M-Polynomial and topological indices of benzene ring embedded in p-type surface network

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Abstract:

The representation of chemical compounds and chemical networks with the M-polynomials is a new idea and it gives nice and good results of the topological indices. These results are used to correlate the chemical compounds and chemical networks with their chemical properties and bioactivities.

Particular attention is paid to the derivation of the M polynomial- for the benzene ring embedded in the P-type surface network in 2D. Furthermore, the topological indices based on the degrees are also derived by using the general form of M-polynomial of benzene ring embedded in the P-type surface network $BR(m, n)$. In the end, the graphical representation and comparison of the M-polynomial and the topological indices of benzene ring embedded in P-type surface network in 2D are described.

Keywords: M-polynomial; Topological indices; Surface network

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1. Introduction

The chemical compounds can be represented by using the mathematical tools of graph theory. The mathematical models that are based on the polynomials of the chemical compounds and crystal structures can be used in order to predict and forecast their chemical properties and bioactivities. Mathematical chemistry is a rich in tools like functions and polynomials which predict the properties of molecular graphs and crystal structures. The topological descriptors are the numerical parameters of the chemical graph which characterize its topology and are usually graph invariants. They explain the structure of chemical compound mathematically and are utilized in the study of quantitative structure properties and activities relationships (QSPR/QSAR).

A topological index is a numerical value which describes and explains an important information about the chemical structure. A great variety of such indices are studied and used in theoretical chemistry, pharmaceutical researchers, in drugs and in different areas of science. The properties like boiling point, strain energy, viscosity, fracture toughness and heat of formation, etc are connected to the chemical structure under study. This fact plays a major role in the field of chemical graph theory [4,5,8,16,17,19,20,21,24,27,37,38,41,42].

The computation of general polynomial is formed whose derivatives or integrals or composition of both, are evaluated at some particular point. Then, the simplified form yields molecular descriptor. For instance, there are polynomials like forgotten polynomials, Zagreb polynomials, Hosoya polynomials but these polynomials gives rise to one or two topological indices [7,13,23,26]. Hosoya polynomial is a polynomial whose derivatives are evaluated at 1 gives Wiener and hyper Wiener index [15]. The Hosoya polynomial and Zagreb polynomials are considered to be the general form of in the determination of distance based and degree based indices respectively. The M-polynomial is a new and recent polynomial. It will open up new results of chemical graphs and insights in the study of topological descriptors based on degrees. The main importance of this polynomial is that it can give exact forms of more than ten degree based molecular descriptors [9,33]. The rapid development and advancements are being made in this

new polynomial. Recently, Young Chel Kwun computed M-polynomial and topological indices of V-phenylenic nanotube and nanotori [30].

The M-polynomial of a graph G is formulated as [9]:

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

where $m_{ij}(G)$ is the number of edges $uv \in E(G)$ such that $(d_u, d_v) = (i, j)$, $\delta = \min d_v \mid v \in V(G)$ and $\Delta = \max d_v \mid v \in V(G)$.

The path number was the first distance based topological index defined by Wiener [43] in 1947. This index is now called as Wiener index. It has many famous mathematical and chemical applications [12,43]. Later on, Milan Randić proposed and formulated the Randić index of a graph G $R_{-\frac{1}{2}}(G)$.

$$R_{-\frac{1}{2}}(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}.$$

The general Randić index was proposed and defined independently by Bollobás et al. [3] and Amic *et al.* [1]. Due to its useful and important results in the field of mathematical chemistry, it has been widely used by both mathematicians and chemists. For a survey of these results, see the references [6,28,31,36]. The general Randić index and inverse Randić index are formulated as:

$$R_\alpha(G) = \sum_{uv \in E(G)} (d_u d_v)^\alpha, \quad RR_\alpha(G) = \sum_{uv \in E(G)} \frac{1}{(d_u d_v)^\alpha}.$$

The first and second Zagreb index is introduced by Gutman and Trinajstić [23,25,40]. Both first and second Zagreb index and the second modified index are formulated as:

$$M_1(G) = \sum_{uv \in E(G)} (d_u + d_v),$$

$$M_2(G) = \sum_{uv \in E(G)} (d_u d_v),$$

$${}^mM_2(G) = \sum_{uv \in E(G)} \frac{1}{d_u d_v}.$$

Recently, the Symmetric division deg index of a graph G is introduced [22]. It is significant index which is used to determine the total surface area of poly-chloro-bi-phenyls [32] and is defined as:

$$SDD(G) = \sum_{uv \in E(G)} \left(\frac{\min(d_u, d_v)}{\max(d_u, d_v)} + \frac{\max(d_u, d_v)}{\min(d_u, d_v)} \right).$$

