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Article

Exploring Kevlar's Chemical Structure through Advanced Topological Co-Indices

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Abstract

Unlocking the secrets of molecular structures has become a paramount pursuit in the realm of scientific inquiry, where the marriage of mathematical models and physical properties plays a pivotal role. Topological co-indices, as mathematical constructs, serve as potent tools to scrutinize the intricate relationship between chemical structures and their properties. By harnessing the power of molecular graphs, where edges represent bonds and points symbolize atoms, these co-indices provide numerical insights into diverse chemical structures. In this study, we delve into the fascinating world of topological co-indices by employing the iconic Kevlar's chemical structure as our focal point. Unlike conventional lab tests, our approach offers a time-efficient alternative, enabling frequent usage without compromising accuracy. The investigation encompasses the derivation and analysis of several topological co-indices tailored to the unique attributes of Kevlar. Furthermore, this research introduces graphical representations that vividly illustrate the comparative landscape of estimated topological indices associated with Kevlar's chemical structure. These visuals serve as a powerful tool for both experts and enthusiasts, enhancing the accessibility and comprehensibility of our findings. Join us on this captivating journey as we unravel the mathematical intricacies intertwined with the physical essence of Kevlar's molecular architecture, shedding light on its distinctive properties through the lens of topological co-indices.

Keywords: Topological co-indices, physical parameters, Zagreb type co-indices, Geometric Randic topological co-indices

1. INTRODUCTION

Chemical graph speculation stands as a captivating realm within mathematical chemistry, dedicated to the nuanced analysis of chemical characteristics, with atoms as vertices and chemical bonds as edges, The graphical representation unveils the intricate architecture of chemical complexes. This unique approach employs mathematical concepts, providing a lens to assess and fathom chemical properties and reactions with precision [1].

The realm of Chemical graph theory, with its far-reaching applications in drug development, materials science, and various branches of chemistry, lays a robust foundation for the exploration of chemical compounds and their nuanced characteristics [2]. It serves as a guiding beacon for chemists, enabling the accurate prediction of the chemical behaviour of a diverse array of substances across all three thermodynamic forms.

In this exploitative journey, substance graphs emerge as invaluable tools, unveiling the spatial arrangement of atoms within a molecule. They play a pivotal role in distinguishing structural isomers of compounds. The consequential numbers derived from the topological intricacies of these graphs are known as topological

indices [3, 4]. Beyond being mere numerical entities, these indices offer a wealth of information on the chemical and structural properties of compounds. Their significance extends to influencing biological activity, solubility, stability, and reactivity, making them indispensable in diverse applications such as drug design, materials research, and chemical informatics [5, 6].

To delve deeper into this fascinating world, the classification of chemical structures involves the computation of topological indices of molecular structures. These indices, rooted in various graph properties, including the count of non-incident edges, degree distribution, and spectrum, contribute to a comprehensive understanding of a compound's nature [7]. Notable examples like the Hosoya index, Estrada index, Randic connection index, and Zagreb indices further enrich the tapestry of topological indices [8, 9].

In essence, this intricate interplay of mathematical chemistry and graph theory unravels a tapestry of molecular intricacies. The significance of this exploration resonates across disciplines, impacting drug design, materials science, and chemical informatics. Beyond numerical abstractions, topological indices become the key to deciphering the language of molecules, unlocking insights that reverberate in the advancement of scientific frontiers.

The calculation of the topological index *TI(G)* follows a well-defined procedure:

$$TI(G) = \sum_{\delta\gamma \in E(G)} F(\Gamma(\delta), \Gamma(\gamma)) \tag{1}$$

Here, the symbol represents the summation across all pairs of neighboring vertices δγ in the edge set E(G). The function F is chosen based on the specific requirements of the analysis [14]. Historically, critical topological indices have proven invaluable in characterizing the structures of numerous compound complexes. However, the field is still evolving, with the continual proposal of new indices that await thorough testing to establish their correlations with various substantial characteristics, substance reactivity, or biological activity. The quest for novel topological indices is propelled by the aspiration to enhance our understanding of molecular structures and their implications in diverse domains.

Kaom et al. employed a valency-based topological descriptor, successfully unravelling the electrical and structural intricacies of diverse hexagonal star networks [15]. Nadeem et al. delved into topological analysis to scrutinize the connectivity and stability of metal-organic systems, showcasing the versatility of this approach in understanding complex molecular architectures [1, 16]. In a parallel exploration, Ahmad et al. conducted an insightful study on the energy variations in phenylene and anthracene molecules, crucial components in materials science and organic electronics. Their findings underscored the influence of molecular conformations and functional groups on energy profiles [17]. Echoing this sentiment, Sun et al. generated diverse topological indices to capture physico-chemical features in the chemical graph of polyphenylene, contributing to a holistic understanding of its molecular characteristics [18].

