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Research Article

M-Polynomial and Topological Indices of Benzene Ring Embedded in P-Type Surface Network

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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. In this article, particular attention will be put on the derivation of 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 the 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 the benzene ring embedded in the P-type surface network in 2D are described.

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 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 compounds mathematically and are utilized in the study of quantitative structure property and activity 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 research, drugs, and different areas of science. The properties like boiling point, strain energy, viscosity, fracture toughness, and heat of formation are connected to the chemical structure under study. This fact plays a major role in the field of chemical graph theory [1–22].

The computation of the general polynomial is formed whose derivatives or integrals or composition of both are evaluated at some particular point. Then, the simplified form yields the molecular descriptor. For instance, there are polynomials like forgotten polynomials, Zagreb polynomials, and Hosoya polynomials, but these polynomials give rise to one or two topological indices [23–26]. The Hosoya polynomial is a polynomial whose derivatives evaluated at 1 give Wiener and hyper Wiener index [27]. The Hosoya polynomial and Zagreb polynomials are considered to be of the general form 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 [28, 29]. Rapid development and advancements are being made in this new polynomial. Recently, Kwun et al. computed M-polynomial and topological indices of V-phenylenic nanotube and nanotori [30].

The M-polynomial of a graph G is formulated as [28]

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

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 [31] in 1947. This index is now called as the Wiener index. It has many famous mathematical and chemical applications [31, 32]. Later on, Milan Randić proposed and formulated the Randić index of a graph $GR_{-(1/2)}(G)$.

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

The general Randić index was proposed and defined independently by Bollobás et al. [33] and Amić et al. [34]. 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 references [35–38]. The general Randić index and inverse Randić index are formulated as

$$\begin{aligned} R_\alpha(G)&=\sum_{uv\in E(G)}(d_u d_v)^\alpha,\\ RR_\alpha(G)&=\sum_{uv\in E(G)}\frac{1}{(d_u d_v)^\alpha}. \end{aligned} \tag{3}$$

The first and second Zagreb indices are introduced by Gutman and Trinajstić [25, 39, 40]. Both first and second Zagreb indices and the second modified index are formulated as

$$\begin{aligned} M_1(G)&=\sum_{uv\in E(G)}(d_u+d_v),\\ M_2(G)&=\sum_{uv\in E(G)}(d_u d_v),\\ {}^{m}M_2(G)&=\sum_{uv\in E(G)}\frac{1}{d_u d_v}. \end{aligned} \tag{4}$$

Recently, the symmetric division deg index of a graph G is introduced [41]. It is the significant index which is used to determine the total surface area of polychlorobiphenyls [42] and is defined as

$$SDD(G)=\sum_{uv\in E(G)}\left(\frac{\min(d_u,d_v)}{\max(d_u,d_v)}+\frac{\max(d_u,d_v)}{\min(d_u,d_v)}\right). \tag{5}$$

The other version of the Randic index is the harmonic index [43] and is defined as

$$H(G)=\sum_{uv\in E(G)}\frac{2}{d_u+d_v}. \tag{6}$$

The inverse sum index is formulated as [44]

$$I(G)=\sum_{uv\in E(G)}\frac{d_u d_v}{d_u+d_v}. \tag{7}$$

The augmented Zagreb index gives best approximation of heat of formation of alkanes [45, 46]. It is formulated as [47]

$$A(G)=\sum_{uv\in E(G)}\left(\frac{d_u d_v}{d_u+d_v-2}\right)^3. \tag{8}$$

Let $M(G;x,y)=f(x,y)$, and then Table 1 relates above described topological indices with M-polynomial [28], where

$$\begin{aligned} Q_\alpha(f(x,y))&=x^\alpha f(x,y),\\ J(f(x,y))&=f(x,x),\\ S_x&=\int_0^x\frac{f(t,y)}{t}dt,\\ S_y&=\int_0^y\frac{f(x,t)}{t}dt,\\ D_x&=x\frac{\partial(f(x,y))}{\partial x},\\ D_y&=y\frac{\partial(f(x,y))}{\partial y}. \end{aligned} \tag{9}$$

2. Main Results and Discussion

O'Keeffe et al. have distributed around a quarter century a letter managing two 3D systems of benzene, and one of the structures was known as 6.82P (or additionally polybenzene) and has a place with the space gather Im3m, compared with the P-type surface [48]. Actually, this is insertion 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. The reader can discover more about this intermittent surface in [49, 50]. This structure was required to be combined as 3D carbon solids and no such combination was accounted before. This has aroused a lot of research enthusiasm of researchers to carbon nanoscience. As much as the graphenes were picked up a moment Nobel prize after C_{60}, fullerenes have also been studied in depth, see detail in [51, 52].

The molecular graph of the benzene ring embedded in the P-type surface network is depicted in Figure 1. The cardinality of vertices and edges of the given molecular graph are $24mn$ and $32mn-2m-2n$, respectively. The vertex set consists of two vertex partitions in the benzene ring embedded in the P-type surface network, as shown in Table 2. 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

Table 1: The relationship of topological indices with M-polynomial.

