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An Algebraic Approach to Find Some Topological Indices of Derived Graphs of the Benzene Ring

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Abstract: Topological indices play a vital role in understanding the chemical and structural properties of the chemical compounds and nanostructures. By finding the M-polynomial of a graph representing a chemical compound, one can obtain the closed forms of some of the commonly known degree-based topological indices of the compound, such as the Zagreb index, general Randić Index and harmonic index. In this article, we obtain the expression for the M-polynomial of the derived graphs of the Benzene ring embedded in the P-type surface network in 2D, namely the line graph, the subdivision graph, and the line graph of its subdivision. Furthermore, some of the degree-based topological indices are obtained for these graphs using their M-polynomials.

Keywords: topological indices; benzene ring; M-polynomial; subdivision; line graph; para-line graph.

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1. Introduction

A chemical graph is the representation of a chemical/molecular structure in terms of a graph, such that each of its atoms is represented by a vertex with an edge representing a bond/multiple bonds between two of its atoms. Such a graph $G = (V, E)$ is simple, undirected, finite, and connected. The order and size of G are, respectively, the number of vertices and edges in it. The length of any shortest path between any two vertices u and v in G is called the distance between them and is denoted $d_G(u, v)$.

The subdivision graph $S(G)$ of a graph G is obtained by replacing each edge $e = uv$ in G with a vertex, say w, of degree two, and then adding two edges of the form uw and vw to it. The line graph $L(G)$ of G is obtained by replacing each edge of G by a vertex and adding edges to it, in such a way that two vertices in $L(G)$ are adjacent if and only if they share a common vertex in G. The para-line graph $L(S(G))$ of G is the line graph of its subdivision graph.

As defined by [1], a Benzene ring is embedded in the P-type surface (6.8^2P) and is derived by condensing truncated-icosahedral C_{60} molecules. In particular, twelve atoms are removed from each C_{60} molecule in such a way that the remaining 48 atoms, in eight hexagonal rings, have cubic symmetry. Further, each of these is joined to six identical structures in the six cubic face directions so that four eight-sided rings are formed at each juncture. The 2D representation of the structure, shortly called the Benzene ring, with m rows and n columns and its subdivision graph is as shown in Figure 1. Further, the line graph and the para-line graph of the structure, taking $m = 3$ and $n = 5$, are depicted in Figure 2.

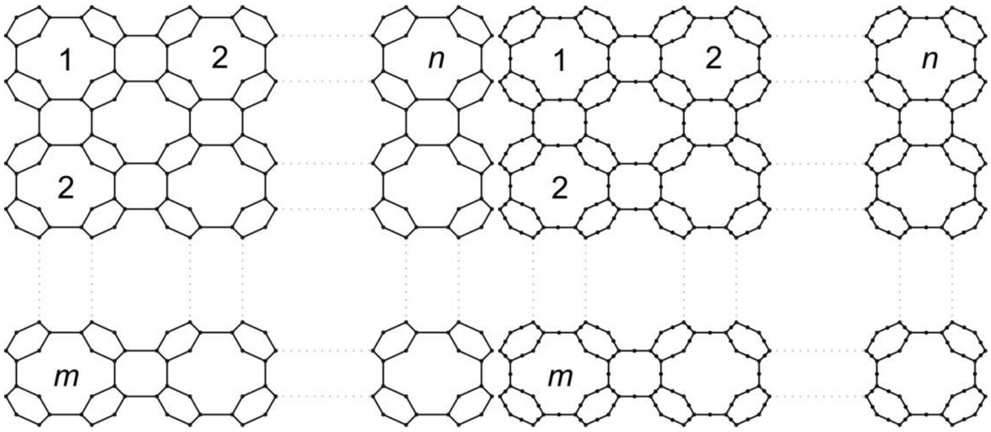

Figure 1. The graphs of the Benzene ring and its subdivision with *m* rows and *n* columns**.**

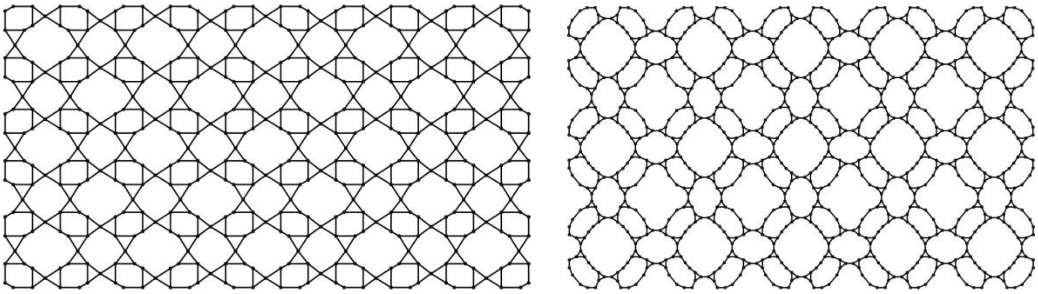

Figure 2. The line and para-line graphs of the Benzene ring with *m* = 3 and *n* = 5**.**