Beyond individual molecular assessments, co-indices such as Randic and Zagreb offer a versatile tool kit for calculating pi electron energy and unravelling geometric properties like inter atomic lengths and bond angles in any chemical compound [19, 20]. These co-indices extend their utility to the analysis of various physiochemical properties, providing nuanced insights into molecular structures and characteristics [21]. Zhang et al., through thermodynamic modelling and experimental data, explored the temperature-dependent heat of formation and entropy of cerium oxide (CeO2), revealing dynamic characteristics influenced by temperature fluctuations [21]. Meanwhile, Gao et al. applied topological indices, including node edition, in the study of nano tubes, unravelling unique structural nuances [22]. In a parallel endeavour, Gao et al. employed the edge set division technique to calculate multiplicative atom-bond connectivity indices for key nano materials, further expanding the spectrum of applications for topological indices in nano-science [23]. The collective efforts showcased here underscore the versatility and applicability of topological indices across diverse domains, from molecular electronics to nano materials research. This mathematical modelling approach is particularly valuable in industrial contexts, as it helps interpret Kevlar's structural behaviour and properties such as tensile strength, thermal stability, and chemical resilience.

In this study, our primary objective is to explore and compute advanced topological co-indices derived from the molecular graph of Kevlar, with the aim of establishing their correlation with the compound's physical and structural properties. By employing mathematical modelling, we seek to provide a time-efficient and analytically

robust alternative to experimental methods for analysing Kevlar's molecular behaviour. Additionally, we aim to visualize these indices through comparative graphical representations, offering intuitive insight into Kevlar's unique topological characteristics. This approach not only broadens the understanding of Kevlar at the molecular level but also contributes to the growing field of chemical graph theory by demonstrating the practical relevance of co-indices in analysing industrially significant material.

2. APPLICATIONS

To date, critical topological indices have proven indispensable in characterizing the designs of various compound complexes. However, many proposed indices await thorough testing to establish their correlations with diverse substantial characteristics, substance reactivity, or biological action. In a notable exploration, Kaom et al. applied a valency-based topological descriptor, successfully elucidating the electrical and structural characteristics of diverse hexagonal star networks [15]. Similarly, Nadeem et al. employed topological analysis to scrutinize the connectivity and stability of metal-organic systems, showcasing the versatility of this approach in understanding complex molecular architectures [1, 16].

In a parallel endeavor, Ahmad et al. delved into the energetic landscape of phenylene and anthracene molecules, pivotal in materials science and organic electronics. Their insightful study unveiled dependencies on molecular conformations and functional groups, offering valuable insights into energy variations [17]. Correspondingly, Sun et al. harnessed topological indices to represent physico-chemical features of polyphenylene, contributing to a comprehensive understanding of its molecular characteristics [18].

A myriad of co-indices, such as the Randic and Zagreb co-indices, have emerged as versatile tools for calculating pi electron energy and unravelling geometric properties like inter atomic lengths and bond angles in chemical compounds [19, 20]. These co-indices extend their utility to the analysis of diverse physicochemical properties, offering nuanced insights into molecular structures and characteristics [21]. Zhang et al., through thermodynamic modelling and experimental data, delved into the temperature-dependent heat of formation and entropy of cerium oxide (CeO_2), revealing dynamic characteristics influenced by temperature fluctuations [21]. In the realm of nanotubes, Gao et al. computed node edition of topological indices, showcasing their applicability in nano-science[22]. In a complementary study, Gao et al. applied the edge set division technique to calculate multiplicative atom-bond connectivity indices for key nanomaterials, further expanding the spectrum of applications for topological indices in nanoscience [23].

This comprehensive implementation of topological indices not only showcases their diverse applications but also underscores their pivotal role in unravelling molecular intricacies across varied scientific domains. Despite the significant advancements in the application of topological indices to a wide range of molecular graphs, a noticeable gap remains in their use for analysing high-performance polymers like Kevlar. While previous studies have focused on simple hydrocarbons, nano structures, or small organic molecules, they often overlook large, rigid, and industrially significant polymers. Moreover, the majority of existing research employs basic indices without extending the analysis to co-indices that can capture finer structural distinctions, such as branching, degree-based interactions, and atom-bond connectivity variations. To the best of our knowledge, no comprehensive study has yet applied advanced co-indices such as ABC, GAC, and GA5 specifically to the chemical graph of Kevlar. This study addresses this gap by systematically deriving and analyzing a broad set of topological co-indices tailored to Kevlar's structure, thereby offering a more nuanced and predictive understanding of its physicochemical properties.

