



M-Polynomial and Degree-Based Topological Indices for Iterative Graphs

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Abstract. Iterative graph have several applications in social network analysis, optimization problems, machine learning, and game theory. Such graphs are also commonly used in chemistry, physics, and mathematics. In this article, we derive the M-polynomial for the fractal growth patterns of benzene (FGB_n , $n \geq 1$), the Pythagoras tree (PT_n , $n \geq 1$), and the benzene dendrimer (DB_n , $n \geq 2$). Moreover, we compute some degree-based topological indices based on the M-polynomials, such as the first Zagreb index, the second Zagreb index, the modified second Zagreb index, the general Randić index, the harmonic index, the inverse sum index, and the symmetric division degree index. Finally, we presented our work graphically and compared the sketches of M-polynomials and degree-based topological indices.

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1. Introduction

Polynomials are tools in chemical graph theory used to collect information about molecular graphs and thus display properties of the molecular graph without using quantum mechanics. A molecular graph is generated by the conversion of a chemical molecule into a graph in which vertices and edges are represented by atoms and bonds, respectively. Let $\mathcal{H}(\mathcal{V}, \mathcal{E})$ be a simple connected undirected graphs, where $\mathcal{V}(\mathcal{H})$ denotes the set of vertices and $\mathcal{E}(\mathcal{H})$ denotes the set of edges. Number of vertices $|V(\mathcal{H})|$ is the order of graph and number of edges $|E(\mathcal{H})|$ is the size of graph. connected graph is a graph in which there exists a path between every pair of vertices. A vertex u 's degree, denoted as d_u , refers

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to the number of edges that are adjacent to vertex u . Topological indices are numerical parameters associated with a molecular graph that characterizes its topology.

The role of algebraic polynomials is central to the development of chemical graph theory, such as the Hosoya polynomial [12], and the acyclic polynomial of a graph [10]. Deutsch and Klavžar [6], introduced the M-polynomial with the aim of achieving similar goals as the Hosoya polynomial, specifically in deriving closed-form expressions for numerous degree-based topological indices. Several researchers have calculated the M-polynomial and associated topological indices for well-known graphs. Examples include the M-polynomial and topological indices of nanostar dendrimers and polyhex nanotubes [17, 18], linear chains of benzene, naphthalene, and anthracene [14], benzene rings embedded in p-type surface networks, zigzag and rhombic benzenoid systems [1], generalized Sierpinski networks [8], hourglass, triangular, as well as jagged-rectangle benzenoid systems detailed [13], Generalized Zegrab index, fourth version of atom-bond connectivity and fifth version of geometric-arithmetic index for an infinite class of Titania nanotubes $\text{TiO}-2[\text{m},\text{n}]$ [15], computation of Benzenoid planar octahedron networks by using topological indices [2], and topological indices of third types of hex-derived networks [3]. In this paper, we derive the M-polynomial for the fractal growth patterns of benzene (FGB_n , $n \geq 1$), the Pythagoras tree (PT_n , $n \geq 1$), and the benzene dendrimer (DB_n , $n \geq 2$). Moreover, we compute some degree-based topological indices based on the M-polynomials.

Definition 1. [6] Let \mathcal{H} be a graph and $m_{\alpha,\beta}$ be the count of edges $e = uv \in \mathcal{E}(\mathcal{H})$ such that $(d_u, d_v) = (\alpha, \beta)$, then the M-polynomial of \mathcal{H} is defined as:

$$M(\mathcal{H}; x, y) = \sum_{\delta \leq \alpha \leq \beta \leq \Delta} m_{\alpha,\beta} x^\alpha y^\beta.$$

Here, δ denotes the minimum degree in \mathcal{H} , while Δ denotes the maximum degree in \mathcal{H} .

Several indices are derived from polynomials. The first index is the Wiener index, also known as the path number, introduced by Wiener in [22]. Gutman and Trinajstić in [11] introduced two new indices labeled as the first Zagreb index, denoted as M_1 , and the second Zagreb index, denoted as M_2 , defined as:

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

$$M_2(\mathcal{H}) = \sum_{uv \in \mathcal{E}(\mathcal{H})} (d_u d_v).$$

Nikolic et al. in [19], studied a modified second Zagreb index MM_2 , formulated as:

$$MM_2(\mathcal{H}) = \sum_{uv \in \mathcal{E}(\mathcal{H})} \frac{1}{(d_u d_v)}.$$

Randic in [20], introduced a bound-additive topological index as:

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

The general Randic index was introduced by Bollobas et. al in [5],

$$R_\gamma(\mathcal{H}) = \sum_{uv \in \mathcal{E}(\mathcal{H})} (d_u d_v)^\gamma.$$

Another Randic index is called harmonic index defined by Fajtlowics in [7], and the inverse sum index established by Vukicevic and Graovac in [21],

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

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

Gupta et al. [9] introduced symmetric division degree index $SSD(\mathcal{H})$, formulated as:

$$SSD(\mathcal{H}) = \sum_{uv \in \mathcal{E}(\mathcal{H})} \left(\frac{\text{Min}(d_u, d_v)}{\text{Max}(d_u, d_v)} + \frac{\text{Max}(d_u, d_v)}{\text{Min}(d_u, d_v)} \right).$$

Computational of degree-based topological indices is immediately from the rules written above or use M-polynomial with next notations to compute degree-based topological indices.

$$D_x = x \frac{\partial M(\mathcal{H}; x, y)}{\partial x}.$$

$$D_y = y \frac{\partial M(\mathcal{H}; x, y)}{\partial y}.$$

$$S_x = \int_0^x \frac{M(\mathcal{H}; x, y)}{t} dt.$$

$$S_y = \int_0^y \frac{M(\mathcal{H}; x, y)}{t} dt.$$

$$JM(\mathcal{H}; x, y) = M(\mathcal{H}; x, x).$$

2. Main Results

This section comprises three subsections, each dedicated to distinct aspects of our analysis. In the first subsection, We investigate the M-polynomial and degree-based topological indices associated with the fractal growth pattern of benzene. Subsection two presents our findings on the M-polynomial of Pythagoras tree as well as the degree-based topological indices of the Pythagoras tree. Finally, we explore the dendrimer of benzene and its associated topological indices in the concluding subsection.