A topological index, or a molecular descriptor, of a graph, is a numerical value associated with a graph. It is useful to correlate the structure of the graph with its physical and chemical properties, and it's QSPR/QSAR analysis. For some applications of topological indices, we cite [2-4]. Since the introduction of the first topological index, namely the Wiener index in the year 1947 by Wiener [5], which is based on the topological distance between vertices in a graph, many indices have been formulated, and later generalized, based on the various parameters of the underlying graph such as degree, distance, and spectrum [6-12]. Further, some of these indices have been obtained for particular chemical graphs and nanostructures [13-18]. Wiener index, Hosoya index, Zagreb index, Randić Index and Estrada index are some of the commonly known topological indeces [6, 19, 20].

In the year 1975, M. Randić [6], during his study of the molecular properties of acyclic structures, formulated the Randić index $R_{-1/2}(G)$ of a graph G as

$$R_{-1/2}(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{deg_G(u)deg_G(v)}}. \quad (1)$$

Later, in the year 1998, Bollobás *et al.* [21] generalized the Randić index, by replacing $-1/2$ by any real number α, as the general Randić index $R_\alpha(G)$ and the inverse Randić index $RR_\alpha(G)$, given by

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

and

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

In the year 1972, Gutman *et al.* [20] introduced the first and second Zagreb indices, $M_1(G)$ and $M_2(G)$ of a graph G, defined as

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

and

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

Further, the second modified Zagreb index ${}^mM_2(G)$ of a graph, G was defined as

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

The symmetric division index $SDD(G)$ of a graph G was defined by Gupta *et al.* [22], in the year 2016, as

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

Zhong, in the year 2012 [23], introduced a variation of the Randić Index called the harmonic index $H(G)$ of a graph G, as

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

As discussed by Vukičević *et al.*, in the year 2010 [24], the inverse sum index $I(G)$ of a graph G was found to be an important indicator to the total surface area of octane isomers and was defined as

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

Formulated by Huang *et al*., in the year 2012 [25], the augmented Zagreb index $A(G)$ of a graph G, found to be very useful in the study of the heat of formation of octanes and heptanes, is defined as

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

2. Materials and Methods

In literature, the study of some of the topological indices has been done by means of constructing graph-related polynomials. Some of the well-known graph polynomials are the Hosoya polynomial, Tutte polynomial, and the Schlutz polynomial [26-28]. In particular, E. Deutsch *et al.* [29] introduced the M-polynomial as

$$M(G; x, y) = \sum_{\delta(G) \le i \le j \le \Delta(G)} m_{ij}(G) x^i y^j \quad (11)$$

where $\boldsymbol{\delta(G)}$ and $\boldsymbol{\Delta(G)}$are the minimum and maximum degrees of any vertex, respectively, in $\boldsymbol{G}$ and $\boldsymbol{m_{ij}(G)}$ is the number of edges $\boldsymbol{e = uv} \in \boldsymbol{E(G)}$ such that $\{\boldsymbol{deg_G(u), deg_G(v)}\} = \{\boldsymbol{i, j}\}$. Further, he showed that the closed-form of some of the degree-based topological indices, such as the Zagreb indices, the general Randić Index and harmonic index can be easily obtained using it, as shown in Table 1. Based on this, several authors have worked on computing the polynomials of various chemical graphs and nanostructures, thereby finding their respective indices [30-40].

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

Topological Index	Expression in terms of $M(G; x, y)$
$M_1(G)$	$(D_x + D_y)(M(G; x, y))\|_{x=y=1}$
$M_2(G)$	$(D_x D_y)(M(G; x, y))\|_{x=y=1}$

Topological Index	Expression in terms of $M(G;x,y)$
$^{m}M_2(G)$	$(S_xS_y)(M(G;x,y))\vert_{x=y=1}$
$R_\alpha(G)$	$(D_x^\alpha D_y^\alpha)(M(G;x,y))\vert_{x=y=1}$
$RR_\alpha(G)$	$(S_x^\alpha S_y^\alpha)(M(G;x,y))\vert_{x=y=1}$
$SSD(G)$	$(D_xS_y+S_xD_y)(M(G;x,y))\vert_{x=y=1}$
H	$2S_xJ(M(G;x,y))\vert_{x=1}$
I	$S_xJD_xD_y(M(G;x,y))\vert_{x=1}$
A	$S_x^3Q_{-2}JD_x^3D_y^3(M(G;x,y))\vert_{x=1}$

