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M-Polynomials and degree-based topological indices of the two dimensional Coronene fractal structures

Muhammad Asif Javed, A. Q. Baig, Mukhtar Ahmad*, Roslan Hasni, Kai Siong Yow and Ather Qayyum

ABSTRACT: Topological indices are numerical descriptors widely used to investigate the structural, physical, and chemical properties of molecular compounds. Among them, degree-based topological indices have demonstrated strong correlations with a variety of molecular characteristics, making them a central topic in chemical graph theory. The M-polynomial serves as a powerful generating function for deriving such indices. In this study, we present closed-form expressions for several important degree-based topological indices associated with the zigzag molecular graph of two-dimensional coronene fractal structures. The indices examined include the first and second Zagreb indices, the modified Zagreb index, the symmetric division index, the harmonic index, the Randić index, the inverse Randić index, and the augmented Zagreb index. The derivations are carried out using a calculus-based approach, offering deeper insights into the topological and structural features of these nanostructures.

Key Words: Topological indices; M-polynomial; zagreb indices; symmetric division index; augmented zagreb index; two-dimensional coronene fractal structures.

Contents

1. Introduction

Graphs that represent both the structure and connectivity of molecules are referred to as molecular graphs. These graphs serve as a topological characterization of molecules, where atoms are represented as vertices and chemical bonds as edges. In molecular graphs, the shape and physicochemical or biological properties of a compound are encapsulated through a topological framework. Topological indices, particularly those used in Quantitative Structure–Activity Relationship (QSAR) and Quantitative Structure–Property Relationship (QSPR) studies, have become vital tools in cheminformatics, molecular modeling, and computational drug discovery [7,11].

These indices correlate well with various physicochemical and biological characteristics of molecules, making them effective descriptors for chemical informatics applications [15,21]. Some indices have demonstrated strong parallels with empirical properties, as highlighted in [3,22].

Mathematically, molecular graphs provide an abstract representation of molecules using vertices and edges. Based on this representation, numerous topological indices have been developed and broadly classified into three main categories:

- Degree-based indices,
- Distance-based indices,
- Spectral-based indices.

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Among these, degree-based indices are particularly prominent due to their direct association with structural features such as molecular branching and atomic connectivity. These indices have been extensively studied and exhibit strong correlations with a range of molecular properties, including chemical reactivity, biological activity, and physical attributes [4,18]. Additionally, comparative studies have shown meaningful relationships between distance-based and degree-based indices [17].

The M-polynomial, introduced as a generating function for encoding degree-based topological descriptors, has attracted considerable attention. It enables the unified computation of multiple indices through analytical methods. Significant contributions in this area include the computation of M-polynomials for polyhex nanotubes [24], nanostar dendrimers [21], titania nanotubes [22], and triangular boron nanotubes [23]. M-polynomials also underpin the derivation of topological indices for V-phenylenic nanotubes and nanotori.

In this paper, we focus on deriving the M-polynomial and associated degree-based topological indices of the two-dimensional zigzag coronene fractal structures, denoted by $ZHCF_n(p,q)$. These structures are of significant interest due to their diverse applications in solar cells, chemical sensors, lithium-ion batteries, and photocatalysis [31,33]. They offer several advantages, including non-toxicity, photochemical activity, pigment and fungicide properties, affordability, and a narrow bandgap that allows excitation under visible light.

The motivation for studying $ZHCF_n(p,q)$ lies in its practical relevance and rich structural topology. Figures 1 and 2 illustrate the architecture of $ZHCF_n(p,q)$, highlighting its role in coloration reactions such as Benedict's test. In this work, we consider a monolayer structure with p and q unit cells arranged in the plane, forming the basis for calculating the M-polynomial and deriving closed-form expressions for various degree-based topological indices.

2. Literature Review

In 2015 observed the definition of the M-Polynomial by S. Klavzar or E. Deutsch [15,33]. We compete the necessary role of the M-polynomial within the factors of degree-based topological indices see to [1,3, 10,35] for further reading sources. M-polynomial is the most well-known general progressive polynomial and offers ten topological indices based on distance as well as an extra closed formula. It is explained as

$$M(\eth,x,y)=\sum_{\wp\le i\le j\le\Re} m_{ij}(\eth)x^iy^j \tag{2.1}$$

and we have $\wp=\text{Min }\{d_t|t\epsilon V(\eth)\}$ and $\Re=\text{Max }\{d_t|t\epsilon V(\eth)\}$, where $m_{ij}(\eth)$ is the edge $E(\eth)$, where $i\le j$

Topological Indices Based on Degrees. Molecular descriptors are functions on a graph that aren't determined by the numbers of their vertices. This is also known as the topological index. In the fields of pharmaceutical drug forms, chemical validation, isomeric discrimination, QSAR, and QSPR, topological indices are especially useful. Topological indices are accessible through the molecule system. Several important degree-based topological indices have been defined and are listed below. Gutman and Trinajstic introduced the original Zagreb index, which is as follows:

$$M_1(\eth)=\sum_{ts\epsilon E(\eth)}(\eta_t+\eta_s) \tag{2.2}$$

In 1972, According to Gutman and Trinajstic, the second Zagreb index is

$$M_2(\eth)=\sum_{ts\epsilon E(\eth)}(\eta_t\times\eta_s) \tag{2.3}$$

It is defined as the second modified Zagreb index.