3. PRELIMINARIES

Suppose P1 represents the molecular structure of Kevlar Poly(azanediyl-1,4-phenyl eneazanediyl terephthaloyl) [24]. The atoms in this molecule are depicted by the node (vertex) set V(P1), and the collection of edges is represented as $E(P_1)$. δ and γ denote two adjacent vertices, and the total number of edges connected to a vertex is known as the degree of the vertex, denoted as Γδ. The complement of the graph is denoted as $\overline{P_1}$ with the vertex set $\overline{V(P_1)}$ and edges $\delta\gamma \in E(\overline{P_1})$ whenever $\delta\gamma \notin E(\overline{P_1})$.

The 1st and 2nd Zagreb indices are denoted as $\overline{M_1}(P_1)$ and $\overline{M_1}(P_2)$, and their revised formulas, transformed into co-indices, are as follows [25, 26]:

$$\overline{MZ}1(P_1) = \sum \delta\gamma \in E(P_1)(\Gamma_\delta + \Gamma_\gamma) \tag{2}$$

The second Zagreb index of the complement of graph $\overline{MZ}2(P_1)$ is defined as follows:

$$\overline{MZ}2(P_1) = \sum \delta\gamma \in E(P_1)(\Gamma\delta \times \Gamma_\gamma) \tag{3}$$

Ghorbani defined the multiple Zagreb indices and multiplicative co-indices as [27][28][29]:

$$\overline{\bigwedge}\,1(P_1) = \prod \delta\gamma \in E(P_1)(\Gamma_\delta + \Gamma_\gamma) \tag{4}$$

The second multiplicative co-index of the complement of graph $\overline{\bigwedge}\,2(P_1)$ is defined as follows:

$$\overline{\bigwedge}\,2(P_1) = \prod \delta\gamma \in E(P_1)(\Gamma\delta \times \Gamma_\gamma) \tag{5}$$

For the diagram P_1, the forgotten index is calculated through $F_C(P_1)$ and is given by:

$$\overline{F_C}(P_1) = \sum_{\delta\gamma \in E(P_1)} (\Gamma_\delta^2 + \Gamma_\gamma^2) \tag{6}$$

Estrada [30] and Fath-tabar [31] established the $\overline{ABCI}(P_1)$ index inequalities. Das and Trinajstic [32] constructed the $\overline{GAC}(P_1)$ index for a substance tree. The Atomic Bond Connectivity co-index [26]is formulated as follows:

$$\overline{ABCI}(P_1) = \sum_{\delta\gamma \in E(P_1)} \sqrt{\frac{(\Gamma_\delta + \Gamma_\gamma - 2)}{(\Gamma_\delta \cdot \Gamma_\gamma)}} \tag{7}$$

$$\overline{GAC}(P_1) = \sum_{\delta\gamma \in E(P_1)} \frac{2\sqrt{(\Gamma_\delta \cdot \Gamma_\gamma)}}{(\Gamma_\delta + \Gamma_\gamma)} \tag{8}$$

The general Randic index [10] is described as the general Randic Co-index [26], formulated as follows:

$$\overline{R}\delta(P_1) = \sum \delta\gamma \in E(P_1)(\Gamma_\delta \cdot \Gamma_\gamma)^\delta; \quad \delta = 1, -1, \frac{1}{2}, -\frac{1}{2} \tag{9}$$

Lemma [33] states, "Let P_1 be an associated graph of order n. Let P_u be the set of vertices of level u, and w_{uv} be the number of edges linking the vertices of degree u and v. Then,"

$$\overline{E}uv = \delta\gamma \in E(\overline{P_1}) : \Gamma\delta = u \text{ and } \Gamma_\gamma = v \tag{10}$$

$$\overline{w}uv = |\overline{E}uv| = \begin{cases} K_u K_v - \overline{w}_{uv}, & \text{if } u \le v \\ \frac{K_u(K_u-1)}{2}, & \text{if } u = v \end{cases} \tag{11}$$

4. KEVLAR STRUCTURE

Kevlar, scientifically known as para-aramid, stands as a remarkable artificial filament renowned for its exceptional durability and fire resistance. This synthetic polymer shares its aramid classification with counterparts like Nomex and Technora, collectively forming a family of robust materials. Its widespread applications span from reinforcing bicycle tires to fortifying bulletproof vehicles, showcasing its versatility and indispensability in various industries.

Kevlar might be able to withstand the outstanding strength due to a huge number of inter-chain links in the molecular chain. This great power of the tensile strength of the polymer is due to the complex structure of bonds of hydrogen between neighbouring molecules. These connections are formed by the reaction of the carbonyl groups and the NH centers, giving a strong network that scaffolds the material with high strength.