Topological descriptor	Derivation from $f(x,y)$
$R_\alpha(G)$, $\alpha \in \mathbb{R}$	$(D_x^\alpha D_y^\alpha)(f(x,y))\vert_{x=y=1}$
$RR_\alpha(G)$, $\alpha \in \mathbb{R}$	$(S_x^\alpha S_y^\alpha)(f(x,y))\vert_{x=y=1}$
$M_1(G)$	$(D_x + D_y)(f(x,y))\vert_{x=y=1}$
$M_2(G)$	$(D_x D_y)(f(x,y))\vert_{x=y=1}$
${}^mM_2(G)$	$(S_x S_y)(f(x,y))\vert_{x=y=1}$
$H(G)$	$2S_x J(f(x,y))\vert_{x=1}$
$SDD(G)$	$(D_x S_y + S_x D_y)(f(x,y))\vert_{x=y=1}$
$I(G)$	$S_x J D_x D_y (f(x,y))\vert_{x=1}$
$A(G)$	$S_x^3 Q_{-2} J D_x^3 D_y^3 (f(x,y))\vert_{x=1}$

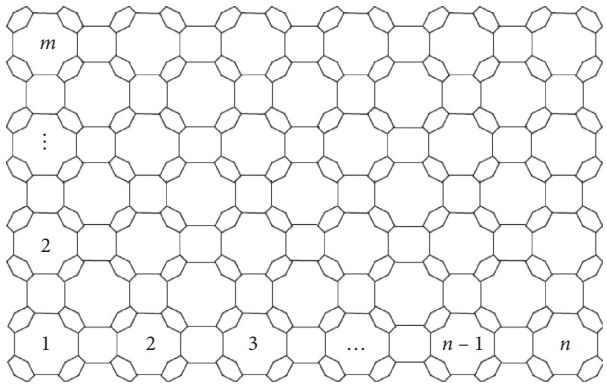

Figure 1: Chemical graph of the benzene ring embedded in a P-type surface network in 2D.

Table 2: Vertex partition of the benzene ring embedded in the P-type surface network based on degrees of each vertex.

d_v	2	3
Frequency	$8mn + 4m + 4n$	$16mn - 4m - 4n$

contains $16mn$ edges uv, where $\deg(u) = 2$ and $\deg(v) = 3$. The third edge partition contains $16mn - 2m - 2n$ edges uv, where $\deg(u) = \deg(v) = 3$. Table 3 shows the edge 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 graphical 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 the benzene ring embedded in the P-type surface network.

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

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

$$M(\mathrm{BR}(m,n);x,y) = (4m+4n)x^2y^2 + (16mn)x^2y^3 + (16mn-6m-6n)x^3y^3. \tag{10}$$

Table 3: Edge partition of the benzene ring embedded in the P-type surface network based on degrees of end vertices of each edge.

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

Proof. Let the graph of a benzene ring embedded in the P-type surface network with m and n being the number of unit cells in the columns and rows, respectively. It consists of two vertices and three edge partitions. From Figure 1, it is easy to observe that

$$\begin{aligned} |V(\mathrm{BR}(m,n))| &= 24mn, \\ |E(\mathrm{BR}(m,n))| &= 32mn - 2m - 2n. \end{aligned} \tag{11}$$

From Table 2, it can be seen that there are two partitions of the vertex set of the benzene ring embedded in the P-type surface network.

$$\begin{aligned} V_1(\mathrm{BR}(m,n)) &= \{u \in V(\mathrm{BR}(m,n)) \mid d_u = 2\}, \\ V_2(\mathrm{BR}(m,n)) &= \{u \in V(\mathrm{BR}(m,n)) \mid d_u = 3\}, \end{aligned} \tag{12}$$

such that

$$\begin{aligned} \left|V_1(\mathrm{BR}(m,n))\right| &= 8mn + 4m + 4n, \\ \left|V_2(\mathrm{BR}(m,n))\right| &= 16mn - 4m - 4n. \end{aligned} \tag{13}$$

From Table 3, it can be seen that there are three partitions of the edge set of the benzene ring embedded in the P-type surface network.

$$\begin{aligned} E_1(\mathrm{BR}(m,n)) &= \{uv \in E(G) \mid d_u = 2, d_v = 2\}, \\ E_2(\mathrm{BR}(m,n)) &= \{uv \in E(G) \mid d_u = 2, d_v = 3\}, \\ E_3(\mathrm{BR}(m,n)) &= \{uv \in E(G) \mid d_u = 3, d_v = 3\}, \end{aligned} \tag{14}$$

such that

$$\begin{aligned} \left|E_1(\mathrm{BR}(m,n))\right| &= 4m + 4n, \\ \left|E_2(\mathrm{BR}(m,n))\right| &= 16mn, \\ \left|E_3(\mathrm{BR}(m,n))\right| &= 16mn - 6m - 6n. \end{aligned} \tag{15}$$