$D_xf(x,y)=x\partial f(x,y)/\partial x$	$D_yf(x,y)=y\partial f(x,y)/\partial y$	$S_xf(x,y)=\int_0^x (f(t,y)/t)dt$
$S_yf(x,y)=\int_0^y (f(x,t)/t)dt$	$Jf(x,y)=f(x,x)$	$Q_\alpha f(x,y)=x^\alpha f(x,y)$

Going in this direction, in this article, we study the M-polynomial of some derived graphs of the Benzene ring embedded in the P-type surface network in 2D and its derived graphs, namely the line graph, the subdivision graph, and the line graph of its subdivision. Using these, we obtain these topological indices for each of the corresponding graph structures. For standard terminologies, we refer to [41-43].

3. Results and Discussion

In this section, we obtain the closed-form of the M-polynomial of subdivision, line graph, and para-line of the Benzene ring embedded in P-type surface network, by means of which, we compute their topological indices.

3.1. M-polynomial of the line graph of the Benzene ring.

Theorem 3.1 Let G be the line graph of the Benzene ring. Then, the M-polynomial of G is given by

$$M(G[m,n];x,y)=4x^2y^2+(8m+8n-8)x^2y^3+(8mn+4)x^3y^3+(32mn-8m-8n)x^3y^4+(16mn-8m-8n)x^4y^4.$$

Proof. Let G be the line graph of the Benzene ring. Since each of the vertices of G is of degree either two, three or four, the vertex set of G has the following three partitions with respect to a degree:

$V_{\{2\}}(G)=\{v\in V(G)|_{deg_G(v)=2}\}$, $V_{\{3\}}(G)=\{v\in V(G)|_{deg_G(v)=3}\}$ and $V_{\{4\}}(G)=\{v\in V(G)|_{deg_G(v)=4}\}$.

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

$E_{\{2,2\}}(G)=\{e=uv\in E(G)|_{deg_G(u)=2,deg_G(v)=2}\}$,

$E_{\{2,3\}}(G)=\{e=uv\in E(G)|_{deg_G(u)=2,deg_G(v)=3}\}$,

$E_{\{3,3\}}(G)=\{e=uv\in E(G)|_{deg_G(u)=3,deg_G(v)=3}\}$,

$E_{\{3,4\}}(G)=\{e=uv\in E(G)|_{deg_G(u)=3,deg_G(v)=4}\}$ and

$E_{\{4,4\}}(G)=\{e=uv\in E(G)|_{deg_G(u)=4,deg_G(v)=4}\}$, such that

$m_{22}(G)=|E_{\{2,2\}}(G)|=4, m_{23}(G)=|E_{\{2,3\}}(G)|=8m+8n-8, m_{33}(G)=|E_{\{3,3\}}(G)|=8mn+4,$

$m_{34}(G) = |E_{\{3,4\}}(G)| = 32mn - 8m - 8nandm_{44}(G) = |E_{\{4,4\}}(G)| = 16mn - 8m - 8n.$

Thus, the M-polynomial of the given graph is

$$M(G;x,y) = \sum_{i\leq j} m_{ij}(G)x^i y^j$$

$$= m_{22}(G)x^2y^2 + m_{23}(G)x^2y^3 + m_{33}(G)x^3y^3 + m_{34}(G)x^3y^4 + m_{44}(G)x^4y^4$$

$$= 4x^2y^2 + (8m + 8n - 8)x^2y^3 + (8mn + 4)x^3y^3$$

$$+(32mn - 8m - 8n)x^3y^4 + (16mn - 8m - 8n)x^4y^4$$

Theorem 3.2 Let G be the line graph of the Benzene ring. Then,

(1) $M_1(G) = 400mn - 80m - 80n$

(2) $M_2(G) = 712mn - 176m - 176n + 4$

(3) $\quad {}^{m}M_2(G) = \frac{41}{9}mn + \frac{1}{6}m + \frac{1}{6}n + \frac{1}{9}$

