Bol. Soc. Paran. Mat.
©SPM – E-ISSN-2175-1188
SPM: www.spm.uem.br/bspm

(3s.) **v. 2025 (43)** : 1–17.
ISSN-0037-8712
doi:10.5269/bspm.76668

Zigzags and rectangular of the two dimensional Coronene fractal by Revan topological indices

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ABSTRACT: Molecular fractals are geometric structures that exhibit self-similarity across multiple scales and are generated through the iterative repetition of a fundamental unit. The natural patterns found in benzenoid compounds provide valuable insights for analyzing the structural and functional properties of these fractals. This study focuses on computing degree-based topological indices, specifically the Revan topological indices, for zigzag Coronene Fractal Structures and rectangular coronene fractals. These indices play a crucial role in characterizing the structural properties of coronene fractals. Additionally, a compatibility analysis was conducted to evaluate the interrelations among different topological indices. The findings of this research contribute to a deeper understanding of molecular topology and hold significance for various scientific fields, including materials science, nanotechnology, and theoretical chemistry.

Key Words:: Molecular fractals; benzenoid compounds; Revan topological indices; Coronene fractal structures; zigzag fractals and rectangular Coronene fractals.

Contents

1. Introduction

Chemical graph theory is a mathematical discipline that applies graph-theoretical principles to the modeling and analysis of molecular structures. In this framework, atoms are represented by vertices and chemical bonds by edges. This approach provides a structural abstraction of chemical compounds and enables the computation of numerical descriptors known as topological indices (TIs), which are used to correlate molecular structure with various physical, chemical, and biological properties.

Topological indices play a pivotal role in the development of Quantitative Structure–Activity Relationships (QSARs), Quantitative Structure–Property Relationships (QSPRs), and Quantitative Structure–Toxicity Relationships (QSTRs). These relationships are fundamental to modern cheminformatics and drug design, providing a pathway to predict molecular behavior without the need for expensive laboratory experiments [6,7,19].

Recent studies have emphasized the significance of advanced topological descriptors, particularly in the context of complex nanostructures such as benzenoid systems, fullerenes, and fractal-like carbon frameworks [14,15,20]. Specifically, coronene-based nanostructures and their zigzag and rectangular variants have been explored due to their remarkable electronic and stability properties, making them promising candidates in nanomaterials research [19,21,23].

In chemical graph theory, several degree-based indices have been introduced, including the Wiener index, Randić index [18,21], and more recently, Revan indices [6,7,8,9,10,11,12,13]. These indices quantify

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2010 *Mathematics Subject Classification:* 35B40, 35L70.
Submitted May 06, 2025. Published September 01, 2025

various aspects of molecular connectivity and have shown strong predictive power for physico-chemical parameters [14,15,22].

This work focuses on computing and analyzing the Omega, Sadhana, and Padmakar–Ivan (PI) polynomials for two-dimensional fractal benzenoid systems, particularly the zigzag coronene fractal structures ($ZHCF_{(m)}$), rectangular coronene fractals ($RCF_{(m)}$), and non-Kekulean benzenoid structures ($\mathbb{k}(p,q,r)$). These polynomials offer compact algebraic forms that encapsulate the edge co-distance structure of molecular graphs, aiding in descriptor generation for QSAR/QSPR applications.

The organization of the paper is as follows. In Section **??**, we describe the structural formation of $ZHCF_{(m)}$ and $RCF_{(m)}$, and compute relevant graph parameters. Sections 3 to 5 are dedicated to the computation of the Omega, Sadhana, and PI polynomials for various nanostructures. The final section outlines the implications of our findings and directions for future research. The first and second Revan indices, introduced by Kulli [7], are defined as follows:

$$R_1(\varpi) = \sum_{\{uv\}\in E(\varpi)} (\mathbb{k}_u + \mathbb{k}_v), \tag{1.1}$$

$$R_2(\varpi) = \sum_{\{uv\}\in E(\varpi)} (\mathbb{k}_u \times \mathbb{k}_v), \tag{1.2}$$

where $\mathbb{k}_u$ denotes the Revan degree of vertex u in the molecular graph ϖ.

The first and second *hyper Revan indices*, as defined by Kulli [8], are given by:

$$HR_1(\varpi) = \sum_{\{uv\}\in E(\varpi)} (\mathbb{k}_u + \mathbb{k}_v)^2, \tag{1.3}$$

$$HR_2(\varpi) = \sum_{\{uv\}\in E(\varpi)} (\mathbb{k}_u \times \mathbb{k}_v)^2. \tag{1.4}$$

The *modified hyper Revan indices*, introduced by Kulli [9,22], are expressed as:

$$mHR_1(\varpi) = \sum_{\{uv\}\in E(\varpi)} \frac{1}{\mathbb{k}_u + \mathbb{k}_v}, \tag{1.5}$$

$$mHR_2(\varpi) = \sum_{\{uv\}\in E(\varpi)} \frac{1}{\mathbb{k}_u \times \mathbb{k}_v}. \tag{1.6}$$

The *overall interconnectedness Revan index*, proposed by Kulli [10], is defined as:

$$OI(\varpi) = \sum_{\{uv\}\in E(\varpi)} \frac{1}{\sqrt{\mathbb{k}_u + \mathbb{k}_v}}. \tag{1.7}$$

The *product connectivity Revan index*, as presented in [11], is given by:

$$PC(\varpi) = \sum_{\{uv\}\in E(\varpi)} \frac{1}{\sqrt{\mathbb{k}_u \times \mathbb{k}_v}}. \tag{1.8}$$

The *ξ-Revan index*, introduced in [12], is:

$$\xi R(\varpi) = \sum_{\{uv\}\in E(\varpi)} \left(\mathbb{k}_u^2 + \mathbb{k}_v^2\right). \tag{1.9}$$