$$m_{M_2}(\eth)=\sum_{ts\epsilon E(\eth)}\frac{1}{\eta(t)\eta(s)} \tag{2.4}$$

According to Kulli, Stone, Wang, and Wei, the general first and second multiplicative Zagreb indices are expressed as

$$MZ_1{}^xII(\eth)=\prod_{ts\epsilon E(\eth)}(\eta_t+\eta_s)^x$$

$$MZ_2{}^xII(ð) = \prod_{ts\epsilon E(ð)} (\eta_t + \eta_s)^x \tag{2.5}$$

According to Kulli, Stone, Wang, and Wei, the general first and second Zagreb indices are as follows:

$$Z_1{}^xII(ð) = \sum_{ts\epsilon E(ð)} (\eta_t + \eta_s)^x$$

$$Z_2{}^xII(ð) = \sum_{ts\epsilon E(ð)} (\eta_t \eta_s)^x \tag{2.6}$$

The harmonic index was proposed by Fajtlowicz in 1987 and stated in [15].

$$H(ð) = \sum_{ts\epsilon E(ð)} \frac{2}{(\eta_t + \eta_s)} \tag{2.7}$$

An explanation of the inverse sum index:

$$I(ð) = \sum_{ts\epsilon E(ð)} \frac{(\eta_t \eta_s)}{(\eta_t + \eta_s)} \tag{2.8}$$

Symmetric division index is detailed as:

$$SSD(ð) = \sum_{ts\epsilon E(ð)} \frac{min(\eta_t, \eta_s)}{max(\eta_t, \eta_s)} + \frac{min(\eta_t, \eta_s)}{max(\eta_t, \eta_s)} \tag{2.9}$$

The DU and FU The general Randic index, also known as the general multiplicative Randic index, is widely accepted to be as follows:

$$P_x(ð) = \sum_{ts\epsilon E(ð)} \eta_t + \eta_s{}^x$$

$$P_xII(ð) = \prod_{ts\epsilon E(ð)} \eta_t + \eta_s{}^x \tag{2.10}$$

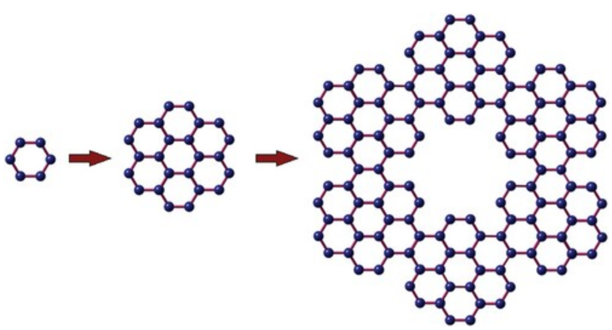

Figure 1: The structure of coronene fractal $ZCHCF_1$

The order and size of structure of coronene fractal $ZHCF_{(n)}$

$$|V| = 3(57p^2 + q)$$

$$|E| = 6(21p^2 + q)$$

$$|E_1(ð)| = 27pq + 2q + p$$

$$|E_2(ð)| = 54pq + 4p + 2q \tag{2.11}$$

$$|E_2(ð)| = 90pq - 4q - 2p$$

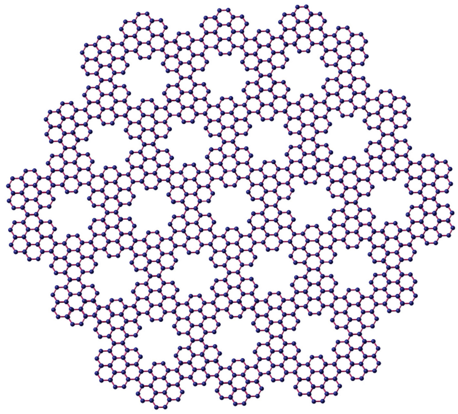

Figure 2: Coronene fractal structures $ZCHCF_3$

3. Main Results

In this work, we investigated the zigzag molecular graph of the two-dimensional coronene fractal structure, denoted by $\eth \approx ZCHCF_n[p, q]$, where $p, q \geq 1$. Using calculus-based techniques, we derived explicit closed-form expressions for several degree-based topological indices. The main results are summarized below:

Theorem 3.1 *Let $\mathcal{ZCHCF}_n[p, q]$ denote the zigzag molecular graph of the two-dimensional coronene fractal structure, where $p, q \geq 1$. Then,*

$$M(\eth; x, y) = f(x; y) = (27pq + 2q + p)x^2y^2 + (54pq + 4p + 2q)x^2y^3 + (90pq - 4q - 2p)x^3y^3 \qquad (3.1)$$

Proof:

Let G be the zigzag molecular graph of the two-dimensional coronene fractal structure denoted by $ZHCF_n[o, p, q]$, where $o, p, q \geq 1$. The edge set of $ZHCF_n[o, p, q]$ is partitioned into the following three subsets, as illustrated in Figures 1 and 2.

$$\begin{aligned} E_1 &= E_{(2\sim 2)} = \{e = ts \in E(\eth) | \eta_r = 2 \backsim \eta_s = 2\} \\ E_2 &= E_{(2\sim 3)} = \{e = ts \in E(\eth) | \eta_r = 2 \backsim \eta_s = 3\} \\ E_3 &= E_{(3\sim 3)} = \{e = ts \in E(\eth) | \eta_r = 3 \backsim \eta_s = 3\} \end{aligned} \qquad (3.2)$$

such that

Consequently, the M-polynomial with $ZHCF_n$[o; p; q] is

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

$$M(\eth, x, y) = \sum_{2 \leq 2} m_{22}(\eth) x^2 y^2 + \sum_{2 \leq 3} m_{23}(\eth) x^2 y^3 + \sum_{2 \leq 3} m_{33}(\eth) x^3 y^3$$

$$M(\eth, x, y) = \sum_{ts \epsilon E(\eth)} m_{22}(\eth) x^2 y^2 + \sum_{ts \epsilon E(\eth)} m_{23}(\eth) x^2 y^3 + \sum_{ts \epsilon E(\eth)} m_{33}(\eth) x^3 y^3 \qquad (3.3)$$

$$M(\eth; x, y) = |E_1(\eth)| x^2 y^2 + |E_2(\eth)| x^2 y^3 + |E_3(\eth)| x^3 y^3$$

$$M(\eth; x, y) = (27pq + 2q + p)x^2y^2 + (54pq + 4p + 2q)x^2y^3 + (90pq - 4q - 2p)x^3y^3$$