(4) $R_\alpha(G) = 2^{2\alpha}(4) + 3^\alpha 2^\alpha(8m + 8n - 8) + 3^{2\alpha}(8mn + 4)$

$$+3^\alpha 4^\alpha(32mn - 8m - 8n) + 4^{2\alpha}(16mn - 8m - 8n)$$

(5) $RR_\alpha(G) = \frac{1}{2^{2\alpha}}(4) + \frac{1}{3^\alpha 2^\alpha}(8m + 8n - 8) + \frac{1}{3^{2\alpha}}(8mn + 4)$

$$+\frac{1}{3^\alpha 4^\alpha}(32mn - 8m - 8n) + \frac{1}{4^{2\alpha}}(16mn - 8m - 8n)$$

(6) $SSD(G) = \frac{344}{3}mn - \frac{46}{3}m - \frac{46}{3}n - \frac{4}{3}$

(7) $H(G) = \frac{332}{21}mn - \frac{38}{35}m - \frac{38}{35}n + \frac{2}{15}$

(8) $I(G) = \frac{692}{7}mn - \frac{704}{35}m - \frac{704}{35}n + \frac{2}{5}$

Proof. From Theorem 3.1, we have

$$M(G;x,y) = 4x^2y^2 + (8m + 8n - 8)x^2y^3 + (8mn + 4)x^3y^3$$
$$+(32mn - 8m - 8n)x^3y^4 + (16mn - 8m - 8n)x^4y^4.$$

Then, we have the following:

$$D_x f(x,y) = 2(4)x^2y^2 + 2(8m + 8n - 8)x^2y^3 + 3(8mn + 4)x^3y^3$$
$$+3(32mn - 8m - 8n)x^3y^4 + 4(16mn - 8m - 8n)x^4y^4,$$
$$D_y f(x,y) = 2(4)x^2y^2 + 3(8m + 8n - 8)x^2y^3 + 3(8mn + 4)x^3y^3$$
$$+4(32mn - 8m - 8n)x^3y^4 + 4(16mn - 8m - 8n)x^4y^4,$$
$$D_y D_x f(x,y) = 4(4)x^2y^2 + 6(8m + 8n - 8)x^2y^3 + 9(8mn + 4)x^3y^3$$
$$+12(32mn - 8m - 8n)x^3y^4 + 16(16mn - 8m - 8n)x^4y^4,$$
$$S_x S_y f(x,y) = \frac{1}{4}(4)x^2y^2 + \frac{1}{6}(8m + 8n - 8)x^2y^3 + \frac{1}{9}(8mn + 4)x^3y^3$$
$$+\frac{1}{12}(32mn - 8m - 8n)x^3y^4 + \frac{1}{16}(16mn - 8m - 8n)x^4y^4,$$
$$D_x^\alpha D_y^\alpha f(x,y) = 4^\alpha(4)x^2y^2 + 6^\alpha(8m + 8n - 8)x^2y^3 + 9^\alpha(8mn + 4)x^3y^3$$
$$+12^\alpha(32mn - 8m - 8n)x^3y^4 + 16^\alpha(16mn - 8m - 8n)x^4y^4,$$
$$S_x^\alpha S_y^\alpha f(x,y) = \frac{1}{4^\alpha}(4)x^2y^2 + \frac{1}{6^\alpha}(8m + 8n - 8)x^2y^3 + \frac{1}{9^\alpha}(8mn + 4)x^3y^3$$
$$+\frac{1}{12^\alpha}(32mn - 8m - 8n)x^3y^4 + \frac{1}{16^\alpha}(16mn - 8m - 8n)x^4y^4,$$

$$S_yD_xf(x,y) = 4x^2y^2 + \frac{2}{3}(8m+8n-8)x^2y^3 + (8mn+4)x^3y^3$$
$$+\tfrac{3}{4}(32mn-8m-8n)x^3y^4 + (16mn-8m-8n)x^4y^4,$$
$$S_xD_yf(x,y) = 4x^2y^2 + \frac{3}{2}(8m+8n-8)x^2y^3 + (8mn+4)x^3y^3$$
$$+\tfrac{4}{3}(32mn-8m-8n)x^3y^4 + (16mn-8m-8n)x^4y^4,$$
$$2S_xJf(x,y) = 2[\frac{1}{4}(4)x^4 + \frac{1}{5}(8m+8n-8)x^5 + \frac{1}{6}(8mn+4)x^6$$
$$+\tfrac{1}{7}(32mn-8m-8n)x^7 + \tfrac{1}{8}(16mn-8m-8n)x^8],$$
$$S_xJD_xD_yf(x,y) = 4x^4 + \frac{6}{5}(8m+8n-8)x^5 + \frac{9}{6}(8mn+4)x^6$$
$$+\tfrac{12}{7}(32mn-8m-8n)x^7 + \tfrac{16}{8}(16mn-8m-8n)x^8,$$
$$S_x^3Q_{-2}JD_x^3D_y^3f(x,y) = 2^3(4)x^2 + 2^3(8m+8n-8)x^3 + \frac{3^6}{4^3}(8mn+4)x^4$$
$$+\frac{4^3 3^3}{5^3}(32mn-8m-8n)x^5 + \frac{4^6}{6^3}(16mn-8m-8n)x^6$$