The *symmetry-based split Revan index*, formulated in [13], is:

$$SDD(\varpi) = \sum_{\{uv\}\in E(\varpi)} \left(\frac{\mathbb{k}_u}{\mathbb{k}_v} + \frac{\mathbb{k}_v}{\mathbb{k}_u}\right). \tag{1.10}$$

The *harmonic Revan index*, as defined in [15], is:

$$H(\varpi) = \sum_{\{uv\}\in E(\varpi)} \frac{2}{\mathbb{k}_u + \mathbb{k}_v}. \tag{1.11}$$

Finally, the *inverse sum Revan index* [13] is given by:

$$I(\varpi) = \sum_{\{uv\}\in E(\varpi)} \frac{\mathbb{k}_u + \mathbb{k}_v}{\mathbb{k}_u \times \mathbb{k}_v}. \tag{1.12}$$

2. Formation and Results for Zigzag Coronene Fractal Structures $ZHCF_{(m)}$ and Rectangular Coronene Fractal $RCF_{(m)}$

This section explores two distinct types of coronene-based fractal structures: the Zigzag Coronene Fractal ($ZHCF_{(m)}$) and the Rectangular Coronene Fractal ($RCF_{(m)}$). Both structures are derived from the basic coronene framework, with their geometric configurations dictated by specific patterns—zigzag in $ZHCF_{(m)}$ and rectangular in $RCF_{(m)}$. These patterns arise due to the connectivity and arrangement of hexagonal units in the molecular graph, often observed in nanostructured periphery cavities.

The parameter $m \geq 1$ represents the fractal iteration or circumscribing order, which controls the size and complexity of the structure.

For the Zigzag Coronene Fractal $ZHCF_{(m)}$, the number of vertices and edges are given by the following expressions:

$$|V(ZHCF_{(m)})| = 3(57m^2 + m),$$
$$|E(ZHCF_{(m)})| = 6(21m^2 + m).$$

The expressions for the number of vertices and edges in the Rectangular Coronene Fractal $RCF_{(m)}$ will be similarly defined, based on the structural growth rules for each successive layer. These parameters serve as the foundation for computing various topological descriptors, including Omega, Sadhana, and PI polynomials, in subsequent sections.

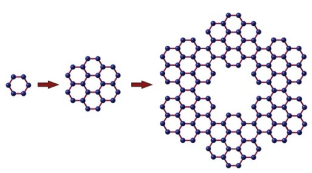


Figure 1: The formation of coronene fractal structures

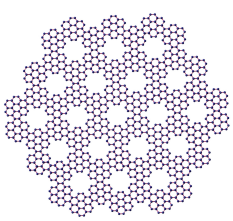


Figure 2: Zigzag hexagonal coronene fractal structures $ZCHCF_3$

The results in this section are derived using the structural configuration shown in Figure 2 and the edge partition details provided in Table 1.

Theorem 2.1 *The first Revan index of the zigzag coronene fractal structures $ZHCF_{(m)}$, where $m \geq 1$, is given by:*

$$R_1(\varpi) = 792m^2 + 72m. \tag{2.1}$$

$(\mathbb{k}_u, \mathbb{k}_v)$	Edge Set	Frequency	$\mathbb{k}_\varpi(u)$	$\mathbb{k}_\varpi(v)$
$(2,2)$	$E_1(\varpi)$	$3(9m^2+m)$	3	3
$(2,3)$	$E_2(\varpi)$	$6(9m^2+m)$	3	2
$(3,3)$	$E_3(\varpi)$	$6(15m^2+m)$	2	2

Table 1: Edge partition of zigzag hexagonal coronene fractals $ZHCF_{(m)}$.

Proof: The first Revan index is defined as:

$$R_1(\varpi) = \sum_{uv \in E(\varpi)} (\mathbb{k}_u + \mathbb{k}_v).$$

Using the edge partition from Table 1, we compute the contribution from each edge type:

$$\begin{aligned} R_1(\varpi) &= \sum_{(2,2)\in E(\varpi)} (\mathbb{k}_u + \mathbb{k}_v) + \sum_{(2,3)\in E(\varpi)} (\mathbb{k}_u + \mathbb{k}_v) + \sum_{(3,3)\in E(\varpi)} (\mathbb{k}_u + \mathbb{k}_v) \\ &= (3+3)\cdot 3(9m^2+m) + (3+2)\cdot 6(9m^2+m) + (2+2)\cdot 6(15m^2+m) \\ &= 6\cdot 3(9m^2+m) + 5\cdot 6(9m^2+m) + 4\cdot 6(15m^2+m) \\ &= 18(9m^2+m) + 30(9m^2+m) + 24(15m^2+m) \\ &= (162m^2+18m) + (270m^2+30m) + (360m^2+24m) \\ &= 792m^2 + 72m. \quad \blacksquare \end{aligned}$$

□

Theorem 2.2 *The second Revan index of the zigzag coronene fractal structures $ZHCF_{(m)}$, where $m \geq 1$, is given by:*

$$R_2(\varpi) = 927m^2 + 87m. \tag{2.2}$$

Proof: The second Revan index is defined as:

$$R_2(\varpi) = \sum_{uv \in E(\varpi)} (\mathbb{k}_u \times \mathbb{k}_v).$$

Using the edge partition from Table 1, we compute the contribution from each type of edge:

$$\begin{aligned} R_2(\varpi) &= \sum_{(2,2)\in E(\varpi)} (\mathbb{k}_u \cdot \mathbb{k}_v) + \sum_{(2,3)\in E(\varpi)} (\mathbb{k}_u \cdot \mathbb{k}_v) + \sum_{(3,3)\in E(\varpi)} (\mathbb{k}_u \cdot \mathbb{k}_v) \\ &= (3\cdot 3)\cdot 3(9m^2+m) + (3\cdot 2)\cdot 6(9m^2+m) + (2\cdot 2)\cdot 6(15m^2+m) \\ &= 9\cdot 3(9m^2+m) + 6\cdot 6(9m^2+m) + 4\cdot 6(15m^2+m) \\ &= 27(9m^2+m) + 36(9m^2+m) + 24(15m^2+m) \\ &= (243m^2+27m) + (324m^2+36m) + (360m^2+24m) \\ &= 927m^2 + 87m. \quad \blacksquare \end{aligned}$$

