$
$R_\alpha(G)$	$(D_x^\alpha D_y^\alpha)(M(G; x, y))\|_{x=y=1}$
$RR_\alpha(G)$	$(S_x^\alpha S_y^\alpha)(M(G; x, y))\|_{x=y=1}$
$SSD(G)$	$(D_x S_y + S_x D_y)(M(G; x, y))\|_{x=y=1}$
H	$2S_x J(M(G; x, y))\|_{x=1}$
I	$S_x J D_x D_y(M(G; x, y))\|_{x=1}$
A	$S_x^3 Q_{-2} J D_x^3 D_y^3(M(G; x, y))\|_{x=1}$

$D_x f(x,y) = x\partial f(x,y)/\partial x, D_y f(x,y) = y\partial f(x,y)/\partial y, S_x f(x,y) = \int_0^x (f(t,y)/t)dt,$ $S_y f(x,y) = \int_0^y (f(x,t)/t)dt, Jf(x,y) = f(x,x), Q_\alpha f(x,y) = x^\alpha f(x,y)$

Table 1: Topological indices in terms of the M-polynomial

Each of the topological indices defined above can be obtained using the M-polynomial as given in Table 1.

3. Main Results

In this section, we obtain the closed form of the M-polynomial of the para-line graphs of $TUC_4C_8(R)[p,q]$ $2D$-lattice, nanotube and nanotorus, by means of which, we compute some of their topological indices.

3.1. M-polynomial of the para-line graph of $TUC_4C_8(R)[p,q]$ $2D$-lattice

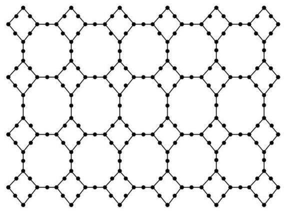

Figure 2: The subdivision graph of the $TUC_4C_8(R)[6,4]$ $2D$-lattice

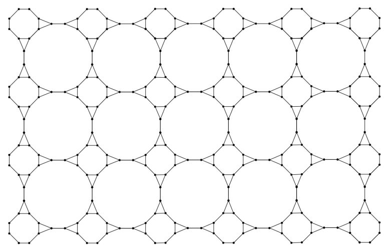

Figure 3: The para-line graph of the $TUC_4C_8(R)[6,4]$ $2D$-lattice

Theorem 3.1. *The M-polynomial of the para-line graph of $TUC_4C_8(R)[p,q]$ $2D$-lattice is* $M(TUC_4C_8(R)[p,q];x,y) = (2p+2q+4)x^2y^2 + (4p+4q-8)x^2y^3 + (18pq-11p-11q+4)x^3y^3$.

Proof. Let G_1 be the para-line graph of $TUC_4C_8(R)[p,q]$ $2D$-lattice. Since each of the vertices of G_1 is of degree either two or three, the vertex set of G_1 has the following two partitions with respect to degree:

$V_{\{2\}}(G_1) = \left\{v \in V(G_1)|_{deg_{G_1}(v)=2}\right\}$ and $V_{\{3\}}(G_1) = \left\{v \in V(G_1)|_{deg_{G_1}(v)=3}\right\}$.

Further, the edge set of G_1 has three partitions based on the degree of the end vertices:

$E_{\{2,2\}}(G_1) = \left\{e = uv \in E(G_1)|_{deg_{G_1}(u)=2, deg_{G_1}(v)=2}\right\}$,

$E_{\{2,3\}}(G_1) = \left\{e = uv \in E(G_1)|_{deg_{G_1}(u)=2, deg_{G_1}(v)=3}\right\}$ and

$E_{\{3,3\}}(G_1) = \left\{ e = uv \in E(G_1)|_{deg_{G_1}(u)=3, deg_{G_1}(v)=3} \right\}$, such that