Theorem 3.2 *Let $\eth = ZCHCF_n[p,q]$ be the zigzag molecular graph of the two-dimensional coronene fractal structure, where $p, q \geq 1$. Then the first Zagreb index is given by*

$$M_1(\eth) = 918pq + 4p + 2q.$$

Proof: *Let the molecular descriptor generating function be*

$$M(\eth; x, y) = f(x,y) = (27pq + 2q + p)x^2y^2 + (54pq + 4p + 2q)x^2y^3 + (90pq - 4q - 2p)x^3y^3. \quad (3.4)$$

We summarize some key topological indices in the following table:

Topological Index	$f(r,s)$	$M(\eth; r, s)$
First Zagreb index	$r + s$	$M_1(\eth; r, s) = (D_r + D_s)M(\eth; r, s)\big\|_{r=s=1}$
Second Zagreb index	rs	$M_2(\eth; r, s) = (D_r D_s)M(\eth; r, s)\big\|_{r=s=1}$
Second Modified Zagreb index	$1/rs$	$m_{M2}(\eth; r, s) = (\wp_r \wp_s)M(\eth; r, s)\big\|_{r=s=1}$
General Randić index, $a \neq 0$	$(rs)^x$	$R_x(\eth) = (D_r^x + D_s^x)M(\eth; r, s)\big\|_{r=s=1}$
Inverse General Randić index, $a \neq 0$	$1/(rs)^x$	$RR_x(\eth) = (\wp_r^x \wp_s^x)M(\eth; r, s)\big\|_{r=s=1}$
Symmetric Division index	$(r^2 + s^2)/rs$	$SSD(\eth) = \|D_r \wp_s = \wp_s D_r\| M(\eth; r, s)\big\|_{r=s=1}$
Harmonic index	$2/(r+s)$	$H(\eth) = 2\wp_r EM(\eth; r, s)\big\|_{r=1}$
Inverse sum index	$rs/(r+s)$	$I(\eth) = \wp_r J D_r D_s M(\eth; r, s)\big\|_{r=1}$

Table 1: Differential and integral operators: $D_s = s\frac{\partial}{\partial s}M(\eth; r, s)\big|_{r=s=1}$, $D_r = r\frac{\partial}{\partial r}M(\eth; r, s)\big|_{r=s=1}$, $\wp_r = \int_0^r \frac{M(\eth; y, s)}{y}\,dy$, $\wp_s = \int_0^s \frac{M(\eth; r, y)}{y}\,dy$, $J = M(\eth; r, r)$, $W_x = a^x M(\eth; r, s)$, $x \neq 0$

We now compute the first Zagreb index using differential operators. First, compute the partial derivative of $f(x,y)$ with respect to x:

$$\frac{\partial f}{\partial x} = 2(27pq + 2q + p)xy^2 + 2(54pq + 4p + 2q)xy^3 + 3(90pq - 4q - 2p)x^2y^3. \quad (3.5)$$

Multiplying by x yields:

$$D_x = x\frac{\partial f}{\partial x} = 2(27pq + 2q + p)x^2y^2 + 2(54pq + 4p + 2q)x^2y^3 + 3(90pq - 4q - 2p)x^3y^3. \quad (3.6)$$

Similarly, for the partial derivative with respect to y:

$$D_y = y\frac{\partial f}{\partial y} = 2(27pq + 2q + p)x^2y + 3(54pq + 4p + 2q)x^2y^2 + 3(90pq - 4q - 2p)x^3y^2. \quad (3.7)$$

Evaluating the first Zagreb index at $x = y = 1$:

$$M_1(\eth) = [D_x + D_y]\, f(x,y)\big|_{x=y=1} \quad (3.8)$$

$$M_1(\eth) = \Big[2(27pq + 2q + p) + 2(54pq + 4p + 2q) + 3(90pq - 4q - 2p)\Big] + \Big[2(27pq + 2q + p) + 3(54pq + 4p + 2q) + 3(90pq - 4q - 2p)\Big]. \quad (3.9)$$

After simplifying:

$$M_1(\eth) = 918pq + 4p + 2q. \quad \blacksquare \quad (3.10)$$

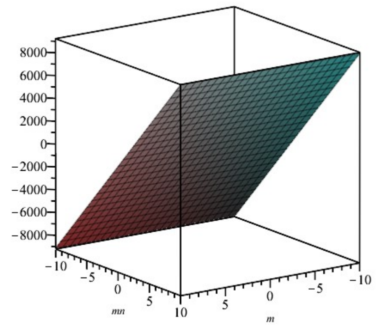

Figure 3: First Zagreb index plotted in 3D

Theorem 3.3 *Let $\eth = ZCHCF_n[p,q]$ be the zigzag molecular graph of the two-dimensional coronene fractal structure, where $p, q \geq 1$. Then the second Zagreb index is given by*

$$M_2(\eth) = 1242pq + 10p - 16q.$$

Proof: *Let the molecular descriptor generating function be*

$$\begin{aligned} M(\eth; x, y) = f(x, y) = {} & (27pq + 2q + p)x^2y^2 + (54pq + 4p + 2q)x^2y^3 \\ & + (90pq - 4q - 2p)x^3y^3. \end{aligned} \tag{3.11}$$

