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Structural Insights into Neighbor Degree-Based Topological Indices for Hexagonal Chain Structures

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Abstract

Background/Objectives: Topological indices serve as essential tools in chemical graph theory, offering numerical descriptors that correlate molecular structure with physicochemical properties. This study introduces and analyzes new topological indices for hexagonal chain-based molecular graphs, focusing on their structural significance and predictive capabilities. **Methods**: We compute the neighbor degree based redefined third Zagreb index, forgotten index, and reduced Zagreb index for three distinct hexagonal chain structures: hammer-like benzenoid chains, linear hexagonal chains, and armchair hexagonal chains. By leveraging degree-based invariants, we establish mathematical formulations that enhance the understanding of molecular connectivity and stability. **Findings**: The results provide a deeper insight into the mathematical foundations of molecular descriptors and their interdisciplinary applications in computational chemistry, drug design, and material science. **Novelty**: Our work provides a simple yet effective way to analyze these graphs and opens new possibilities for studying their applications in chemistry.

Keywords: Neighborhood Degree; Redefined third Zagreb index; Forgotten index; Reduced Zagreb index; Hexagonal chains

1 Introduction

A graph can be described as mathematical structure consisting of two sets: a set V of entities called vertices (or nodes) and a set E of pairs of vertices, known as edges. The degree of a vertex in a graph is the count of edges that are directly connected to it and is represented as $deg(v)$ [(1)]. Nowadays the idea of the neighbor degree sum has drawn substantial scholarly attention and has been extensively studied by researchers. The neighbor degree sum of a vertex v is defined as, $\delta_G(v) = \sum_{u \in N_G(v)} d_G(u)$ and it is used to define various topological indices like Redefined third Zagreb index $ReZ(G)$ and Reduced Zagreb index $RM_2(G)$ [(2)].

$$ReZ(G) = \sum_{u \in V(G)} d_G(u)^2 \delta_G(u). \quad (1)$$

$$RM_2(G) = m + \frac{1}{2}\sum_{u\in V(G)} \delta_G(u)(d_G(u)-2). \quad (2)$$

Topological indices are important numerical measures derived from the graph models of chemical structures. These indices help chemists understand and predict various molecular properties, including boiling point, strain energy, stability, and biological activity. One area where these indices have been particularly useful is in the study of benzenoid systems, which are widely found in organic compounds.

Alongside introducing several neighbor degree indices, Mondal[3],[4] has discussed their key mathematical features, highlighting their relevance in graph theoretic analysis. These indices contribute to a deeper understanding of network structures and offer valuable tools for ongoing research.

Later, inspired from the Forgotten topological indices Mondal introduced neighborhood version of Forgotten topological index $F_N(G)$ [4] as follows:

$$F_N(G) = \sum_{u\in V(G)} \delta_G(u)^3. \quad (3)$$

Among benzenoid structures, hexagonal chains have drawn considerable interest. These chains can take different forms, such as *hammer-like benzenoid chains*, *linear hexagonal chains* and *armchair hexagonal chains*. Each type of chain is built from hexagonal rings joined in specific ways, giving rise to different shapes and properties. For example, linear hexagonal chains resemble a straight sequence of hexagons, while armchair and hammer-like forms show more complex branching and arrangements. These variations are important when designing new organic materials, including nanoribbons and molecular wires. So far, most studies on topological indices have focused on simpler or more regular structures. However, detailed investigations of indices for hexagonal chains like the hammer-like and armchair types are still limited. This lack of data leaves a gap in understanding how these specific structures influence molecular properties as described by topological indices. Our study aims to provide a more intuitive characterization of the molecular structure of these chains, seeking to bridge existing gaps in chemical theory and computational approaches using graph theory.

Hammer-like benzenoid chains, **Figure 1 (a)** are molecular structures that integrate both catacondensed and pericondensed features. Structurally, they consist of a central linear polyacene comprising *n* linearly fused benzene rings flanked by two pyrene-like fragments at each end. These terminal units are pericondensed, meaning they share more than one edge with adjacent rings, giving the molecule its characteristic "hammer" shape. The corresponding molecular graph features vertices representing carbon atoms and edges as bonds, with vertex degrees of 2 at the periphery and 3 in the interior. These chains are highly symmetric and serve as ideal compounds for theoretical analyses involving topological indices. Their hybrid topology and predictable symmetry are useful in computational chemistry and molecular modelling.