2.1. Fractal Growth of Benzene

The term fractal was coined in 1975 by Benoit Mandelbrot to describe a new idea in geometry. Geometric figures in regular shapes are characterized by mathematical equations that define their dimensions such as length, width, and height. Irregular shapes can not be measured in this way. A Fractal is a type of mathematical shape that are infinitely complex. In essence, a Fractal is a pattern that repeats forever, and every part of the Fractal, regardless of how zoomed in, or zoomed out you are, it looks very similar to the whole image. Fractals are currently employed in various applications to generate textured landscapes and images resembling natural scenes, including lunar surfaces and mountain ranges [4, 16]. Moreover, the order and size of all graphs is given by geometric series.

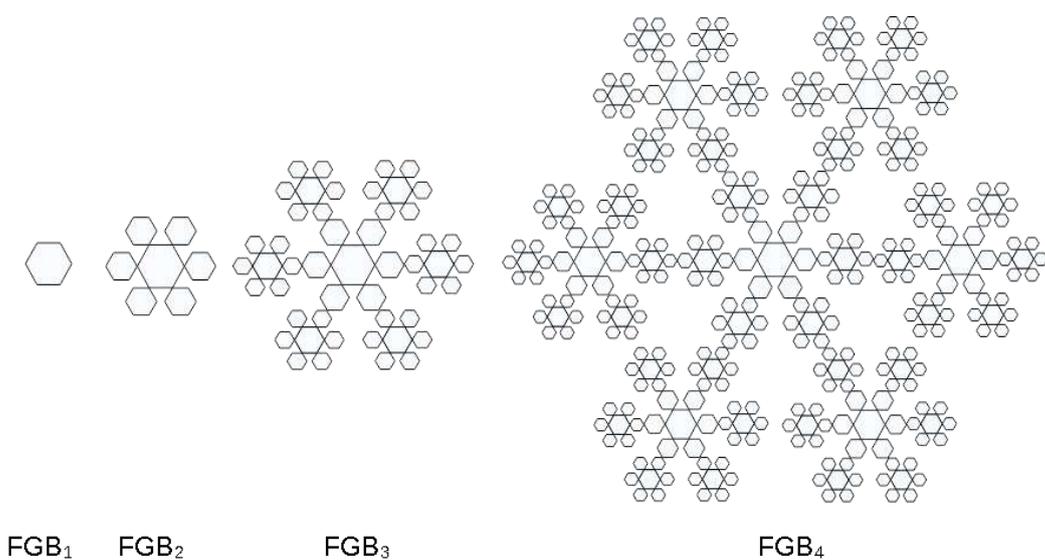


Figure 1: Fractal Growth of Benzene FGB_1 , FGB_2 , FGB_3 and FGB_4 .

The following theorem computes the M-polynomial of fractal growth of benzene.

Theorem 1. *Let FGB_n be a fractal growth of benzene where n is the number of iterative fractal growth.*

(i) *If $n = 1$, then $M(FGB_1; x, y) = 6x^2y^2$.*

(ii) *If $n \geq 2$, then $M(FGB_n; x, y) = [20(7^{n-2}) + 4]x^2y^2 + [16(7^{n-2}) - 4]x^2y^4 + 6(7^{n-2})x^4y^4$.*

Proof. Assume that FGB_n is the fractal growth of benzene as shown in Figure 4, $|\mathcal{V}(FGB_n)| = |\mathcal{V}(FGB_{n-1})| + 6|\mathcal{V}(FGB_{n-1}) - 1|$ and $|\mathcal{E}(FGB_n)| = 6(7^{n-1})$, where $n \geq 2$.

(i) For $n = 1$, the edge set $\mathcal{E}(FGB_1)$ has only one partition

$$|\mathcal{E}(2, 2)| = |e = uv \in \mathcal{E}(FGB_1) : d_u = 2 \text{ and } d_v = 2| = 6.$$

Hence, the M-polynomial for FGB_1 is

$$\begin{aligned} M(FGB_1; x, y) &= \sum_{\delta \leq \alpha \leq \beta \leq \Delta} m_{\alpha, \beta} x^\alpha y^\beta \\ &= \sum_{2 \leq 2} m_{2, 2} x^2 y^2 \\ &= 6x^2 y^2. \end{aligned}$$

(ii) For $n \geq 2$, the edge set $\mathcal{E}(FGB_n)$ can be divided into the following three parts $|\mathcal{E}(2, 2)| = |e = uv \in \mathcal{E}(FGB_n) : d_u = 2 \text{ and } d_v = 2| = 20(7^{n-2}) + 4$, $|\mathcal{E}(2, 4)| = |e = uv \in \mathcal{E}(FGB_n) : d_u = 2 \text{ and } d_v = 4| = 16(7^{n-2}) - 4$, and $|\mathcal{E}(4, 4)| = |e = uv \in \mathcal{E}(FGB_n) : d_u = 4 \text{ and } d_v = 4| = 6(7^{n-2})$.

