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M-POLYNOMIALS AND TOPOLOGICAL INDICES OF BENZENE RING EMBEDDED IN P TYPE SURFACE IN 2D NETWORK

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Abstract. M-Polynomials of different molecular structures helps to compute few topological indices namely first Zagreb index, second Zagreb index, second modified Zagreb index, general Randic index, general inverse Randic index, symmetric division degree index. In this article M-polynomial of benzene ring embedded in p type surface in 2D network and find some topological indices. Adopting similar technique for its subdivision graph and semi total point graph.

1. Introduction and Terminologies

Throughout this paper all graphs G will be assumed undirected and without any self loops or parallel edges, having the vertex set $V(G)$ and the edge set $E(G)$. Unless stated otherwise the cardinality of $V(G)$ will be considered n while the cardinality of $E(G)$ will be considered m. The degree of any vertex v in G is denoted by $d_G(v)$ (or shortly d_v). A topological index is a numerical descriptor of a molecule based on a certain topological feature of the corresponding molecular graph. The advantage of topological indices is that they may be used directly as simple numerical descriptors in a comparison with physical, chemical or biological parameters of molecules in quantitative structure activity relationship (QSAR) and structure property relationship (QSPR).

Several polynomials have useful applications in chemistry. The Hosoya polynomial is perhaps the best well known example [6] and it plays a vital role in determining distance based topological indices. Among other algebraic polynomials, M-polynomial [3] was introduced in 2015 and plays the same role in determining closed forms of many degree based topological indices. These indices are actually score functions that capture a variety of physco-chmical properties of chemical compounds such as boiling point, heat of evaporation, heat of formation, chromatographic retention times, surface tension and vapour pressure [14].

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Definition 1.1([3]) *LetG be simple connected graph. The M-polynomial of G is defined as*

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

where m_{ij} is the number of edges $uv \in E(G)$ such that $d_u, d_v = i, j$.

Among the various degree-based topological indices, the first and second Zagreb indices of a graph G are one of the oldest and most studied topological indices that are firstly introduced by Gutman and Trinajstic in [7] which are defined respectively as

$$M_1(G) = \sum_{u \in V(G)} d_u^2 \quad \text{and} \quad M_2(G) = \sum_{u,v \in E(G)} d_u d_v \,.$$

The second modified Zagreb index is defined as

$$m_{M_2(G)} = \sum_{u,v \in E(G)} \frac{1}{d_u d_v}$$

The general Randic index is defined as [9]

$$R_\alpha(G) = \sum_{u,v \in E(G)} (d_u d_v)^\alpha$$

The reciprocal general Randic index is defined as [9]

$$RR_\alpha(G) = \sum_{u,v \in E(G)} \frac{1}{(d_u d_v)^\alpha}$$

The symmetric division degree index is defined as

$$SDD(G) = \sum_{u,v \in E(G)} \{\frac{min(d_u d_v)}{max(d_u d_v)} + \frac{max(d_u d_v)}{min(d_u d_v)}\}$$

The harmonic index is defined as

$$H(G) = \sum_{u,v \in E(G)} \frac{2}{d_u + d_v}$$

The inverse sum index is defined as

$$I(G) = \sum_{u,v \in E(G)} \frac{d_u d_v}{d_u + d_v}$$

These topological indexes can be recovered from M-polynomial, see Table 1 for details.

This paper consists of 2 main sections. In section 1, is introductory in nature. In section 2 consists of main results and discussion.

TABLE 1. Derivation of some degree-based topological indices from M-polynomial

Topological index	Derivation from $M(G;x,y)$
First Zagreb	$(D_x + D_y)(M(G;x,y)) \|_{x=y=1}$
Second Zagreb	$D_x D_y(M(G;x,y)) \|_{x=y=1}$
Second modified Zagreb	$S_x S_y(M(G;x,y)) \|_{x=y=1}$
General Randic	$(D_x^\alpha D_y^\alpha)(M(G;x,y)) \|_{x=y=1}$
Inverse General Randic	$(S_x^\alpha S_y^\alpha)(M(G;x,y)) \|_{x=y=1}$
Symmetric Division Degree	$(D_x S_y + S_x D_y)(M(G;x,y)) \|_{x=y=1}$
Harmonic	$2S_x J(M(G;x,y)) \|_{x=1}$
Inverse sum	$S_x J D_x D_y(M(G;x,y)) \|_{x=1}$