A linear hexagonal benzenoid chain, **Figure 1 (b)** is a planar catacondensed molecular structure composed of benzene rings fused edge-to-edge in a straight alignment. Each unit in the chain shares a side with its neighboring hexagon, creating a honeycomb-like strip that extends horizontally or vertically, depending on orientation. The geometry is remarkably symmetric, with no ring sharing more than one edge ensuring the absence of internal vertices with higher connectivity. This configuration supports a pattern of alternating single and double carbon-carbon bonds, promoting extensive π -electron delocalization across the molecule. These chains are foundational in modeling polyacenes, making them a staple in computational chemistry and molecular graph theory, particularly in evaluating aromatic stability, toological indices and quantum descriptors.

An armchair hexagonal benzenoid chain, **Figure 1 (c)** is a structural variation of the linear type, characterized by a periodic zigzag arrangement of fused benzene rings. Unlike the straight configuration of linear chains, the fusion pattern here alternated in an up and down fashion, giving rise to a distinctive edge shape often referred to as the "armchair" edge. This arrangement preserves symmetry across the molecule and introduces alternating bond angles, contributing to its unique electronic and mechanical properties. The design is especially significant in the study of graphene nanoribbons and carbon-based materials, where such geometries influence conductivity, aromaticity and edge-state behaviors.

In recent years, many studies have focused on some degree and neighborhood degree-based complex chemical networks, chains, and drug-related molecular structures. Kulli VR. defined leap Kepler Banhatti indices of molecular structure such as remdesivir, chloroquine and hydroxychloroquine[5]. Asghar A. investigated the neighborhood degree-based topological indices of cellulose, amylopectin and some complex networks[6],[7]. Chen R. delt with square-hexagonal chains and their structural properties[8]. Further works are carried out on degree-based topological indices on molecular structures of cardiac drugs, TriCF network, hexagonal phenylene chain network and dominating David derived networks and explored new applications[9],[10],[11],[12].

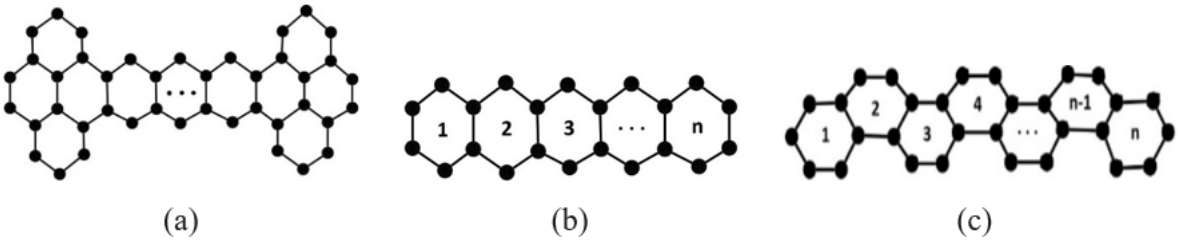

Fig 1. Hammer-like benzenoid chain, (b) Linear hexagonal chain, (c) Armchair hexagonal chain

2 Methodology

In this work, we analyze three types of hexagonal chains distinguished by their structural arrangements and vertex classifications based on the neighbor degree sum.

Type 1: **Hammer-like benzenoid chain:**

Table 1. The values of $d_G(u)$ when $\delta_G(u) = 4,5,6,7,8,9$ in hammer-like benzenoid chain

$\delta_G(u)$	4	5	6	7	8	9
$d_G(u)$	2	2	2	3	3	3

Table 2. Cardinality of the vertex set when neighbor degree sum $\delta_G(u) = 4,5,6,7,8,9$ with corresponding $n \geq 9$ hexagonal faces in order $m \in N = \{1,2,3,4,\ldots\}$ in hammer-like benzenoid chain