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

$$\begin{aligned} M(\mathrm{BR}(m,n);x,y) &= \sum_{i\le j} m_{ij} x^i y^j \\ &= \sum_{i\le j} m_{ij} x^i y^j \\ &= \sum_{uv\in E_1(G)} m_{22} x^2 y^2 + \sum_{uv\in E_2(G)} m_{23} x^2 y^3 \\ &\quad + \sum_{uv\in E_3(G)} m_{33} x^3 y^3 \\ &= \left|E_1(G)\right| x^2 y^2 + \left|E_2(G)\right| x^2 y^3 \\ &\quad + \left|E_3(G)\right| x^3 y^3, \\ M(\mathrm{BR}(m,n);x,y) &= (4m+4n)x^2y^2 + (16mn)x^2y^3 \\ &\quad + (16mn-6m-6n)x^3y^3. \end{aligned} \tag{16}$$

The 3D graphical representation of M-polynomial of the benzene ring embedded in the P-type surface network $BR(m,n)$ is depicted in Figure 2. 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. If 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 Figures 3(a) and 3(b). If the parameter x is taken to be the 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 the benzene ring embedded in the P-type surface network.

Proposition 1. *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) ${}^{m}M_2(G) = (40mn + 3m + 3n)/9$

(4) $SDD(G) = (200mn - 12m - 12n)/3$

(5) $H(G) = 176mn/15$

(6) $I(G) = (24mn - 25m - 25n)/5$

(7) $A(G) = (9928mn - 1163m - 1163n)/32$

(8) $RR_\alpha(G) = (16mn)((2^\alpha + 3^\alpha)/2^\alpha 3^{2\alpha}) + (m+n)((4(3^{2\alpha}) - 6(2^{2\alpha}))/6^{2\alpha})$

(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 following:

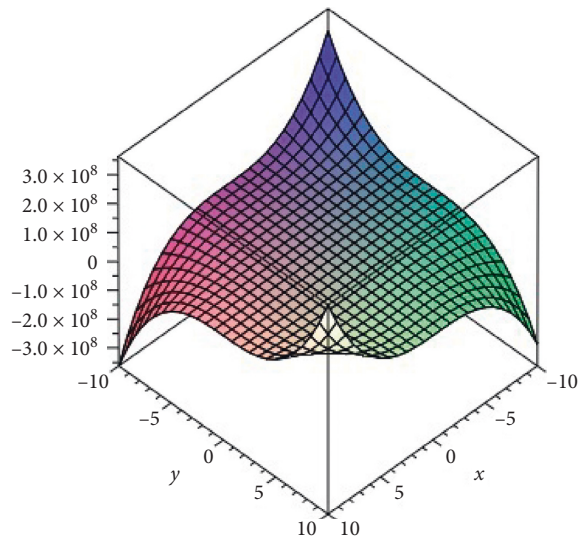

Figure 2: The 3D plot of M-polynomial of the benzene ring embedded in the P-type surface network.

$$M(G;x,y) = f(x,y),$$
$$f(x,y) = (4m+4n)x^2y^2 + (16mn)x^2y^3 + (16mn - 6m - 6n)x^3y^3. \quad (17)$$

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

$$Q_\alpha(f(x,y)) = x^\alpha f(x,y),$$
$$J(f(x,y)) = f(x,x),$$
$$S_x = \int_0^x \frac{f(t,y)}{t}\,dt,$$
$$S_y = \int_0^y \frac{f(x,t)}{t}\,dt, \quad (18)$$
$$D_x = x\frac{\partial(f(x,y))}{\partial x},$$
$$D_y = y\frac{\partial(f(x,y))}{\partial y}.$$

Now, we have the following computations:

$$D_x(f(x,y)) = 2(4m+4n)x^2y^2 + 2(16mn)x^2y^3 + 3(16mn - 6m - 6n)x^3y^3, \quad (19)$$

$$D_y(f(x,y)) = 2(4m+4n)x^2y^2 + 3(16mn)x^2y^3 + 3(16mn - 6m - 6n)x^3y^3, \quad (20)$$

$$D_xD_y(f(x,y)) = 4(4m+4n)x^2y^2 + 6(16mn)x^2y^3 + 9(16mn - 6m - 6n)x^3y^3, \quad (21)$$

$$S_x(f(x,y)) = \frac{(4m+4n)}{2}x^2y^2 + \frac{(16mn)}{2}x^2y^3 + \frac{(16mn - 6m - 6n)}{3}x^3y^3, \quad (22)$$