2. Results and Discussion

A network is a simply connected graph having no multiple edges and loops. OKeeffe et al. [11] have distributed around a quarter century a letter managing two 3D systems of benzene one of the structure was called 6.82p (additionally polybenzene) and has a place with the space gather 1m 3m, comparing to the P-type surface. The P-type surface is coordinated to the Cartesian arranges in the Euclidean space. More about this intermittent surface can discover in [4,5].This structure was required to be combined as 3D carbon solids: be that as it may, in our best learning, no such a combination was accounted for as such.

Ali [1] computed some topological indices of benzene ring embedded in P-type-surface in 2D network. There is a relation connecting three graph operators [2] and calculated some topological indices of nanostructures using Q(G)and R(G) [10].

2.1. M-polynomial and Topological Indices on Subdivision Graph of G

Recall that, [12] for a simple graph G, the subdivision graph $S(G)$ is obtained from G by replacing each of its edges with a path of length two or, equivalently, by inserting an additional vertex into each edge of G.

Theorem 2.1. *Let G be a benzene ring embedded in the P-type-surface network. Then the M-polynomial of $S(G)$ is given by*

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

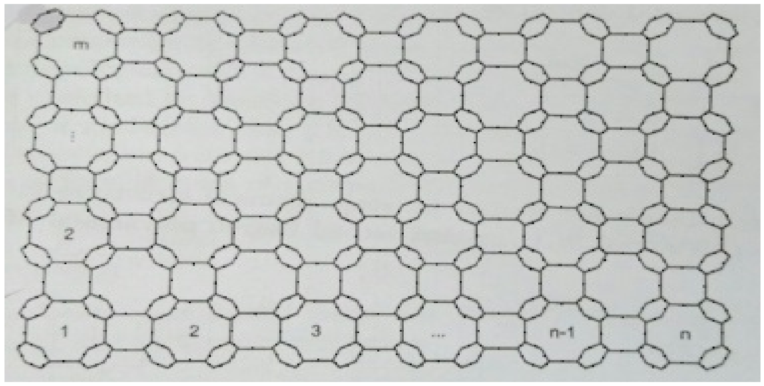

FIGURE 1. The subdivision graph of benzene ring embedded in P-type surface network

Proof. Let G be a benzene ring embedded in the P-type-surface network. Then the number of the edges of types are given bellow:

$$E_1 = \{uv \in E(S(G)) : d_{S(G)}(u) = 2, d_{S(G)}(v) = 2\}.$$
$$E_2 = \{uv \in E(S(G)) : d_{S(G)}(u) = 2, d_{S(G)}(v) = 3\}.$$

One can calculate easily that $|E_1(S(G))| = (8m + 8n + 16^{mn})$, $|E_2(S(G))| = 48mn - 12m - 12n$,

By the definition of M-polynomial,

$$\begin{aligned} M(S(G), x, y) &= \sum_{i \leq j} m_{ij}(S(G))x^i y^j \\ &= m_{22}x^2y^2 + m_{23}x^2y^3 \\ &= (8m + 8n + 16mn)x^2y^2 + (48mn - 12m - 12n)x^2y^3. \end{aligned}$$

□

Proposition 2.2. *Let G be a benzene ring embedded in the P-type-surface network. Then*

(1) $M_1S(G) = 304mn - 28m - 28n$;

(2) $M_2S(G) = 352mn - 40m - 40n$;

(3) $m_{M_2S(G)} = 12mn$;

(4) $R_\alpha S(G) = 4^{\alpha+1}(2m + 2n + 4mn) + 6^{\alpha+1}(8mn - 2m - 2n)$;

(5) $RR_\alpha S(G) = \frac{1}{4^\alpha}(8m + 8n + 16mn) + \frac{1}{6^\alpha}(48mn - 12m - 12n)$;

(6) $SDD(S(G)) = 136mn - 10m - 10n$;

(7) $H(G) = \frac{1}{5}(136mn - 4m - 4n)$;

(8) $I(G) = \frac{1}{5}(368mn - 32m - 32n)$.