No. of hexagonal faces	V_0 $(\delta_G(u)=4)$	V_1 $(\delta_G(u)=5)$	V_2 $(\delta_G(u)=6)$	V_3 $(\delta_G(u)=7)$	V_4 $(\delta_G(u)=8)$	V_5 $(\delta_G(u)=9)$
9	4	12	2	4	8	4
10	4	12	4	6	8	4
11	4	12	6	8	8	4
12	4	12	8	10	8	4
13	4	12	10	12	8	4
.	.	.	.	.	.	.
.	.	.	.	.	.	.
.	.	.	.	.	.	.
n	4	12	2m	4n-2m-30	8	4

Type 2: Linear hexagonal chain:

Table 3. The values of $d_G(u)$ when $\delta_G(u) = 4,5,6,7$ in linear hexagonal chain

$\delta_G(u)$	4	5	6	7
$d_G(u)$	2	2	2	3

Type 3: Armchair hexagonal chain:

3 Results and Discussion

In this section we computed $ReZ(G)$, $RM_2(G)$, $F_N(G)$ for three types of chemical hexagonal chains as shown in Figure 1.

Theorem 2.1 Let G be the hammer-like benzenoid chain with $n \geq 9$ hexagonal faces. Then,

$$ReZ(G) = 252n - 78m - 686$$
$$RM_2(G) = 44n - 7m - 73$$
$$F_N(G) = 2(686n - 127m - 761)$$

Table 4. Cardinality of the vertex set when neighbor degree sum $\delta_G(u) = 4, 5, 6, 7$ with corresponding $n \geq 3$ hexagonal faces in linear hexagonal chain

Number of hexagonal faces	V_0 $(\delta_G(u) = 4)$	V_1 $(\delta_G(u) = 5)$	V_2 $(\delta_G(u) = 6)$	V_3 $(\delta_G(u) = 7)$
3	4	4	2	4
4	4	4	4	6
5	4	4	6	8
6	4	4	8	10
.	.	.	.	.
.	.	.	.	.
.	.	.	.	.
n	4	4	2n-4	2n-2

Table 5. The values of $d_G(u)$ when $\delta_G(u) = 4, 5, 7, 8$ in armchair hexagonal chain

$\delta_G(u)$	4	5	7	8
$d_G(u)$	2	2	3	3

Table 6. Cardinality of the vertex set when neighbor degree sum $\delta_G(u) = 4, 5, 7, 8$ with corresponding $n \geq 3$ hexagonal faces in armchair hexagonal chain

Number of hexagonal faces	V_0 $(\delta_G(u) = 4)$	V_1 $(\delta_G(u) = 5)$	V_2 $(\delta_G(u) = 7)$	V_3 $(\delta_G(u) = 8)$
3	4	6	2	2
4	4	8	2	4
5	4	10	2	6
6	4	12	2	8
.	.	.	.	.
.	.	.	.	.
.	.	.	.	.
n	4	2n	2	2(n-2)

Proof: By substituting the values from the Table 1 and Table 2 in **Equation 1, Equation 2 and Equation 3**. We obtain,

$$\begin{aligned} ReZ(G) &= \sum_{u\in V_0(G)} 2^2(4) + \sum_{u\in V_1(G)} 2^2(5) + \sum_{u\in V_2(G)} 2^2(6) + \sum_{u\in V_3(G)} 3^2(7) + \sum_{u\in V_4(G)} 3^2(8) \\ &\quad + \sum_{u\in V_5(G)} 3^2(9) = 252n - 78m - 686 \\ RM_2(G) &= (5n-3) + (5n-3) + (5n-3) + \left((5n-3) + \tfrac{1}{2}\sum_{u\in V_3(G)} 7\right) + \left((5n-3) + \tfrac{1}{2}\sum_{u\in V_4(G)} 8\right) \\ &\quad + \left((5n-3) + \tfrac{1}{2}\sum_{u\in V_5(G)} 9\right) = 44n - 7m - 73 \\ F_N(G) &= \sum_{u\in V_0(G)} 4^3 + \sum_{u\in V_1(G)} 5^3 + \sum_{u\in V_2(G)} 6^3 + \sum_{u\in V_3(G)} 7^3 + \sum_{u\in V_4(G)} 8^3 + \sum_{u\in V_5(G)} 9^3 \\ &= 2(686n - 127m - 761) \end{aligned}$$