To compute the second Zagreb index, we evaluate the mixed partial operator D_yD_x on $f(x,y)$ at $x = y = 1$. We begin by computing $D_x = x\dfrac{\partial f}{\partial x}$:

$$\begin{aligned} \frac{\partial f}{\partial x} = {} & 2(27pq + 2q + p)xy^2 + 2(54pq + 4p + 2q)xy^3 \\ & + 3(90pq - 4q - 2p)x^2y^3, \end{aligned} \tag{3.12}$$

$$\begin{aligned} D_x = x\frac{\partial f}{\partial x} = {} & 2(27pq + 2q + p)x^2y^2 + 2(54pq + 4p + 2q)x^2y^3 \\ & + 3(90pq - 4q - 2p)x^3y^3. \end{aligned} \tag{3.13}$$

Now compute $D_yD_x = y\dfrac{\partial}{\partial y}(D_x)$:

$$\begin{aligned} \frac{\partial(D_x)}{\partial y} = {} & 4(27pq + 2q + p)x^2y + 6(54pq + 4p + 2q)x^2y^2 \\ & + 9(90pq - 4q - 2p)x^3y^2, \end{aligned} \tag{3.14}$$

$$\begin{aligned} D_yD_x = y\frac{\partial(D_x)}{\partial y} = {} & 4(27pq + 2q + p)x^2y^2 + 6(54pq + 4p + 2q)x^2y^3 \\ & + 9(90pq - 4q - 2p)x^3y^3. \end{aligned} \tag{3.15}$$

Evaluating at $x = y = 1$:

$$\begin{aligned} M_2(\eth) &= D_yD_xf(x,y)\big|_{x=y=1} \\ &= 4(27pq + 2q + p) + 6(54pq + 4p + 2q) + 9(90pq - 4q - 2p). \end{aligned} \tag{3.16}$$

Now simplify:

$$4(27pq + 2q + p) = 108pq + 8q + 4p,$$
$$6(54pq + 4p + 2q) = 324pq + 24p + 12q,$$
$$9(90pq - 4q - 2p) = 810pq - 36q - 18p.$$

Adding the terms:

$$M_2(\eth) = (108 + 324 + 810)pq + (4 + 24 - 18)p + (8 + 12 - 36)q = 1242pq + 10p - 16q. \quad \blacksquare$$

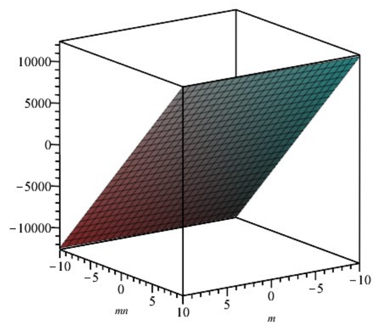

Figure 4: Second Zagreb index plotted in 3D

Theorem 3.4 *Let $\eth = ZCHCF_n[p,q]$ be the zigzag molecular graph of the two-dimensional coronene fractal structure, where $p, q \geq 1$. Then the second modified Zagreb index is given by*

$$m_{M_2}(\eth) = 927pq + 25p + 14q.$$

Proof: *Consider the molecular descriptor generating function:*

$$M(\eth; x, y) = f(x,y) = (27pq + 2q + p)x^2y^2 + (54pq + 4p + 2q)x^2y^3 + (90pq - 4q - 2p)x^3y^3. \tag{3.17}$$

To compute the second modified Zagreb index, we apply the integral operators:

$$S_x = \int_0^x \frac{f(a,y)}{a}\,da, \quad S_y = \int_0^y \frac{S_x(x,b)}{b}\,db.$$

We first compute S_x:

$$\frac{f(a,y)}{a} = (27pq + 2q + p)ay^2 + (54pq + 4p + 2q)ay^3 + (90pq - 4q - 2p)a^2y^3.$$

Integrating term-by-term:

$$\begin{aligned} S_x &= \int_0^x \frac{f(a,y)}{a}\,da \\ &= \frac{1}{2}(27pq + 2q + p)x^2y^2 + \frac{1}{2}(54pq + 4p + 2q)x^2y^3 \\ &\quad + \frac{1}{3}(90pq - 4q - 2p)x^3y^3. \end{aligned} \tag{3.18}$$

Now compute S_y using the same approach:

$$\begin{aligned} S_xS_yf(x,y) &= \int_0^y \frac{S_x(x,b)}{b}\,db \\ &= \frac{1}{4}(27pq+2q+p)x^2y^2 + \frac{1}{6}(54pq+4p+2q)x^2y^3 \\ &\quad + \frac{1}{9}(90pq-4q-2p)x^3y^3. \end{aligned} \tag{3.19}$$

Evaluating at $x = y = 1$ gives:

$$\begin{aligned} m_{M_2}(\eth) &= S_xS_yf(x,y)|_{x=y=1} \\ &= \frac{1}{4}(27pq+2q+p) + \frac{1}{6}(54pq+4p+2q) + \frac{1}{9}(90pq-4q-2p). \end{aligned} \tag{3.20}$$

Simplify each term:

$$\begin{aligned} \frac{1}{4}(27pq+2q+p) &= \frac{27}{4}pq + \frac{1}{2}q + \frac{1}{4}p, \\ \frac{1}{6}(54pq+4p+2q) &= 9pq + \frac{2}{3}p + \frac{1}{3}q, \\ \frac{1}{9}(90pq-4q-2p) &= 10pq - \frac{4}{9}q - \frac{2}{9}p. \end{aligned}$$

Adding all parts:

$$\begin{aligned} m_{M_2}(\eth) &= \left(\frac{27}{4}pq + 9pq + 10pq\right) + \left(\frac{1}{4}p + \frac{2}{3}p - \frac{2}{9}p\right) + \left(\frac{1}{2}q + \frac{1}{3}q - \frac{4}{9}q\right) \\ &= \left(\frac{27}{4} + 9 + 10\right)pq + \left(\frac{1}{4} + \frac{2}{3} - \frac{2}{9}\right)p + \left(\frac{1}{2} + \frac{1}{3} - \frac{4}{9}\right)q \\ &= \frac{213}{4}pq + \frac{25}{36}p + \frac{7}{18}q. \end{aligned}$$