Proof. Let $f(x,y) = M(S(G);x,y)$ be the M-polynomial of $S(G)$. Then

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

Now the partial derivatives and integrals are obtained as

$$D_xf(x,y) = 2(8m+8n+16mn)x^2y^2 + 2(48mn-12m-12n)x^2y^3,$$
$$D_yf(x,y) = 2(8m+8n+16mn)x^2y^2 + 3(48mn-12m-12n)x^2y^3,$$
$$S_xf(x,y) = \frac{1}{2}(8m+8n+16mn)x^2y^2 + \frac{1}{2}(48mn-12m-12n)x^2y^3,$$
$$S_yf(x,y) = \frac{1}{2}(8m+8n+16mn)x^2y^2 + \frac{1}{3}(48mn-12m-12n)x^2y^3,$$
$$D_xD_yf(x,y) = 4(8m+8n+16mn)x^2y^2 + 6(48mn-12m-12n)x^2y^3,$$
$$S_xS_yf(x,y) = \frac{1}{4}(8m+8n+16mn)x^2y^2 + \frac{1}{6}(48mn-12m-12n)x^2y^3,$$
$$D_x^\alpha D_y^\alpha f(x,y) = 4^\alpha(8m+8n+16mn)x^2y^2 + 6^\alpha(48mn-12m-12n)x^2y^3,$$
$$S_x^\alpha S_y^\alpha f(x,y) = \frac{1}{4^\alpha}(8m+8n+16mn)x^2y^2 + \frac{1}{6^\alpha}(48mn-12m-12n)x^2y^3,$$
$$D_xS_yf(x,y) = (8m+8n+16mn)x^2y^2 + \frac{2}{3}(48mn-12m-12n)x^2y^3,$$
$$S_xD_yf(x,y) = (8m+8n+16mn)x^2y^2 + \frac{3}{2}(48mn-12m-12n)x^2y^3,$$
$$S_xJf(x,y) = \frac{1}{4}(8m+8n+16mn)x^4 + \frac{1}{5}(48mn-12m-12n)x^5,$$
$$S_xJD_xD_yf(x,y) = (8m+8n+16mn)x^4 + \frac{6}{5}(48mn-12m-12n)x^5.$$

Using above facts in the definitions of topological indices we obtained the corresponding required results. □

2.2 M-Polynomial and Topological Indices on Semi-Total Point Graph $R(G)$

We know that,[12] for a simple graph G, the semi total point graph $R(G)$ is the graph obtained from G by adding a new vertex corresponding to each edge of G and by joining each new vertex to the end vertices of the edge corresponding to it. Figure 2 shows the semi total point graph of benzene ring embedded in the P-type-surface in 2D network.

Let G be a benzene ring embedded in the P-type-surface network. Then the number of the edges of types are given bellow:

$$E_1 = \{uv \in E(R(G)) : d_{R(G)}(u) = 4, d_{R(G)}(v) = 2\},$$
$$E_2 = \{uv \in E(R(G)) : d_{R(G)}(u) = 4, d_{R(G)}(v) = 4\},$$
$$E_3 = \{uv \in E(R(G)) : d_{R(G)}(u) = 4, d_{R(G)}(v) = 6\},$$
$$E_4 = \{uv \in E(R(G)) : d_{R(G)}(u) = 2, d_{R(G)}(v) = 6\},$$
$$E_5 = \{uv \in E(R(G)) : d_{R(G)}(u) = 6, d_{R(G)}(v) = 6\}.$$

