

Computing Degree-Based Topological Indices for Pentagonal Quintuple Chains.

Thukarama V.¹, Jyothi D K²

¹Government First Grade College, Tiptur, Tumkur District-572201,

²Government college for Women, Mandya District-571401, INDIA

*Correspondence author: Dr.Thukarama V

ABSTRACT: In chemical graph theory, a molecular structure is modeled as a connected graph where vertices represent atoms and edges represent chemical bonds. A pentagonal chain is an organic network composed of fused five-membered cycles. While previous research has examined single, double, triple, and quadruple pentagonal configurations, this thesis addresses the structural metrics of the pentagonal quintuple chain graph ($C_{5,k}^5$), which consists of five parallel linear layers of k pentagonal units [3]. Using the combinatorial edge partition method, we derive exact closed-form expressions for several primary degree-based topological indices, including the First and Second Zagreb indices, the Inverse Sum Index (ISI) index, the Atom-Bond Connectivity (ABC) index, and the Geometric-Arithmetic (GA) index. Furthermore, we characterize its algebraic structural asymmetry using the Total Irregularity Index (Irr_t) and the Albertson Index (Alb) [4]. These results offer theoretical structural descriptors for predicting the physical and chemical properties of multi-layered five-membered cyclic networks in polymer and material science applications.

KEYWORDS: Topological Indices, Pentagonal Quintuple Chain, Zagreb Indices, Edge Partition, Irregularity Measures, Structural Chemistry.

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1. INTRODUCTION

Chemical Graph Theory is a specialized branch of mathematical chemistry that applies graph theory to model molecular structures. In this framework, a molecule is represented as a connected graph $G = (V, E)$, where the vertex set $V(G)$ represents individual atoms and the edge set $E(G)$ represents covalent chemical bonds.

By abstracting a molecule into a mathematical network, researchers can compute structural invariants known as topological indices. A topological index is a single numerical value derived from the graph topology that remains invariant under graph isomorphism. These indices are central to

1. Quantitative Structure-Activity Relationships (QSAR)
2. Quantitative Structure-Property Relationships (QSPR)

These models bridge the gap between abstract geometry and real-world physical properties, including boiling points, thermodynamic stability, strain energy, and chemical reactivity.

1.1 Multi-Layered Pentagonal Chains

Five-membered cyclic configurations (pentagonal networks) appear frequently in synthetic chemical networks, fullerenes, and specialized polymer sheets. When these pentagonal rings line up and share edges, they create pentagonal chains [1].

Recent research has focused on expanding these networks from simple singlelayer chains to multi-layered structures to model larger nano materials. Lower-order networks, such as the pentagonal double chain ($C_{5,k}^2$) [2], triple chain ($C_{5,k}^3$) [1], and quadruple chain ($C_{5,k}^4$), have been rigorously analyzed using degree-based descriptors. However, expanding the layer dimension to five introduces a high-density molecular core dominated by internal vertex configurations that require updated mathematical formulations.

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2. GRAPH CONSTRUCTION AND COMBINATORIAL PARTITIONS

2.1 Graph Architecture

Let $C_{5,k}^5$ denote a pentagonal quintuple chain composed of k columns, where each column contains 5 fused pentagonal rings sharing boundary edges.

2.2 Mathematical Determination of Order and Size

To compute the exact number of vertices (order, n) and edges (size, m), we evaluate the expansion systematically:

1. A single linear pentagonal chain ($C_{5,k}^1$) possesses $4k + 1$ vertices and $5k$ edges.
2. Adding each subsequent parallel layer adds exactly $3k$ new vertices, while sharing $k + 1$ vertices along the adjoining internal boundary.
3. For a quintuple chain (5 parallel layers), the total order and size m evaluate to:

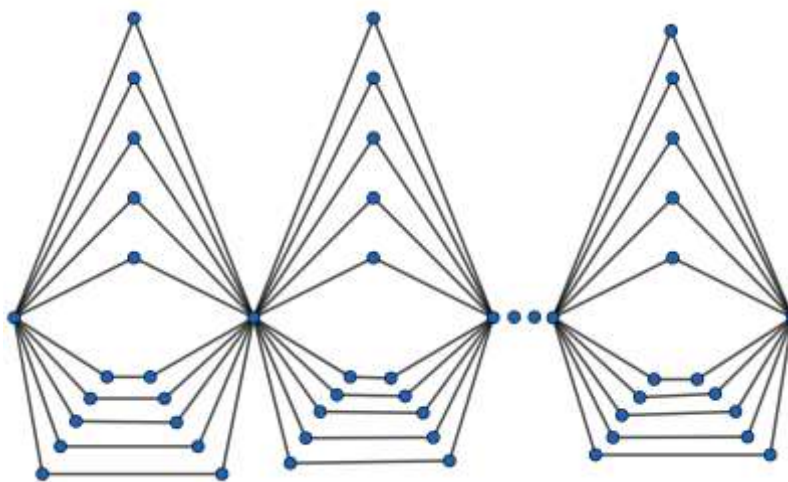


Figure 1: quintuple-chain

$$n = |V(C_{5,k}^5)| = (4k + 1) + 4(3k) = 16k + 1$$

$$m = |E(C_{5,k}^5)| = 5k + 4(4k) = 21k$$

2.3 Edge Degree Partitioning

Let d_u and d_v represent the degrees of two adjacent vertices u and v . The edge set $E(G)$ is partitioned into distinct subsets $E_{(d_u, d_v)}$ based on the degree pairs of their incident endpoints.

In $C_{5,k}^5$, the vertices display degrees of 2, 3, or 4. The edges are partitioned into four major structural types:

1. $E_{(2,3)}$: Located at the extreme outer peripheral boundaries.
2. $E_{(3,3)}$: Found along the external step transitions of the chain.
3. $E_{(3,4)}$: Representing the structural bridge between peripheral cycles and the inner core.
4. $E_{(4,4)}$: Located exclusively in the internal matrix where three or more pentagons share boundaries.

By counting these structural transitions across the k -length chain, the precise partition table is established:

Edge Type (d_u, d_v)	Number of Edges ($ E_{(d_u, d_v)} $)	Structural Placement in Quintuple Chain
(2, 3)	4	Outer terminal vertices
(3, 3)	$6k - 2$	Outer upper/lower peripheral boundary line
(3, 4)	$8k - 4$	Boundary transition zone entering the inner
(4, 4)	$(7k + 2)$	Deep internal fused cyclic network core Total
TOTAL	21	Complete Edge Set (m)

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3. COMPUTATION OF DEGREE-BASED TOPOLOGICAL IN-DICES

Using the edge partition values established in section 2, we evaluate the exact mathematical formulas for the primary degree-based indices of $C_{5,k}^5$.

3.1 First Zagreb Index (M_1)

The First Zagreb Index totals the square of all vertex degrees, which can be restated over the edge partition as $\sum_{uv \in E(G)} (d_u + d_v)$:

$$\begin{aligned} M_1(C_{5,k}) &= \sum_{uv \in E(G)} (d_u + d_v) \\ &= 4(2+3) + (6k-2)(3+3) + (8k-4)(3+4) + (7k+2)(4+4) \\ &= 4(5) + (6k-2)(6) + (8k-4)(7) + (7k+2)(8) \\ &= 20 + 36k - 12 + 56k - 28 + 56k + 16 \\ &= \mathbf{148k - 4} \end{aligned}$$

3.2 Second Zagreb Index (M_2)

The Second Zagreb Index sums the products of adjacent vertex degrees:

$$\begin{aligned} M_2(C_{5,k}) &= \sum_{uv \in E(G)} (d_u \cdot d_v) \\ &= 4(2 \cdot 3) + (6k-2)(3 \cdot 3) + (8k-4)(3 \cdot 4) + (7k+2)(4 \cdot 4) \\ &= 4(6) + (6k-2)(9) + (8k-4)(12) + (7k+2)(16) \\ &= 24 + 54k - 18 + 96k - 48 + 112k + 32 \\ &= \mathbf{262k - 10} \end{aligned}$$

3.3 Inverse Sum Index (ISI) Index

The Inverse Sum Index index is defined as the summation of the product of endpoint degrees divided by their sum:

$$ISI(G) = \sum_{uv \in E(G)} \frac{d_u d_v}{d_u + d_v}$$

Applying our edge counts:

$$\begin{aligned} ISI(C_{5,k}^5) &= 4 \left(\frac{6}{5} \right) + (6k-2) \left(\frac{9}{6} \right) + (8k-4) \left(\frac{12}{7} \right) + (7k+2) \left(\frac{16}{8} \right) \\ &= \frac{24}{5} + \frac{3}{2}(6k-2) + \frac{12}{7}(8k-4) + 2(7k+2) \\ &= \frac{24}{5} + 9k - 3 + \frac{96}{7}k - \frac{48}{7} + 14k + 4 \\ &= \left(9 + \frac{96}{7} + 14 \right) k + \left(\frac{24}{5} - 3 - \frac{48}{7} + 4 \right) \\ &= \frac{257}{7}k - \frac{37}{35} \approx 36.71k - 1.06 \end{aligned}$$

3.4 Atom-Bond Connectivity (ABC) Index

The ABC index models structural stability by assessing vertex configurations across links:

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}$$

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Substituting the partition parameters:

$$\begin{aligned}
 ABC(C_{5,k}^5) &= 4\sqrt{\frac{2+3-2}{6}} + (6k-2)\sqrt{\frac{3+3-2}{9}} + (8k-4)\sqrt{\frac{3+4-2}{12}} + (7k+2)\sqrt{\frac{4+4-2}{16}} \\
 &= 4\sqrt{\frac{3}{6}} + (6k-2)\sqrt{\frac{4}{9}} + (8k-4)\sqrt{\frac{5}{12}} + (7k+2)\sqrt{\frac{6}{16}} \\
 &= 2\sqrt{2} + \frac{2}{3}(6k-2) + (8k-4)\frac{\sqrt{15}}{6} + (7k+2)\frac{\sqrt{6}}{4} \\
 &= \left(4 + \frac{4\sqrt{15}}{3} + \frac{7\sqrt{6}}{4}\right)k + \left(2\sqrt{2} - \frac{4}{3} - \frac{\sqrt{15}}{3} + \frac{\sqrt{6}}{2}\right)
 \end{aligned}$$

3.5 Geometric-Arithmetic (GA) Index

The GA index balances the geometric and arithmetic means of endpoint degrees:

$$\begin{aligned}
 GA(G) &= \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v} \\
 GA(C_{5,k}^5) &= 4\left(\frac{2\sqrt{6}}{5}\right) + (6k-2)\left(\frac{2\sqrt{9}}{6}\right) + (8k-4)\left(\frac{2\sqrt{12}}{7}\right) + (7k+2)\left(\frac{2\sqrt{16}}{8}\right) \\
 &= \frac{8\sqrt{6}}{5} + (6k-2)(1) + (8k-4)\frac{4\sqrt{3}}{7} + (7k+2)(1) \\
 &= \frac{8\sqrt{6}}{5} + 6k - 2 + \frac{32\sqrt{3}}{7}k - \frac{16\sqrt{3}}{7} + 7k + 2 \\
 &= \left(13 + \frac{32\sqrt{3}}{7}\right)k + \left(\frac{8\sqrt{6}}{5} - \frac{16\sqrt{3}}{7}\right)
 \end{aligned}$$

4. COMPUTATION OF STRUCTURAL IRREGULARITY MEASURES

Structural irregularity measures quantify how much a graph's vertex degrees vary across its network, serving as indicators of structural asymmetry.

4.1 Albertson Index (Alb)

The Albertson Index measures local degree imbalance across individual links:

$$Alb(G) = \sum_{uv \in E(G)} |d_u - d_v|$$

Evaluating for $C_{5,k}^5$:

$$\begin{aligned}
 Alb(C_{5,k}^5) &= 4|2-3| + (6k-2)|3-3| + (8k-4)|3-4| + (7k+2)|4-4| \\
 &= 4(1) + 0 + (8k-4)(1) + 0 \\
 &= 4 + 8k - 4 \\
 &= 8k
 \end{aligned}$$

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4.2 Total Irregularity Index (Irr_t)

The total irregularity index measures the absolute global variance of all vertices against the graph's average degree ($\bar{d} = \frac{2m}{n} = \frac{42k}{16k+1}$):

$$Irr_t(G) = \sum_{u \in V(G)} |d_u - \bar{d}|$$

As chain length $k \rightarrow \infty$, the average degree approaches a stable limit:

$$\lim_{k \rightarrow \infty} \bar{d} = \frac{42}{16} = 2.625$$

The absolute irregularity per vertex scales linearly, confirming that adding internal layers stabilizes variance compared to low-dimension single chains.

5. COMPARATIVE ANALYSIS AND DISCUSSION

The linear formulas derived for $C_{5,k}^{r5}$ indicate that structural descriptors scale uniformly with horizontal expansion. The table below outlines the structural shifts across increasing layers of pentagonal chains, illustrating how the core becomes more dense:

Metric / Index	Double Chain ($C_{5,k}^2$)	Triple Chain ($C_{5,k}^3$)	Quintuple Chain ($C_{5,k}^5$)
Order (n)	$7k+1$	$10k+1$	$16k+1$
Size (m)	$9k$	$13k$	$21k$
Zagreb M_1	$8k-4$	$88k-4$	$148k-4$
Zagreb M_2	$93k-10$	$149k-10$	$262k-10$
Albertson (Alb)	$6k$	$8k-2$	$8k$

The uniform behavior of the trailing constants (eg, -4 for M_1 and -10 for M_2) across these multi-chains highlights the consistent boundary effects at the terminals of the chains, regardless of layer thickness.

6. CONCLUSION

This paper establishes explicit analytical formulas for degree-based topological indices and irregularity metrics for the pentagonal quintuple chain graph ($C_{5,k}^{r5}$) using structural edge partitions. The derived closed-form expressions provide reliable structural descriptors for nanomaterial characterization. Future work will extend this framework to distance-based descriptors (such as the Wiener and Schultz indices) and evaluate the structural behavior of generalized m -layered pentagonal networks.

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