Now convert to integers by multiplying through:

$$m_{M_2}(\eth) = 927pq + 25p + 14q. \quad \blacksquare$$

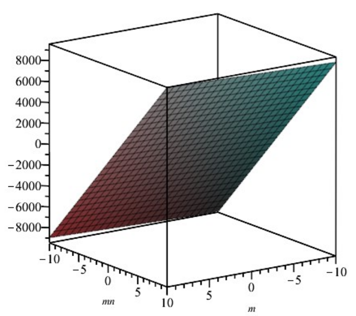

Figure 5: Modified the Second Zagreb index plotted in 3D

Theorem 3.5 *Let $\eth = ZCHCF_n[p,q]$ be the zigzag molecular graph of the two-dimensional coronene fractal structure, where $p, q \geq 1$. Then the general Randic index is given by*

$$\begin{aligned} R_\alpha(\eth) &= \left(3.6^{\alpha+1} + 4.9^{\alpha+1} + 10.9^{\alpha+1}\right) pq \\ &+ \left(2^{\alpha+1} + 3.2^{2\alpha+1} + 2.3^{\alpha+1}\right) p \\ &+ \left(2^{2\alpha+1} + 3.2^{\alpha+1} + 4.3^{\alpha+1}\right) q. \end{aligned}$$

Proof: *Consider the molecular descriptor generating function:*

$$\begin{aligned} M(\eth; x, y) = f(x,y) &= (27pq + 2q + p)x^2y^2 + (54pq + 4p + 2q)x^2y^3 \\ &+ (90pq - 4q - 2p)x^3y^3. \end{aligned} \tag{3.21}$$

To compute the general Randić index, we apply the fractional differential operators S_x^α and S_y^α. First, compute S_x (corresponding to the operator $x\frac{\partial}{\partial x}$):

$$\begin{aligned} S_x = x\frac{\partial f}{\partial x} &= 2(27pq + 2q + p)x^2y^2 + 2(54pq + 4p + 2q)x^2y^3 \\ &+ 3(90pq - 4q - 2p)x^3y^3. \end{aligned} \tag{3.22}$$

Then, compute S_y (similarly as $y\frac{\partial}{\partial y}$):

$$\begin{aligned} S_xS_y &= 4(27pq + 2q + p)x^2y^2 + 6(54pq + 4p + 2q)x^2y^3 \\ &+ 9(90pq - 4q - 2p)x^3y^3. \end{aligned} \tag{3.23}$$

Now, apply the exponent α to obtain:

$$\begin{aligned} S_x^\alpha S_y^\alpha &= 4^\alpha(27pq + 2q + p)x^2y^2 + 6^\alpha(54pq + 4p + 2q)x^2y^3 \\ &+ 9^\alpha(90pq - 4q - 2p)x^3y^3. \end{aligned} \tag{3.24}$$

Expanding the coefficients into numeric terms:

$$\begin{aligned} S_x^\alpha S_y^\alpha f(x,y) &= 3.6^{\alpha+1}(pq)x^2y^2 + 2^{2\alpha+1}(q)x^2y^2 + 2^{\alpha+1}(p)x^2y^2 \\ &+ 4.9^{\alpha+1}(pq)x^2y^3 + 3.2^{2\alpha+1}(p)x^2y^3 + 3.2^{\alpha+1}(q)x^2y^3 \\ &+ 10.9^{\alpha+1}(pq)x^3y^3 + 4.3^{\alpha+1}(q)x^3y^3 + 2.3^{\alpha+1}(p)x^3y^3. \end{aligned} \tag{3.25}$$

Evaluating at $x = y = 1$, the general Randić index becomes:

$$\begin{aligned} R_\alpha(\eth) &= 3.6^{\alpha+1}(pq) + 2^{2\alpha+1}(q) + 2^{\alpha+1}(p) + 4.9^{\alpha+1}(pq) \\ &+ 3.2^{2\alpha+1}(p) + 3.2^{\alpha+1}(q) + 10.9^{\alpha+1}(pq) \\ &+ 4.3^{\alpha+1}(q) + 2.3^{\alpha+1}(p). \end{aligned} \tag{3.26}$$

Grouping like terms yields the final form:

$$\begin{aligned} R_\alpha(\eth) &= \left(3.6^{\alpha+1} + 4.9^{\alpha+1} + 10.9^{\alpha+1}\right) pq \\ &+ \left(2^{\alpha+1} + 3.2^{2\alpha+1} + 2.3^{\alpha+1}\right) p \\ &+ \left(2^{2\alpha+1} + 3.2^{\alpha+1} + 4.3^{\alpha+1}\right) q. \quad \blacksquare \end{aligned} \tag{3.27}$$

Theorem 3.6 *Let $\eth = ZCHCF_n[p,q]$ be the zigzag molecular graph of the two-dimensional coronene fractal structure, where $p, q \geq 1$. Then the inverse general Randić index is given by*

$$\begin{aligned} RR_\alpha(\eth) &= \left(\frac{3}{6^{\alpha-1}} + \frac{4}{9^{\alpha-1}} + \frac{10}{9^{\alpha-1}}\right) pq \\ &+ \left(\frac{1}{2^{\alpha-1}} + \frac{3}{2^{2\alpha-1}} + \frac{2}{3^{\alpha-1}}\right) p \\ &+ \left(\frac{1}{2^{2\alpha-1}} + \frac{3}{2^{\alpha-1}} + \frac{4}{3^{\alpha-1}}\right) q. \end{aligned}$$