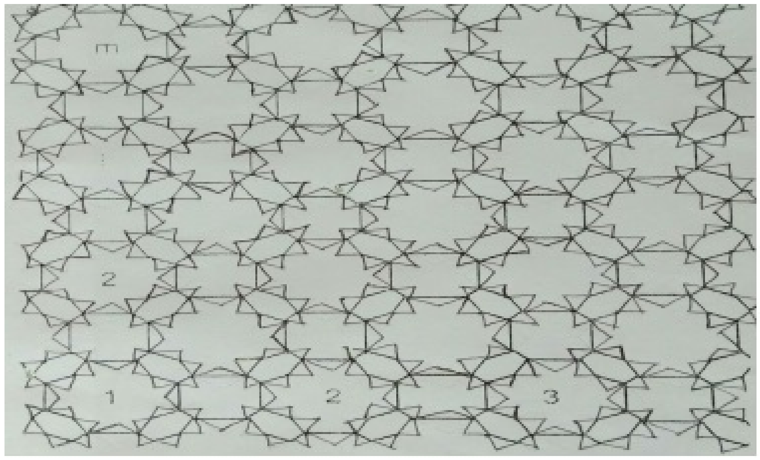

FIGURE 2. The semi total point graph of benzene ring embedded in P-type surface network

One can calculate easily that $|E_1(R(G))| = 8m + 8n + 16mn$, $|E_2(R(G))| = 4m + 4n$, $|E_3(R(G))| = 16mn$, $|E_4(R(G))| = 48mn - 12m - 12n$, $|E_5(R(G))| = 96mn - 6m - 6n$.

Now we calculate the M-polynomial.

Theorem 2.3. *Let G be a benzene ring embedded in the P-type-surface network. Then the M-polynomial of $R(G)$ is given by*

$$\begin{aligned} M(R(G); x, y) &= (8m + 8n + 16mn)x^2y^4 + (4m + 4n)x^4y^4 + 16mnx^4y^6 \\ &\quad +(48mn - 12m - 12n)x^2y^6 + (16mn - 6m - 6n)x^6y^6. \end{aligned}$$

Proof. By the definition of M-polynomial,

$$\begin{aligned} M(R(G), x, y) &= \sum_{i\leq j} m_{ij}(R(G))x^iy^j \\ &= m_{24}x^2y^4 + m_{44}x^4y^4 + m_{46}x^4y^6 + m_{26}x^2y^6 + m_{66}x^6y^6 \\ &= (8m + 8n + 16mn)x^2y^4 + (4m + 4n)x^4y^4 + 16mnx^4y^6 \\ &\quad +(48mn - 12m - 12n)x^2y^6 + (16mn - 6m - 6n)x^6y^6. \end{aligned}$$

□

Proposition 2.4. *Let G be a benzene ring embedded in the P-type-surface network. Then*

(1) $M_1(R(G)) = 832mn - 88m - 88n$;

(2) $M_2(R(G)) = 1644mn - 232m - 232n$;

(3) $m_{M_2}(R(G)) = \frac{64}{9}mn - \frac{m}{12} - \frac{n}{12}$;

(4) $R_\alpha(R(G)) = 8^{\alpha+1}(m + n + 2mn) + 16^\alpha(4m + 4n) + 24^\alpha 16mn$
$+12^{\alpha+1}(4mn - m - n) + 36^\alpha(16mn - 6m - 6n)$;

(5) $RR_\alpha(R(G)) = \frac{1}{8^\alpha}(8m+8n+16mn) + \frac{1}{16^\alpha}(4m+4n) + \frac{1}{24^\alpha}16mn$
$+\frac{1}{12^\alpha}(48mn-12m-12n) + \frac{1}{36^\alpha}(16mn-6m-6n);$

(6) $SDD(R(G)) = \frac{800}{3}mn - 24m - 24n;$

(7) $H(R(G)) = \frac{348}{15}mn - \frac{1}{3}m - \frac{1}{3}n;$

(8) $I(R(G)) = \frac{2696}{155}mn - \frac{52}{3}m - \frac{52}{3}n.$

Proof. Let $f(x,y) = M(S(G);x,y)$ be the M-polynomial of $R(G)$. Then

$$\begin{aligned} f(x,y) &= (8m+8n+16mn)x^2y^4 + (4m+4n)x^4y^4 + 16mnx^4y^6 \\ &\quad +(48mn-12m-12n)x^2y^6 + (16mn-6m-6n)x^6y^6. \end{aligned}$$