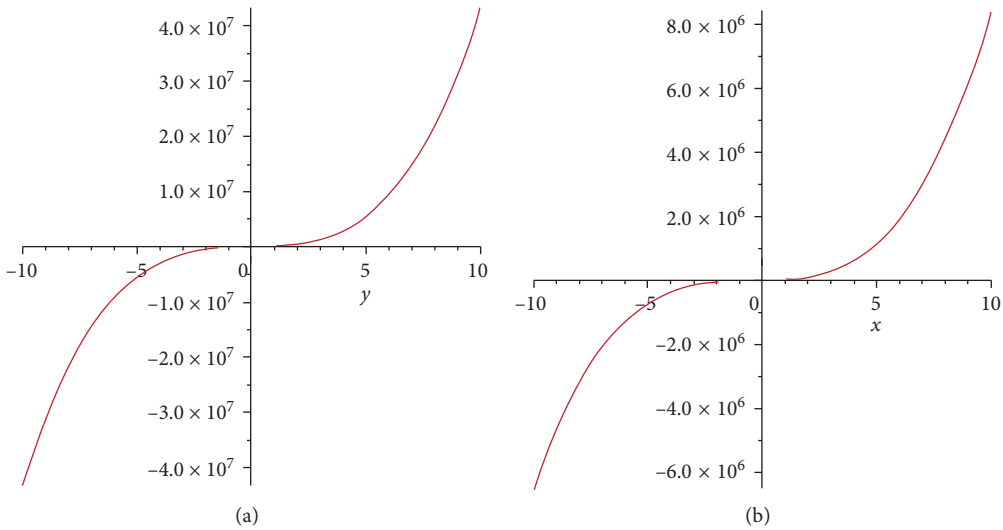

FIGURE 3: (a) The 2D plot of M-polynomial of the benzene ring embedded in the P-type surface network by fixing the parameter x. (b) The 2D plot of M-polynomial of the benzene ring embedded in the P-type surface network by fixing the parameter y.

$$S_xS_y(f(x,y)) = \frac{(4m+4n)}{4}x^2y^2 + \frac{(16mn)}{6}x^2y^3 + \frac{(16mn-6m-6n)}{9}x^3y^3, \tag{23}$$

$$S_xD_y(f(x,y)) = (4m+4n)x^2y^2 + \frac{3(16mn)}{2}x^2y^3 + (16mn-6m-6n)x^3y^3, \tag{24}$$

$$D_xS_y(f(x,y)) = (4m+4n)x^2y^2 + \frac{2(16mn)}{3}x^2y^3 + (16mn-6m-6n)x^3y^3, \tag{25}$$

$$D_x^{\alpha}D_y^{\alpha}(f(x,y)) = 2^{2\alpha}(4m+4n)x^2y^2 + 6^{\alpha}(16mn)x^2y^3 + 3^{2\alpha}(16mn-6m-6n)x^3y^3, \tag{26}$$

$$S_x^{\alpha}S_y^{\alpha}(f(x,y)) = \frac{(4m+4n)}{2^{2\alpha}}x^2y^2 + \frac{(16mn)}{6^{\alpha}}x^2y^3 + \frac{(16mn-6m-6n)}{3^{2\alpha}}x^3y^3, \tag{27}$$

$$S_xJ(f(x,y)) = \frac{(4m+4n)}{4}x^4 + \frac{(16mn)}{5}x^5 + \frac{(16mn-6m-6n)}{6}x^6, \tag{28}$$

$$S_xJD_xD_y(f(x,y)) = (4m+4n)x^4 + \frac{6(16mn)}{5}x^5 + \frac{3(16mn-6m-6n)}{2}x^6, \tag{29}$$

$$S_x^3Q_{-2}JD_x^3D_y^3(f(x,y)) = 8(4m+4n)x^2 + 8(16mn)x^3 + \frac{729(16mn-6m-6n)}{64}x^4. \tag{30}$$

Now, by using all the aforementioned values from equations (19)–(30) in Table 1, the topological indices defined in Table 1 are obtained.

(1) $M_1(G) = 176mn - 20m - 20n$

(2) $M_2(G) = 240mn - 38m - 38n$

(3) ${}^mM_2(G) = (40mn + 3m + 3n)/9$

(4) $SDD(G) = (200mn - 12m - 12n)/3$

(5) $H(G) = 176mn/15$

(6) $I(G) = (24mn - 25m - 25n)/5$

(7) $A(G) = (9928mn - 1163m - 1163n)/32$

(8) $RR_{\alpha}(G) = (16mn)((2^{\alpha} + 3^{\alpha})/2^{\alpha}3^{2\alpha}) + (m+n)((4(3^{2\alpha}) - 6(2^{2\alpha}))/6^{2\alpha})$

(9) $R_{\alpha}(G) = (16mn)(3^{2\alpha} + 6^{\alpha}) + (m+n)(4(2^{2\alpha}) - 6(3^{2\alpha}))$

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 colors show the symmetric division, harmonic, inverse sum, and augmented Zagreb indices, respectively, as depicted in Figure 4(a). Figure 4(b) illustrates