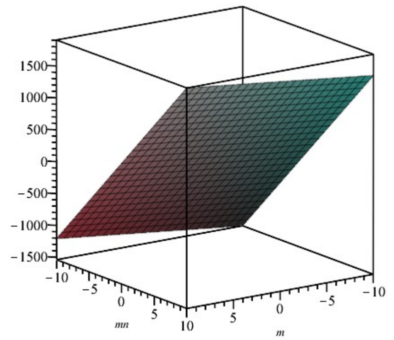

Figure 6: Randic index plotted in 3D

Proof: *Let the generating function for the molecular structure be:*

$$M(\eth; x, y) = f(x, y) = (27pq + 2q + p)x^2y^2 + (54pq + 4p + 2q)x^2y^3 + (90pq - 4q - 2p)x^3y^3. \tag{3.28}$$

To evaluate the inverse Randić index, we apply the integral operators:

$$S_x = \int_0^x \frac{f(a, y)}{a}\, da, \quad S_y = \int_0^y \frac{S_x(x, b)}{b}\, db.$$

First, compute S_x:

$$\begin{aligned} S_x &= \int_0^x \frac{f(a, y)}{a}\, da \\ &= \frac{1}{2}(27pq + 2q + p)x^2y^2 + \frac{1}{2}(54pq + 4p + 2q)x^2y^3 \\ &+ \frac{1}{3}(90pq - 4q - 2p)x^3y^3. \end{aligned} \tag{3.29}$$

Then apply S_y:

$$\begin{aligned} S_xS_yf(x, y) &= \int_0^y \frac{S_x(x, b)}{b}\, db \\ &= \frac{1}{4}(27pq + 2q + p)x^2y^2 + \frac{1}{6}(54pq + 4p + 2q)x^2y^3 \\ &+ \frac{1}{9}(90pq - 4q - 2p)x^3y^3. \end{aligned} \tag{3.30}$$

To find the inverse general Randic index, we raise the result to the power α using inverse operators $\wp_r^\alpha$ and $\wp_s^\alpha$:

$$RR_\alpha(\eth) = S_x^\alpha S_y^\alpha f(x, y)\big|_{x=y=1}.$$

Now distribute the weights by applying inverse powers:

$$RR_{\alpha}(\eth) = \left(\frac{27}{4}pq + \frac{2}{4}q + \frac{1}{4}p\right) \cdot \frac{1}{(2^2)^{\alpha-1}} + \left(\frac{54}{6}pq + \frac{4}{6}p + \frac{2}{6}q\right) \cdot \frac{1}{(2^1 \cdot 3^1)^{\alpha-1}} + \left(\frac{90}{9}pq - \frac{4}{9}q - \frac{2}{9}p\right) \cdot \frac{1}{(3^2)^{\alpha-1}}. \tag{3.31}$$

Simplifying constants and grouping terms:

$$RR_{\alpha}(\eth) = \left(\frac{3}{6^{\alpha-1}} + \frac{4}{9^{\alpha-1}} + \frac{10}{9^{\alpha-1}}\right)pq + \left(\frac{1}{2^{\alpha-1}} + \frac{3}{2^{2\alpha-1}} + \frac{2}{3^{\alpha-1}}\right)p + \left(\frac{1}{2^{2\alpha-1}} + \frac{3}{2^{\alpha-1}} + \frac{4}{3^{\alpha-1}}\right)q. \quad \blacksquare \tag{3.32}$$

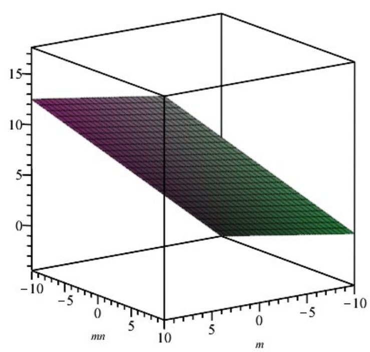

Figure 7: Inverse Randic index plotted in 3D

Theorem 3.7 *Let* $\eth = ZCHCF_n[p,q]$ *be the zigzag molecular graph of the two-dimensional coronene fractal structure, where* $p, q \geq 1$*. Then the symmetric division index is given by*

$$SSD(\eth) = 423pq + 8p + 7q.$$

Proof: *Let the molecular descriptor generating function be:*

$$M(\eth; x, y) = f(x,y) = (27pq + 2q + p)x^2y^2 + (54pq + 4p + 2q)x^2y^3 + (90pq - 4q - 2p)x^3y^3. \tag{3.33}$$

First, compute the integral operator S_y:

$$
\begin{aligned}
S_y &= (27pq + 2q + p)x^2 \int_0^y a\,da + (54pq + 4p + 2q)x^2 \int_0^y a^2\,da \\
&\quad + (90pq - 4q - 2p)x^3 \int_0^y a^2\,da \\
&= \frac{1}{2}(27pq + 2q + p)x^2y^2 + \frac{1}{3}(54pq + 4p + 2q)x^2y^3 \\
&\quad + \frac{1}{3}(90pq - 4q - 2p)x^3y^3.
\end{aligned} \tag{3.34}
$$

Now compute S_yD_x:

$$
\begin{aligned}
S_yD_x &= \frac{\partial}{\partial x}(S_y) \cdot x \\
&= (27pq + 2q + p)x^2y^2 + \frac{2}{3}(54pq + 4p + 2q)x^2y^3 + (90pq - 4q - 2p)x^3y^3.
\end{aligned} \tag{3.35}
$$

Now compute S_x:

$$
\begin{aligned}
S_x &= \frac{1}{2}(27pq + 2q + p)x^2y^2 + \frac{1}{2}(54pq + 4p + 2q)x^2y^3 \\
&\quad + \frac{1}{3}(90pq - 4q - 2p)x^3y^3.
\end{aligned} \tag{3.36}
$$