□

Theorem 2.3 *The hyper first Revan index of the zigzag coronene fractal structures $ZHCF_{(m)}$, where $m \geq 1$, is given by:*

$$HR_1(\varpi) = 3762m^2 + 354m. \tag{2.3}$$

Proof: By definition, the hyper first Revan index is:

$$HR_1(\varpi) = \sum_{uv \in E(\varpi)} (\Bbbk_u + \Bbbk_v)^2 .$$

Using the edge partition data from Table 1, we compute:

$$\begin{aligned} HR_1(\varpi) &= \sum_{(2,2)} (3+3)^2 \cdot 3(9m^2+m) + \sum_{(2,3)} (3+2)^2 \cdot 6(9m^2+m) + \sum_{(3,3)} (2+2)^2 \cdot 6(15m^2+m) \\ &= 36 \cdot 3(9m^2+m) + 25 \cdot 6(9m^2+m) + 16 \cdot 6(15m^2+m) \\ &= 108(9m^2+m) + 150(9m^2+m) + 96(15m^2+m) \\ &= (972m^2+108m) + (1350m^2+150m) + (1440m^2+96m) \\ &= 3762m^2 + 354m. \quad \blacksquare \end{aligned}$$

□

Theorem 2.4 *The hyper second Revan index of the zigzag coronene fractal structures $ZHCF_{(m)}$, where $m \geq 1$, is given by:*

$$HR_2(\varpi) = 5571m^2 + 555m. \tag{2.4}$$

Proof: By definition, the hyper second Revan index is:

$$HR_2(\varpi) = \sum_{uv \in E(\varpi)} (\Bbbk_u \cdot \Bbbk_v)^2 .$$

Using the edge partition from Table 1, we compute:

$$\begin{aligned} HR_2(\varpi) &= \sum_{(2,2)} (3 \cdot 3)^2 \cdot 3(9m^2+m) + \sum_{(2,3)} (3 \cdot 2)^2 \cdot 6(9m^2+m) + \sum_{(3,3)} (2 \cdot 2)^2 \cdot 6(15m^2+m) \\ &= 81 \cdot 3(9m^2+m) + 36 \cdot 6(9m^2+m) + 16 \cdot 6(15m^2+m) \\ &= 243(9m^2+m) + 216(9m^2+m) + 96(15m^2+m) \\ &= (2187m^2+243m) + (1944m^2+216m) + (1440m^2+96m) \\ &= 5571m^2 + 555m. \quad \blacksquare \end{aligned}$$

□

Theorem 2.5 *The modified hyper first Revan index of the zigzag coronene fractal structures $ZHCF_{(m)}$, where $m \geq 1$, is given by:*

$$mHR_1(\varpi) = \frac{189}{5}m^2 + \frac{16}{5}m. \tag{2.5}$$

Proof: By definition, the modified hyper first Revan index is:

$$mHR_1(\varpi) = \sum_{uv \in E(\varpi)} \frac{1}{\Bbbk_u + \Bbbk_v}.$$

Using the edge classification from Table 1, we compute:

$$\begin{aligned}
mHR_1(\varpi) &= \sum_{(2,2)} \frac{1}{3+3} \cdot 3(9m^2+m) + \sum_{(2,3)} \frac{1}{2+3} \cdot 6(9m^2+m) + \sum_{(3,3)} \frac{1}{2+2} \cdot 6(15m^2+m) \\
&= \frac{3(9m^2+m)}{6} + \frac{6(9m^2+m)}{5} + \frac{6(15m^2+m)}{4} \\
&= \left(\frac{27m^2+3m}{6}\right) + \left(\frac{54m^2+6m}{5}\right) + \left(\frac{90m^2+6m}{4}\right) \\
&= \frac{27m^2+3m}{6} + \frac{54m^2+6m}{5} + \frac{90m^2+6m}{4} \\
&= \frac{90m^2+10m+324m^2+36m+675m^2+45m}{60} \\
&= \frac{1089m^2+91m}{60} \\
&= \frac{189}{5}m^2 + \frac{16}{5}m. \quad \blacksquare
\end{aligned}$$

□

Theorem 2.6 *The modified second Revan index of the zigzag coronene fractal structures $ZHCF_{(m)}$, where $m \geq 1$, is given by:*

$$mHR_2(\varpi) = \frac{69}{2}m^2 + \frac{17}{6}m. \tag{2.6}$$

Proof: By definition, the modified second Revan index is:

$$mHR_2(\varpi) = \sum_{uv \in E(\varpi)} \frac{1}{\Bbbk_u \times \Bbbk_v}.$$

Using the edge classification from Table 1, we compute:

$$\begin{aligned}
mHR_2(\varpi) &= \sum_{(2,2)} \frac{1}{3 \times 3} \cdot 3(9m^2+m) + \sum_{(2,3)} \frac{1}{3 \times 2} \cdot 6(9m^2+m) + \sum_{(3,3)} \frac{1}{2 \times 2} \cdot 6(15m^2+m) \\
&= \frac{3(9m^2+m)}{9} + \frac{6(9m^2+m)}{6} + \frac{6(15m^2+m)}{4} \\
&= (9m^2+m) + (9m^2+m) + \frac{90m^2+6m}{4} \\
&= 18m^2 + 2m + \frac{90m^2+6m}{4} \\
&= 18m^2 + 2m + 22.5m^2 + 1.5m \\
&= \left(18 + \frac{90}{4}\right)m^2 + \left(2 + \frac{6}{4}\right)m \\
&= \frac{36}{2}m^2 + \frac{90}{4}m^2 + \frac{4}{2}m + \frac{6}{4}m \\
&= \frac{69}{2}m^2 + \frac{17}{6}m. \quad \blacksquare
\end{aligned}$$