In addition to hydrogen bonding, the second important source of strength in Kevlar is aromatic stacking of

adjacent strands. These are interactions of aligning aromatic rings in the molecule. This results in a stacking effect. This lamination also increases the strength of the entire material, and this is why it is a favorite to use in industries where extra tensile and mechanical strength is an essential requirement.

Kevlar structural strength is created by complex level hydrogen intermolecular bonding and aromatic intermolecular stacking interactions. Such molecular properties do not only render it with notable tensile strength but also allow its use in a variety of ways across many industry branches.

5. RESULTS FOR CHEMICAL GRAPH

A unit cell of Kevlar is shown in Figure 1 (a), and its molecular structure is also shown on the right. The structure consists of a total of $28n$ vertices and $30n - 1$ edges. The degrees of the vertices are labeled as v_1, v_2, and v_3. Further details about the degrees of vertices and edges are provided in Table 1 and 2.

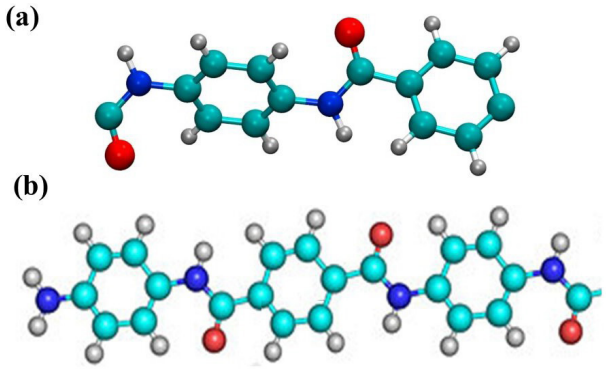

Figure 1: *(a) unit cell of Kevlar molecule and (b) long chain of Kevlar*

5.1 Vertex classes:

Table 1: *Classes of vertices are shown*

n	1	2	3	4	5	Rate or frequency	Classes of vertices
v_1	12	24	36	48	60	$12n$	n_1
v_2	2	2	2	2	2	2	n_2
v_3	14	30	46	62	78	$16n-2$	n_3

5.2 Degree of edges

Table 2: *Degree of edges is represented*

$(\Gamma_\delta, \Gamma_\gamma)$	1	2	3	4	5	Frequency	Class of edge
(1, 2)	2	2	2	2	2	2	w_{12}
(1, 3)	10	22	34	46	58	$12n-2$	w_{13} w_{23}
(2, 3)	2	2	2	2	2	2	
(3, 3)	15	33	51	69	87	$18n-3$	w_{33}

Using Lemma from [33], we will locate the preliminary outcome for $\Gamma_\delta = 1$ and $\Gamma_\gamma = 2$:

$$\overline{w}_{12} = n_1 n_2 - w_{12}$$

$$\overline{w}_{12} = 12n \times 2 - 2$$

$$\overline{w}_{12} = 24n - 2$$

For $\Gamma_\delta = 1$ and $\Gamma_\gamma = 3$:

$$\overline{w}_{13} = n_1 n_{3-} w_{13}$$

$$\overline{w}_{13} = 12n \times (16n-2) - (12n-2)$$

$$\overline{w}_{13} = 192n^2 - 36n + 2$$

For $\Gamma_\delta = 2$ and $\Gamma_\gamma = 3$:

$$\overline{w}_{23} = n_2 n_{3-} w_{23}$$

$$\overline{w}_{23} = 2(16n-2) - 2$$

$$\overline{w}_{23} = 32n - 6$$

For $\Gamma_\delta = 3$ and $\Gamma_\gamma = 3$:

$$\overline{w}_{33} = n_3 n_{3-} w_{33}\, w_{33} = 12n \times 2 - 2$$

$$\overline{w}_{33} = (16n-2)^2 - (18n-3)$$

$$\overline{w}_{33} = 256n^2 - 82n + 7$$

5.3 First Zagreb Co-index

$$\overline{MZ}_1(P_1) = \sum_{\delta\gamma \in E(P_1)} (\Gamma_\delta + \Gamma_\gamma)$$
$$\overline{MZ}_1(P_1) = (1+2)\overline{w}_{12} + (1+3)\overline{w}_{13} + (2+3)\overline{w}_{23} + (3+3)\overline{w}_{33}$$
$$\overline{MZ}_1(P_1) = 3(24n-2) + 4(192n^2 - 36n + 2) + 5(32n-6) + 6(256n^2 - 82n + 7)$$
$$\overline{MZ}_1(P_1) = 230n^2 - 404n + 14$$