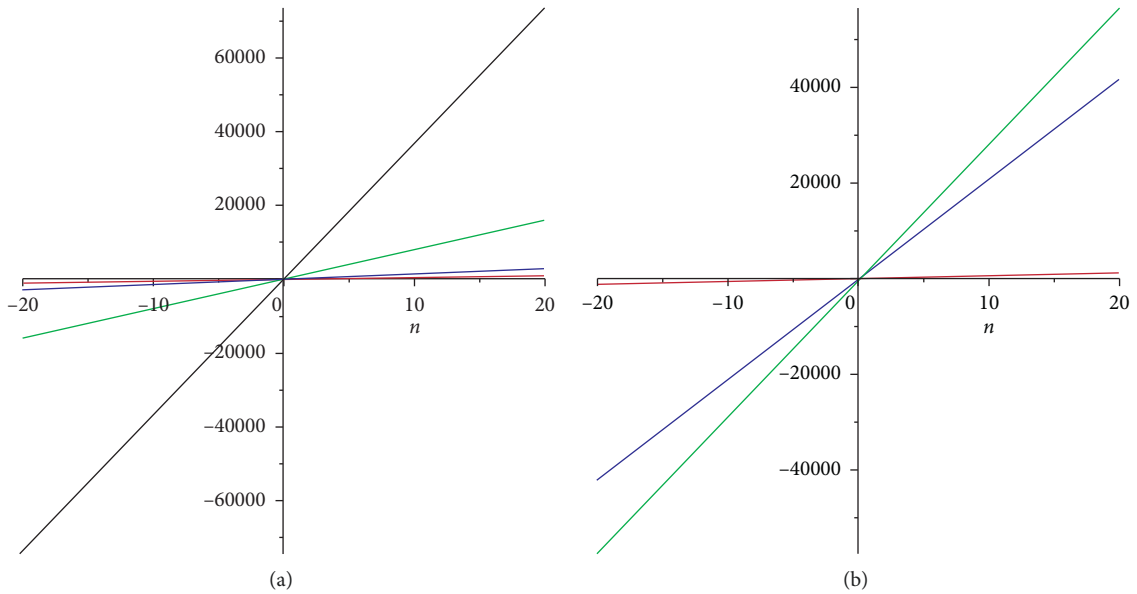

Figure 4: (a) Plot of symmetric division, harmonic, inverse sum, and augmented Zagreb index for fix n parameter. (b) Plot of first Zagreb, second Zagreb, and modified Zagreb index for fix m parameter.

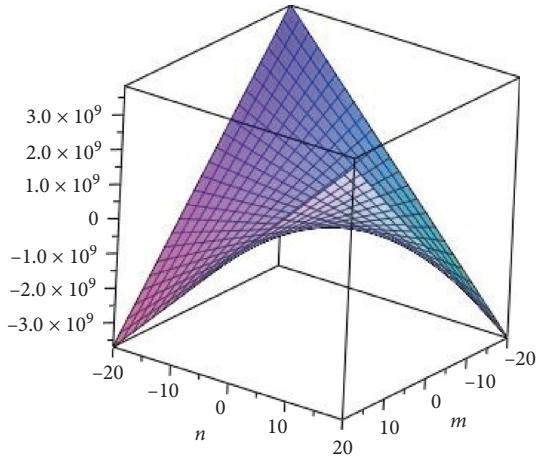

Figure 5: The 3D plot of Randić index for BR(m,n).

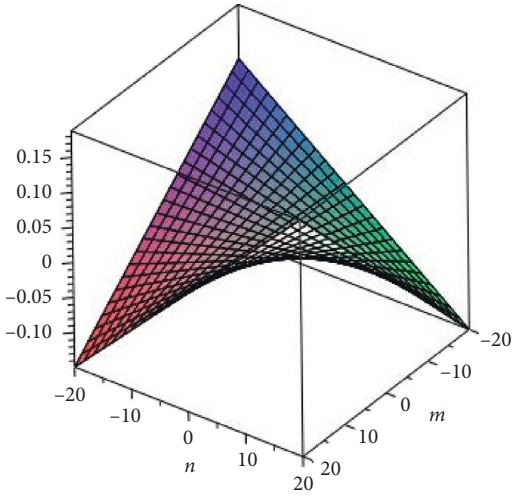

Figure 6: The 3D plot of the inverse Randić index for BR(m,n).