□

Theorem 2.7 *The harmonic Revan index of the zigzag coronene fractal structures $ZHCF_{(m)}$, where $m \geq 1$, is given by:*

$$H(\varpi) = \frac{378}{5}m^2 + \frac{32}{5}m. \tag{2.7}$$

Proof: By definition, the harmonic Revan index is:

$$H(\varpi) = \sum_{uv \in E(\varpi)} \frac{2}{\Bbbk_u + \Bbbk_v}.$$

Using the edge classification from Table 1, we compute:

$$\begin{aligned} H(\varpi) &= \frac{2}{6} \cdot 3(9m^2 + m) + \frac{2}{5} \cdot 6(9m^2 + m) + \frac{2}{4} \cdot 6(15m^2 + m) \\ &= \frac{1}{3}(27m^2 + 3m) + \frac{12}{5}(9m^2 + m) + \frac{1}{2}(90m^2 + 6m) \\ &= 9m^2 + m + \frac{108m^2 + 12m}{5} + 45m^2 + 3m \\ &= \left(9 + \frac{108}{5} + 45\right) m^2 + \left(1 + \frac{12}{5} + 3\right) m \\ &= \frac{45}{5}m^2 + \frac{108}{5}m^2 + \frac{225}{5}m^2 + \frac{5}{5}m + \frac{12}{5}m + \frac{15}{5}m \\ &= \frac{378}{5}m^2 + \frac{32}{5}m. \quad \blacksquare \end{aligned}$$

□

Theorem 2.8 *The sum division Revan index of the zigzag coronene fractal structures $ZHCF_{(m)}$, where $m \geq 1$, is given by:*

$$SDR(\varpi) = 351m^2 + 31m. \tag{2.8}$$

Proof: The sum division Revan index is defined as:

$$SDR(\varpi) = \sum_{uv \in E(\varpi)} \left(\frac{\Bbbk_u}{\Bbbk_v} + \frac{\Bbbk_v}{\Bbbk_u}\right).$$

Using the edge partitioning from Table 1, we compute:

$$\begin{aligned} SDR(\varpi) &= \left(\frac{3}{3} + \frac{3}{3}\right) \cdot 3(9m^2 + m) + \left(\frac{3}{2} + \frac{2}{3}\right) \cdot 6(9m^2 + m) + \left(\frac{2}{2} + \frac{2}{2}\right) \cdot 6(15m^2 + m) \\ &= 2 \cdot 3(9m^2 + m) + \frac{13}{6} \cdot 6(9m^2 + m) + 2 \cdot 6(15m^2 + m) \\ &= 6(9m^2 + m) + 13(9m^2 + m) + 12(15m^2 + m) \\ &= (54m^2 + 6m) + (117m^2 + 13m) + (180m^2 + 12m) \\ &= 351m^2 + 31m. \quad \blacksquare \end{aligned}$$

□

Theorem 2.9 *The inverse Revan index of the zigzag coronene fractal structures $ZHCF_{(m)}$, where $m \geq 1$, is given by:*

$$IR(\varpi) = \frac{1953}{10}m^2 + \frac{177}{10}m. \tag{2.9}$$

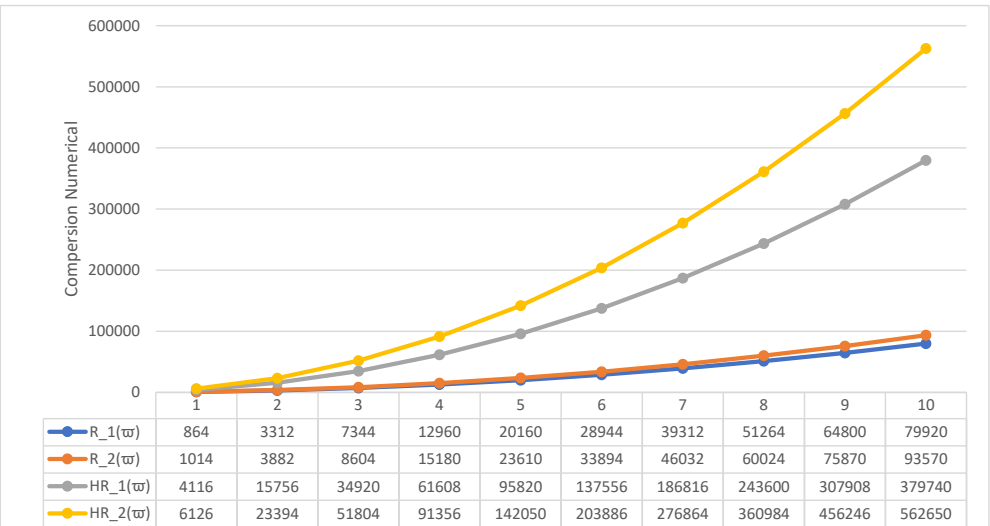
Proof: The inverse Revan index is defined as:

$$IR(\varpi) = \sum_{uv \in E(\varpi)} \frac{\Bbbk_u \cdot \Bbbk_v}{\Bbbk_u + \Bbbk_v}.$$