Hence, the M-polynomial of FGB_n is

$$\begin{aligned} M(FGB_n; x, y) &= \sum_{\delta \leq \alpha \leq \beta \leq \Delta} m_{\alpha, \beta} x^\alpha y^\beta \\ &= \sum_{2 \leq 2} m_{2, 2} x^2 y^2 + \sum_{2 \leq 4} m_{2, 4} x^2 y^4 + \sum_{4 \leq 4} m_{4, 4} x^4 y^4 \\ &= [20(7^{n-2}) + 4]x^2 y^2 + [16(7^{n-2}) - 4]x^2 y^4 + 6(7^{n-2})x^4 y^4. \end{aligned}$$

Degree-based topological indices of fractal growth of benzene $FGB_n, n \geq 2$ are given in the next proposition.

Proposition 1. *Let FGB_n be a fractal growth of benzene where $n \geq 2$, then*

$$(i) \quad M_1(FGB_n) = 32(7^{n-1}) - 8.$$

$$(ii) \quad M_2(FGB_n) = 304(7^{n-2}) - 16.$$

$$(iii) \quad MM_2(FGB_n) = \frac{59}{8}(7^{n-2}) + \frac{1}{2}.$$

$$(iv) \quad R_\gamma(FGB_n) = [5(2^{2\gamma+2}) + 2^{3\gamma+4} + 3(2^{4\gamma+1})](7^{n-2}) + 2^{2\gamma+2} - 2^{3\gamma+2}.$$

$$(v) \quad SSD(FGB_n) = 92(7^{n-2}) - 2.$$

$$(vi) \quad H(FGB_n) = \frac{101}{6}(7^{n-2}) + \frac{2}{3}.$$

$$(vii) \quad I(FGB_n) = \frac{160}{3}(7^{n-2}) - \frac{4}{3}.$$

Proof. Since, $M(FGB_n; x, y) = [20(7^{n-2}) + 4]x^2 y^2 + [16(7^{n-2}) - 4]x^2 y^4 + 6(7^{n-2})x^4 y^4$, using above operators we get:

$$\begin{aligned}
 D_x(FGB_n) &= 2[20(7^{n-2}) + 4]x^2y^2 + 2[16(7^{n-2}) - 4]x^2y^4 + 24(7^{n-2})x^4y^4, \\
 D_y(FGB_n) &= 2[20(7^{n-2}) + 4]x^2y^2 + 4[16(7^{n-2}) - 4]x^2y^4 + 24(7^{n-2})x^4y^4, \\
 D_xD_y(FGB_n) &= 4[20(7^{n-2}) + 4]x^2y^2 + 8[16(7^{n-2}) - 4]x^2y^4 + 96(7^{n-2})x^4y^4, \\
 S_x(FGB_n) &= [10(7^{n-2}) + 2]x^2y^2 + [8(7^{n-2}) - 2]x^2y^4 + \frac{3}{2}(7^{n-2})x^4y^4, \\
 S_y(FGB_n) &= [10(7^{n-2}) + 2]x^2y^2 + [4(7^{n-2}) - 1]x^2y^4 + \frac{3}{2}(7^{n-2})x^4y^4, \\
 S_xS_y(FGB_n) &= [5(7^{n-2}) + 1]x^2y^2 + \frac{1}{2}[4(7^{n-2}) - 1]x^2y^4 + \frac{3}{8}(7^{n-2})x^4y^4, \\
 S_xD_y(FGB_n) &= [20(7^{n-2}) + 4]x^2y^2 + 2[16(7^{n-2}) - 4]x^2y^4 + 6(7^{n-2})x^4y^4, \\
 S_yD_x(FGB_n) &= [20(7^{n-2}) + 4]x^2y^2 + \frac{1}{2}[16(7^{n-2}) - 4]x^2y^4 + 6(7^{n-2})x^4y^4, \\
 S_xJ(FGB_n) &= [5(7^{n-2}) + 1]x^4 + \frac{2}{3}[4(7^{n-2}) - 1]x^6 + \frac{3}{4}(7^{n-2})x^8, \\
 S_xJ(D_xD_y(FGB_n)) &= [20(7^{n-2}) + 4]x^4 + \frac{4}{3}[16(7^{n-2}) - 4]x^6 + 12(7^{n-2})x^8, \\
 D_x^\gamma D_y^\gamma(FGB_n) &= 2^{2\gamma+2}[5(7^{n-2}) + 1]x^2y^2 + 2^{3\gamma+2}[4(7^{n-2}) - 1]x^2y^4 + 3(2^{4\gamma+1})(7^{n-2})x^4y^4.
 \end{aligned}$$