The other version of Randic index is harmonic index [44] and is defined as:

$$H(G) = \sum_{uv \in E(G)} \frac{2}{d_u + d_v}.$$

The inverse sum index is formulated as [35]:

$$I(G) = \sum_{uv \in E(G)} \frac{d_u d_v}{d_u + d_v}.$$

The augmented Zagreb index gives best approximation of heat of formation of alkanes [14,18]. It is formulated as [29]:

$$A(G) = \sum_{uv \in E(G)} \left(\frac{d_u d_v}{d_u + d_v - 2} \right)^3$$

Let $M(G; x, y) = f(x, y)$ then the following Table 1.1 relates above described topological indices with M-polynomial [9].

Where

$$Q_\alpha(f(x, y)) = x^\alpha f(x, y), \quad J(f(x, y)) = f(x, x)$$

,

$$S_x = \int_0^x \frac{f(t, y)}{t} dt, \quad S_y = \int_0^y \frac{f(x, t)}{t} dt$$

$$D_x = x \frac{\partial(f(x, y))}{\partial x}, \quad D_y = y \frac{\partial(f(x, y))}{\partial y}$$

Topological Descriptor	Derivation from $f(x, y)$
$R_\alpha(G), \alpha \in R$	$(D_x^\alpha D_y^\alpha)(f(x, y)) _{x=y=1}$
$RR_\alpha(G), \alpha \in R$	$(S_x^\alpha S_y^\alpha)(f(x, y)) _{x=y=1}$
$M_1(G)$	$(D_x + D_y)(f(x, y)) _{x=y=1}$
$M_2(G)$	$(D_x D_y)(f(x, y)) _{x=y=1}$
${}^m M_2(G)$	$(S_x S_y)(f(x, y)) _{x=y=1}$
$H(G)$	$2S_x J(f(x, y)) _{x=1}$
$SDD(G)$	$(D_x S_y + S_x D_y)(f(x, y)) _{x=y=1}$
$I(G)$	$S_x J D_x D_y(f(x, y)) _{x=1}$
$A(G)$	$S_x^3 Q_{-2} J D_x^3 D_y^3(f(x, y)) _{x=1}$

Table 1.1: The relationship of topological indices with M-polynomial.

2. Main Results and Discussion

O'Keeffe et al. have distributed around a quarter century a letter managing two 3D systems of benzene, one of the structure was known as 6.82P (or additionally polybenzene) and has a place with the space gather Im3m, comparing to the P-type surface [34]. Actually, this is inserting of the hexagon fix in the surface of negative ebb and flow P. The P-type surface is coordinated to the cartesian arranges in the Euclidean space. More about this intermittent surface the reader can discover in [10,11]. 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. This goal was to awaken the enthusiasm of researchers to the atomic acknowledgment of such pleasant thoughts in carbon nanoscience, as much as the graphenes were picked up a moment Nobel prize after C_{60} , also the immediate union of fullerenes is currently a reality, see detail in [2,39].

Figure 2.1: Chemical graph of benzene ring embedded in P-type surface network in 2D.

The molecular graph of benzene ring embedded in the P-type surface network is depicted in fig. 2. The cardinality of vertices and edges of the given molecular graph are $24mn$ and $32m - 2m - 2n$ respectively. The vertex set consists of two vertex partitions in the benzene ring embedded in the P-type surface network. The table 2.1. Furthermore, the edge set consists of three edge partitions. The first edge partition contains $4m + 4n$ edges uv , where $\deg(u) = \deg(v) = 2$. The second edge partition contains $16mn$ edges uv , where $\deg(u) = 2$ and $\deg(v) = 3$. The third edge partition contains $16mn - 2m - 2n$ edges uv , where $\deg(u) = \deg(v) = 3$. The table 2.2 shows the edges partition in the benzene ring embedded in the P-type surface network. We compute the M-polynomial of the benzene ring embedded in the P-type surface network. Also, we present the graphically representation of this graph in 2D and 3D by using Maple 13. In the end, we compute and simplify the topological indices by using the M-polynomial of benzene ring embedded in the P-type surface network.

d_v	2	3
<i>Frequency</i>	$8mn + 4m + 4n$	$16mn - 4m - 4n$

Table 2.1: Vertex partition of benzene ring embedded in the P-type surface network based on degrees of each vertex.