$m_{22}(G_1) = \left| E_{\{2,2\}}(G_1) \right| = 2p + 2q + 4$, $m_{23}(G_1) = \left| E_{\{2,3\}}(G_1) \right| = 4p + 4q - 8$ and

$$m_{33}(G_1) = \left| E_{\{3,3\}}(G_1) \right| = 18pq - 11p - 11q + 4.$$

Thus, the M-polynomial of the given graph is

$$\begin{aligned} M(G_1; x, y) &= \sum_{2 \le i \le j \le 3} m_{ij}(G_1) x^i y^j \\ &= m_{22}(G_1) x^2 y^2 + m_{23}(G_1) x^2 y^3 + m_{33}(G_1) x^3 y^3 \\ &= (2p + 2q + 4) x^2 y^2 + (4p + 4q - 8) x^2 y^3 + (18pq - 11p - 11q + 4) x^3 y^3. \end{aligned}$$

Theorem 3.2. *Let G_1 be the para-line graph of $TUC_4C_8(R)[p, q]$ $2D$-lattice. Then,*

(1) $M_1(G_1) = 108pq - 38p - 38q$

(2) $M_2(G_1) = 162pq - 67p - 67q + 4$

(3) ${}^m M_2(G_1) = 2pq - \frac{1}{18} p - \frac{1}{18} q + \frac{1}{9}$

(4) $R_\alpha(G_1) = 4^\alpha(2p + 2q + 4) + 3^\alpha 2^\alpha(4p + 4q - 8) + 9^\alpha(18pq - 11p - 11q + 4)$

(5) $RR_\alpha(G_1) = \frac{1}{4^\alpha}(2p + 2q + 4) + \frac{1}{3^\alpha 2^\alpha}(4p + 4q - 8) + \frac{1}{9^\alpha}(18pq - 11p - 11q + 4)$

(6) $SSD(G_1) = 36pq - \frac{28}{3} p - \frac{28}{3} q - \frac{4}{3}$

(7) $H(G_1) = 6pq - \frac{16}{15} p - \frac{16}{15} q + \frac{2}{15}$

(8) $I(G_1) = 27pq - \frac{97}{10} p - \frac{97}{10} q + \frac{2}{5}$

(9) $A(G_1) = \frac{6561}{32} pq - \frac{4947}{64} p - \frac{4947}{64} q + \frac{217}{16}$

Proof. From Theorem 3.1, we have
$M(G_1; x, y) = f(x, y) = (2p + 2q + 4) x^2 y^2 + (4p + 4q - 8) x^2 y^3 + (18pq - 11p - 11q + 4) x^3 y^3$.
Then, we have the following:

$D_x f(x,y) = 2(2p+2q+4)x^2y^2 + 2(4p+4q-8)x^2y^3 + 3(18pq-11p-11q+4)x^3y^3,$

$D_y f(x,y) = 2(2p+2q+4)x^2y^2 + 3(4p+4q-8)x^2y^3 + 3(18pq-11p-11q+4)x^3y^3,$

$D_yD_x f(x,y) = 4(2p+2q+4)x^2y^2 + 6(4p+4q-8)x^2y^3 + 9(18pq-11p-11q+4)x^3y^3,$

$S_xS_y f(x,y) = \frac{1}{4}(2p+2q+4)x^2y^2 + \frac{1}{6}(4p+4q-8)x^2y^3 + \frac{1}{9}(18pq-11p-11q+4)x^3y^3,$

$D_x^\alpha D_y^\alpha f(x,y) = 4^\alpha(2p+2q+4)x^2y^2 + 6^\alpha(4p+4q-8)x^2y^3 + 9^\alpha(18pq-11p-11q+4)x^3y^3,$

$S_x^\alpha S_y^\alpha f(x,y) = \frac{1}{4^\alpha}(2p+2q+4)x^2y^2 + \frac{1}{3^\alpha 2^\alpha}(4p+4q-8)x^2y^3 + \frac{1}{9^\alpha}(18pq-11p-11q+4)x^3y^3,$

