Mathematical Biosciences and Engineering

http://www.aimspress.com/journal/MBE

MBE, 17(3): 2384–2398.
DOI: 10.3934/mbe.2020127
Received: 15 October 2019
Accepted: 31 December 2019
Published: 14 February 2020

Research article

M-polynomials and topological indices of linear chains of benzene, napthalene and anthracene

Cheng-Peng Li[1], **Cheng Zhonglin**[2], **Mobeen Munir**[3,*], **Kalsoom Yasmin**[4] **and Jia-bao Liu**[5]

[1] Techanical and Electrical Engineering Department, Anqing Vocational and Technical College , Anqing 246003, P.R. China

[2] Teaching Department of Public Basic Course, Anhui International University, Hefei 231201, China

[3] Department of Mathematics, Division of Science and Technology, University of Education, Lahore-54590, Pakistan

[4] Department of Mathematics, Division of Science and Technology, University of Education, Lahore-54590, Pakistan

[5] School of Mathematics, Southeast University, Nanjing 210096, China

* **Correspondence:** Email: mmunri@ue.edu.pk; Tel:+92320-9472-635.

Abstract: The universality of M-polynomial paves way towards establishing closed forms of many leading degree-based topological indices as it is done by Hosoya polynomial for distance-based indices. The study of topological indices is recently one of the most active research areas in chemical graph theory. The aim of this paper is to establish closed formulas for M-polynomials of Linear chains of benzene, napthalene, and anthracene graphs. From this polynomial we also compute as many as nine degree-based topological indices for these three chains. Our results will potentially play an important role in pharmacy, drug design, and many other applied areas of molecular sciences.

Keywords: M-polynomial; degree-based index; linear chain of benzene; napthalene; anthracene

1. Introduction

Chemical graph theory is an emerging subfield of Mathematical Chemistry which helps in providing us tools such as polynomials and functions [1] to characterize properties of substances [2]. Wiener index has been largely used in [3]. A general modelling of some vertex-based indices of benzenoid systems has been presented in [4] and hexagonal systems in [5]. These tools carry potential information relating the structural properties of a molecular substance. Mathematicians are actively developing structural polynomials and functions that can take structural parameters such as number of atoms or molecules in a certain unit or number of bonds etc. as inputs to these functions and the out put information will be related to the properties of these molecular substances [6]. The main problem comes in the development of a very general polynomial that can generate these key functions after successive operations of differentiation and integration. The Hosoya polynomial is one such ingredient in the context of distance-based topological indices and key functions obtained from it are Weiner index, hyper Weiner index, and Harary index [6]. The M-polynomial is quite similar to the Hosoya polynomial except the fact that it produces degree-based topological indices.

A similar breakthrough was obtained recently by Deutsch and Klavzar [7] in 2015 in the form of M-polynomial which is extensively used nowadays to obtain many degree-based indices of different structures. The Authors established closed forms of degree-based indices of some famous structures like nanostar dendrimers in [8], titania nanotubes in [9], V-phenylenic nanotubes and nanotori in [10], boron nanotubes in [11], polyhex nanoubes in [12] and benzenoid systems in [13]. These indices have been closely linked with properties of chemical substances [14]. Wiener indices of trees have been computed in [15] which have a lots of applications. Benzenoid hydrocarbons play a vital role in our environment, food and chemical industries. In this article we are concerned about some linear chains of hydrocarbon in which benzene is an integral element. All considered graphs are simple and connected. We fix G for a connected simple graph with edge set $E(G)$ and vertex set $V(G)$, d_u is the degree of vertex u, $\delta = min\{d_u : u \in V(G)\}$ and $\Delta = max\{d_u : u \in V(G)\}$. The M- Polynomial of G is defined as

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

where m_{ij} is the number of edges $uv \epsilon E(G)$ such that $i \leq j$ [7]. For the sake of mere computation, we prefer to notate $M(x, y) = f(x, y)$. In 1975 Milan Randic introduced the Randic index $R_{-1/2}(G)$ and he defined it as

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

the generalized Randic index is defined as

$$R_\alpha(G) = \sum_{uv \epsilon E(G)} (1/d_u d_v)^\alpha$$

,[16]. Randic used this index to study molecular attributes in [17]. Bollobas et al. discussed graphs with maximal weight using Randic index in [18]. New look of this index is presented in [19]. Authors discussed some molecular graphs with Randic index in [20] and with maximal Randic index in [21]. The Inverse Randic index [22], is defined as

$$RR_\alpha(G) = \sum_{uv \epsilon E(G)} (d_u d_v)^\alpha.$$

It is clear that $R_{-1/2}(G)$ is a special case of $R_\alpha(G)$ where $\alpha = -1/2$. This index has vast application in diverse areas [23] and [24]. Some recent results about Randic index can be traced from [25]. Gutman and Trinajstic defined two other indices as