Combining these results, using Table 1, we have the following:

(1) The first Zagreb index

$$M_1(G) = (D_x + D_y)(f(x,y))|_{x=y=1} = 400mn - 80m - 80n$$

(2) The second Zagreb index

$$M_2(G) = D_yD_x(f(x,y))|_{x=y=1} = 712mn - 176m - 176n + 4$$

(3) The modified second Zagreb index

$${}^{m}M_2(G) = S_xS_y(f(x,y))|_{x=y=1} = \tfrac{41}{9}mn + \tfrac{1}{6}m + \tfrac{1}{6}n + \tfrac{1}{9}$$

(4) The generalized Randić index

$$R_\alpha(G) = D_x^\alpha D_y^\alpha(f(x,y))|_{x=y=1}$$
$$= 2^{2\alpha}(4) + 3^\alpha 2^\alpha(8m+8n-8) + 3^{2\alpha}(8mn+4)$$
$$+3^\alpha 4^\alpha(32mn-8m-8n) + 4^{2\alpha}(16mn-8m-8n)$$

(5) The inverse Randić index

$$RR_\alpha(G) = \frac{1}{2^{2\alpha}}(4) + \frac{1}{3^\alpha 2^\alpha}(8m+8n-8) + \frac{1}{3^{2\alpha}}(8mn+4)$$
$$+\frac{1}{3^\alpha 4^\alpha}(32mn-8m-8n) + \frac{1}{4^{2\alpha}}(16mn-8m-8n)$$

(6) The symmetric division index

$$SSD(G) = \tfrac{344}{3}mn - \tfrac{46}{3}m - \tfrac{46}{3}n - \tfrac{4}{3}$$

(7) The harmonic index

$$H(G) = 2S_xJf(x,y)|_{x=1} = 2[\tfrac{1}{4}(4)x^4 + \tfrac{1}{5}(8m+8n-8)x^5 + \tfrac{1}{6}(8mn+4)x^6$$
$$+\frac{1}{7}(32mn-8m-8n)x^7 + \frac{1}{8}(16mn-8m-8n)x^8]_{x=1}$$
$$= \frac{332}{21}mn - \frac{38}{35}m - \frac{38}{35}n + \frac{2}{15}$$

(8) The inverse sum index

$$I(G) = S_xJD_xD_yf(x,y)|_{x=1} = [4x^4 + \tfrac{5}{6}(8m+8n-8)x^5 + \tfrac{9}{6}(8mn+4)x^6$$

$$+\frac{12}{7}(32mn-8m-8n)x^7+\frac{16}{8}(16mn-8m-8n)x^8]_{x=1}$$
$$=\frac{692}{7}mn-\frac{704}{35}m-\frac{704}{35}n+\frac{2}{5}$$

3.2. M-polynomial of the subdivision graph of the Benzene ring.

Theorem 3.3 Let G_1 be the subdivision graph of the Benzene ring. Then the M-polynomial of G_1 is

$$M(G_1[m,n];x,y)=(16mn+8m+8n)x^2y^2+(48mn-12m-12n)x^2y^3.$$

Proof. Let G_1 be the subdivision graph of the Benzene ring. 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 a degree:

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

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

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

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

$m_{22}(G_1)=|E_{\{2,2\}}(G_1)|=16mn+8m+8n$ *and* $m_{23}(G_1)=|E_{\{2,3\}}(G_1)|=48mn-12m-12n.$

Thus, the M-polynomial of the given graph is

$$M(G_1;x,y)=\sum_{i\le j}m_{ij}(G_1)x^iy^j=m_{22}(G_1)x^2y^2+m_{23}(G_1)x^2y^3$$
$$=(16mn+8m+8n)x^2y^2+(48mn-12m-12n)x^2y^3$$

Theorem 3.4 Let G_1 be the subdivision graph of the Benzene ring. Then,

(1) $M_1(G_1)=304mn-28m-28n$

(2) $M_2(G_1)=352mn-40m-40n$

(3) ${}^{m}M_2(G_1)=12mn$

(4) $R_\alpha(G_1)=2^{2\alpha}(16mn+8m+8n)+3^\alpha 2^\alpha(48mn-12m-12n)$

(5) $RR_\alpha(G_1)=\frac{1}{2^{2\alpha}}(16mn+8m+8n)+\frac{1}{3^\alpha 2^\alpha}(48mn-12m-12n)$