(d_u, d_v)	(2, 2)	(2, 3)	(3, 3)
<i>Frequency</i>	$4m + 4n$	$16mn$	$16mn - 6m - 6n$

Table 2.2: Edge partition of benzene ring embedded in the P-type surface network based on degrees of end vertices of each edge.

3. M-Polynomial of Benzene Ring Embedded in P-Type Network

Consider the graph of a benzene ring embedded in the P-type surface network $BR(m, n)$ with $m, n > 1$, then the M-polynomial of this graph is given by,

$$M(BR(m, n); x, y) = (4m + 4n)x^2y^2 + (16mn)x^2y^3 + (16mn - 6m - 6n)x^3y^3$$

Proof. Let the graph of a benzene ring embedded in the P-type surface network with m and n are the number of unit cells in the columns and rows respectively. It consists of two vertex and three edge partitions.

From the fig.1, it is easy to observe that

$$|V(BR(m, n))| = 24mn$$

$$|E(BR(m, n))| = 32mn - 2m - 2n$$

From table 2.1, it can be seen that there are two partitions of the vertex set of benzene ring embedded in the P-type surface network.

$$V_1(BR(m, n)) = \{u \in V(BR(m, n)) \mid d_u = 2\},$$

$$V_2(BR(m, n)) = \{u \in V(BR(m, n)) \mid d_u = 3\}$$

such that

$$|V_1(BR(m, n))| = 8mn + 4m + 4n, |V_2(BR(m, n))| = 16mn - 4m - 4n$$

From table 2.2, it can be seen that there are three partitions of the edge set of benzene ring embedded in the P-type surface network.

$$E_1(BR(m, n)) = \{uv \in E(G) \mid d_u = 2, d_v = 2\},$$

$$E_2(BR(m, n)) = \{uv \in E(G) \mid d_u = 2, d_v = 3\},$$

$$E_3(BR(m, n)) = \{uv \in E(G) \mid d_u = 3, d_v = 3\},$$

such that

$$|E_1(BR(m, n))| = 4m + 4n, \quad |E_2(BR(m, n))| = 16mn$$

$$|E_3(BR(m, n))| = 16mn - 6m - 6n$$

Now, applying the definition of M-polynomial to the graph of benzene ring P-type network, we have

$$\begin{aligned} M(BR(m, n); x, y) &= \sum_{i \leq j} m_{ij} x^i y^j \\ &= \sum_{i \leq j} m_{ij} x^i y^j = \sum_{2 \leq 2} m_{22} x^2 y^2 + \sum_{2 \leq 3} m_{23} x^2 y^3 + \sum_{3 \leq 3} m_{33} x^3 y^3 \\ &= \sum_{uv \in E_1(G)} m_{22} x^2 y^2 + \sum_{uv \in E_2(G)} m_{23} x^2 y^3 + \sum_{uv \in E_3(G)} m_{33} x^3 y^3 \\ &= |E_1(G)| x^2 y^2 + |E_2(G)| x^2 y^3 + |E_3(G)| x^3 y^3 \end{aligned}$$

$$M(BR(m, n); x, y) = (4m+4n)x^2y^2 + (16mn)x^2y^3 + (16mn-6m-6n)x^3y^3.$$

Figure 3.1: The 3D plot of M-polynomial of benzene ring P-type surface network.

Figure 3.2: (a) The 2D plot of M-polynomial of benzene ring P-type surface network by fixing the parameter x . (b) The 2D plot of M-polynomial of benzene ring P-type surface network by fixing the parameter y .

The 3D graphical representation of M-polynomial of benzene ring embedded in the P-type surface network $BR(m, n)$ is depicted in fig. 3.1. This is plotted by using Maple 13. The graph shows different behavior by fixing the values of m and n and changing the parameters x and y . The 2D

graphical representation of M-polynomial of $BR(m, n)$ can be formed by considering the parameter x to be the positive value, then the graph increases by increasing the values of x and the graph lies in the first and third quadrant. The same behavior occurs for positive values of y , as depicted in fig. 3.2(a) and 3.2(b). If the parameter x is taken to be negative value, then the graph increases by increasing the values of x and the graph lies in the second and fourth quadrant. The same behavior occurs for negative values of y .