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

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

and the modified second Zagreb index is

$$M_2^m(G) = \sum_{uv\epsilon E(G)} 1/d_u d_v.$$

For details about these indices we refer to [26] and [27]. Some properties of Zagreb index have been outlined in [28] The Symetric Division index is also an important index given as

$$SSD(G) = \sum_{uv\epsilon E(G)} \{(min(d_u, d_v))/(max(d_u, d_v)) + (max(d_u, d_v))/(min(d_u, d_v))\}$$

Harmonic Index is

$$H(G) = \sum_{uv\epsilon E(G)} 2/d_u + d_v,$$

the inverse sum index is

$$I(G) = \sum_{uv\epsilon E(G)} d_u d_v/(d_u d_v),$$

and the augmented Zagreb index is

$$A(G) = \sum_{uv\epsilon E(G)} \{d_u d_v/(d_u + d_v - 2)\}^3.$$

For further details of these indices, we refer to [29] and [30] where Zagreb indices and some of its variants have been provided. We use the following notations for the operations

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

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

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

$$\delta_y = \int_0^y \frac{f(t, y)}{t} dt,$$

$$Jf(x, y) = f(x, x),$$

and

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

Benzenoid graphs play important part in industry of hydrocarbons. Saturation numbers of benzenoid graphs have been computed in [31]. Linear chains of these benzene contribute in formation of many other important hydrocarbons. In 1981 Graovac et al. studied about benzenoid system with zero Energy gap [32]. In 2001 Gutman discussed Hosoya polynomial of benzenooid graphs [33]. In 2004 Vukicevic et al. gave the results about the Wiener indices of Benzenoid graph [34]. In 2006 Gutman et al. computed the formula for calculating resonance energy of benzenoid hydrocarbons [35]. In 2009 vesel studied about 4-tiling of benzenoid graphs [36]. In 2011 Das et al. gave the spectral properties of some matrix of benzenoid systems [37].

In the present article we focus on the combinatorial and topological aspects of Linear chains of Benzene, Nepthalene and Anthracene graphs. In particular we establish closed results for M-polynomials of these systems and then using successive operations of calculus, we derive formulas for topological indices of these systems.

2. The main results

In this section we will compute M Polynomial of linear chains of benzene, napthalene and anthracene graphs and also some topological indices related to these graphs. We start with the linear chains of benzene.

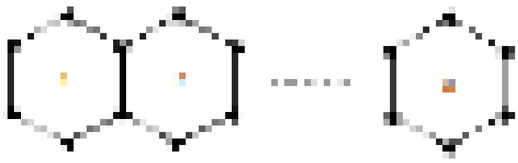

Figure 1. Linear chain of benzene graph.

.

Theorem 2.1.1 The M-Polynomial of linear chain of benzene graph is

$$M(B_n, x, y) = 6x^2y^2 + 4(n-1)x^3y^2 + (n-1)x^3y^3.$$

Proof. Let B_n be the linear chain of benzene graph. Then from Figure 1 we have

$$|V(B_n)| = 4n + 2$$

$$|E(B_n)| = 5n + 1$$

The edge set $E(B_n$ has following three partitions

$$|E_{2,2}| = \{e = uv\epsilon E(B_n)|d_u = 2d_v = 2\},$$
$$|E_{3,2}| = \{e = uv\epsilon E(B_n)|d_u = 3d_v = 2\},$$
$$|E_{3,3}| = \{e = uv\epsilon E(B_n)|d_u = 3d_v = 3\},$$

and

$$|E_{2,2}| \quad = \quad 6,$$

$$
\begin{aligned}
|E_{3,2}| &= 4(n-1), \\
|E_{3,3}| &= n-1.
\end{aligned}
$$

Thus , M polynomial of B_n is

$$
\begin{aligned}
M(B_n, x, y) &= \sum_{i \geq j} m_{ij}(B_n) x^i y^j \\
&= \sum_{2 \geq 2} m_{22}(B_n) x^2 y^2 + \sum_{3 \geq 2} m_{32}(B_n) x^3 y^2 + \sum_{3 \geq 3} m_{33}(B_n) x^3 y^3 \\
&= \sum_{2 \geq 2} m_{22}(B_n) x^2 y^2 + \sum_{3 \geq 2} m_{32}(B_n) x^3 y^2 + \sum_{3 \geq 3} m_{33}(B_n) x^3 y^3 \\
&= |E_{2,2}| x^2 y^2 + |E_{3,2}| x^3 y^2 + |E_{3,3}| x^3 y^3 \\
&= 6x^2 y^2 + 4(n-1) x^3 y^2 + (n-1) x^3 y^3.
\end{aligned}
$$

□

Now using the operations discussed in introduction we have the following results,
proposition 2.1.2 Let B_n be linear chain of benzene graph then