(6) $SSD(G_1)=136mn-10m-10n$

(7) $H(G_1)=\frac{136}{5}mn-4m-4n$

(8) $I(G_1)=\frac{368}{5}mn-\frac{32}{5}m-\frac{32}{5}n$

(9) $A(G_1)=512mn-32m-32n$

Proof. From Theorem 3.2, we have

$M(G_1;x,y)=(16mn+8m+8n)x^2y^2+(48mn-12m-12n)x^2y^3.$

Then, we have the following:

$D_xf(x,y)=2(16mn+8m+8n)x^2y^2+2(48mn-12m-12n)x^2y^3,$

$$D_y f(x,y) = 2(16mn + 8m + 8n)x^2y^2 + 3(48mn - 12m - 12n)x^2y^3,$$

$$D_y D_x f(x,y) = 4(16mn + 8m + 8n)x^2y^2 + 6(48mn - 12m - 12n)x^2y^3,$$

$$S_x S_y f(x,y) = \frac{1}{4}(16mn + 8m + 8n)x^2y^2 + \frac{1}{6}(48mn - 12m - 12n)x^2y^3,$$

$$D_x^\alpha D_y^\alpha f(x,y) = 4^\alpha(16mn + 8m + 8n)x^2y^2 + 6^\alpha(48mn - 12m - 12n)x^2y^3,$$

$$S_x^\alpha S_y^\alpha f(x,y) = \frac{1}{4^\alpha}(16mn + 8m + 8n)x^2y^2 + \frac{1}{6^\alpha}(48mn - 12m - 12n)x^2y^3,$$

$$S_y D_x f(x,y) = (16mn + 8m + 8n)x^2y^2 + \frac{2}{3}(48mn - 12m - 12n)x^2y^3,$$

$$S_x D_y f(x,y) = (16mn + 8m + 8n)x^2y^2 + \frac{3}{2}(48mn - 12m - 12n)x^2y^3,$$

$$2S_x J f(x,y) = 2[\frac{1}{4}(16mn + 8m + 8n)x^4 + \frac{1}{5}(48mn - 12m - 12n)x^5],$$

$$S_x J D_x D_y f(x,y) = (16mn + 8m + 8n)x^4 + \frac{6}{5}(48mn - 12m - 12n)x^5,$$

$$S_x^3 Q_{-2} J D_x^3 D_y^3 f(x,y) = 8(16mn + 8m + 8n)x^2 + 8(48mn - 12m - 12n)x^3$$

Using Table 1 and the above expressions, we have

(1) The first Zagreb index

$$M_1(G_1) = (D_x + D_y)(f(x,y))|_{x=y=1} = 304mn - 28m - 28n$$

(2) The second Zagreb index

$$M_2(G_1) = D_y D_x(f(x,y))|_{x=y=1} = 352mn - 40m - 40n$$

(3) The modified second Zagreb index

$$^mM_2(G_1) = S_x S_y(f(x,y))|_{x=y=1} = 12mn$$

(4) The generalized Randić index

$$R_\alpha(G_1) = D_x^\alpha D_y^\alpha(f(x,y))|_{x=y=1} = 2^{2\alpha}(16mn + 8m + 8n) + 3^\alpha 2^\alpha(48mn - 12m - 12n)$$

(5) The inverse Randić index

$$RR_\alpha(G_1) = \frac{1}{2^{2\alpha}}(16mn + 8m + 8n) + \frac{1}{3^\alpha 2^\alpha}(48mn - 12m - 12n)$$

(6) The symmetric division index

$$SSD(G_1) = 136mn - 10m - 10n$$

(7) The harmonic index

$$H(G_1) = 2S_x J f(x,y)|_{x=1} = 2[\frac{1}{4}(16mn + 8m + 8n)x^4 + \frac{1}{5}(48mn - 12m - 12n)x^5]_{x=1}$$

$$= \frac{136}{5}mn - 4m - 4n$$

(8) The inverse sum index

$$I(G_1) = S_x J D_x D_y f(x,y)|_{x=1} = [(16mn + 8m + 8n)x^4 + \frac{6}{5}(48mn - 12m - 12n)x^5]_{x=1}$$

$$= \frac{368}{5}mn - \frac{32}{5}m - \frac{32}{5}n$$

(9) The augmented Zagreb index

$$A(G_1) = S_x^3 Q_{-2} J D_x^3 D_y^3 f(x,y)|_{x=1} = [8(16mn + 8m + 8n) + 8(48mn - 12m - 12n)]_{x=1}$$