$S_yD_x f(x,y) = (2p+2q+4)x^2y^2 + \frac{2}{3}(4p+4q-8)x^2y^3 + (18pq-11p-11q+4)x^3y^3,$

$S_xD_y f(x,y) = (2p+2q+4)x^2y^2 + \frac{3}{2}(4p+4q-8)x^2y^3 + (18pq-11p-11q+4)x^3y^3,$

$2S_xJ f(x,y) = 2\Big[\frac{1}{4}(2p+2q+4)x^4 + \frac{1}{5}(4p+4q-8)x^5 + \frac{1}{6}(18pq-11p-11q+4)x^6\Big],$

$S_xJD_xD_y f(x,y) = (2p+2q+4)x^4 + \frac{6}{5}(4p+4q-8)x^5 + \frac{3}{2}(18pq-11p-11q+4)x^6,$

$S_x^3Q_{-2}JD_x^3D_y^3 f(x,y) = 2^3(2p+2q+4)x^2 + 2^3(4p+4q-8)x^3 + \frac{3^6}{4^3}(18pq-11p-11q+4)x^4.$

Using Table 1,

(1) The first Zagreb index

$$M_1(G_1) = (D_x + D_y)(f(x,y))\Big|_{x=y=1} = 108pq - 38p - 38q$$

(2) The second Zagreb index

$$M_2(G_1) = D_yD_x(f(x,y))\Big|_{x=y=1} = 162pq - 67p - 67q + 4.$$

(3) The modified second Zagreb index

$$^{m}M_2(G_1) = S_x S_y(f(x,y))\Big|_{x=y=1} = 2pq - \frac{1}{18}p - \frac{1}{18}q + \frac{1}{9}.$$

(4) The generalized Randić index

$$R_\alpha(G_1) = D_x^\alpha D_y^\alpha(f(x,y))\Big|_{x=y=1}$$
$$= 4^\alpha(2p+2q+4) + 3^\alpha 2^\alpha(4p+4q-8) + 9^\alpha(18pq-11p-11q+4).$$

(5) The inverse Randić index

$$RR_\alpha(G_1) = S_x^\alpha S_y^\alpha(f(x,y))\Big|_{x=y=1}$$
$$= \frac{1}{4^\alpha}(2p+2q+4) + \frac{1}{3^\alpha 2^\alpha}(4p+4q-8) + \frac{1}{9^\alpha}(18pq-11p-11q+4).$$

(6) The symmetric division index

$$SSD(G_1) = (S_y D_x + S_x D_y)f(x,y)\Big|_{x=y=1} = 36pq - \frac{28}{3}p - \frac{28}{3}q - \frac{4}{3}.$$

(7) The harmonic index

$$H(G_1) = 2S_x J f(x,y)\Big|_{x=1}$$
$$= 2\Big[\frac{1}{4}(2p+2q+4)x^4 + \frac{1}{5}(4p+4q-8)x^5 + \frac{1}{6}(18pq-11p-11q+4)x^6\Big]_{x=1}$$
$$= 6pq - \frac{16}{15}p - \frac{16}{15}q + \frac{2}{15}$$

(8) The inverse sum index

$$I(G_1) = S_x J D_x D_y f(x,y)\Big|_{x=1}$$
$$= \Big[(2p+2q+4)x^4 + \frac{6}{5}(4p+4q-8)x^5 + \frac{3}{2}(18pq-11p-11q+4)x^6\Big]_{x=1}$$
$$= 27pq - \frac{97}{10}p - \frac{97}{10}q + \frac{2}{5}.$$

(9) The augmented Zagreb index

$$A(G_1) = S_x^3 Q_{-2} J D_x^3 D_y^3 f(x,y)\Big|_{x=1}$$
$$= \left[2^3(2p+2q+4)x^2 + 2^3(4p+4q-8)x^3 + \frac{3^6}{4^3}(18pq-11p-11q+4)x^4\right]_{x=1}$$
$$= \frac{6561}{32}pq - \frac{4947}{64}p - \frac{4947}{64}q + \frac{217}{16}.$$