1. $M_1(B_n) = 26n - 2$
2. $M_2(B_n) = 33n - 9$
3. $M_2^m(B_n) = 7n/9 + 13/8$
4. $R\alpha(B_n) = (3^\alpha.2^{\alpha+2} + 3^{2\alpha})n + (2^{2\alpha+1}.3 - 3^\alpha.2^{\alpha+2} - 3^{2\alpha})$
5. $RR\alpha(B_n) = (1/3^\alpha.2^{\alpha-1} + 1/3^{2\alpha})n + (3/2^{2\alpha-1} - 1/3^\alpha.2^{\alpha-2} - 1/3^{2\alpha})$
6. $SSD(B_n) = 32n/3 + 2$
7. $H(B_n) = 29n/15 + 16/15$
8. $I(B_n) = 63n/10 - 3/10$
9. $A(B_n) = 2777n/64 + 295/64$

Proof. Let

$$M(B_n, x, y) = 6x^2 y^2 + 4(n-1) x^3 y^2 + (n-1) x^3 y^3.$$

Then ,

$$
\begin{aligned}
D_x(f(x,y)) &= 12x^2 y^2 + 12(n-1) x^3 y^2 + 3(n-1) x^3 y^3. \\
D_y(f(x,y)) &= 12x^2 y^2 + 8(n-1) x^3 y^2 + 3(n-1) x^3 y^3. \\
D_y D_x(f(x,y)) &= 24x^2 y^2 + 24(n-1) x^3 y^2 + 9(n-1) x^3 y^3. \\
\delta_x(f(x,y)) &= 3x^2 y^2 + 4/3(n-1) x^3 y^2 + 1/3(n-1) x^3 y^3.
\end{aligned}
$$

$$\begin{aligned}
\delta_x\delta_y(f(x,y)) &= 3/2x^2y^2 + 2/3(n-1)x^3y^2 + 1/9(n-1)x^3y^3.\\
D_x^{\alpha}D_y^{\alpha}(f(x,y)) &= 2^{2\alpha+1}.3x^2y^2 + 3^{\alpha}.2^{\alpha+2}(n-1)x^3y^2 + 3^{2\alpha}(n-1)x^3y^3.\\
\delta_x^{\alpha}\delta_y^{\alpha}(f(x,y)) &= 3/2^{2\alpha-1}x^2y^2 + 1/3^{\alpha}.2^{\alpha-2}(n-1)x^3y^2 + 1/3^{2\alpha}(n-1)x^3y^3.\\
\delta_yD_x(f(x,y)) &= 6x^2y^2 + 6(n-1)x^3y^2 + (n-1)x^3y^3.\\
\delta_xD_y(f(x,y)) &= 6x^2y^2 + 6(n-1)x^3y^2 + (n-1)x^3y^3.\\
\delta_xJ(f(x,y)) &= 3/2x^4 + 4/5(n-1)x^5 + 1/6(n-1)x^6.\\
\delta_xJ(D_yD_x(f(x,y))) &= 6x^4 + 24/5(n-1)x^5 + 3/2(n-1)x^6.\\
\delta_x^3Q_{-2}J(D_x^3D_y^3(f(x,y))) &= 48x^2 + 32(n-1)x^3 + 729/64(n-1)x^4
\end{aligned}$$

1. First zagreb Index :

$$M_1(B_n) = (D_x + D_y)f(x,y)|_{x=y=1} = 26n - 2,$$

2. Second Zagreb Index :

$$M_2(B_n) = (D_yD_x)f(x,y)|_{x=y=1} = 33n - 9,$$

3. Modified Second Zagreb Index :

$$M_2^m(B_n) = (\delta_x\delta_y)f(x,y)|_{x=y=1} = 7n/9 + 13/8,$$

4. Generalized Randic Index :

$$R\alpha(B_n) = D_x^{\alpha}D_y^{\alpha}(f(x,y))|_{x=y=1} = (3^{\alpha}.2^{\alpha+2} + 3^{2\alpha})n + (2^{2\alpha+1}.3 - 3^{\alpha}.2^{\alpha+2} - 3^{2\alpha}),$$

5. Inverse randic Index :

$$RR\alpha(B_n) = \delta_x^{\alpha}\delta_y^{\alpha}(f(x,y))|_{x=y=1} = (1/3^{\alpha}.2^{\alpha-1} + 1/3^{2\alpha})n + (3/2^{2\alpha-1} - 1/3^{\alpha}.2^{\alpha-2} - 1/3^{2\alpha}),$$

6.Symmetric division Index:

$$SSD(B_n) = (\delta_xD_x + \delta_yD_y)f(x,y)|_{x=y=1} = 32n/3 + 2,$$

7.Harmonic Index:

$$H(B_n) = 2\delta_xJ(f(x,y))|_{x=1} = 29n/15 + 16/15,$$

8.Inverse Sum Index :

$$I(B_n) = \delta_xJ(D_yD_x(f(x,y)))|_{x=1} = 63n/10 - 3/10,$$

9. Augmented zagreb Index :

$$A(B_n) = \delta_x^3Q_{-2}J(D_x^3D_y^3(f(x,y)))|_{x=1} = 2777n/64 + 295/64,$$

□

2.1. Aspects of linear chains of nepthalene graphs

Now we move towards the second main object of this article. Figure 2 is a linear chain of Napthalene graphs.