Using the edge partition of $ZHCF_{(m)}$, we compute:

$$\begin{aligned}
IR(\varpi) &= \left(\frac{3\cdot 3}{3+3}\right)\cdot 3(9m^2+m) + \left(\frac{3\cdot 2}{3+2}\right)\cdot 6(9m^2+m) + \left(\frac{2\cdot 2}{2+2}\right)\cdot 6(15m^2+m)\\
&= \left(\frac{9}{6}\right)\cdot 3(9m^2+m) + \left(\frac{6}{5}\right)\cdot 6(9m^2+m) + \left(\frac{4}{4}\right)\cdot 6(15m^2+m)\\
&= \frac{3}{2}\cdot 3(9m^2+m) + \frac{6}{5}\cdot 6(9m^2+m) + 1\cdot 6(15m^2+m)\\
&= \frac{9}{2}(9m^2+m) + \frac{36}{5}(9m^2+m) + 6(15m^2+m)\\
&= \left(\frac{729}{10}+\frac{1188}{10}+\frac{360}{10}\right)m^2 + \left(\frac{81}{10}+\frac{396}{10}+\frac{90}{10}\right)m\\
IR(\varpi) &= \frac{1953}{10}m^2 + \frac{177}{10}m. \quad \blacksquare
\end{aligned}$$

□

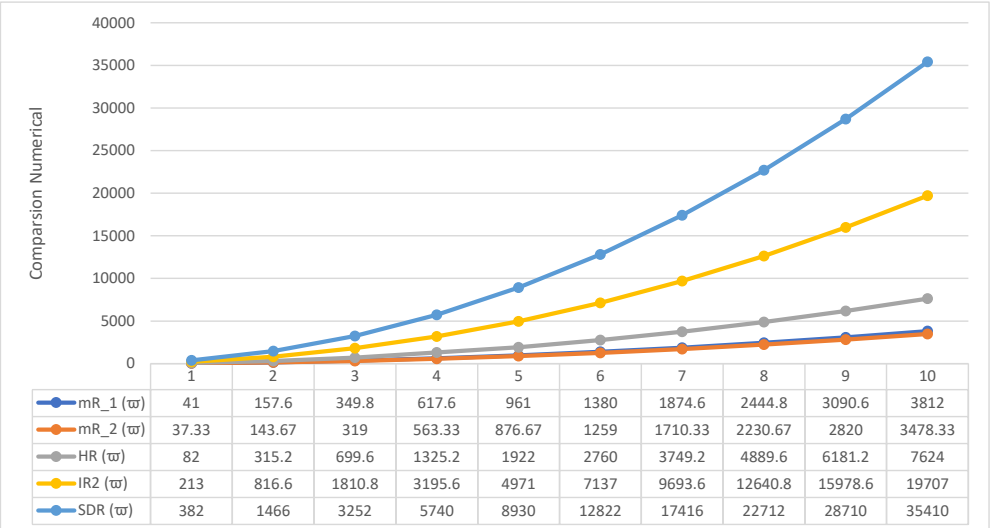


	1	2	3	4	5	6	7	8	9	10
R_1(ϖ)	864	3312	7344	12960	20160	28944	39312	51264	64800	79920
R_2(ϖ)	1014	3882	8604	15180	23610	33894	46032	60024	75870	93570
HR_1(ϖ)	4116	15756	34920	61608	95820	137556	186816	243600	307908	379740
HR_2(ϖ)	6126	23394	51804	91356	142050	203886	276864	360984	456246	562650

Figure 3: Comparison of $R_1(\varpi)$, $R_2(\varpi)$, $HR_1(\varpi)$, $HR_2(\varpi)$

3. Rectangular Coronene Fractal Structures $RCF_{(m)}$

The results in this section are obtained using Figure 5 and Table 2.



	1	2	3	4	5	6	7	8	9	10
mR_1 (ϖ)	41	157.6	349.8	617.6	961	1380	1874.6	2444.8	3090.6	3812
mR_2 (ϖ)	37.33	143.67	319	563.33	876.67	1259	1710.33	2230.67	2820	3478.33
HR (ϖ)	82	315.2	699.6	1325.2	1922	2760	3749.2	4889.6	6181.2	7624
IR2 (ϖ)	213	816.6	1810.8	3195.6	4971	7137	9693.6	12640.8	15978.6	19707
SDR (ϖ)	382	1466	3252	5740	8930	12822	17416	22712	28710	35410

Figure 4: Comparison of $m_{R_1}(\varpi)$, $m_{R_2}(\varpi)$, $HR(\varpi)$, $IR(\varpi)$, $SDR_(\varpi)$

The number of vertices and edges in $RCF_{(m)}$, for $m \geq 1$, are given by:

$$|V| = 12(7m^2 + 4m),$$

$$|E| = 6(19m^2 + 10m).$$

Edge Class	Vertex Degrees	Frequency	$\Bbbk_\varpi(u)$	$\Bbbk_\varpi(v)$
$E_1(\varpi)$	(2,2)	$6(3m^2 + 2m)$	3	3
$E_2(\varpi)$	(2,3)	$12(3m^2 + 2m)$	3	2
$E_3(\varpi)$	(3,3)	$12(5m^2 + 2m)$	2	2