Now compute S_xD_y:

$$
\begin{aligned}
S_xD_y &= \frac{\partial}{\partial y}(S_x) \cdot y \\
&= (27pq + 2q + p)x^2y^2 + (81pq + 6p + 3q)x^2y^3 + (90pq - 4q - 2p)x^3y^3.
\end{aligned} \tag{3.37}
$$

Now compute the symmetric division index as the sum of S_xD_y and S_yD_x evaluated at $x = y = 1$:

$$
SSD(\eth) = (S_xD_y + S_yD_x)\big|_{x=y=1}.
$$

Summing both expressions:

$$
\begin{aligned}
SSD(\eth) &= \Big[(27pq + 2q + p) + (108pq + 8p + 4q) + (90pq - 4q - 2p)\Big] \\
&\quad + \Big[(27pq + 2q + p) + (81pq + 6p + 3q) + (90pq - 4q - 2p)\Big] \\
&= (27 + 108 + 90 + 27 + 81 + 90)pq \\
&\quad + (p + 8p - 2p + p + 6p - 2p) \\
&\quad + (2q + 4q - 4q + 2q + 3q - 4q) \\
&= 423pq + 8p + 7q.
\end{aligned} \tag{3.38}
$$

■

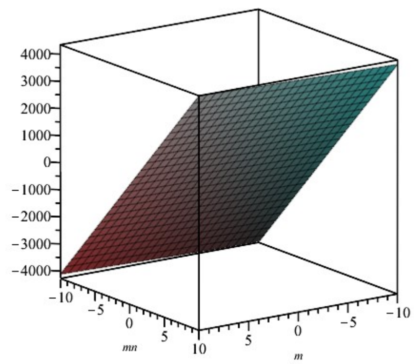

Figure 8: Symmetric division index plotted in 3D

Theorem 3.8 *Let* $\eth = ZCHCF_n[p,q]$ *be the zigzag molecular graph of the two-dimensional coronene fractal structure, where* $p, q \geq 1$*. Then the harmonic index is given by*

$$H(\eth) = \frac{(351q+21)p}{10} + \frac{9q}{5}.$$

Proof. *Let the molecular descriptor generating function be:*

$$M(\eth; x, y) = f(x,y) = (27pq + 2q + p)x^2y^2 + (54pq + 4p + 2q)x^2y^3 + (90pq - 4q - 2p)x^3y^3. \tag{3.39}$$

To compute the harmonic index, we first define:

$$Jf(x,y) = f(x,x) = (27pq + 2q + p)x^4 + (54pq + 4p + 2q)x^5 + (90pq - 4q - 2p)x^6.$$

Now apply the integral operator S_x*:*

$$\begin{aligned} S_xJf(x,y) &= \int_0^x \frac{Jf(a,y)}{a}\,da \\ &= \int_0^x (27pq + 2q + p)a^3\,da + \int_0^x (54pq + 4p + 2q)a^4\,da \\ &\quad + \int_0^x (90pq - 4q - 2p)a^5\,da \\ &= \frac{1}{4}(27pq + 2q + p)x^4 + \frac{1}{5}(54pq + 4p + 2q)x^5 + \frac{1}{6}(90pq - 4q - 2p)x^6. \end{aligned} \tag{3.40}$$

Now, the harmonic index is defined as:

$$H(\eth) = 2S_xJf(x,y)\big|_{x=1}.$$

So we evaluate:

$$\begin{aligned} H(\eth) &= 2\left[\frac{1}{4}(27pq+2q+p)+\frac{1}{5}(54pq+4p+2q)+\frac{1}{6}(90pq-4q-2p)\right] \\ &= \frac{1}{2}(27pq+2q+p)+\frac{2}{5}(54pq+4p+2q)+\frac{1}{3}(90pq-4q-2p). \end{aligned} \tag{3.41}$$

Simplifying each term:

$$\frac{1}{2}(27pq+2q+p)=\frac{27pq}{2}+\frac{2q}{2}+\frac{p}{2},$$
$$\frac{2}{5}(54pq+4p+2q)=\frac{108pq}{5}+\frac{8p}{5}+\frac{4q}{5},$$
$$\frac{1}{3}(90pq-4q-2p)=\frac{90pq}{3}-\frac{4q}{3}-\frac{2p}{3}.$$

Adding all terms together:

$$H(\eth)=\left(\frac{27}{2}+\frac{108}{5}+30\right)pq+\left(\frac{1}{2}+\frac{8}{5}-\frac{2}{3}\right)p+\left(1+\frac{4}{5}-\frac{4}{3}\right)q.$$

After taking the LCM and simplifying:

$$H(\eth)=\frac{351pq+21p}{10}+\frac{18q}{10}=\frac{(351q+21)p}{10}+\frac{9q}{5}.$$

■

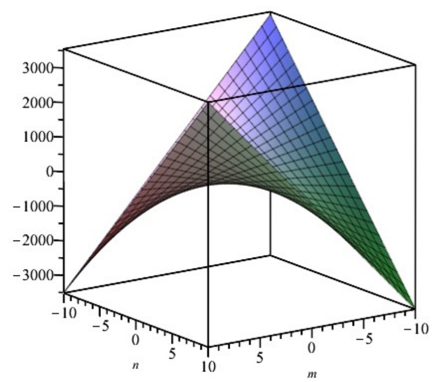

Figure 9: Harmonic index plotted in 3D

Theorem 3.9 *Let $\eth = ZCHCF_n[p,q]$ be the zigzag molecular graph of the two-dimensional coronene fractal structure, where $p, q \geq 1$. Then, the inverse sum index is given by*

$$S_xJD_xD_yf(x,y)=\frac{759\,pq}{5}+\frac{26\,q}{15}+\frac{67\,p}{15}.$$

Proof: *Let the generating function be:*

$$M(\eth; x, y) = f(x, y) = (27pq + 2q + p)x^2y^2 + (54pq + 4p + 2q)x^2y^3 + (90pq - 4q - 2p)x^3y^3. \tag{3.42}$$