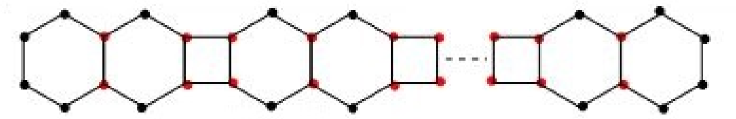

Figure 2. Linear chain of napthalene graphs.

. **Theorem 2.1.3** The M-Polynomial of linear napthalene $L.N_n$ graph is

$$M(L.N_n, x, y) = 6x^2y^2 + 4(2n - 1)x^3y^2 + (5n - 4)x^3y^3.$$

Proof. Let $L.N_n$ be the linear napthalene graph. Then from Figure 2 we have

$$|V(L.N_n)| = 10n$$

$$|E(L.N_n)| = 13n - 2.$$

The edge set $E(L.N_n$ has following three partitions

$$\begin{aligned}
|E_{2,2}| &= \{e = uv\epsilon E(L.N_n)|d_u = 2d_v = 2\},\\
|E_{3,2}| &= \{e = uv\epsilon E(L.N_n)|d_u = 3d_v = 2\},\\
|E_{3,3}| &= \{e = uv\epsilon E(L.N_n)|d_u = 3d_v = 3\},
\end{aligned}$$

and

$$\begin{aligned}
|E_{2,2}| &= 6,\\
|E_{3,2}| &= 8n - 4 = 4(2n - 1),\\
|E_{3,3}| &= 5n - 4.
\end{aligned}$$

Thus , M polynomial of $L.N_n$ is

$$
\begin{aligned}
M(B_n,x,y) &= \sum_{i\geq j} m_{ij}(L.N_n)x^iy^j\\
&= \sum_{2\geq 2} m_{22}(L.N_n)x^2y^2 + \sum_{3\geq 2} m_{32}(L.N_n)x^3y^2 + \sum_{3\geq 3} m_{33}(L.N_n)x^3y^3\\
&= \sum_{2\geq 2} m_{22}(L.N_n)x^2y^2 + \sum_{3\geq 2} m_{32}(L.N_n)x^3y^2 + \sum_{3\geq 3} m_{33}(L.N_n)x^3y^3\\
&= |E_{2,2}|x^2y^2 + |E_{3,2}|x^3y^2 + |E_{3,3}|x^3y^3\\
&= 6x^2y^2 + 4(2n-1)x^3y^2 + (5n-4)x^3y^3.
\end{aligned}
$$

□

proposition 2.1.4 Let $L.N_n$ be linear napthalene graph then,

1. $M_1(L.N_n) = 70n - 20$,
2. $M_2(L.N_n) = 93n - 36$,
3. $M_2^m(L.N_n) = 17n/9 + 7/18$,
4. $R\alpha(L.N_n) = (5.3^{2\alpha} + 3^{\alpha}.2^{\alpha+3})n + (2^{2\alpha+1}.3 - 3^{\alpha}.2^{\alpha+2} - 4.3^{2\alpha})$,
5. $RR\alpha(L.N_n) = (5/3^{2\alpha} + 1/3^{\alpha}.2^{\alpha-2})n + (3/2^{2\alpha-1} - 1/3^{\alpha}.2^{\alpha-2} - 4/3^{2\alpha})$,
6. $SSD(L.N_n) = 82n/3 - 14/3$,
7. $H(L.N_n) = 73n/15 + 1/15$,
8. $I(L.N_n) = 171n/10 - 24/5$,
9. $A(L.N_n) = 7741n/64 - 473/16$.