3.2. M-polynomial of the Para-line Graph of $TUC_4C_8(R)[p,q]$ Nanotube

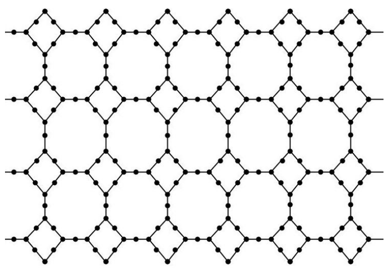

Figure 4: The subdivision graph of the $TUC_4C_8(R)[6,4]$ nanotube

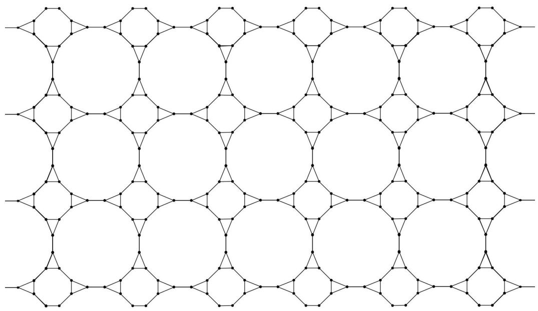

Figure 5: The para-line graph of the $TUC_4C_8(R)[6,4]$ nanotube

Theorem 3.3. *The M-polynomial of the para-line graph of $TUC_4C_8(R)[p,q]$ nanotube is*
$M(TUC_4C_8(R)[p,q]; x, y) = (2p)x^2y^2 + (4p)x^2y^3 + (18pq-11p)x^3y^3.$

Proof. Let G_2 be the para-line graph of $TUC_4C_8(R)[p,q]$ nanotube. Since each of the vertices of G_2 is of degree either two or three, the vertex set of G_2 has the following two partitions with respect to degree:
$V_{\{2\}}(G_2) = \left\{v \in V(G_2)|_{deg_{G_2}(v)=2}\right\}$ and $V_{\{3\}}(G_2) = \left\{v \in V(G_2)|_{deg_{G_2}(v)=3}\right\}$.
Further, the edge set of G_2 has three partitions based on the degree of the end vertices:
$E_{\{2,2\}}(G_2) = \left\{e = uv \in E(G_2)|_{deg_{G_2}(u)=2, deg_{G_2}(v)=2}\right\}$,
$E_{\{2,3\}}(G_2) = \left\{e = uv \in E(G_2)|_{deg_{G_2}(u)=2, deg_{G_2}(v)=3}\right\}$ and
$E_{\{3,3\}}(G_2) = \left\{e = uv \in E(G_2)|_{deg_{G_2}(u)=3, deg_{G_2}(v)=3}\right\}$, such that
$m_{22}(G_2) = \left|E_{\{2,2\}}(G_2)\right| = 2p$, $m_{23}(G_2) = \left|E_{\{2,3\}}(G_2)\right| = 4p$ and
$m_{33}(G_2) = \left|E_{\{3,3\}}(G_2)\right| = 18pq - 11p.$

Thus, the M-polynomial of the given graph is

$$M(G_2;x,y) = \sum_{2\leq i\leq j\leq 3} m_{ij}(G_2)x^iy^j = m_{22}(G_2)x^2y^2 + m_{23}(G_2)x^2y^3 + m_{33}(G_2)x^3y^3$$
$$= (2p)x^2y^2 + (4p)x^2y^3 + (18pq - 11p)x^3y^3.$$

Theorem 3.4. *Let G_2 be the para-line graph of $TUC_4C_8(R)[p,q]$ nanotube. Then,*

(1) $M_1(G_2) = 108pq - 38p$

(2) $M_2(G_2) = 162pq - 67p$

(3) ${}^mM_2(G_2) = 2pq - \frac{1}{18}p$

(4) $R_\alpha(G_2) = 4^\alpha(2p) + 3^\alpha 2^\alpha(4p) + 9^\alpha(18pq - 11p)$