5.4 Second Zagreb Co-index:

$$\overline{MZ}_2(P_1) = \sum_{\delta\gamma \in E(P_1)} (\Gamma_\delta \times \Gamma_\gamma)$$
$$\overline{MZ}_2(P_1) = (1 \times 2)\overline{w}_{12} + (1 \times 3)\overline{w}_{13} + (2 \times 3)\overline{w}_{23} + (3 \times 3)\overline{w}_{33}$$
$$\overline{MZ}_2(P_1) = 2(24n-2) + 3(192n^2 - 36n + 2) + 6(32n-6) + 9(256n^2 - 82n + 7)$$
$$\overline{MZ}_2(P_1) = 2880n^2 - 606n + 23$$

5.5 First multiplicative Zagreb Co-index:

$$\overline{\bigwedge}_2(P_1) = \prod_{\delta\gamma \in E(P_1)} (\Gamma_\delta \times \Gamma_\gamma)$$
$$\overline{\bigwedge}_2(P_1) = (1 \times 2)\overline{w}_{12} \times (1 \times 3)\overline{w}_{13} \times (2 \times 3)\overline{w}_{23} \times (3 \times 3)\overline{w}_{33}$$
$$\overline{\bigwedge}_2(P_1) = 2(24n-2) \times 3(192n^2 - 36n + 2) \times 6(32n-6) \times 9(256n^2 - 82n + 7)$$
$$\overline{\bigwedge}_2(P_1) = 324(24n-2)(32n-6)(192n^2 - 36n + 2)(256n^2 - 82n + 7)$$

5.6 Second multiplicative Zagreb Co-index:

$$\overline{\bigwedge}_2(P_1) = \prod_{\delta\gamma \in E(P_1)} (\Gamma_\delta \times \Gamma_\gamma)$$
$$\overline{\bigwedge}_2(P_1) = (1\times 2)\overline{w}_{12} \times (1\times 3)\overline{w}_{13} \times (2\times 3)\overline{w}_{23} \times (3\times 3)\overline{w}_{33}$$
$$\overline{\bigwedge}_2(P_1) = 2(24n-2) \times 3(192n^2 - 36n + 2) \times 6(32n-6) \times 9(256n^2 - 82n + 7)$$
$$\overline{\bigwedge}_2(P_1) = 324(24n-2)(32n-6)(192n^2 - 36n + 2)(256n^2 - 82n + 7)$$

5.7 Forgotten topological Co-index:

$$\overline{F}_C(P_1) = \sum_{\delta\gamma \in E(P_1)} (\Gamma_\delta^2 + \Gamma_\gamma^2)$$
$$\overline{F}_C(P_1) = (1^2+2^2)\overline{w}_{12} + (1^2+3^2)\overline{w}_{13} + (2^2+3^2)\overline{w}_{23} + (3^2+3^2)\overline{w}_{33}$$
$$\overline{F}_C(P_1) = 5(24n-2) + 10(192n^2 - 36n + 2) + 13(32n-6) + 18(256n^2 - 82n + 7)$$
$$\overline{F}_C(P_1) = 65n^2 - 1300n + 58$$

5.8 Atom bond connectivity topological Co-indices:

$$\overline{ABCI}(P_1) = \sum_{\delta\gamma \in E(P_1)} \sqrt{\frac{(\Gamma_\delta + \Gamma_\gamma - 2)}{\Gamma_\delta \Gamma_\gamma}}$$
$$\overline{ABCI}(P_1) = \sqrt{\frac{(1+2-2)}{(1\times 2)}}\overline{w}_{12} + \sqrt{\frac{(1+3-2)}{(1\times 3)}}\overline{w}_{13} + \sqrt{\frac{(2+3-2)}{(2\times 3)}}\overline{w}_{23} + \sqrt{\frac{(3+3-2)}{(2\times 3)}}\overline{w}_{33}$$
$$\overline{ABCI}(P_1) = \frac{1}{\sqrt{2}}(24n-2) + \sqrt{\frac{2}{3}}(192n^2 - 36n + 2) + \sqrt{\frac{3}{2}}(32n-6) + \frac{2}{3}(256n^2 - 82n + 7)$$

5.9 Geometric arithmetic topological Co-indices:

$$\overline{GAC}(P_1) = \sum_{\delta\gamma \in E(P_1)} \frac{2\sqrt{\Gamma_\delta \Gamma_\gamma}}{\Gamma_\delta + \Gamma_\gamma}$$
$$\overline{GAC}(P_1) = \frac{2\sqrt{1\times 2}}{1+2}\overline{w}_{12} + \frac{2\sqrt{1\times 3}}{1+3}\overline{w}_{13} + \frac{2\sqrt{2\times 3}}{2+3}\overline{w}_{23} + \frac{2\sqrt{3\times 3}}{3+3}\overline{w}_{33}$$
$$\overline{GAC}(P_1) = \frac{2\sqrt{2}}{3}(24n-2) + \sqrt{\frac{3}{2}}(192n^2 - 36n + 2) + \frac{2\sqrt{6}}{5}(32n-6) + (256n^2 - 82n + 7)$$