4. Topological Indices Derived From M-Polynomial of $BR(m, n)$

The following proposition computes the degree based topological indices that are derived from the M-polynomial of the molecular graph of benzene ring P-type surface network.

Consider the graph G be a benzene ring embedded in the P-type surface network with $m, n > 1$, then we have the following degree based topological indices,

1. $M_1(G) = 176mn - 20m - 20n$
2. $M_2(G) = 240mn - 38m - 38n$
3. ${}^mM_2(G) = \frac{40mn+3m+3n}{9}$
4. $SDD(G) = \frac{200mn-12m-12n}{3}$
5. $H(G) = \frac{176mn}{15}$
6. $I(G) = \frac{24mn-25m-25n}{5}$
7. $A(G) = \frac{9928mn-1163m-1163n}{32}$
8. $RR_\alpha(G) = (16mn) \left(\frac{2^\alpha+3^\alpha}{2^\alpha 3^{2\alpha}} \right) + (m+n) \left(\frac{4(3^{2\alpha})-6(2^{2\alpha})}{6^{2\alpha}} \right)$
9. $R_\alpha(G) = (16mn) (3^{2\alpha} + 6^\alpha) + (m+n) (4(2^{2\alpha}) - 6(3^{2\alpha}))$

Proof. Consider the molecular graph of G be a benzene ring embedded in the P-type surface network with $m, n > 1$, its M-polynomial is simplified in the first theorem. Now, consider the

$$M(G; x, y) = f(x, y)$$

$$f(x, y) = (4m + 4n)x^2y^2 + (16mn)x^2y^3 + (16mn - 6m - 6n)x^3y^3$$

In order to prove the above nine results, we use the following formulas.

$$Q_\alpha(f(x, y)) = x^\alpha f(x, y), \quad J(f(x, y)) = f(x, x),$$

$$S_x = \int_0^x \frac{f(t, y)}{t} dt, \quad S_y = \int_0^y \frac{f(x, t)}{t} dt$$

$$D_x = x \frac{\partial(f(x, y))}{\partial x}, \quad D_y = y \frac{\partial(f(x, y))}{\partial y}$$

Now, we have the following computations

$$(4.1) \quad D_x(f(x, y)) = 2(4m + 4n)x^2y^2 + 2(16mn)x^2y^3 + 3(16mn - 6m - 6n)x^3y^3$$

$$(4.2) \quad D_y(f(x, y)) = 2(4m + 4n)x^2y^2 + 3(16mn)x^2y^3 + 3(16mn - 6m - 6n)x^3y^3$$

$$(4.3) \quad D_x D_y(f(x, y)) = 4(4m + 4n)x^2y^2 + 6(16mn)x^2y^3 + 9(16mn - 6m - 6n)x^3y^3$$

$$(4.4) \quad S_x(f(x, y)) = \frac{(4m + 4n)}{2}x^2y^2 + \frac{(16mn)}{2}x^2y^3 + \frac{(16mn - 6m - 6n)}{3}x^3y^3$$

$$(4.5) \quad S_x S_y(f(x, y)) = \frac{(4m + 4n)}{4}x^2y^2 + \frac{(16mn)}{6}x^2y^3 + \frac{(16mn - 6m - 6n)}{9}x^3y^3$$

$$(4.6) \quad S_x D_y(f(x, y)) = (4m + 4n)x^2y^2 + \frac{3(16mn)}{2}x^2y^3 + (16mn - 6m - 6n)x^3y^3$$

$$(4.7) \quad D_x S_y(f(x, y)) = (4m + 4n)x^2y^2 + \frac{2(16mn)}{3}x^2y^3 + (16mn - 6m - 6n)x^3y^3$$

$$D_x^\alpha D_y^\alpha(f(x, y)) = 2^{2\alpha}(4m+4n)x^2y^2 + 6^\alpha(16mn)x^2y^3 + 3^{2\alpha}(16mn-6m-6n)x^3y^3 \quad (4.8)$$

$$S_x^\alpha S_y^\alpha(f(x, y)) = \frac{(4m+4n)}{2^{2\alpha}}x^2y^2 + \frac{(16mn)}{6^\alpha}x^2y^3 + \frac{(16mn-6m-6n)}{3^{2\alpha}}x^3y^3 \quad (4.9)$$