(5) $RR_\alpha(G_2) = \frac{1}{4^\alpha}(2p) + \frac{1}{3^\alpha 2^\alpha}(4p) + \frac{1}{9^\alpha}(18pq - 11p)$

(6) $SSD(G_2) = 36pq - \frac{28}{3}p$

(7) $H(G_2) = 6pq - \frac{16}{15}p$

(8) $I(G_2) = 27pq - \frac{97}{10}p$

(9) $A(G_2) = \frac{6561}{32}pq - \frac{4947}{64}p$

Proof. From Theorem 3.3, we have $M(G_2;x,y) = f(x,y) = (2p)x^2y^2 + (4p)x^2y^3 + (18pq - 11p)x^3y^3$. Then, we have the following:

$$D_xf(x,y) = 2(2p)x^2y^2 + 2(4p)x^2y^3 + 3(18pq - 11p)x^3y^3,$$

$$D_yf(x,y) = 2(2p)x^2y^2 + 3(4p)x^2y^3 + 3(18pq - 11p)x^3y^3,$$

$$D_yD_xf(x,y) = 4(2p)x^2y^2 + 6(4p)x^2y^3 + 9(18pq - 11p)x^3y^3,$$

$$S_xS_yf(x,y) = \frac{1}{4}(2p)x^2y^2 + \frac{1}{6}(4p)x^2y^3 + \frac{1}{9}(18pq - 11p)x^3y^3,$$

$$D_x^\alpha D_y^\alpha f(x,y) = 4^\alpha(2p)x^2y^2 + 6^\alpha(4p)x^2y^3 + 9^\alpha(18pq - 11p)x^3y^3,$$

$$S_x^\alpha S_y^\alpha f(x,y) = \frac{1}{4^\alpha}(2p)x^2y^2 + \frac{1}{3^\alpha 2^\alpha}(4p)x^2y^3 + \frac{1}{9^\alpha}(18pq-11p)x^3y^3,$$

$$S_yD_xf(x,y) = (2p)x^2y^2 + \frac{2}{3}(4p)x^2y^3 + (18pq-11p)x^3y^3,$$

$$S_xD_yf(x,y) = (2p)x^2y^2 + \frac{3}{2}(4p)x^2y^3 + (18pq-11p)x^3y^3,$$

$$2S_xJf(x,y) = 2\Big[\frac{1}{4}(2p)x^4 + \frac{1}{5}(4p)x^5 + \frac{1}{6}(18pq-11p)x^6\Big],$$

$$S_xJD_xD_yf(x,y) = (2p)x^4 + \frac{6}{5}(4p)x^5 + \frac{3}{2}(18pq-11p)x^6,$$

$$S_x^3Q_{-2}JD_x^3D_y^3f(x,y) = 2^3(2p)x^2 + 2^3(4p)x^3 + \frac{3^6}{4^3}(18pq-11p)x^4.$$

Using Table 1,

(1) The first Zagreb index

$$M_1(G_2) = (D_x+D_y)(f(x,y))\Big|_{x=y=1} = 108pq - 38p.$$

(2) The second Zagreb index

$$M_2(G_2) = D_yD_x(f(x,y))\Big|_{x=y=1} = 162pq - 67p.$$

(3) The modified second Zagreb index

$$^mM_2(G_2) = S_xS_y(f(x,y))\Big|_{x=y=1} = 2pq - \frac{1}{18}p$$

(4) The generalized Randić index

$$R_\alpha(G_2) = D_x^\alpha D_y^\alpha(f(x,y))\Big|_{x=y=1} = 4^\alpha(2p) + 3^\alpha 2^\alpha(4p) + 9^\alpha(18pq-11p).$$