Now, the desired result can be obtained from the following.

$$\begin{aligned} D_xf(x,y) &= 2(8m+8n+16mn)x^2y^4 + 4(4m+4n)x^4y^4 + 4x16mnx^4y^6 \\ &\quad + 2(48mn-12m-12n)x^2y^6 + 6(16mn-6m-6n)x^6y^6, \end{aligned}$$

$$\begin{aligned} D_yf(x,y) &= 4(8m+8n+16mn)x^2y^4 + 4(4m+4n)x^4y^4 + 6x16mnx^4y^6 \\ &\quad + 6(48mn-12m-12n)x^2y^6 + 6(16mn-6m-6n)x^6y^6, \end{aligned}$$

$$\begin{aligned} S_xf(x,y) &= \frac{1}{2}(8m+8n+16mn)x^2y^4 + \frac{1}{4}(4m+4n)x^4y^4 + \frac{1}{4}x16mnx^4y^6 \\ &\quad + \frac{1}{2}(48mn-12m-12n)x^2y^6 + \frac{1}{6}(16mn-6m-6n)x^6y^6, \end{aligned}$$

$$\begin{aligned} S_yf(x,y) &= \frac{1}{4}(8m+8n+16mn)x^2y^4 + \frac{1}{4}(4m+4n)x^4y^4 + \frac{1}{6}x16mnx^4y^6 \\ &\quad + \frac{1}{6}(48mn-12m-12n)x^2y^6 + \frac{1}{6}(16mn-6m-6n)x^6y^6, \end{aligned}$$

$$\begin{aligned} D_xD_yf(x,y) &= 8(8m+8n+16mn)x^2y^4 + 16(4m+4n)x^4y^4 + 24x16mnx^4y^6 \\ &\quad + 12(48mn-12m-12n)x^2y^6 + 36(16mn-6m-6n)x^6y^6, \end{aligned}$$

$$\begin{aligned} S_xS_yf(x,y) &= \frac{1}{8}(8m+8n+16mn)x^2y^4 + \frac{1}{16}(4m+4n)x^4y^4 + \frac{1}{24}x16mnx^4y^6 \\ &\quad + \frac{1}{12}(48mn-12m-12n)x^2y^6 + \frac{1}{36}(16mn-6m-6n)x^6y^6, \end{aligned}$$

$$\begin{aligned} D_xD_yf(x,y) &= 8^\alpha(8m+8n+16mn)x^2y^4 + 16^\alpha(4m+4n)x^4y^4 + 24^\alpha16mnx^4y^6 \\ &\quad + 12^\alpha(48mn-12m-12n)x^2y^6 + 36^\alpha(16mn-6m-6n)x^6y^6, \end{aligned}$$

$$S_xS_yf(x,y) = \frac{1}{8^\alpha}(8m+8n+16mn)x^2y^4 + \frac{1}{16^\alpha}(4m+4n)x^4y^4 + \frac{1}{24^\alpha}16mnx^4y^6 + \frac{1}{12^\alpha}(48mn-12m-12n)x^2y^6 + \frac{1}{36^\alpha}(16mn-6m-6n)x^6y^6.$$

$$D_xS_yf(x,y) = \frac{1}{2}(8m+8n+16mn)x^2y^4 + (4m+4n)x^4y^4 + \frac{2}{3}x16mnx^4y^6 + \frac{1}{3}(48mn-12m-12n)x^2y^6 + (16mn-6m-6n)x^6y^6,$$

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

$$S_xJf(x,y) = \frac{1}{6}(8m+8n+16mn)x^6 + \frac{1}{8}(4m+4n)x^8 + \frac{1}{10}16mnx^{10} + \frac{1}{8}(48mn-12m-12n)x^8 + \frac{1}{12}(16mn-6m-6n)x^{12},$$

$$S_xJD_xD_yf(x,y) = \frac{4}{3}(8m+8n+16mn)x^6 + 2(4m+4n)x^8 + \frac{12}{5}16mnx^{10} + \frac{3}{2}(48mn-12m-12n)x^8 + 3(16mn-6m-6n)x^{12}.$$

This completes the proof. □

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