Theorem 2.2 Let G be the linear hexagonal chain with $n \geq 3$ hexagonal faces. Then,

$$\begin{aligned} ReZ(G) &= 2(87n - 39) \\ RM_2(G) &= 3(9n - 1) \\ F_N(G) &= 2(559n - 397) \end{aligned}$$

Proof: By substituting the values from the Table 3 and Table 4 in **Equation 1, Equation 2 and Equation 3**. We obtain,

$$\begin{aligned} ReZ(G) &= \sum_{u\in V_0(G)} 2^2(4) + \sum_{u\in V_1(G)} 2^2(5) + \sum_{u\in V_2(G)} 2^2(6) + \sum_{u\in V_3(G)} 3^2(7) = 2(87n - 39) \\ RM_2(G) &= (5n+1) + (5n+1) + (5n+1) + \left((5n+1) + \tfrac{1}{2}\sum_{u\in V_3(G)} 7\right) = 3(9n - 1) \\ F_N(G) &= \sum_{u\in V_0(G)} 4^3 + \sum_{u\in V_1(G)} 5^3 + \sum_{u\in V_2(G)} 6^3 + \sum_{u\in V_3(G)} 7^3 = 2(559n - 397) \end{aligned}$$

Theorem 2.3 Let G be the armchain hexagonal chain with $n \geq 3$ hexagonal faces. Then,

$$ReZ(G) = 2(92n-49)$$
$$RM_2(G) = 28n-5$$
$$F_N(G) = 2(637n-553)$$

Proof: By substituting the values from the Table 5 and Table 6 in **Equation 1, Equation 2 and Equation 3**. We obtain,

$$\begin{aligned} ReZ(G) &= \sum_{u\in V_0(G)} 2^2(4) + \sum_{u\in V_1(G)} 2^2(5) + \sum_{u\in V_2(G)} 3^2(7) + \sum_{u\in V_3(G)} 3^2(8) = 2(92n-49) \\ RM_2(G) &= (5n+1)+(5n+1)+\left((5n+1)+\tfrac{1}{2}\sum_{u\in V_3(G)} 7\right)+\left((5n+1)+\tfrac{1}{2}\sum_{u\in V_4(G)} 8\right) = 28n-5 \\ F_N(G) &= \sum_{u\in V_0(G)} 4^3 + \sum_{u\in V_1(G)} 5^3 + \sum_{u\in V_2(G)} 7^3 + \sum_{u\in V_3(G)} 8^3 = 2(637n-553) \end{aligned}$$

4 Application of the topological descriptors to the QSPR /QSAR of molecular structure

In this section, we have analysed the QSPR data- strain energy and boiling point of the different benzenoid chains using their molecular structure's topological descriptors, studied above.

Table 7. Strain energy and boiling point for hammer-like benzenoid chains, linear hexagonal chains, armchair hexagonal chains based on available research

Hammer-like benzenoid chains (11 to 23 hexagonal faces)					
Hexagonal Faces (n)	**Strain Energy (kJ/mol)**	**Boiling Point (°C)**	$ReZ(G)$	$RM_2(G)$	$F_N(G)$
11	120.5	80	1852	390	12808
12	135.2	95	2026	427	13926
13	150.8	110	2200	464	15044
14	165.4	125	2374	501	16162
15	180.1	140	2548	538	17280
16	195.7	155	2722	575	18398
17	210.3	170	2896	612	19516
18	225.9	185	3070	649	20634
19	241.5	200	3244	686	21752
20	257.1	215	3418	723	22870
21	272.7	230	3592	760	23988
22	288.3	245	3766	797	25106
23	303.9	260	3940	834	26224
Linear hexagonal chains (3 to 15 hexagonal faces)					
Hexagonal Faces (n)	**Strain Energy (kJ/mol)**	**Boiling Point (°C)**	$ReZ(G)$	$RM_2(G)$	$F_N(G)$
3	115.3	78	444	78	2560
4	130.1	92	618	105	3678
5	145.6	107	792	132	4796
6	160.9	122	966	159	5914
7	176.2	137	1140	186	7032
8	191.5	152	1314	213	8150
9	206.8	167	1488	240	9268
10	222.1	182	1662	267	10386
11	237.4	197	1836	294	11504
12	252.7	212	2010	321	12622
13	268.0	227	2184	348	13740
14	283.3	242	2358	375	14858
15	298.6	257	2532	402	15976