(5) The inverse Randić index

$$RR_\alpha(G_2) = S_x^\alpha S_y^\alpha(f(x,y))\Big|_{x=y=1} = \frac{1}{4^\alpha}(2p) + \frac{1}{3^\alpha 2^\alpha}(4p) + \frac{1}{9^\alpha}(18pq-11p).$$

(6) The symmetric division index

$$SSD(G_2) = (S_yD_x + S_xD_y)f(x,y)\Big|_{x=y=1} = 36pq - \frac{28}{3}p.$$

(7) The harmonic index

$$H(G_2) = 2S_xJf(x,y)\Big|_{x=1} = 2\Big[\frac{1}{4}(2p)x^4 + \frac{1}{5}(4p)x^5 + \frac{1}{6}(18pq-11p)x^6\Big]_{x=1}$$
$$= 6pq - \frac{16}{15}p.$$

(8) The inverse sum index

$$I(G_2) = S_xJD_xD_yf(x,y)\Big|_{x=1} = \Big[(2p)x^4 + \frac{6}{5}(4p)x^5 + \frac{3}{2}(18pq-11p)x^6\Big]_{x=1}$$
$$= 27pq - \frac{97}{10}p.$$

(9) The augmented Zagreb index

$$A(G_2) = S_x^3Q_{-2}JD_x^3D_y^3f(x,y)\Big|_{x=1}$$
$$= \Big[2^3(2p)x^2 + 2^3(4p)x^3 + \frac{3^6}{4^3}(18pq-11p)x^4\Big]_{x=1} = \frac{6561}{32}pq - \frac{4947}{64}p.$$

3.3. M-polynomial of the Para-line Graph of $TUC_4C_8(R)[p,q]$ Nanotorus

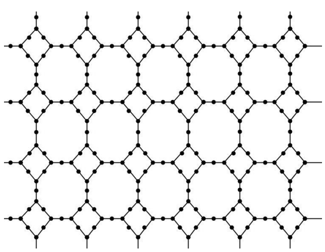

Figure 6: The subdivision graph of the $TUC_4C_8(R)[6,4]$ nanotorus

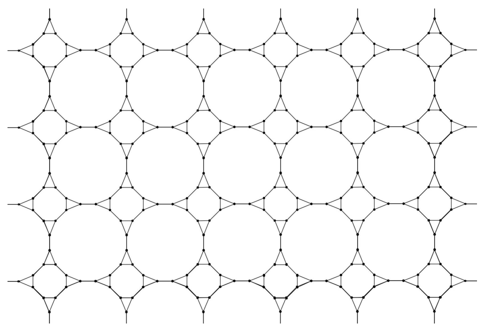

Figure 7: The para-line graph of the $TUC_4C_8(R)[6,4]$ nanotorus

Theorem 3.5. *The M-polynomial of the para-line graph of $TUC_4C_8(R)[p,q]$ nanotorus is $M(TUC_4C_8(R)[p,q];x,y) = (18pq)x^3y^3$.*
Proof. Let G_3 be the para-line graph of $TUC_4C_8(R)[p,q]$ nanotorus. Since each of the vertices of G_3 is of degree three, the vertex set of G_3 has the partition with respect to degree:
$V_{\{3\}}(G_3) = \left\{v \in V(G_3)|_{deg_{G_3}(v)=3}\right\}$.
Further, the edge set of G_3 has the partition based on the degree of the end vertices:
$E_{\{3,3\}}(G_3) = \left\{e = uv \in E(G_3)|_{deg_{G_3}(u)=3, deg_{G_3}(v)=3}\right\}$, such that,
$m_{33}(G_3) = \left|E_{\{3,3\}}(G_3)\right| = 18pq$. Thus, the M-polynomial of the given graph is

$$\begin{aligned} M(G_3;x,y) &= \sum_{3\le i\le j\le 3} m_{ij}(G_3)x^iy^j \\ &= (18pq)x^3y^3. \end{aligned}$$