Thus,

- (i) $M_1(FGB_n) = (D_x + D_y)(M(FGB_n; x, y))|_{x=y=1} = 32(7^{n-1}) - 8.$
- (ii) $M_2(FGB_n) = (D_xD_y)(M(FGB_n; x, y))|_{x=y=1} = 304(7^{n-2}) - 16.$
- (iii) $MM_2(FGB_n) = (S_xS_y)(M(FGB_n; x, y))|_{x=y=1} = \frac{59}{8}(7^{n-2}) + \frac{1}{2}.$
- (iv) $R_\gamma(FGB_n) = (D_x^\gamma D_y^\gamma)(M(FGB_n; x, y))|_{x=y=1} = [5(2^{2\gamma+2}) + 2^{3\gamma+4} + 3(2^{4\gamma+1})](7^{n-2}) + 2^{2\gamma+2} - 2^{3\gamma+2}.$
- (v) $SSD(FGB_n) = (S_yD_x + S_xD_y)(M(FGB_n; x, y))|_{x=y=1} = 92(7^{n-2}) - 2.$
- (vi) $H(FGB_n) = (2S_xJ)(M(FGB_n; x, y))|_{x=1} = \frac{101}{6}(7^{n-2}) + \frac{2}{3}.$
- (vii) $I(FGB_n) = (S_xJ)(D_xD_y(M(FGB_n; x, y)))|_{x=1} = \frac{160}{3}(7^{n-2}) - \frac{4}{3}.$

2.2. Pythagoras tree

Pythagoras tree (PT_n), $n \geq 1$ is a fractal that begins with a square. It involves creating a right isosceles triangle with its hypotenuse along the top edge of the square. Squares are then constructed along the other two sides of this triangle. This process is repeated recursively for each new square created. See Figure 2.

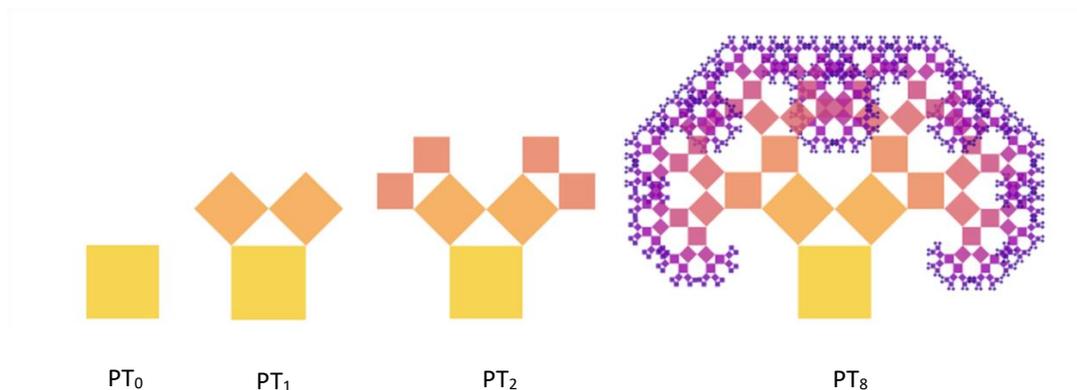


Figure 2: Pythagoras tree PT_0 , PT_1 , PT_2 and PT_8 .

In the rest of this subsection, we determine the M-polynomial of the Pythagoras tree and with the help of the M-polynomial, we find some degree-based topological indices. The next theorem presents the calculation of the M-polynomial for the Pythagoras tree.

Theorem 2. Let $PT_n, n \geq 1$ be the Pythagoras tree. Then, $M(PT_n; x, y) = (1 + 2^n)x^2y^2 + (2 + 2^{n+1})x^2y^4 + (5 \cdot 2^n - 7)x^4y^4$.

Proof. Let $PT_n, n \geq 1$ be the Pythagoras tree as shown in Figure 2. Then,

$$|\mathcal{V}(PT_n)| = 5 \cdot 2^n - 1 \text{ and } |\mathcal{E}(PT_n)| = (2^{n+3} - 4).$$

The edge set $\mathcal{E}(PT_n)$ can be divided into the following three parts:

$$|\mathcal{E}(2, 2)| = |e = uv \in \mathcal{E}(PT_n) : d_u = 2 \text{ and } d_v = 2| = 1 + 2^n,$$

$$|\mathcal{E}(2, 4)| = |e = uv \in \mathcal{E}(PT_n) : d_u = 2 \text{ and } d_v = 4| = 2 + 2^{n+1}, \text{ and}$$

$$|\mathcal{E}(4, 4)| = |e = uv \in \mathcal{E}(PT_n) : d_u = 4 \text{ and } d_v = 4| = 5 \cdot 2^n - 7.$$

Thus, the M-polynomial of PT_n is given as:

$$\begin{aligned} M(PT_n; x, y) &= \sum_{\delta \leq \alpha \leq \beta \leq \Delta} m_{\alpha, \beta} x^\alpha y^\beta \\ &= \sum_{2 \leq 2} m_{2, 2} x^2 y^2 + \sum_{2 \leq 4} m_{2, 4} x^2 y^4 + \sum_{4 \leq 4} m_{4, 4} x^4 y^4 \\ &= |\mathcal{E}(2, 2)| x^2 y^2 + |\mathcal{E}(2, 4)| x^2 y^4 + |\mathcal{E}(4, 4)| x^4 y^4 \\ &= (1 + 2^n)x^2 y^2 + (2 + 2^{n+1})x^2 y^4 + (5 \cdot 2^n - 7)x^4 y^4. \end{aligned}$$

Now, We provide several topological indices based on degrees using the M-polynomial of the Pythagoras tree.