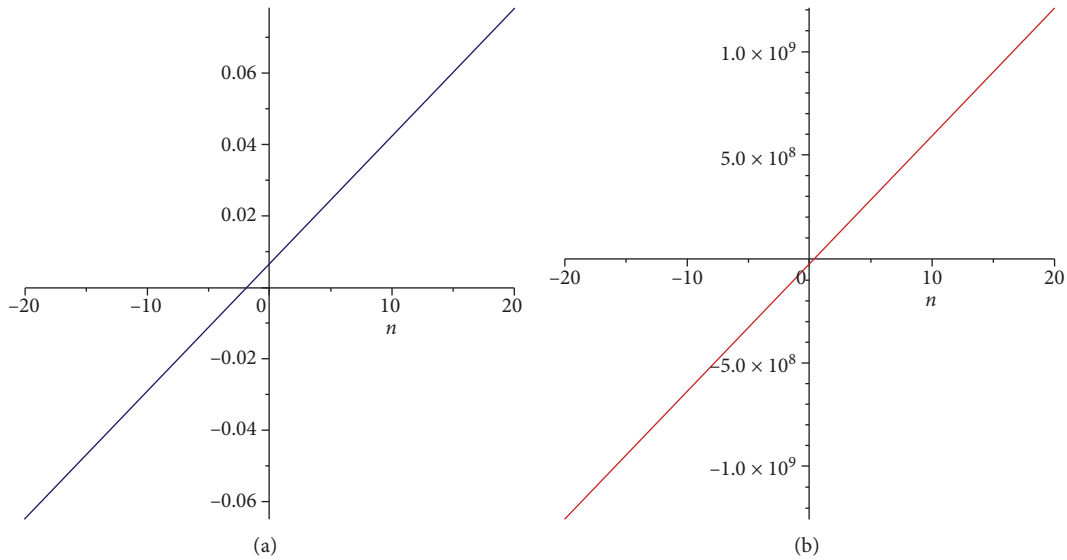

Figure 7: (a) The 2D plot of the Randić index for BR(m,n). (b) The 2D plot of the inverse Randić index for BR(m,n).

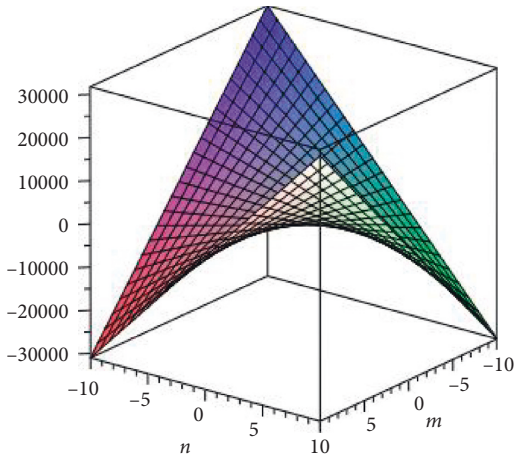

Figure 8: The 3D plot of the augmented Zagreb index for BR(m,n).

the first Zagreb index in blue color, second Zagreb index in green color, and modified Zagreb index in red color.

The 3D plot of the Randić index and inverse Randić index is illustrated in Figures 5 and 6, respectively. It is clearly seen from the graphs that by increasing the values of the parameters m and n, the graph of 5 increases faster than the graph of 6. It can be concluded that the Randić index increases faster than the inverse Randić index.

The 2D plot of the inverse Randić index is depicted in Figure 7(a). This is achieved by using Maple 13 and fixing the value of the parameter m or n. In both cases, if values of the parameter increases then the graph increases gradually and shows different behavior. The 2D plot of the Randić index is depicted in Figure 7(b). By increasing the values of the parameters, the graph increases and depicts different behavior.

Figure 8 illustrates the 3D plot of the 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) increase by changing the values of parameters m and n. The indices derived here are the functions that depend on the values of parameters, where m and n are the independent parameters and the index is the dependent parameter. □

5. Conclusions

We have computed the general form of M-polynomial for the molecular graph of the 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.

Data Availability

The data used to support the findings of this study are available from the corresponding author upon request.

Conflicts of Interest

The authors declare that there are no conflicts of interest regarding the publication of this paper.

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References

[1] A. Q. Baig, M. Imran, and H. Ali, "On topological indices of poly oxide, poly silicate, DOX, and DSL networks," *Canadian Journal of Chemistry*, vol. 93, no. 7, pp. 730–739, 2015.

[2] A. Q. Baig, M. Imran, W. Khalid, and M. Naeem, "Molecular description of carbon graphite and crystal cubic carbon structures," *Canadian Journal of Chemistry*, vol. 95, no. 6, pp. 674–686, 2017.

[3] H. Deng, J. Yang, and F. Xia, "A general modeling of some vertex-degree based topological indices in benzenoid systems and phenylenes," *Computers and Mathematics with Applications*, vol. 61, no. 10, pp. 3017–3023, 2011.

[4] W. Gao, M. R. Farahani, and L. Shi, "Forgotten topological index of some drug structures," *Acta Medica Mediterranea*, vol. 32, pp. 579–585, 2016.

[5] W. Gao and M. R. Farahani, "Degree-based indices computation for special chemical molecular structures using edge dividing method," *Applied Mathematics and Nonlinear Sciences*, vol. 1, no. 1, pp. 94–117, 2015.

[6] I. Gutman and O. E. Polansky, *Mathematical Concepts in Organic Chemistry*, Springer-Verlag New York, New York, NY, USA, 1986.

[7] W. Gao, M. K. Siddiqui, M. Imran, M. K. Jamil, and M. R. Farahani, "Forgotten topological index of chemical structure in drugs," *Saudi Pharmaceutical Journal*, vol. 24, no. 3, pp. 258–264, 2016.