Theorem 3.6. *Let G_3 be the para-line graph of $TUC_4C_8(R)[p,q]$ nanotorus. Then,*

(1) $M_1(G_3) = 108pq$

(2) $M_2(G_3) = 162pq$

(3) ${}^mM_2(G_3) = 2pq$

(4) $R_\alpha(G_3) = 9^\alpha(18pq)$

(5) $RR_\alpha(G_3) = \frac{1}{9^\alpha}(18pq)$

(6) $SSD(G_3) = 36pq$

(7) $H(G_3) = 6pq$

(8) $I(G_3) = 27pq$

(9) $A(G_3) = \frac{6561}{32}pq$

Proof. From Theorem 3.5, we have $M(G_3;x,y) = f(x,y) = (18pq)x^3y^3$. Then, we have the following:

$D_xf(x,y) = 3(18pq)x^3y^3$,

$D_yf(x,y) = 3(18pq)x^3y^3$,

$D_yD_xf(x,y) = 9(18pq)x^3y^3,$

$S_xS_yf(x,y) = \frac{1}{9}(18pq)x^3y^3,$

$D_x^\alpha D_y^\alpha f(x,y) = 9^\alpha(18pq)x^3y^3,$

$S_x^\alpha S_y^\alpha f(x,y) = \frac{1}{9^\alpha}(18pq)x^3y^3,$

$S_yD_xf(x,y) = (18pq)x^3y^3,$

$S_xD_yf(x,y) = (18pq)x^3y^3,$

$2S_xJf(x,y) = 2\left[\frac{1}{6}(18pq)x^6\right],$

$S_xJD_xD_yf(x,y) = \frac{3}{2}(18pq)x^6,$

$S_x^3Q_{-2}JD_x^3D_y^3f(x,y) = \frac{3^6}{4^3}(18pq)x^4.$

Using Table 1,

(1) The first Zagreb index

$$M_1(G_3) = (D_x + D_y)(f(x,y))\Big|_{x=y=1} = 108pq.$$

(2) The second Zagreb index

$$M_2(G_3) = D_yD_x(f(x,y))\Big|_{x=y=1} = 162pq.$$

(3) The modified second Zagreb index

$$^mM_2(G_3) = S_xS_y(f(x,y))\Big|_{x=y=1} = \frac{1}{9}(18pq).$$

(4) The generalized Randić index

$$R_\alpha(G_3) = D_x^\alpha D_y^\alpha(f(x,y))\Big|_{x=y=1} = 9^\alpha(18pq).$$

(5) The inverse Randić index

$$RR_\alpha(G_3) = S_x^\alpha S_y^\alpha(f(x,y))\Big|_{x=y=1} = \frac{1}{9^\alpha}(18pq).$$

(6) The symmetric division index

$$SSD(G_3) = (S_y D_x + S_x D_y) f(x,y)\Big|_{x=y=1} = 36pq.$$

(7) The harmonic index

$$\begin{aligned} H(G_3) &= 2S_x J f(x,y)\Big|_{x=1} \\ &= 6pq. \end{aligned}$$

(8) The inverse sum index

$$\begin{aligned} I(G_3) &= S_x J D_x D_y f(x,y)\Big|_{x=1} \\ &= 27pq. \end{aligned}$$

(9) The augmented Zagreb index

$$\begin{aligned} A(G_3) &= S_x^3 Q_{-2} J D_x^3 D_y^3 f(x,y)\Big|_{x=1} \\ &= \frac{6561}{32} pq. \end{aligned}$$

4. Conclusion

In this paper, we have obtained the closed form of the M-polynomial of the para-line graphs of the $TUC_4C_8(R)\,[p,q]$ $2D$-lattice, nanotube and nanotorus. Using these, we have computed some of their important topological indices such as the general Randić index, Zagreb indices and harmonic index. The study of these topological indices, in turn, is helpful in understanding many of their physico-chemical properties as seen in literature.

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