Table 3: Comparison of $\overline{M}Z_1(P_1)$, $\overline{M}Z_2(P_1)$, $\overline{\Lambda}_1(P_1)$, and $\overline{\Lambda}_2(P_1)$

n	$\overline{MZ}_1(P_1)$	$\overline{MZ}_2(P_1)$	$\overline{\bigwedge}_1(P_1)$	$\overline{\bigwedge}_2(P_1)$
1	1,914	2,297	5,888,900,160	5,300,010,144
2	8,422	10,331	581,249,839,680	523,124,855,712
3	19,538	24,125	7,596,507,240,000	6,836,856,516,000
4	35,262	43,679	45,664,085,160,000	41,097,676,644,000
5	55,594	68,993	181,329,815,177,280	163,196,833,659,552
6	80,534	100,067	556,048,816,580,160	500,443,934,922,144
7	110,082	136,901	1,428,945,848,930,880	1,286,051,264,037,792

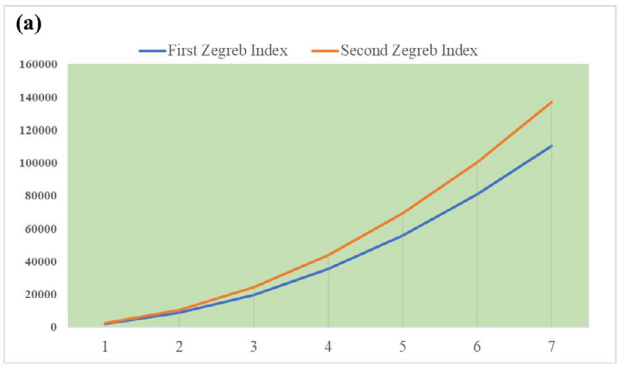

Figure 2: *Comparison of first Zegreb index and second zegreb index*

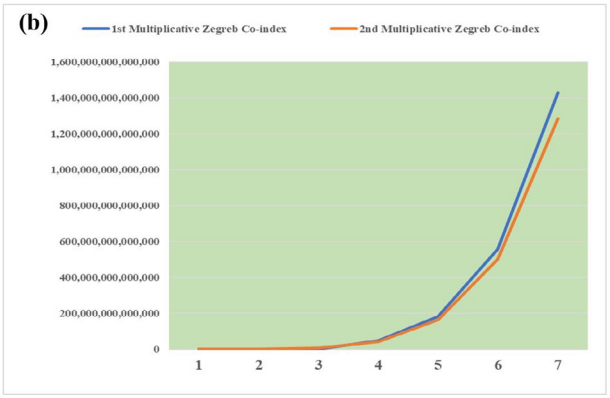

Figure 3: *Comparison of first and second multiplicative Zegreb Co-indices*

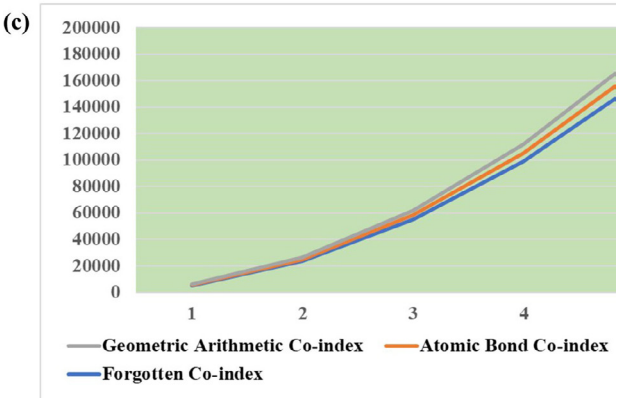

Figure 4: *comparison of Geometric Arithmetic, Atomic Bond and Forgotten Co-indices*

6. GOMETRIC RANDIC TOPOLOGICAL CO-INDICES:

$$\bar{R}_\delta(P_1) = \sum_{\delta\gamma \in E(P_1)} (\Gamma_\delta \times \Gamma_\gamma)^\delta, \quad \delta = 1, -1, \frac{1}{2}, -\frac{1}{2}$$