[8] X. Zhang, H. Jiang, J.-B. Liu, and Z. Shao, "The cartesian product and join graphs on edge-version atom-bond connectivity and geometric arithmetic indices," *Molecules*, vol. 23, no. 7, p. 1731, 2018.

[9] X. Zhang, X. Wu, S. Akhter, M. Jamil, J.-B. Liu, and M. Farahani, "Edge-version atom-bond connectivity and geometric arithmetic indices of generalized bridge molecular graphs," *Symmetry*, vol. 10, no. 12, p. 751, 2018.

[10] J.-B. Liu and X.-F. Pan, "Minimizing Kirchhoff index among graphs with a given vertex bipartiteness," *Applied Mathematics and Computation*, vol. 291, pp. 84–88, 2016.

[11] J.-B. Liu, X.-F. Pan, F.-T. Hu, and F.-F. Hu, "Asymptotic Laplacian-energy-like invariant of lattices," *Applied Mathematics and Computation*, vol. 253, pp. 205–214, 2015.

[12] J.-B. Liu, X.-F. Pan, L. Yu, and D. Li, "Complete characterization of bicyclic graphs with minimal Kirchhoff index," *Discrete Applied Mathematics*, vol. 200, pp. 95–107, 2016.

[13] Y. W. Zhu, Y. Zhang, J. B. Yuan, and X. M. Wang, "FTP: an approximate fast privacy-preserving equality test protocol for authentication in Internet of things," *Security and Communication Networks*, vol. 2018, Article ID 6909703, 9 pages, 2018.

[14] Y. Zhu, X. Li, J. Wang, Y. Liu, and Z. Qu, "Practical secure naïve Bayesian classification over encrypted big data in cloud," *International Journal of Foundations of Computer Science*, vol. 28, no. 6, pp. 683–703, 2017.

[15] X. Li, Y. Zhu, J. Wang, and J. Zhang, "Efficient and secure multi-dimensional geometric range query over encrypted data in cloud," *Journal of Parallel and Distributed Computing*, vol. 131, pp. 44–54, 2019.

[16] Y. Gao, E. Zhu, Z. Shao, I. Gutman, and A. Klobučar, "Total domination and open packing in some chemical graphs," *Journal of Mathematical Chemistry*, vol. 56, no. 5, pp. 1481–1492, 2018.

[17] Z. Shao, P. Wu, X. Zhang, D. Dimitrov, and J.-B. Liu, "On the maximum ABC index of graphs with prescribed size and without pendent vertices," *IEEE Access*, vol. 6, pp. 27604–27616, 2018.

[18] Z. Shao, P. Wu, Y. Gao, I. Gutman, and X. Zhang, "On the maximum ABC index of graphs without pendent vertices," *Applied Mathematics and Computation*, vol. 315, pp. 298–312, 2017.

[19] M. R. Farahani, W. Gao, A. Q. Baig, and W. Khalid, "Molecular description of copper(II) oxide," *Macedonian Journal of Chemistry and Chemical Engineering*, vol. 36, no. 1, pp. 93–99, 2017.

[20] S. Hayat, M. A. Malik, and M. Imran, "Computing topological indices of honeycomb derived networks," *Romanian Journal of Information Science and Technology*, vol. 18, pp. 144–165, 2015.

[21] G. Rücker and C. Rücker, "On topological indices, boiling points, and cycloalkanes," *Journal of Chemical Information and Computer Sciences*, vol. 39, no. 5, pp. 788–802, 1999.

[22] D. Vukičević and A. Graovac, "Valence connectivities versus Randić, Zagreb, and modified Zagreb index: a linear algorithm to check discriminative properties of indices in acyclic molecular graphs," *Croatica Chemica Acta*, vol. 77, pp. 501–508, 2004.

[23] K. C. Das and I. Gutman, "Some properties of the second Zagreb index," *Match-Communications in Mathematical and in Computer Chemistry*, vol. 52, pp. 103–112, 2004.

[24] M. Eliasi and B. Taeri, "Hosoya polynomial of zigzag polyhex nanotorus," *Journal of the Serbian Chemical Society*, vol. 73, pp. 313–319, 2008.

[25] I. Gutman and K. C. Das, "The first Zagreb index 30 years after," *Match-Communications in Mathematical and in Computer Chemistry*, vol. 50, pp. 83–92, 2004.

[26] H. Hosoya, "On some counting polynomials in chemistry," *Discrete Applied Mathematics*, vol. 19, no. 1–3, pp. 239–257, 1988.

[27] M. R. Farahani, "Hosoya polynomial, wiener and hyper wiener indices of some regular graphs," *Informatics Engineering, an International Journal (IEIJ)*, vol. 1, no. 1, pp. 9–13, 2013.

[28] E. Deutsch and S. Klavzar, "M-Polynomial and degree-based topological indices," *Iranian Journal of Mathematical Chemistry*, vol. 6, pp. 93–102, 2015.