Table 2: Edge partition of rectangular coronene fractal structures $RCF_{(m)}$

Theorem 3.1 *The first Revan index of rectangular coronene fractal structures $RCF_{(m)}$, where $m \geq 1$, is given by:*

$$R_1(\varpi) = 528m^2 + 228m. \tag{3.1}$$

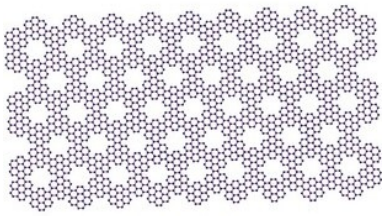


Figure 5: Rectangular coronene fractal structures $RCF_{(m)}$

Proof: Let

$$\begin{aligned}
R_1(\varpi) &= \sum_{\upsilon\nu\in E(\varpi)} (\Bbbk_\upsilon + \Bbbk_\nu) \\
&= \sum_{(2,2)\in E(\varpi)} (\Bbbk_\upsilon + \Bbbk_\nu) + \sum_{(2,3)\in E(\varpi)} (\Bbbk_\upsilon + \Bbbk_\nu) + \sum_{(3,3)\in E(\varpi)} (\Bbbk_\upsilon + \Bbbk_\nu) \\
&= (3+3)\cdot 6(3m^2+2m) + (3+2)\cdot 12(3m^2+2m) + (2+2)\cdot 12(5m^2+2m) \\
&= 6\cdot 6(3m^2+2m) + 5\cdot 12(3m^2+2m) + 4\cdot 12(5m^2+2m) \\
&= 36(3m^2+2m) + 60(3m^2+2m) + 48(5m^2+2m) \\
&= [108m^2+72m] + [180m^2+120m] + [240m^2+96m] \\
&= (108+180+240)m^2 + (72+120+96)m \\
&= 528m^2 + 228m.
\end{aligned} \tag{3.2}$$

□

Theorem 3.2 *The second Revan index of rectangular coronene fractal structures $RCF_{(m)}$, where $m \geq 1$, is given by:*

$$R_2(\varpi) = 618m^2 + 348m. \tag{3.3}$$

Proof: Let

$$\begin{aligned}
R_2(\varpi) &= \sum_{\upsilon\nu\in E(\varpi)} (\Bbbk_\upsilon \times \Bbbk_\nu) \\
&= \sum_{(2,2)\in E(\varpi)} (\Bbbk_\upsilon \times \Bbbk_\nu) + \sum_{(2,3)\in E(\varpi)} (\Bbbk_\upsilon \times \Bbbk_\nu) + \sum_{(3,3)\in E(\varpi)} (\Bbbk_\upsilon \times \Bbbk_\nu) \\
&= (3\times 3)\cdot 6(3m^2+2m) + (3\times 2)\cdot 12(3m^2+2m) + (2\times 2)\cdot 12(5m^2+2m) \\
&= 9\cdot 6(3m^2+2m) + 6\cdot 12(3m^2+2m) + 4\cdot 12(5m^2+2m) \\
&= 54(3m^2+2m) + 72(3m^2+2m) + 48(5m^2+2m) \\
&= [162m^2+108m] + [216m^2+144m] + [240m^2+96m] \\
&= (162+216+240)m^2 + (108+144+96)m \\
&= 618m^2 + 348m.
\end{aligned} \tag{3.4}$$

□

The number of vertices and edges in the rectangular coronene fractal structure $RCF_{(n)}$, where $n \geq 1$, are given by:

$$|V| = 12(7n^2 + 4n)$$

$$|E| = 6(19n^2 + 10n)$$

Theorem 3.3 *The hyper first Revan index of rectangular coronene fractal structures $RCF_{(m)}$, where $m \geq 1$, is given by:*

$$HR_1(\varpi) = 2508m^2 + 1416m \tag{3.5}$$

Proof: Let

$$\begin{aligned} HR_1(\varpi) &= \sum_{\upsilon\nu \in E(\varpi)} (\Bbbk_\upsilon + \Bbbk_\nu)^2 \\ &= \sum_{(2,2)\in E(\varpi)} (\Bbbk_\upsilon + \Bbbk_\nu)^2 + \sum_{(2,3)\in E(\varpi)} (\Bbbk_\upsilon + \Bbbk_\nu)^2 + \sum_{(3,3)\in E(\varpi)} (\Bbbk_\upsilon + \Bbbk_\nu)^2 \\ &= [3+3]^2 \cdot 6(3m^2 + 2m) + [3+2]^2 \cdot 12(3m^2 + 2m) + [2+2]^2 \cdot 12(5m^2 + 2m) \\ &= 36 \cdot 6(3m^2 + 2m) + 25 \cdot 12(3m^2 + 2m) + 16 \cdot 12(5m^2 + 2m) \\ &= 2508m^2 + 1416m \end{aligned} \tag{3.6}$$

□

Theorem 3.4 *The hyper second Revan index of rectangular coronene fractal structures $RCF_{(m)}$, where $m \geq 1$, is given by:*

$$HR_2(\varpi) = 3714m^2 + 2220m \tag{3.7}$$

Proof: Let

$$\begin{aligned} HR_2(\varpi) &= \sum_{\upsilon\nu \in E(\varpi)} (\Bbbk_\upsilon \times \Bbbk_\nu)^2 \\ &= \sum_{(2,2)\in E(\varpi)} (\Bbbk_\upsilon \times \Bbbk_\nu)^2 + \sum_{(2,3)\in E(\varpi)} (\Bbbk_\upsilon \times \Bbbk_\nu)^2 + \sum_{(3,3)\in E(\varpi)} (\Bbbk_\upsilon \times \Bbbk_\nu)^2 \\ &= [3\times 3]^2 \cdot 6(3m^2 + 2m) + [3\times 2]^2 \cdot 12(3m^2 + 2m) + [2\times 2]^2 \cdot 12(5m^2 + 2m) \\ &= 81 \cdot 6(3m^2 + 2m) + 36 \cdot 12(3m^2 + 2m) + 16 \cdot 12(5m^2 + 2m) \\ &= 3714m^2 + 2220m \end{aligned} \tag{3.8}$$