Proof. Let

$$M(L.N_n,x,y) = 6x^2y^2 + 4(2n-1)x^3y^2 + (5n-4)x^3y^3.$$

Then,

$$
\begin{aligned}
D_x(f(x,y)) &= 12x^2y^2 + 12(2n-1)x^3y^2 + 3(5n-4)x^3y^3,\\
D_y(f(x,y)) &= 12x^2y^2 + 8(2n-1)x^3y^2 + 3(5n-4)x^3y^3,\\
D_yD_x(f(x,y)) &= 24x^2y^2 + 24(2n-1)x^3y^2 + 9(5n-4)x^3y^3,\\
\delta_x(f(x,y)) &= 3x^2y^2 + 4/3(2n-1)x^3y^2 + 1/3(5n-4)x^3y^3,\\
\delta_x\delta_y(f(x,y)) &= 3/2x^2y^2 + 2/3(2n-1)x^3y^2 + 1/9(5n-4)x^3y^3,\\
D_x^{\alpha}D_y^{\alpha}(f(x,y)) &= 2^{2\alpha+1}.3x^2y^2 + 3^{\alpha}.2^{\alpha+2}(2n-1)x^3y^2 + 3^{2\alpha}(5n-4)x^3y^3,\\
\delta_x^{\alpha}\delta_y^{\alpha}(f(x,y)) &= 3/2^{2\alpha-1}x^2y^2 + 1/3^{\alpha}.2^{\alpha-2}(2n-1)x^3y^2 + 1/3^{2\alpha}(5n-4)x^3y^3,\\
\delta_yD_x(f(x,y)) &= 6x^2y^2 + 6(n-1)x^3y^2 + (5n-4)x^3y^3,\\
\delta_xD_y(f(x,y)) &= 6x^2y^2 + 8/3(2n-1)x^3y^2 + (5n-4)x^3y^3,\\
\delta_xJ(f(x,y)) &= 3/2x^4 + 4/5(2n-1)x^5 + 1/6(5n-4)x^6,\\
\delta_xJ(D_yD_x(f(x,y))) &= 6x^4 + 24/5(2n-1)x^5 + 3/2(5n-4)x^6,
\end{aligned}
$$

$$\delta_x^3 Q_{-2} J(D_x^3 D_y^3(f(x,y))) \;=\; 48x^2 + 32(2n-1)x^3 + 729/64(5n-4)x^4.$$

1. First zagreb Index :

$$M_1(L.N_n) = (D_x + D_y)f(x,y)|_{x=y=1} = 70n - 20.$$

2. Second Zagreb Index :

$$M_2(L.N_n) = (D_y D_x)f(x,y)|_{x=y=1} = 93n - 36.$$

3. Modified Second Zagreb Index :

$$M_2^m(L.N_n) = (\delta_x \delta_y)f(x,y)|_{x=y=1} = 17n/9 + 7/18.$$

4. Generalized randic Index :

$$R\alpha(L.N_n) = D_x^\alpha D_y^\alpha(f(x,y))|_{x=y=1} = (5.3^{2\alpha} + 3^\alpha.2^{\alpha+3})n + (2^{2\alpha+1}.3 - 3^\alpha.2^{\alpha+2} - 4.3^{2\alpha}).$$

5. Inverse randic Index :

$$RR\alpha(L.N_n) = \delta_x^\alpha \delta_y^\alpha(f(x,y))|_{x=y=1} = (5/3^{2\alpha} + 1/3^\alpha.2^{\alpha-2})n + (3/2^{2\alpha-1} - 1/3^\alpha.2^{\alpha-2} - 4/3^{2\alpha}).$$

6.Symmetric division Index:

$$SSD(L.N_n) = (\delta_x D_x + \delta_y D_y)f(x,y)|_{x=y=1} = 82n/3 - 14/3.$$

7.Harmonic Index:

$$H(L.N_n) = 2\delta_x J(f(x,y))|_{x=1} = 73n/15 + 1/15.$$

8.Inverse Sum Index :

$$I(L.N_n) = \delta_x J(D_y D_x(f(x,y)))|_{x=1} = 171n/10 - 24/5.$$

9. Augmented zagreb Index :

$$A(L.N_n) = \delta_x^3 Q_{-2} J(D_x^3 D_y^3(f(x,y)))|_{x=1} = 7741n/64 - 473/16.$$

2.2. Aspects of linear chains of anthracene graphs

Now we move towards the theoretical aspects of linear chain of anthracene graphs. Following Figure 3 gives a mathematical pattern of carbon atoms sequencing. □

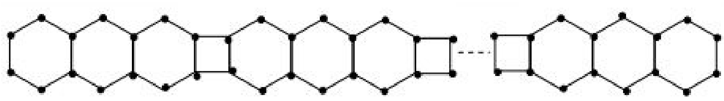

Figure 3. Linear chain of anthracene graph.

.