Proposition 2. Let $PT_n, n \geq 1$ be the Pythagoras tree. Then,

$$(i) M_1(PT_n) = 56 \cdot 2^n - 40.$$

$$(ii) M_2(PT_n) = 100 \cdot 2^n - 92.$$

$$(iii) MM_2(PT_n) = \frac{13}{16} \cdot 2^n + \frac{1}{16}.$$

$$(iv) R_\gamma(PT_n) = (1 + 2^{\gamma+1} - 7 \cdot 2^{2\gamma})2^{2\gamma} + (1 + 2^{\gamma+1} + 5 \cdot 2^{2\gamma})2^{2\gamma+n}.$$

$$(v) SSD(PT_n) = 17 \cdot 2^n - 7.$$

$$(vi) H(PT_n) = \frac{29}{12}(2^n) - \frac{7}{12}.$$

$$(vii) I(PT_n) = \frac{41}{3}2^n - \frac{31}{3}.$$

Proof. Since, $M(PT_n; x, y) = (1 + 2^n)x^2y^2 + (2 + 2^{n+1})x^2y^4 + (5 \cdot 2^n - 7)x^4y^4$. Then, we have

$$D_x(PT_n) = 2(1 + 2^n)x^2y^2 + 2(2 + 2^{n+1})x^2y^4 + 4(5 \cdot 2^n - 7)x^4y^4,$$

$$D_y(PT_n) = 2(1 + 2^n)x^2y^2 + 4(2 + 2^{n+1})x^2y^4 + 4(5 \cdot 2^n - 7)x^4y^4,$$

$$D_x D_y(PT_n) = 4(1 + 2^n)x^2y^2 + 8(2 + 2^{n+1})x^2y^4 + 16(5 \cdot 2^n - 7)x^4y^4,$$

$$D_x^3 D_y^3(PT_n) = 64(1 + 2^n)x^2y^2 + 512(2 + 2^{n+1})x^2y^4 + 4096(5 \cdot 2^n - 7)x^4y^4,$$

$$S_x(PT_n) = \frac{1}{2}(1 + 2^n)x^2y^2 + \frac{1}{2}(2 + 2^{n+1})x^2y^4 + \frac{1}{4}(5 \cdot 2^n - 7)x^4y^4,$$

$$S_y(PT_n) = \frac{1}{2}(1 + 2^n)x^2y^2 + \frac{1}{4}(2 + 2^{n+1})x^2y^4 + \frac{1}{4}(5 \cdot 2^n - 7)x^4y^4,$$

$$S_x S_y(PT_n) = \frac{1}{4}(1 + 2^n)x^2y^2 + \frac{1}{8}(2 + 2^{n+1})x^2y^4 + \frac{1}{16}(5 \cdot 2^n - 7)x^4y^4,$$

$$S_x D_y(PT_n) = (1 + 2^n)x^2y^2 + 2(2 + 2^{n+1})x^2y^4 + (5 \cdot 2^n - 7)x^4y^4,$$

$$S_y D_x(PT_n) = (1 + 2^n)x^2y^2 + \frac{1}{2}(2 + 2^{n+1})x^2y^4 + (5 \cdot 2^n - 7)x^4y^4,$$

$$S_x J(PT_n) = \frac{i}{4}(1 + 2^n)x^4 + \frac{1}{6}(2 + 2^{n+1})x^6 + \frac{1}{8}(5 \cdot 2^n - 7)x^8,$$

$$S_x J(D_x D_y(PT_n)) = (1 + 2^n)x^4 + \frac{4}{3}(2 + 2^{n+1})x^6 + 2(5 \cdot 2^n - 7)x^8,$$

$$D_x^\gamma D_y^\gamma(PT_n) = 2^{2\gamma}(1 + 2^n)x^2y^2 + 2^{3\gamma}(2 + 2^{n+1})x^2y^4 + 2^{4\gamma}(5 \cdot 2^n - 7)x^4y^4,$$

Thus,

$$(i) M_1(PT_n) = (D_x + D_y)(M(FGB_n; x, y))|_{x=y=1} = 56 \cdot 2^n - 40.$$

$$(ii) M_2(PT_n) = (D_x D_y)(M(FGB_n; x, y))|_{x=y=1} = 100 \cdot 2^n - 92.$$

$$(iii) MM_2(PT_n) = (S_x S_y)(M(FGB_n; x, y))|_{x=y=1} = \frac{13}{16} \cdot 2^n + \frac{1}{16}.$$

$$(iv) R_\gamma(PT_n) = (D_x^\gamma D_y^\gamma)(M(FGB_n; x, y))|_{x=y=1} = (1 + 2^{\gamma+1} - 7 \cdot 2^{2\gamma})2^{2\gamma} + (1 + 2^{\gamma+1} + 5 \cdot 2^{2\gamma})2^{2\gamma+n}.$$

$$(v) SSD(PT_n) = (S_y D_x + S_x D_y)(M(FGB_n; x, y))|_{x=y=1} = 17 \cdot 2^n - 7.$$

$$(vi) H(PT_n) = (2S_x J)(M(FGB_n; x, y))|_{x=1} = \frac{29}{12}(2^n) - \frac{7}{12}.$$

$$(vii) I(PT_n) = S_x J(D_x D_y(M(FGB_n; x, y)))|_{x=1} = \frac{41}{3}2^n - \frac{31}{3}.$$

2.3. Dendrimer of Benzene

A dendrimer is also one kind of a graph that is never-ending in its iterative growth, it possesses molecular architecture has three domains central, branches, and terminal. As shown in next Figure 3.