For $\delta = 1$:

$$\bar{R}_\delta(P_1) = 2880n^2 - 606n + 23$$

For $\delta = -1$:

$$\begin{aligned}\bar{R}_\delta(P_1) &= \sum_{\delta\gamma \in E(P_1)} (\Gamma_\delta \times \Gamma_\gamma)^{-1} \\ &= \frac{1}{2}\bar{w}_{12} + \frac{1}{3}\bar{w}_{13} + \frac{1}{6}\bar{w}_{23} + \frac{1}{3}\bar{w}_{33} \\ &= \frac{1}{2}(24n-2) + \frac{1}{3}(192n^2 - 36n + 2) + \frac{1}{6}(32n-6) + \frac{1}{3}(256n^2 - 82n + 7) \\ &= \frac{832}{9}n^2 - \frac{34}{9}n - \frac{5}{9}\end{aligned}$$

For $\delta = \frac{1}{2}$:

$$\begin{aligned}\bar{R}_\delta(P_1) &= \sum_{\delta\gamma \in E(P_1)} (\Gamma_\delta \times \Gamma_\gamma)^{\frac{1}{2}} \\ &= \sqrt{2}\bar{w}_{12} + \sqrt{3}\bar{w}_{13} + \sqrt{6}\bar{w}_{23} + \sqrt{3}\bar{w}_{33} \\ &= \sqrt{2}(24n-2) + \sqrt{3}(192n^2 - 36n + 2) + \sqrt{6}(32n-6) + \sqrt{3}(256n^2 - 82n + 7)\end{aligned}$$

For $\delta = -\frac{1}{2}$:

$$\begin{aligned}\bar{R}_\delta(P_1) &= \sum_{\delta\gamma \in E(P_1)} (\Gamma_\delta \times \Gamma_\gamma)^{-\frac{1}{2}} \\ &= \frac{1}{\sqrt{2}}\bar{w}_{12} + \frac{1}{\sqrt{3}}\bar{w}_{13} + \frac{1}{\sqrt{6}}\bar{w}_{23} + \frac{1}{\sqrt{3}}\bar{w}_{33} \\ &= \frac{1}{\sqrt{2}}(24n-2) + \frac{1}{\sqrt{3}}(192n^2 - 36n + 2) + \frac{1}{\sqrt{6}}(32n-6) + \frac{1}{\sqrt{3}}(256n^2 - 82n + 7)\end{aligned}$$

n	$\overline{F_C}(P_1)$	$\overline{ABCI}(P_1)$	$\overline{GAC}(P_1)$
1	5286	344	364
2	23,570	1489	1572
3	54,910	3436	3624
4	99,306	6184	6521
5	156,758	9735	10,262
6	227,266	14088	14,848
7	310,830	19243	20,278

Table 4: Comparison of $\overline{F_C}(P_1)$, $\overline{ABCI}(P_1)$, and $\overline{GAC}(P_1)$

n	$\overline{R}_1(P_1)$	$\overline{R}_{-1}(P_1)$	$\overline{R}_{1/2}(P_1)$	$\overline{R}_{-1/2}(P_1)$
1	2297	88	921	178
2	10,331	362	4053	748
3	24,125	820	9405	1711
4	43,679	1463	16,975	3066
5	68,993	2292	26,766	4814
6	100,067	3305	38775	6954
7	136,901	4503	52,562	9486

Table 5: Comparison of $\overline{R}_1(P_1)$, $\overline{R}_{-1}(P_1)$, $\overline{R}_{1/2}(P_1)$, and $\overline{R}_{-1/2}(P_1)$

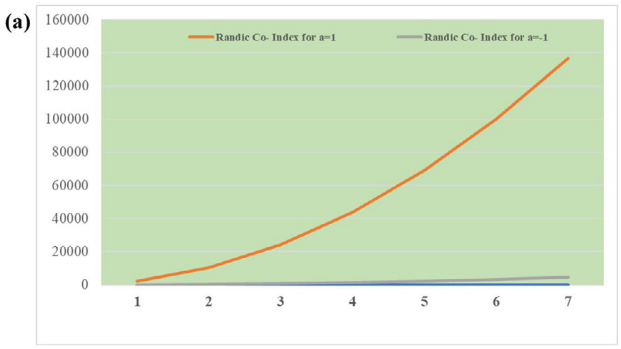

Figure 5: *comparison of Geometric Arithmetic, Atomic Bond and Forgotten Co-indices*