Theorem 2.1.5 The M-Polynomial of linear anthracene $L.A_n$ graph is

$$M(L.A_n, x, y) = 6x^2y^2 + 4(3n-1)x^3y^2 + 2(3n-2)x^3y^3.$$

Proof. Let $L.A_n$ be the linear anthracene graph. Then from figure 3 we have

$$|V(L.A_n)| = 14n,$$

$$|E(L.A_n)| = 18n - 2,$$

The edge set $E(L.A_n$ has following three partitions

$$\begin{aligned}
|E_{2,2}| &= \{e = uv\epsilon E(L.A_n)|d_u = 2d_v = 2\},\\
|E_{3,2}| &= \{e = uv\epsilon E(L.A_n)|d_u = 3d_v = 2\},\\
|E_{3,3}| &= \{e = uv\epsilon E(L.A_n)|d_u = 3d_v = 3\},
\end{aligned}$$

and

$$\begin{aligned}
|E_{2,2}| &= 6,\\
|E_{3,2}| &= 4(3n-1),\\
|E_{3,3}| &= 2(3n-2).
\end{aligned}$$

Thus, M polynomial of $L.A_n$ is

$$\begin{aligned}
M(B_n, x, y) &= \sum_{i\geq j} m_{ij}(L.A_n)x^iy^j,\\
&= \sum_{2\geq 2} m_{22}(L.A_n)x^2y^2 + \sum_{3\geq 2} m_{32}(L.A_n)x^3y^2 + \sum_{3\geq 3} m_{33}(L.A_n)x^3y^3,\\
&= \sum_{2\geq 2} m_{22}(L.A_n)x^2y^2 + \sum_{3\geq 2} m_{32}(L.A_n)x^3y^2 + \sum_{3\geq 3} m_{33}(L.A_n)x^3y^3,\\
&= |E_{2,2}|x^2y^2 + |E_{3,2}|x^3y^2 + |E_{3,3}|x^3y^3
\end{aligned}$$

$$= \quad 6x^2y^2 + 4(3n-1)x^3y^2 + 2(3n-2)x^3y^3,$$

□

proposition 2.1.6 Let $L.A_n$ be linear anthracene graph then,

1. $M_1(L.A_n) = 96n - 20$,
2. $M_2(L.A_n) = 126n - 36$,
3. $M_2^m(L.A_n) = 8n/3 + 7/18$,
4. $R\alpha(L.A_n) = (3^{2\alpha+1}.2 + 3^{\alpha+1}.2^{\alpha+2})n + (2^{2\alpha+1}.3 - 3^{\alpha}.2^{\alpha+2} - 3^{2\alpha}.2^2)$,
5. $RR\alpha(L.A_n) = (1/3^{\alpha-1}.2^{\alpha-2} + 2/3^{2\alpha-1})n + (3/2^{2\alpha-1} - 1/3^{\alpha}.2^{\alpha-2} - 4/3^{2\alpha})$,
6. $SSD(L.A_n) = 38n - 14/3$,
7. $H(L.A_n) = 34n/5 + 1/15$,
8. $I(L.A_n) = 117n/5 - 24/5$,
9. $A(L.A_n) = 825n - 473/16$.

Proof. Let

$$M(L.A_n, x, y) = 6x^2y^2 + 4(3n-1)x^3y^2 + 2(3n-2)x^3y^3.$$

Then ,

$$\begin{aligned}
D_x(f(x,y)) &= 12x^2y^2 + 12(3n-1)x^3y^2 + 6(3n-2)x^3y^3,\\
D_y(f(x,y)) &= 12x^2y^2 + 8(3n-1)x^3y^2 + 6(3n-2)x^3y^3,\\
D_yD_x(f(x,y)) &= 24x^2y^2 + 24(3n-1)x^3y^2 + 18(3n-2)x^3y^3,\\
\delta_x(f(x,y)) &= 3x^2y^2 + 4/3(3n-1)x^3y^2 + 2/3(3n-2)x^3y^3,\\
\delta_x\delta_y(f(x,y)) &= 3/2x^2y^2 + 2/3(3n-1)x^3y^2 + 2/9(3n-2)x^3y^3,\\
D_x^{\alpha}D_y^{\alpha}(f(x,y)) &= 2^{2\alpha+1}.3x^2y^2 + 3^{\alpha}.2^{\alpha+2}(3n-1)x^3y^2 + 3^{2\alpha}.2(3n-2)x^3y^3,\\
\delta_x^{\alpha}\delta_y^{\alpha}(f(x,y)) &= 3/2^{2\alpha-1}x^2y^2 + 1/3^{\alpha}.2^{\alpha-2}(3n-1)x^3y^2 + 2/3^{2\alpha}(3n-2)x^3y^3,\\
\delta_yD_x(f(x,y)) &= 6x^2y^2 + 6(3n-1)x^3y^2 + 2(3n-2)x^3y^3,\\
\delta_xD_y(f(x,y)) &= 6x^2y^2 + 8/3(3n-1)x^3y^2 + 2(3n-2)x^3y^3,\\
\delta_xJ(f(x,y)) &= 3/2x^4 + 4/5(3n-1)x^5 + 1/3(3n-2)x^6,\\
\delta_xJ(D_yD_x(f(x,y))) &= 6x^4 + 24/5(3n-1)x^5 + 3(3n-2)x^6,\\
\delta_x^3Q_{-2}J(D_x^3D_y^3(f(x,y))) &= 48x^2 + 32(3n-1)x^3 + 729/32(3n-2)x^4.
\end{aligned}$$