□

Theorem 3.5 *The modified first Revan index of rectangular coronene fractal structures $RCF_{(m)}$, where $m \geq 1$, is given by:*

$$m_{R_1}(\varpi) = \frac{126}{5}m^2 + \frac{64}{5}m \tag{3.9}$$

Proof: Let

$$\begin{aligned} m_{R_1}(\varpi) &= \sum_{\upsilon\nu\in E(\varpi)} \frac{1}{\Bbbk_\upsilon + \Bbbk_\nu} \\ &= \sum_{(2,2)\in E(\varpi)} \frac{1}{\Bbbk_\upsilon + \Bbbk_\nu} + \sum_{(2,3)\in E(\varpi)} \frac{1}{\Bbbk_\upsilon + \Bbbk_\nu} + \sum_{(3,3)\in E(\varpi)} \frac{1}{\Bbbk_\upsilon + \Bbbk_\nu} \\ &= \frac{6(3m^2+2m)}{6} + \frac{12(3m^2+2m)}{5} + \frac{12(5m^2+2m)}{4} \\ &= \frac{126}{5}m^2 + \frac{64}{5}m \end{aligned} \tag{3.10}$$

□

Theorem 3.6 *The modified second Revan index of rectangular coronene fractal structures $RCF_{(m)}$, where $m \geq 1$, is given by:*

$$m_{R_2}(\varpi) = 23m^2 + \frac{34}{3}m \tag{3.11}$$

Proof: Let

$$\begin{aligned} m_{R_2}(\varpi) &= \sum_{\upsilon\nu\in E(\varpi)} \frac{1}{\Bbbk_\upsilon \cdot \Bbbk_\nu} \\ &= \sum_{(2,2)\in E(\varpi)} \frac{1}{\Bbbk_\upsilon \cdot \Bbbk_\nu} + \sum_{(2,3)\in E(\varpi)} \frac{1}{\Bbbk_\upsilon \cdot \Bbbk_\nu} + \sum_{(3,3)\in E(\varpi)} \frac{1}{\Bbbk_\upsilon \cdot \Bbbk_\nu} \\ &= \frac{6(3m^2+2m)}{9} + \frac{12(3m^2+2m)}{6} + \frac{12(5m^2+2m)}{4} \\ &= 23m^2 + \frac{34}{3}m \end{aligned} \tag{3.12}$$

□

Theorem 3.7 *The harmonic Revan index of rectangular coronene fractal structures $RCF_{(m)}$, where $m \geq 1$, is given by:*

$$HR(\varpi) = \frac{252}{5}m^2 + \frac{128}{5}m \tag{3.13}$$

Proof: Let

$$\begin{aligned} HR(\varpi) &= \sum_{\upsilon\nu\in E(\varpi)} \frac{2}{\Bbbk_\upsilon + \Bbbk_\nu} \\ &= \sum_{(2,2)\in E(\varpi)} \frac{2}{\Bbbk_\upsilon + \Bbbk_\nu} + \sum_{(2,3)\in E(\varpi)} \frac{2}{\Bbbk_\upsilon + \Bbbk_\nu} + \sum_{(3,3)\in E(\varpi)} \frac{2}{\Bbbk_\upsilon + \Bbbk_\nu} \\ &= \frac{2\cdot 6(3m^2+2m)}{6} + \frac{2\cdot 12(3m^2+2m)}{5} + \frac{2\cdot 12(5m^2+2m)}{4} \\ &= \frac{252}{5}m^2 + \frac{128}{5}m \end{aligned} \tag{3.14}$$

□

Theorem 3.8 *The sum division Revan index of rectangular coronene fractal structures $RCF_{(m)}$, where $m \geq 1$, is given by:*

$$SDR(\varpi) = 234m^2 + 124m \tag{3.15}$$

Proof: Let

$$\begin{aligned} SDR(\varpi) &= \sum_{\upsilon_i\nu_j \in E(\varpi)} \left(\frac{\Bbbk_\upsilon}{\Bbbk_\nu} + \frac{\Bbbk_\nu}{\Bbbk_\upsilon}\right) \\ &= \sum_{(2,2)\in E(\varpi)} \left(\frac{3}{3} + \frac{3}{3}\right)(6(3m^2+2m)) \\ &\quad + \sum_{(2,3)\in E(\varpi)} \left(\frac{3}{2} + \frac{2}{3}\right)(12(3m^2+2m)) \\ &\quad + \sum_{(3,3)\in E(\varpi)} \left(\frac{2}{2} + \frac{2}{2}\right)(12(5m^2+2m)) \\ &= 2\cdot 6(3m^2+2m) + \frac{13}{6}\cdot 12(3m^2+2m) + 2\cdot 12(5m^2+2m) \\ &= 234m^2 + 124m \end{aligned} \tag{3.16}$$

□

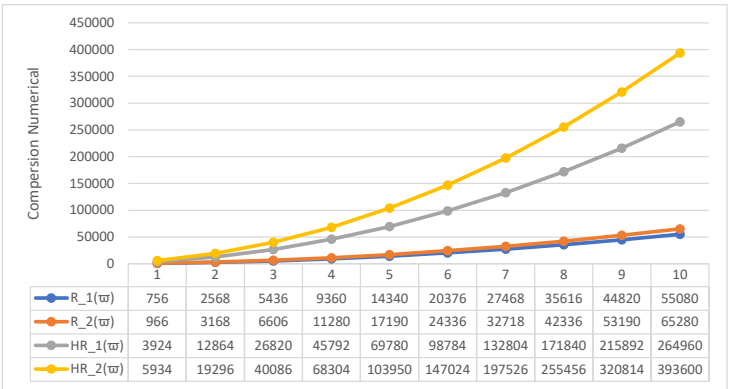
Theorem 3.9 *The inverse Revan index of Rectangular coronene fractal structures $RCF_{(m)}$, where $m \geq 1$, is given by:*