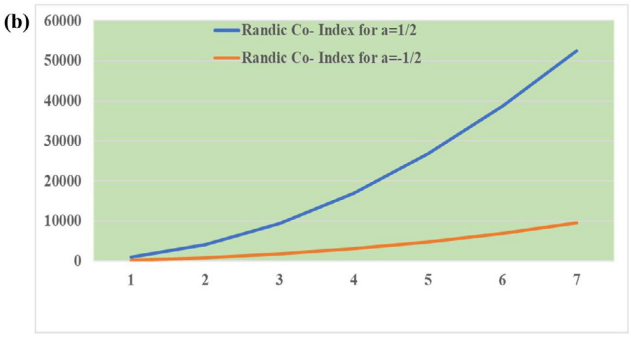

Figure 6: *Evaluation of Randic Co-index for a = 1/2anda = −1/2*

6.1 Comparison

We compare here the values for $\bar{M}Z_1(P_1)$, $\bar{M}Z_2(P_1)$, $\bar{\Lambda}_1(P_1)$ and $\bar{\Lambda}_2(P_1)$ in table 3. Additionally, in Table 4, we present a comparison for $\bar{F}_C(P_1)$, $\bar{A}BCI(P_1)$, and $\bar{G}AC(P_1)$. Furthermore, in Table 5, we explore the relationships of the Randic Co-index for the values $\delta = 1, \delta = -1, \delta = \frac{1}{2}, and\ \delta = -\frac{1}{2}$ for the Kevlar structure is done and in Table 5 relationship of Randicc Co-index for1, 1, 1/2*and*(1)/2 for Kevlar structure.

6.2 Physico-Mathematical Analysis and Practical Implications of Kevlar: Unveiling the Science Behind Extraordinary Properties

Kevlar, also known as paraaramid, stands as a testament to the convergence of chemistry and physics, showcasing its remarkable properties through a combination of intricate molecular structure and practical applications. This polymeric material, formally Poly(azanediyl-1,4-phenyl eneazanediyl terephthaloyl) [24], is more than just a substance; it's a marvel of scientific ingenuity.

Synthesis and Structure:

Kevlar's journey begins with a meticulous condensation procedure involving the monomers 1,4-phenylenediamine and terephthaloyl chloride. This chemical ballet creates a robust molecular structure, forming the backbone of Kevlar's legendary strength and resilience.

Versatility in Applications:

Designed in various grades to cater to specific needs, Kevlar finds itself at the heart of diverse applications. From manufacturing to ballistic defense, Kevlar plays a pivotal role in crafting cables, supports, and protective gear. Its versatility extends to sporting goods like canoes, bike tires, and rackets, making it an indispensable material in various industries.

Mathematical Insights:

The betrothal between mathematics and physics can better explain the characteristics of Kevlar. In keeping with the boiling points, through the Randic index, finding correlation with the Kovats index, which is intricately linked to boiling points, is possible. On the other hand, ABC co-index offers a measure of stability in a compound. Optical details of the genome are disclosed through the physico-mathematical analysis of connections which may be nonlinear and even chaotic within the molecular structure of Kevlar.

Topological Co-Indices:

Topological co-indices are efficient to derive and open the unlock to the discovery of beneficial physical advantages. These co-indices are in addition to the fact that they are time and cost saving methods of testing the properties of Kevlar that have gone beyond the standard fields of experimentation. Examining indexes like the second multiplicative Zagreb co-index and Randic co-index of $\delta = -1$, we can get understand the behaviour of the material.

Practical Implications:

A study of physico-mathematical complexity of Kevlar gives a guideline on the prediction of Kevlar boiling and melting temperature, stability, strain energy, surface tension, vapor pressure, and heat of formation. This knowledge could be used by scientists and engineers so as to streamline their application which can save time and resources. To sum up, Kevlar is rather a scientific wonder that unites mathematics and physics. The world that is revealed in its physico-mathematical analysis opens up the world of possibilities, leading to its tremendous impact on both the theoretical and practical use. The legacy of Kevlar still exists and continues to transform industries as well as redefine what can be done in materials science.

7. CONCLUSION

This study presents a comprehensive analysis of the chemical structure of Kevlar using advanced topological co-indices. By translating the molecular architecture into mathematical form, we derived indices that correlate with physical properties such as melting point, boiling point, and density. These indices not only enhance our theoretical understanding but also have practical relevance in QSAR and QSPR modeling. Our findings offer valuable insights into the complex structure of Kevlar, highlighting how topological descriptors reflect its unique strength and stability. The tabulated results and graphical representations provide a clear comparative framework, supporting further research in materials science.

In essence, this work bridges mathematical graph theory and chemical structure analysis, emphasizing the potential of co-indices to predict and explain material behaviour. While this study focuses on Kevlar, the methodology holds promise for broader applications to other industrially significant polymers. The journey into molecular topology continues, with each index bringing us closer to unlocking the deeper secrets of matter.

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Availability of Data and Materials

The data supporting this study are available upon request.

Declaration of Conflict

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Clinical Trial Number

Not Applicable.

Human Ethics and Consent to Participate

The study did not involve any clinical interventions or experiments requiring formal ethical approval.

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