$= 512mn - 32m - 32n$

3.3. M-polynomial of the para-line graph of the Benzene ring.

Theorem 3.5 Let G_2 be the para-line graph of the Benzene ring. Then the M-polynomial of G_2 is

$$M(G_2[m,n];x,y) = (8mn + 8m + 8n)x^2y^2 + (16mn)x^2y^3 + (64mn - 18m - 18n)x^3y^3.$$

Proof. Let G_2 be the para-line graph of the Benzene ring. 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 a degree:

$V_{\{2\}}(G_2) = \{v \in V(G_2)|_{deg_{G_2}(v)=2}\}$ and $V_{\{3\}}(G_2) = \{v \in V(G)|_{deg_{G_2}(v)=3}\}$.

Further, the edge set of G_2 has three partitions based on the degree of the end vertices:

$E_{\{2,2\}}(G_2) = \{e = uv \in E(G_2)|_{deg_{G_2}(u)=2, deg_{G_2}(v)=2}\}$,

$E_{\{2,3\}}(G_2) = \{e = uv \in E(G_2)|_{deg_{G_2}(u)=2, deg_{G_2}(v)=3}\}$and

$E_{\{3,3\}}(G_2) = \{e = uv \in E(G_2)|_{deg_{G_2}(u)=3, deg_{G_2}(v)=3}\}$, such that

$$m_{22}(G_2) = |E_{\{2,2\}}(G_2)| = 8mn + 8m + 8n \;, m_{23}(G_2) = |E_{\{2,3\}}(G_2)| = 16mn \;\; and$$

$$m_{33}(G_2) = |E_{\{3,3\}}(G_2)| = 64mn - 18m - 18n.$$

Thus, the M-polynomial of the given graph is

$M(G_2;x,y) = \sum_{i\le j} m_{ij}(G_2)x^iy^j = m_{22}(G_2)x^2y^2 + m_{23}(G_2)x^2y^3 + m_{33}(G_2)x^3y^3$

$$= (8mn + 8m + 8n)x^2y^2 + (16mn)x^2y^3 + (64mn - 18m - 18n)x^3y^3$$

Theorem 3.6 Let G_2 be the para-line graph of the Benzene ring. Then,

(1) $M_1(G_2) = 496mn - 76m - 76n$

(2) $M_2(G_2) = 704mn - 130m - 130n$

(3) ${}^mM_2(G_2) = \frac{106}{9}mn$

(4) $R_\alpha(G_2) = 2^{2\alpha}(8mn + 8m + 8n) + 3^\alpha 2^\alpha(16mn) + 3^{2\alpha}(64mn - 18m - 18n)$

(5) $RR_\alpha(G_2) = \frac{1}{2^{2\alpha}}(8mn + 8m + 8n) + \frac{1}{3^\alpha 2^\alpha}(16mn) + \frac{1}{3^{2\alpha}}(64mn - 18m - 18n)$

(6) $SSD(G_2) = \frac{536}{3}mn - 20m - 20n$

(7) $H(G_2) = \frac{476}{15}mn - 2m - 2n$

(8) $I(G_2) = \frac{616}{5}mn - 19m - 19n$

(9) $A(G_2) = 921mn - \frac{4513}{32}m - \frac{4513}{32}n$

Proof. From Theorem 3.3, we have

$M(G_2;x,y) = (8mn + 8m + 8n)x^2y^2 + (16mn)x^2y^3 + (64mn - 18m - 18n)x^3y^3.$

Then, we have the following:

$D_x f(x,y) = 2(8mn + 8m + 8n)x^2y^2 + 2(16mn)x^2y^3 + 3(64mn - 18m - 18n)x^3y^3,$

$D_y f(x,y) = 2(8mn + 8m + 8n)x^2y^2 + 3(16mn)x^2y^3 + 3(64mn - 18m - 18n)x^3y^3,$

$D_y D_x f(x,y) = 4(8mn + 8m + 8n)x^2y^2 + 6(16mn)x^2y^3 + 9(64mn - 18m - 18n)x^3y^3,$

$S_x S_y f(x,y) = \frac{1}{4}(8mn + 8m + 8n)x^2y^2 + \frac{1}{6}(16mn)x^2y^3 + \frac{1}{9}(64mn - 18m - 18n)x^3y^3,$