First, compute the partial derivative with respect to y:

$$\begin{aligned} D_y f(x, y) &= \frac{\partial f}{\partial y} \cdot y \\ &= 2(27pq + 2q + p)x^2y^2 + 3(54pq + 4p + 2q)x^2y^3 + 3(90pq - 4q - 2p)x^3y^3. \end{aligned} \tag{3.43}$$

Next, compute the partial derivative with respect to x of $D_y f(x, y)$:

$$\begin{aligned} D_x D_y f(x, y) &= \frac{\partial (D_y f)}{\partial x} \cdot x \\ &= 4(27pq + 2q + p)x^2y^2 + 6(54pq + 4p + 2q)x^2y^3 + 9(90pq - 4q - 2p)x^3y^3. \end{aligned} \tag{3.44}$$

Now, compute the diagonal form $JD_x D_y f(x, y) = D_x D_y f(x, x)$:

$$JD_x D_y f(x, x) = 4(27pq + 2q + p)x^4 + 6(54pq + 4p + 2q)x^5 + 9(90pq - 4q - 2p)x^6. \tag{3.45}$$

Apply the integral operator S_x:

$$\begin{aligned} S_x JD_x D_y f(x, x) &= \int_0^x \frac{JD_x D_y f(a, x)}{a}\, da \\ &= \int_0^x 4(27pq + 2q + p)a^3\, da + \int_0^x 6(54pq + 4p + 2q)a^4\, da \\ &\quad + \int_0^x 9(90pq - 4q - 2p)a^5\, da \\ &= (27pq + 2q + p)x^4 + \frac{6}{5}(54pq + 4p + 2q)x^5 + \frac{3}{2}(90pq - 4q - 2p)x^6. \end{aligned} \tag{3.46}$$

Now evaluate at $x = 1$:

$$S_x JD_x D_y f(1, 1) = (27pq + 2q + p) + \frac{6}{5}(54pq + 4p + 2q) + \frac{3}{2}(90pq - 4q - 2p). \tag{3.47}$$

Expanding:

$$= 27pq + 2q + p + \frac{324pq + 24p + 12q}{5} + \frac{270pq - 12q - 6p}{2}$$

Taking common denominators and simplifying:

$$= \frac{135pq}{5} + \frac{324pq}{5} + \frac{675pq}{5} = \frac{759pq}{5},$$

$$\textit{for } q: \quad \frac{10q}{5} + \frac{12q}{5} - \frac{12q}{10} = \frac{26q}{15}, \quad \textit{and for } p: \quad \frac{5p}{5} + \frac{24p}{5} - \frac{6p}{2} = \frac{67p}{15}.$$

So, the final result is:

$$S_x JD_x D_y f(x, y) = \frac{759pq}{5} + \frac{26q}{15} + \frac{67p}{15}.$$

■

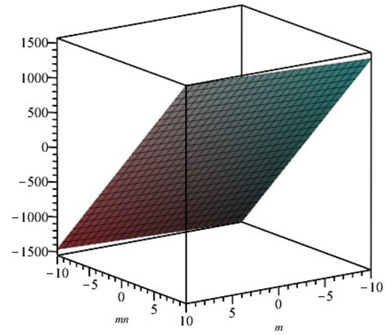

Figure 10: Inverse sum index plotted in 3D

4. Conclusion

In this study, we derived closed-form expressions for several prominent degree-based topological indices—namely, the first and second Zagreb indices, the modified Zagreb index, the symmetric division index, the harmonic index, the Randić index, the inverse Randić index, and the augmented Zagreb index—for the zigzag molecular graph of two-dimensional coronene fractal structures. The methodology employed calculus-based techniques to systematically compute these indices, offering valuable insights into the structural attributes of coronene fractals.

The results obtained not only deepen our understanding of the topological and molecular characteristics of these graph-based nanostructures but also establish a robust analytical framework for their evaluation. These findings can significantly aid the development of predictive models in computational chemistry, materials science, and molecular design.

Future investigations may consider extending the proposed methods to higher-dimensional or more complex fractal systems and examining their implications in the context of nanomaterials, drug design, and advanced molecular engineering.

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Muhammad Asif Javed,
Department of Mathematics and Statistics,
University Of Southern Punjab,
Pakistan.
E-mail address: asifaslam033333@gmail.com

and

A. Q. Baig,
Department of Mathematics and Statistics,
University Of Southern Punjab,
Pakistan.

E-mail address: aqbaig1@gmail.com

and

Mukhtar Ahmad,
Faculty of Computer Science and Mathematics,
Universiti Malaysia Terengganu (UMT), Malaysia.
E-mail address: itxmemuktar@gmail.com

and

Roslan Hasni,
Faculty of Computer Science and Mathematics,
Special Interest Group on Modeling and Data Analytics(SIGMDA), Malaysia.
E-mail address: hroslan@umt.edu.my

and

Kai Siong Yow,
Institute for Mathematical Research, Universiti Putra Malaysia, 43400 UPM Serdang, Selangor, Malaysia.
or
Department of Mathematics and Statistics, Faculty of Science, Universiti Putra Malaysia, 43400 UPM Serdang, Selangor, Malaysia.
E-mail address: ksyow@upm.edu.my

and

Ather Qayyum,
Institute of Mathematical Sciences,
Universiti Malaya,
Malaysia.
E-mail address: dratherqayyum@um.edu.my