1. First zagreb Index :

$$M_1(L.A_n) = (D_x + D_y)f(x,y)|_{x=y=1} = 96n - 20$$

2. Second Zagreb Index :

$$M_2(L.A_n) = (D_yD_x)f(x,y)|_{x=y=1} = 126n - 36$$

3. Modified Second Zagreb Index :

$$.M_2^m(L.A_n) = (\delta_x\delta_y)f(x,y)|_{x=y=1} = 8n/3 + 7/18$$

4. Generalized randic Index :

$$R\alpha(L.A_n) = D_x^\alpha D_y^\alpha(f(x,y))|_{x=y=1} = (3^{2\alpha+1}.2 + 3^{\alpha+1}.2^{\alpha+2})n + (2^{2\alpha+1}.3 - 3^\alpha.2^{\alpha+2} - 3^{2\alpha}.2^2)$$

5. Inverse randic Index :

$$RR\alpha(L.A_n) = \delta_x^\alpha\delta_y^\alpha(f(x,y))|_{x=y=1} = (1/3^{\alpha-1}.2^{\alpha-2} + 2/3^{2\alpha-1})n + (3/2^{2\alpha-1} - 1/3^\alpha.2^{\alpha-2} - 4/3^{2\alpha})$$

6.Symmetric division Index:

$$SSD(L.A_n) = (\delta_x D_x + \delta_y D_y)f(x,y)|_{x=y=1} = 38n - 14/3$$

7.Harmonic Index:

$$H(L.A_n) = 2\delta_x J(f(x,y))|_{x=1} = 34n/5 + 1/15$$

8.Inverse Sum Index :

$$I(L.A_n) = \delta_x J(D_y D_x(f(x,y)))|_{x=1} = 117n/5 - \text{‘}24/5$$

9. Augmented zagreb Index :

$$A(L.A_n) = \delta_x^3 Q_{-2} J(D_x^3 D_y^3(f(x,y)))|_{x=1} = 825n - 473/16.$$

□

3. Conclusions

In this paper we derived M-polynomials and closed forms of some degree-based topological indices of linear chains of benzene, napthalene and anthracene graphs. Actual features about these results are the correlation of these indices on the basic units of these three chains. These indices could potentially play a significant role in determining properties of these compounds and others in which these compounds are used. It is important to mention here that some of these topological indices are derived directly by using techniques and definitions available in the literature.

Authors contributions

Conceptualization, Mobeen Munir and Jiabao Liu; Investigation, Cheng Zhonglin and Cheng-Peng Li; Writing original draft, Kalsoom Yasmin.

Acknowledegements

We are highly thankful to reviewer’s comments to improve the quality of article.

Funding

This research is funded from Major natural science research projects in Colleges and universities of Anhui Province in 2019 (No. KJ2019 ZD77).

Conflict of interest

The authors declare that they have no competing interests.

References

1. G. Rucker, C. Rucker, On topological indices, boiling points, and cycloalkanes, *J. Chem. Inf. Comput. Sci.*, **39** (1999), 788–802.
2. S. Klavzar, I. Gutman, A comparison of the schultz molecular topological index with the wiener index, *J. Chem. Inf. Comput. Sci.*, **36** (1996), 1001–1003.
3. F. M. Bruckler, C. T. Dosli, A. Graovac, I. Gutman, On a class of distance-based molecular structure descriptors, *Chem. Phys. Lett.*, **503** (2011), 336–338.
4. H. Deng, J. Yang, F. Xia , A general modeling of some vertex-degree based topological indices in benzenoid systems and phenylenes, *Comput. Math. Appl.*, **61** (2011), 3017–3023.
5. H. Zhang, F. Zhang, The clar covering polynomial of hexagonal systems I, *Discrete Appl. Math.*, **69** (1996), 147–167.
6. I. Gutman, Some properties of the Wiener polynomial, *Graph. Theory Notes N. Y.*, **125** (1993), 13–18.
7. E. Deutsch, S. Klavzar, M-polynomial and degreebased topological indices,*Iran. J. Math. Chem*, **6** (2015), 93-102.
8. M. Munir, W. Nazeer, S. Rafique, S. M. Kang, M-polynomial and related topological indices of nanostar dendrimers, *Symmetry*, **8** (2016), 97.
9. M. Munir, W.Nazeer, S.Rafique, A. R. Nizami, S. M. Kang, M-polynomial and degree-based topological indices of titaniananotubes, *Symmetry*, **8** (2016), 117.
10. Y. Kwun, M. Munir, W. Nazeer, S. Rafique, S. M. Kang, M-polynomial and degree-based topological indices of Vphenylenic nanotubes and nanotori, *Sci. Rep.*, **7** (2017), 8756.
11. M. Munir, W. Nazeer, S. Rafique, A. R. Nizami, S. M. Kang, Some computational aspects of triangular boron nanotubes, *Symmetry*, **9** (2016), 6.
12. M. Munir, W. Nazeer, S. Rafique, S. M. Kang, M-polynomial and degree-based topological indices of polyhex nanotubes, *Symmetry*, **8** (2016), 149.
13. A. Ali, W. Nazeer, M. Munir, S. M. Kang, M-Polynomials and topological indices of zigzag and rhombic benzenoidsystems, *Open Chem.*, **16** (2018), 73–78.
14. H. Wiener, Structural determination of paran boiling points, *JACS*, **69** (1947), 17–20.
15. A. A. Dobrynin, R. Entringer, I. Gutman, Wiener index of trees: Theory and applications, *Acta Appl. Math.*, **66** (2001), 211–249.