$D_x^\alpha D_y^\alpha f(x,y) = 4^\alpha(8mn + 8m + 8n)x^2y^2 + 6^\alpha(16mn)x^2y^3 + 9^\alpha(64mn - 18m - 18n)x^3y^3,$

$S_x^\alpha S_y^\alpha f(x,y) = \frac{1}{4^\alpha}(8mn + 8m + 8n)x^2y^2 + \frac{1}{6^\alpha}(16mn)x^2y^3 + \frac{1}{9^\alpha}(64mn - 18m - 18n)x^3y^3,$

$S_y D_x f(x,y) = (8mn + 8m + 8n)x^2y^2 + \frac{2}{3}(16mn)x^2y^3 + (64mn - 18m - 18n)x^3y^3,$

$S_x D_y f(x,y) = (8mn + 8m + 8n)x^2y^2 + \frac{3}{2}(16mn)x^2y^3 + (64mn - 18m - 18n)x^3y^3,$

$2S_x J f(x,y) = 2[\frac{1}{4}(8mn + 8m + 8n)x^4 + \frac{1}{5}(16mn)x^5 + \frac{1}{6}(64mn - 18m - 18n)x^6],$

$S_x J D_x D_y f(x,y) = (8mn + 8m + 8n)x^4 + \frac{6}{5}(16mn)x^5 + \frac{9}{6}(64mn - 18m - 18n)x^6,$

and $S_x^3 Q_{-2} J D_x^3 D_y^3 f(x,y) = 8(8mn + 8m + 8n)x^2 + 8(16mn)x^3 + \frac{3^6}{64}(64mn - 18m - 18n)x^4$

Using Table 1, we have

(1) The first Zagreb index

$$M_1(G_2) = (D_x + D_y)(f(x,y))|_{x=y=1} = 496mn - 76m - 76n$$

(2) The second Zagreb index

$$M_2(G_2) = D_y D_x(f(x,y))|_{x=y=1} = 704mn - 130m - 130n$$

(3) The modified second Zagreb index

$$^m M_2(G_2) = S_x S_y(f(x,y))|_{x=y=1} = \frac{106}{9}mn$$

(4) The generalized Randić index

$$R_\alpha(G_2) = D_x^\alpha D_y^\alpha(f(x,y))|_{x=y=1}$$
$$= 2^{2\alpha}(8mn + 8m + 8n) + 3^\alpha 2^\alpha(16mn) + 3^{2\alpha}(64mn - 18m - 18n)$$

(5) The inverse Randić index

$$RR_\alpha(G_2) = \frac{1}{2^{2\alpha}}(8mn + 8m + 8n) + \frac{1}{3^\alpha 2^\alpha}(16mn) + \frac{1}{3^{2\alpha}}(64mn - 18m - 18n)$$

(6) The symmetric division index

$$SSD(G_2) = \frac{536}{3}mn - 20m - 20n$$

(7) The harmonic index

$$H(G_2) = 2S_x J f(x,y)|_{x=1}$$
$$= 2[\frac{1}{4}(8mn + 8m + 8n)x^4 + \frac{1}{5}(16mn)x^5 + \frac{1}{6}(64mn - 18m - 18n)x^6]_{x=1}$$
$$= \frac{476}{15}mn - 2m - 2n$$

(8) The inverse sum index

$$I(G_2) = S_x J D_x D_y f(x,y)|_{x=1}$$

$$= [(8mn + 8m + 8n)x^4 + \frac{6}{5}(16mn)x^5 + \frac{9}{6}(64mn - 18m - 18n)x^6]_{x=1}$$
$$= \frac{616}{5}mn - 19m - 19n$$

(9) The augmented Zagreb index

$$A(G_2) = S_x^3 Q_{-2} J D_x^3 D_y^3 f(x, y)|_{x=1}$$
$$= [2^3(8mn + 8m + 8n)x^2 + 2^3(16mn)x^3 + \frac{3^6}{4^3}(64mn - 18m - 18n)x^4]_{x=1}$$
$$= 8(8mn + 8m + 8n) + 8(16mn) + \frac{3^6}{4^3}(64mn - 18m - 18n)$$
$$= 921mn - \frac{4513}{32}m - \frac{4513}{32}n$$

4. Conclusions

In this paper, we have obtained the closed form of the M-polynomial of some derived graphs of the Benzene ring embedded in P-type surface network in 2D. Using these, we have computed some of their degree-based topological indices. As seen in literature, the study of these topological indices, in turn, helps understand many of their physicochemical properties.

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Conflicts of Interest

The authors declare no conflict of interest.

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