Continued on next page

Table 7 continued

Armchair hexagonal chains (3 to 15 hexagonal faces) Hexagonal Faces (n)	**Strain Energy (kJ/mol)**	**Boiling Point (°C)**	$ReZ(G)$	$RM_2(G)$	$F_N(G)$
3	118.2	82	454	79	2716
4	132.8	97	638	107	3990
5	147.5	112	822	135	5264
6	162.1	127	1006	163	6538
7	176.7	142	1190	191	7812
8	191.3	157	1374	219	9086
9	205.9	172	1558	247	10360
10	220.5	187	1742	275	11634
11	235.1	202	1926	303	12908
12	249.7	217	2110	331	14182
13	264.3	232	2294	359	15456
14	278.9	247	2478	387	16730
15	293.5	262	2662	415	18004

Table 8. Correlation coefficients of $ReZ(G)$, $RM_2(G)$ and $F_N(G)$ with Strain energy and boiling point

	ReZ(G)	***$F_N(G)$***	***$RM_2(G)$***
Strain Energy (Hammer)	0.999946	0.999946	0.999946
Strain Energy (Linear)	0.999999	0.999999	0.999999
Strain Energy (Armchair)	1	1	1
Boiling point (Hammer)	1	1	1
Boiling point (Linear)	0.999991	0.999991	0.999991
Boiling point (Armchair)	1	1	1

Table 8 was obtained using python plots for the first 13 molecular structures of three type of hexagonal chains under our study. We observe a strong correlation between the variables, given the $\mathbf{R^2}$ value of **1** (signifies a perfect fit) for all the three models for correlation with the forgotten index, $F_N(G)$ of armchair structural model, hammer like benzenoid chains and the linear chain model with their respective boiling points. The model equations are **y = 84.933x - 4248.5**, **y = 74.533x + 6845.3** and **y = 74.696x – 3212** respectively. Similarly, the regression correlation model of Redefined third Zagreb index $ReZ(G)$ of all the three hexagonal chain structures mentioned above v/s their boiling points depict strong linear relationships with perfect $\mathbf{R^2}$ values of **1**(perfect fit), confirming precise fits. Each model follows a distinct trend, with equations **y = 74.533x + 6845.3**, **y = 12.267x - 551.87**, and **y = 11.625x - 454.33**, respectively. All the three chain models scatter plots under Reduced Zagreb index $RM_2(G)$ showcase strong linear relationships, each with an $\mathbf{R^2}$ value of **1** once again. The trend equations **y = 1.8667x - 74.067**, **y = 2.4667x + 192.67**, and **y = 1.8039x - 61.396.** likewise, the three topological index models (**$F_N(G)$, $ReZ(G)$, $RM_2(G)$**) of armchair, hammer like and hexagonal chain molecular structure suggest a good correlation ranging from R^2 value of **0.9999** to **1** with their stability energy.

5 Conclusion

This work presents three novel benzenoid chains, hammer-like, linear and armchair hexagonal chains for evaluating their respective topological descriptors-the Redefined Third Zagreb index, the Reduced Zagreb index and the neighborhood version of the Forgotten topological index. The novelty of these findings lies in introducing these indices to capture intricate structural characteristics of hexagonal molecular graphs and establishing regression models that link these indices to key physicochemical properties such as strain energy and boiling point. Looking ahead, these indices offer promising potential for enhancing QSPR and QSAR predictions, enabling more accurate modeling of molecular behavior in materials science and pharmaceutical chemistry. This work will form a good base for future researchers to extend these indices to other classes of polycyclic aromatic hydrocarbons, compare their predictive performance with existing topological measures and explore their integration for improved chemical informatics.

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