$$IR(\varpi) = \frac{576}{5}m^2 + \frac{304}{5}m \tag{3.17}$$

Proof: Let

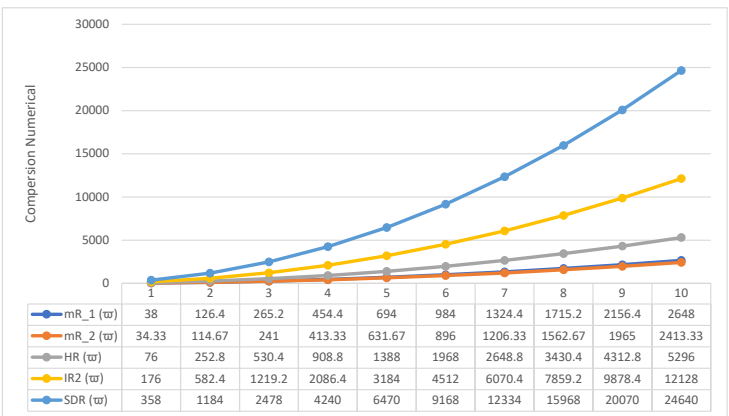
$$\begin{aligned} IR(\varpi) &= \sum_{\upsilon_i\nu_j \in E(\varpi)} \frac{\Bbbk_\upsilon \times \Bbbk_\nu}{\Bbbk_\upsilon + \Bbbk_\nu} \\ &= \sum_{(2,2)\in E(\varpi)} \left(\frac{3\times 3}{3+3}\right)(6(3m^2+2m)) \\ &\quad + \sum_{(2,3)\in E(\varpi)} \left(\frac{3\times 2}{3+2}\right)(12(3m^2+2m)) \\ &\quad + \sum_{(3,3)\in E(\varpi)} \left(\frac{2\times 2}{2+2}\right)(12(5m^2+2m)) \\ &= \frac{9}{6}\cdot 6(3m^2+2m) + \frac{6}{5}\cdot 12(3m^2+2m) + \frac{4}{4}\cdot 12(5m^2+2m) \\ &= \frac{3}{1}\cdot(3m^2+2m) + \frac{72}{5}(3m^2+2m) + 12(5m^2+2m) \\ &= \left[3 + \frac{216}{5} + 60\right]m^2 + \left[6 + \frac{144}{5} + 24\right]m \\ &= \frac{576}{5}m^2 + \frac{304}{5}m \end{aligned} \tag{3.18}$$

□



	1	2	3	4	5	6	7	8	9	10
R_1(ϖ)	756	2568	5436	9360	14340	20376	27468	35616	44820	55080
R_2(ϖ)	966	3168	6606	11280	17190	24336	32718	42336	53190	65280
HR_1(ϖ)	3924	12864	26820	45792	69780	98784	132804	171840	215892	264960
HR_2(ϖ)	5934	19296	40086	68304	103950	147024	197526	255456	320814	393600

Figure 6: Comparison of $R_1(\varpi)$, $R_2(\varpi)$, $HR_1(\varpi)$, $HR_2(\varpi)$



	1	2	3	4	5	6	7	8	9	10
mR_1 (ϖ)	38	126.4	265.2	454.4	694	984	1324.4	1715.2	2156.4	2648
mR_2 (ϖ)	34.33	114.67	241	413.33	631.67	896	1206.33	1562.67	1965	2413.33
HR (ϖ)	76	252.8	530.4	908.8	1388	1968	2648.8	3430.4	4312.8	5296
IR2 (ϖ)	176	582.4	1219.2	2086.4	3184	4512	6070.4	7859.2	9878.4	12128
SDR (ϖ)	358	1184	2478	4240	6470	9168	12334	15968	20070	24640

Figure 7: Comparison of $m_{R_1}(\varpi)$, $m_{R_2}(\varpi)$, $HR(\varpi)$, $IR(\varpi)$, $SDR_(\varpi)$

4. Numerical and Graphical Representation

The computed results for the Zigzags Coronene Fractal and Rectangular Coronene Fractal structures are presented both numerically and graphically.

For the Zigzags Coronene Fractal, the topological indices derived in the previous section are summarized mathematically in Table 1, while their numerical behavior is illustrated in Figures 3 and 4. As observed in the figures, all index values exhibit a consistent increasing trend as the parameter n increases. This upward trajectory confirms that the topological indices listed in Table 1 grow proportionally with n.

Similarly, the results for the Rectangular Coronene Fractal are shown in Table 2, with their graphical representation provided in Figures 6 and 7. The graphs clearly demonstrate that all topological index values increase steadily with the parameter m. This observation supports the conclusion that the indices given in Table 2 follow an ascending trend as m grows.

These numerical and graphical validations affirm the mathematical behavior and monotonic growth of the Revan-type topological indices for both types of coronene fractal structures.

5. Conclusion

In this study, we computed a range of degree-based topological indices—specifically the Revan-type indices—for both Zigzag Coronene Fractal Structures and Rectangular Coronene Fractals. These computations offer meaningful insights into the structural characterization of coronene-based molecular graphs. A compatibility analysis was also conducted to evaluate the relationships among the various indices, reinforcing their effectiveness and relevance in structural analysis. The outcomes of this research contribute to the growing understanding of molecular topology and its potential applications in chemistry and material science. Future work may focus on extending these analyses to more intricate and higher-dimensional fractal structures. Additional topological indices could be incorporated to further refine molecular characterization. Moreover, investigating the correlations between topological indices and physical, chemical, or electronic properties may reveal deeper insights into molecular behavior and stability. Integrating machine learning techniques for predicting such properties based on topological features presents another promising direction. Potential applications in fields such as drug discovery, nanotechnology, and computational materials science make this a fertile area for continued interdisciplinary exploration.

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