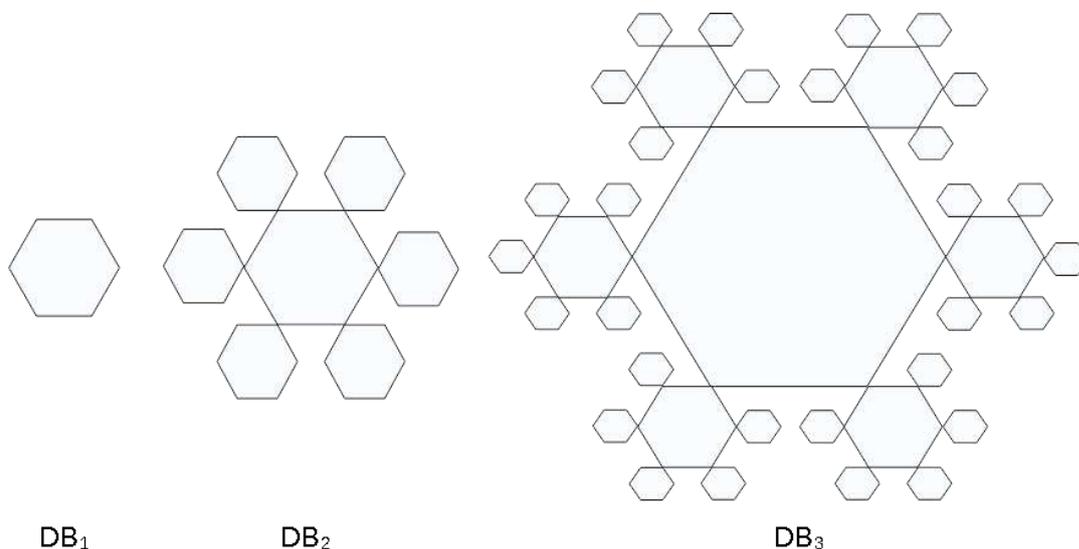


Figure 3: Dendrimer of Benzene DB_1 , DB_2 and DB_3 .

M-polynomial of dendrimer graph is given in theorem 3.

Theorem 3. Let DB_n be a dendrimer of benzene where n is the number of iterative growth of the dendrimer.

(i) If $n = 1$, then $M(DB_1; x, y) = 6x^2y^2$.

(ii) If $n \geq 2$, then $M(DB_n; x, y) = 24(5^{n-2})x^2y^2 + 12(5^{n-2})x^2y^4 + (9 \cdot 5^{n-2} - 3)x^4y^4$.

Proof. Let $DB_n, n \geq 1$ is the dendrimer of benzene as shown in Figure 3, then $|\mathcal{V}(DB_n)| = \frac{3}{2}(5^n - 1)$ and $|\mathcal{E}(DB_n)| = 6 + 9 \cdot 5^{n-1} - 3$.

(i) For $n = 1$, the prove is same as in theorem 1.

(ii) For $n \geq 2$, the edge set $\mathcal{E}(DB_n)$ has three partitions:

$$|\mathcal{E}_{(2,2)}| = |e = uv \in \mathcal{E}(FGB_n) : d_u = 2 \text{ and } d_v = 2| = 24(5^{n-2}). \quad |\mathcal{E}_{(2,4)}| = |e = uv \in \mathcal{E}(FGB_n) : d_u = 2 \text{ and } d_v = 4| = 12(5^{n-2}). \quad |\mathcal{E}_{(4,4)}| = |e = uv \in \mathcal{E}(FGB_n) : d_u = 4 \text{ and } d_v = 4| = 6 + 9 \cdot 5^{n-2} - 3.$$

Hence, the M-polynomial of DB_n is

$$\begin{aligned} M(DB_n; x, y) &= \sum_{\delta \leq \alpha \leq \beta \leq \Delta} m_{\alpha, \beta} x^\alpha y^\beta \\ &= \sum_{2 \leq 2} m_{2,2} x^2 y^2 + \sum_{2 \leq 4} m_{2,4} x^2 y^4 + \sum_{4 \leq 4} m_{4,4} x^4 y^4 \\ &= 24(5^{n-2})x^2 y^2 + 12(5^{n-2})x^2 y^4 + [6 + 9(5^{n-2} - 1)]x^4 y^4. \end{aligned}$$

The following proposition provides the degree-based topological indices for the benzene dendrimer $DB_n, n \geq 2$.

Proposition 3. *Let DB_n be a dendrimer of benzene where $n \geq 2$, then*

- (i) $M_1(DB_n) = 48(5^{n-1}) - 24.$
- (ii) $M_2(DB_n) = 336(5^{n-2}) - 48.$
- (iii) $MM_2(DB_n) = \frac{129}{16}(5^{n-2}) - \frac{3}{16}.$
- (iv) $R_\gamma(DB_n) = 3 \cdot 2^{2\gamma} \cdot 5^{n-2} [8 + 2^{\gamma+2} + 3 \cdot 2^{2\gamma}] - 3 \cdot 2^{4\gamma}.$
- (v) $SSD(DB_n) = 96(5^{n-2}) - 6.$
- (vi) $H(DB_n) = \frac{73}{4}(5^{n-2}) - \frac{3}{4}.$
- (vii) $I(DB_n) = 58(5^{n-2}) - 6.$