[29] M. Munir, W. Nazeer, S. Rafique, and S. Kang, "M-polynomial and related topological indices of nanostar dendrimers," *Symmetry*, vol. 8, no. 9, p. 97, 2016.

[30] Y. C. Kwun, M. Munir, W. Nazeer, S. Rafique, and S. Min Kang, "M-Polynomials and topological indices of V-phenylenic nanotubes and nanotori," *Scientific Reports*, vol. 7, no. 1, 2017.

[31] H. Wiener, "Structural determination of paraffin boiling points," *Journal of the American Chemical Society*, vol. 69, no. 1, pp. 17–20, 1947.

[32] A. A. Dobrynin, R. Entringer, and I. Gutman, "Wiener index of trees: theory and applications," *Acta Applicandae Mathematicae*, vol. 66, no. 3, pp. 211–249, 2001.

[33] B. Bollobás and P. Erdös, "Graphs of extremal weights," *Ars Combinatoria*, vol. 50, pp. 225–233, 1998.

[34] D. Amić, D. Bešlo, B. Lučić, S. Nikolić, and N. Trinajstić, "The vertex-connectivity index revisited," *Journal of Chemical Information and Computer Sciences*, vol. 38, no. 5, pp. 819–822, 1998.

[35] G. Caporossi, I. Gutman, P. Hansen, and L. Pavlović, "Graphs with maximum connectivity index," *Computational Biology and Chemistry*, vol. 27, no. 1, pp. 85–90, 2003.

[36] Y. Hu, X. Li, Y. Shi, T. Xu, and I. Gutman, "On molecular graphs with smallest and greatest zeroth-order general Randić index," *Match-Communications in Mathematical and in Computer Chemistry*, vol. 54, pp. 425–434, 2005.

[37] I. Gutman, M. Randić, and X. Li, "Mathematical aspects of Randić type molecular structure descriptors," *Mathematical Chemistry Monographs No. 1*, University of Kragujevac, Kragujevac, Serbia, 2006.

[38] M. Randić, "On history of the Randić index and emerging hostility toward chemical graph theory," *Match-Communications in Mathematical and in Computer Chemistry*, vol. 59, pp. 5–124, 2008.

[39] I. Gutman and N. Trinajstić, "Graph theory and molecular orbitals. Total φ-electron energy of alternant hydrocarbons," *Chemical Physics Letters*, vol. 17, no. 4, pp. 535–538, 1972.

[40] N. Trinajstic, S. Nikolic, A. Milicevic, and I. Gutman, "On Zagreb indices," *Kemija u Industriji*, vol. 59, pp. 577–589, 2010.

[41] C. K. Gupta, V. Lokesha, B. S. Shetty, and P. S. Ranjini, "On the symmetric division deg index of graph," *Southeast Asian Bulletin of Mathmatics*, vol. 41, no. 1, pp. 1–23, 2016.

[42] V. Lokesha and T. Deepika, "Symmetric division deg index of tricyclic and tetracyclic graphs," *International Journal of Scientific & Engineering Research*, vol. 7, no. 5, pp. 53–55, 2016.

[43] L. Zhong, "The harmonic index for graphs," *Applied Mathematics Letters*, vol. 25, no. 3, pp. 561–566, 2012.

[44] K. Pattabiraman, "Inverse sum indeg index of graphs," *AKCE International Journal of Graphs and Combinatorics*, vol. 15, no. 2, pp. 155–167, 2018.

[45] E. Estrada, L. Torres, L. Rodríguez, and I. Gutman, "An atom-bond connectivity index: modelling the enthalpy of formation of alkanes," *Indian Journal of Chemistry*, vol. 37A, no. 10, pp. 849–855, 1998.

[46] B. Furtula, A. Graovac, and D. Vukičević, "Augmented Zagreb index," *Journal of Mathematical Chemistry*, vol. 48, no. 2, pp. 370–380, 2010.

[47] Y. Huang, B. Liu, and L. Gan, "Augmented Zagreb index of connected graphs," *Match-Communications in Mathematical and in Computer Chemistry*, vol. 67, pp. 483–494, 2012.

[48] M. ÓKeeffe, G. B. Adams, and O. F. Sankey, "Predicted new low energy forms of carbon," *Physical Review Letters*, vol. 68, pp. 232–328, 1992.

[49] M. V. Diudea, *Nanostructures, Novel Architecture*, NOVA, New York, NY, USA, 2005.

[50] M. V. Diudea and C. L. Nagy, *Periodic Nanostructures*, Springer, Dordrecht, Netherlands, 2007.

[51] K. Y. Amsharov and M. Jansen, "A C_{78} fullerene precursor: toward the direct synthesis of higher fullerenes," *Journal of Organic Chemistry*, vol. 73, no. 7, pp. 293–934, 2008.

[52] Y. Shi, "Note on two generalizations of the Randić index," *Applied Mathematics and Computation*, vol. 265, pp. 1019–1025, 2015.