$$(4.10) \quad S_x J(f(x, y)) = \frac{(4m+4n)}{4}x^4 + \frac{(16mn)}{5}x^5 + \frac{(16mn-6m-6n)}{6}x^6$$

$$(4.11) \quad S_x J D_x D_y(f(x, y)) = (4m+4n)x^4 + \frac{6(16mn)}{5}x^5 + \frac{3(16mn-6m-6n)}{2}x^6$$

$$S_x^3 Q_{-2} J D_x^3 D_y^3(f(x, y)) = 8(4m+4n)x^2 + 8(16mn)x^3 + \frac{729(16mn-6m-6n)}{64}x^4 \quad (4.12)$$

Now by using the above all values from equation 4.1 to 4.12 in table 1.1 to get the topological indices defined in the table 1.1 are obtained.

1. $M_1(G) = 176mn - 20m - 20n$
2. $M_2(G) = 240mn - 38m - 38n$
3. ${}^m M_2(G) = \frac{40mn+3m+3n}{9}$
4. $SDD(G) = \frac{200mn-12m-12n}{3}$
5. $H(G) = \frac{176mn}{15}$
6. $I(G) = \frac{24mn-25m-25n}{5}$
7. $A(G) = \frac{9928mn-1163m-1163n}{32}$
8. $RR_\alpha(G) = (16mn)\left(\frac{2^\alpha+3^\alpha}{2^\alpha 3^{2\alpha}}\right) + (m+n)\left(\frac{4(3^{2\alpha})-6(2^{2\alpha})}{6^{2\alpha}}\right)$
9. $R_\alpha(G) = (16mn)(3^{2\alpha} + 6^\alpha) + (m+n)(4(2^{2\alpha}) - 6(3^{2\alpha}))$

□

Figure 4.1: (a) Plot of symmetric division, harmonic, inverse sum and augmented Zagreb index for fix n parameter. (b) Plot of first Zagreb, second Zagreb and modified Zagreb index for fix m parameter.

Figure 4.2: The 3D plot of Randić index for $BR(m, n)$.

The symmetric division, harmonic, inverse sum and augmented Zagreb indices are plotted by using Maple 13. The graphical representation depicts different behavior of indices by changing the parameters m and n . The blue, green, red and black shows the symmetric division, harmonic, inverse sum and augmented Zagreb indices respectively, as depicted in fig. 4.1(a). The fig. 4.1(b) illustrates the first Zagreb index in blue color, second Zagreb index in green color and modified Zagreb index in red color.

The 3d plot of Randić index and inverse Randić index are illustrated in the fig. 4.2 and fig. 4.3 respectively. It is clearly seen from the graphs that by increasing the values of the parameters m and n , the graph of 4.2 increases faster as compared to the graph 4.3. It can be concluded that the Randić index increases faster than the inverse Randić index.

Figure 4.3: The 3D plot of inverse Randić index for $BR(m, n)$.

The 2D plot of inverse Randić index is depicted in fig. 4.4(a). This is achieved by using Maple 13 and fixing the value of the parameter m or n . In both cases, if values of parameter increases then graph increases gradually and shows different behavior. The 2D plot of Randić index is depicted in fig. 4.4(b). By increasing the values of the parameters, the graph increases and depicts different behavior.

Figure 4.4: (a) The 2D plot of Randić for $BR(m, n)$. (b) The 2D plot of inverse Randić index for $BR(m, n)$.

The fig. 4.5 illustrates the 3D plot of augmented Zagreb index for the molecular graph $BR(m, n)$. By increasing the values of the given parameters, the value of indices increases. The value indices of $BR(m, n)$ increases by changing the values of parameters m and n . The indices derived here are the functions that depends on the values of parameters, where m and n are the independent parameters and the index is dependent parameter.

Figure 4.5: The 3D plot of augmented Zagreb index for $BR(m, n)$.

Conclusion

We have computed the general form of M-polynomial for the molecular graph of benzene ring embedded in the P-type surface network $BR(m, n)$ for the first time. The graphical representation of M-polynomial of $BR(m, n)$ and some of its indices have plotted for different values of the given parameters. Furthermore, we have derived and simplified the exact results for degree based topological indices of $BR(m, n)$ from the M-polynomial of $BR(m, n)$.

In future, we will sketch and design some new chemical graphs/networks and compute their M-polynomial and examine their underlying topological properties.

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