Proof. Since, $M(DB_n; x, y) = 24(5^{n-2})x^2 y^2 + 12(5^{n-2})x^2 y^4 + (9 \cdot 5^{n-2} - 3)x^4 y^4.$, using above operators we get:

$$\begin{aligned} D_x(DB_n) &= 48(5^{n-2})x^2 y^2 + 24(5^{n-2})x^2 y^4 + 4(9 \cdot 5^{n-2} - 3)x^4 y^4., \\ D_y(DB_n) &= 48(5^{n-2})x^2 y^2 + 48(5^{n-2})x^2 y^4 + 4(9 \cdot 5^{n-2} - 3)x^4 y^4., \\ D_x D_y(DB_n) &= 96(5^{n-2})x^2 y^2 + 96(5^{n-2})x^2 y^4 + 16(9 \cdot 5^{n-2} - 3)x^4 y^4., \\ S_x(DB_n) &= 12(5^{n-2})x^2 y^2 + 6(5^{n-2})x^2 y^4 + \frac{1}{4}(9 \cdot 5^{n-2} - 3)x^4 y^4., \\ S_y(DB_n) &= 12(5^{n-2})x^2 y^2 + 3(5^{n-2})x^2 y^4 + \frac{1}{4}(9 \cdot 5^{n-2} - 3)x^4 y^4., \\ S_x S_y(DB_n) &= 6(5^{n-2})x^2 y^2 + \frac{3}{2}(5^{n-2})x^2 y^4 + \frac{1}{16}(9 \cdot 5^{n-2} - 3)x^4 y^4., \\ S_x D_y(DB_n) &= 24(5^{n-2})x^2 y^2 + 24(5^{n-2})x^2 y^4 + (9 \cdot 5^{n-2} - 3)x^4 y^4., \\ S_y D_x(DB_n) &= 24(5^{n-2})x^2 y^2 + 6(5^{n-2})x^2 y^4 + (9 \cdot 5^{n-2} - 3)x^4 y^4., \\ S_x J(DB_n) &= 6(5^{n-2})x^2 y^2 + 2(5^{n-2})x^2 y^4 + \frac{1}{8}(9 \cdot 5^{n-2} - 3)x^4 y^4., \\ S_x J(D_x D_y(DB_n)) &= 24(5^{n-2})x^2 y^2 + 16(5^{n-2})x^2 y^4 + 2(9 \cdot 5^{n-2} - 3)x^4 y^4., \\ D_x^\gamma D_y^\gamma(DB_n) &= 3 \cdot 2^{2\gamma+3} \cdot 5^{n-2} x^2 y^2 + 3 \cdot 2^{3\gamma+2} \cdot 5^{n-2} x^2 y^4 + 2^{4\gamma}(9 \cdot 5^{n-2} - 3)x^4 y^4.. \end{aligned}$$

Thus,

- (i) $M_1(FGB_n) = (D_x + D_y)(M(FGB_n; x, y))|_{x=y=1} = 48(5^{n-1}) - 24.$
- (ii) $M_2(FGB_n) = (D_x D_y)(M(FGB_n; x, y))|_{x=y=1} = 336(5^{n-2}) - 48.$
- (iii) $MM_2(FGB_n) = (S_x S_y)(M(FGB_n; x, y))|_{x=y=1} = \frac{129}{16}(5^{n-2}) - \frac{3}{16}.$
- (iv) $R_\gamma(FGB_n) = (D_x^\gamma D_y^\gamma)(M(FGB_n; x, y))|_{x=y=1} = 3 \cdot 2^{2\gamma} \cdot 5^{n-2} [8 + 2^{\gamma+2} + 3 \cdot 2^{2\gamma}] - 3 \cdot 2^{4\gamma}.$
- (v) $SSD(FGB_n) = (S_y D_x + S_x D_y)(M(FGB_n; x, y))|_{x=y=1} = 96(5^{n-2}) - 6.$
- (vi) $H(FGB_n) = (2S_x J)(M(FGB_n; x, y))|_{x=1} = \frac{73}{4}(5^{n-2}) - \frac{3}{4}.$
- (vii) $I(FGB_n) = (S_x J)(D_x D_y(M(FGB_n; x, y)))|_{x=1} = 58(5^{n-2}) - 6.$

Remark 1. The order and size of all graphs is given by geometric series.

2.4. Plotting Representation

Our figures 2D and 3D of M-polynomials and topological indices are obtained by *Wolfram Mathematica*.

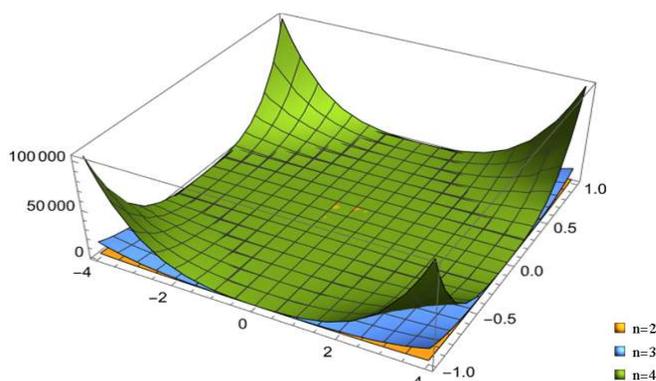


Figure 4: A 3D representation of the M-polynomial for benzene's fractal growth with n=2,3 and 4.

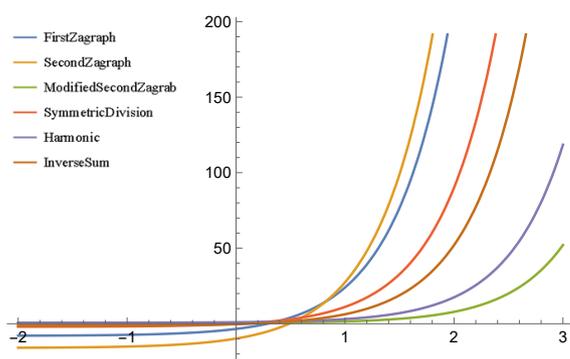


Figure 5: A 2D representation of degree-based topological indices derived from the M-polynomial of benzene's fractal growth.