16. I. Gutman, O. E. Polansky , Mathematical concepts in organic chemistry, *Springer Science and Business Media, Berlin, Germany*, (2012).
17. M. Randic, On characterization of molecular attributes, *Acta Chim. Slov.*, **45** (1998), 239.
18. B. Bollobas, P. Erdos, Graphs of extremal weights, *Ars Combinatoria*, **50** (1998), 225–233.
19. D. Amic, D. Beslo, B. Lucic, S. Nikolic, N. Trinajstic, The vertex-connectivity index revisited, *J. Chem. Inf. Comput. Sci.*, **38** (1998), 819–822.
20. Y. Hu, X. Li, Y. Shi, T. Xu, I.Gutman, On molecular graphs with smallest and greatest zeroth-order general Randic index, *Match-Commun. Math. Co.*, **54** (2005), 425–434.
21. G. Caporossi, I. Gutman, P. Hansen, L. Pavlovic, Graphs with maximum connectivity index, *Comput. Biol. Chem.*, **27**(2003), 85–90.
22. X. Li, I. Gutman, Mathematical chemistry monographs no. 1, *Kragujevac*, **330** (2006), 6.
23. L. Kier, Molecular connectivity in chemistry and drug research, *Elsevier, NY. USA*, **14** (2012).
24. L. B. Kierand, L. H. Hall, Molecular connectivity in structure activity analysis, research studies, chemometrics research studies press, 1st edition, (1986).
25. I. Gutman, B. Furtula, Recent Results in the Theory of Randic Index, University of Kragujevac and Faculty of Science Kragujevac, *Kragujevac, Serbia*, (2008).
26. S. Nikolic, G. Kovacevic, A. Milicevic, N. Trinajstic, The Zagreb indices 30 years after, *Croa. Chem. Acta*, **76** (2003), 113–124.
27. I. Gutman, K. C. Das, The first Zagreb index 30 years after, *Math. Commun. Math. Comput. Chem.*, **50** (2004), 83–92.
28. K. C. Das, I. Gutman, Some properties of the second Zagreb index, *Match-Commun. Math. Co.*, **52** (2004), 1–3.
29. N. Trinajstic, S. Nikolic, A. Milicevic, I. Gutman, About the Zagreb Indices, *Kemija u Industriji: Casopis Kemicara i Kemijskih Inzenjera Hrvatske*, **59** (2010), 577–589.
30. D. Vukicevic, A. Graovac, Valence connectivity versus Randic, Zagreb and modified Zagreb index, a linear algorithm to check discriminative properties of indices in acyclic molecular graphs, *Croa. Chem. Acta*, **77** (2004), 501–508.
31. T. Doslic, I. Zubac, Saturation number of benzenoid graphs, *Math. Commun. Math. Comput. Chem.*, (2015).
32. A. Graovac, N. Trinjstic, Graph thoretical search for benzenoid polymers with zero energy gap, *Croat. Chem. Acta*, **4** (1981), 571–579.
33. I. Gutman, M. Petkovsek, R. Z. pleterselt, On Hosoya polynomial of benzenoid Graph, *Math. Commun.*, (2001).
34. D. Vukicevic, N. Trinajstic, Wiener indices of benzenoid graph, *Bull. Chem. Technol. Macedon.*, **23** (2004), 113–129.
35. I. Gutman, S. Radenkovic, Simple formula for calculating resonance energy of benzenoid hydrocarbons, *Bull. Chem. Technol. Macedon.*, **25** (2006), 17–21.
36. A. vesel, 4-tilings of benzenoid graphs *Math. Commun Math. Comput. Chem.*, **62** (2009), 221–234.

37. K. C. Das, F. M. Bhatti, S. G. lee, I. Gutman, Spectral properties of the he matrix of hexagonal systems, *Math. Commun Math. Comput. Chem.*, **65** (2011), 753–774.

AIMS Press