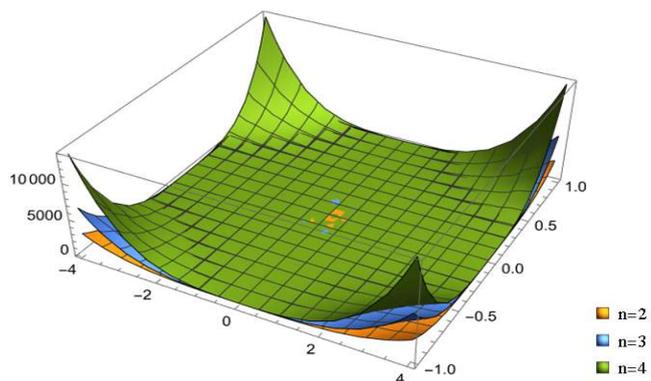


Figure 6: A 3D representation of the M-polynomial for a Pythagoras tree with $n=2,3$ and 4.

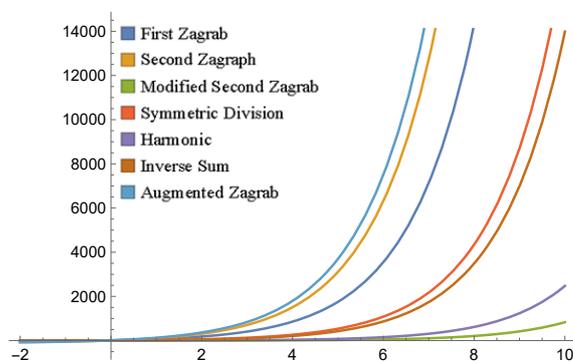


Figure 7: A 2D representation of degree-based topological indices derived from the M-polynomial of a Pythagoras tree.

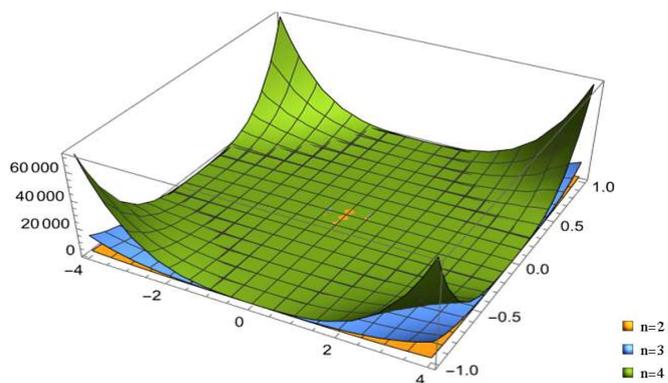


Figure 8: A 3D representation of the M-polynomial for a benzene dendrimer with $n=2,3$ and 4.

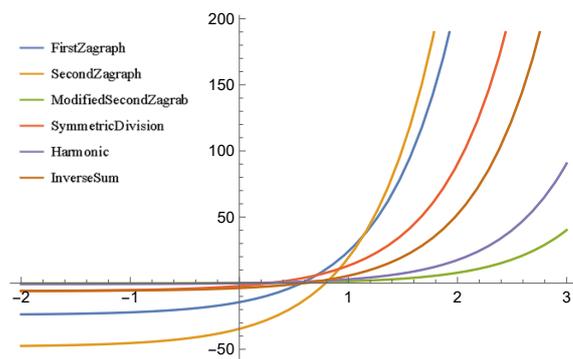


Figure 9: A 2D representation of degree-based topological indices derived from the M-polynomial of a benzene dendrimer.

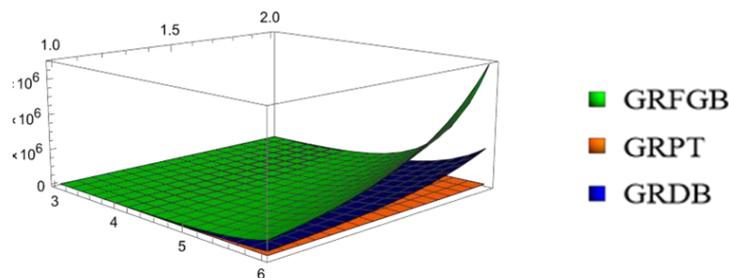


Figure 10: A 3D representation of the general Randic index for above three graphs with $n=3,6$ and $\gamma=1,2$

3. Conclusions

In this article, we have derived the general forms of the M-polynomials for the fractal growth patterns of benzene ($FGB_n, n \geq 1$), the Pythagoras tree ($PT_n, n \geq 1$), and the benzene dendrimer ($DB_n, n \geq 2$). Additionally, we computed degree-based topological indices associated with these polynomials. The graphical representations in Figures (4, 6, 8) illustrate the M-polynomial graphs for the fractal growth patterns of benzene FGB_n , the Pythagoras tree PT_n , and the benzene dendrimer DB_n for $n = 2, 3, 4$. It is evident that as n increases, the graph in Figure 4 becomes larger than that in Figure 8, and both surpass the graph in Figure 8. Similarly, the topological indices shown in Figure 5 are greater than those in Figure 7, which in turn are larger than those in Figure 9. These findings highlight the trends in graph growth and the corresponding indices as the fractal structure evolves.

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