International Journal of Basic and Applied Sciences, 14 (3) (2025) 361-372

International Journal of Basic and Applied Sciences

Website: www.sciencepubco.com/index.php/IJBAS
https://doi.org/10.14419/1hbdss79
Research paper

Chemical Relevance and Expected Values of K-Banhatti Indices for Random Cyclodecane Chains

Priyanka Agarwal *, A. Bharali

Department of Mathematics, Dibrugarh University, Dibrugarh, India, 786004
**Corresponding author E-mail: priyanka.agarwal0012@gmail.com*

Received: June 13, 2025, Accepted: July 19, 2025, Published: July 27, 2025

Abstract

Cyclodecane, a remarkable cyclic hydrocarbon, comprises larger molecular structures or polymers formed by interlinking multiple cyclodecane rings. These interactions are crucial in pharmacogenomics, as the strategic design of a compound decisively influences its interactions with gene products, including enzymes and receptors. In the dynamic field of mathematical chemistry, chemical graph theory plays a crucial role in enhancing our understanding of the complex properties of chemical compounds. Currently, one of the most promising areas of research involves the calculation of topological indices. Among these indices, the First K hyper-Banhatti index, Second K hyper-Banhatti index, Modified first K-Banhatti index, and Modified second K-Banhatti index serve as important topological descriptors that significantly contribute to our analysis of the physicochemical, biological, and structural characteristics of chemical compounds. This article aims to determine the expected values of these topological descriptors for random cyclodecane chains, presenting our findings in significant numerical tables and insightful graphical representations. Through this exploration, we aim to deepen our appreciation of how these descriptors impact the fundamental properties of chemical compounds, paving the way for future discoveries in this compelling field.

Keywords: *Chemical Graph Theory; Topological Indices; Cyclodecane Chains; Genes; Pharmacogenomics; Expected Values; Comparisons.*

1. Introduction

Chemical graph theory constitutes an important branch of mathematical chemistry that examines the complex structures of chemical compounds. It unveils a remarkable pathway to understand the fundamental physical properties of these compounds. The chemical insights gleaned from molecular descriptors differ across various algorithms, each offering its unique perspective [1 - 3]. A pivotal technique lies in skillfully encoding the information from these descriptors through the very architecture of the molecule itself. Visionaries such as Alexandru Balaban, Iv́an Gutman, Milan Randić, and Nenad Trinajstić have been instrumental in shaping this dynamic field, which continues to influence new explorations and discoveries [4 - 7].

The application of topological indices, often referred to as connectivity indices, as molecular descriptors associated with the molecular graph of chemical compounds represents a significant advancement in scientific research [8 - 11]. These indices open up a world of possibilities across diverse fields, including engineering, materials science, and pharmaceutical development. By developing a range of topological indices, researchers can effectively depict the complex details of chemical structures. They stand out not just for their mathematical elegance but also for their impact on quantitative structure-property relationship (QSPR) and quantitative structure-activity relationship (QSAR) studies, which delve into the relationship between the physicochemical properties and biological activities of chemical compounds. The success of these studies hinges on a precise understanding of molecular structures and their defining parameters [12 - 14]. Topological indices have recently emerged as a powerful tool for extracting valuable information from the molecular structures of various compounds. While there is a wealth of degree- and distance-based topological indices available in the literature, some indices have demonstrated particularly strong correlations with important chemical properties such as boiling point, strain energy, and stability. This highlights the importance of topological indices, an invaluable tool in the quest for innovation and discovery in chemistry [15 - 19].

Let G be a simple graph adorned with n vertices and m edges. We denote the vertex set as $V(G)$ and the edge set as $E(G)$. The degree $d(v)$ of a vertex v is the count of vertices that share an adjacency with v, showcasing its connectivity within the graph. An edge e that bridges the vertices u and v is represented as uv. When we say $e = uv$ is an edge of G, it implies that u and e are intimately linked, just as v shares this connection with edge e. We can denote the degree of an edge e within G as $d(e)$, defined with the formula $d(e) = d(u) + d(v) - 2$ for the edge $e = uv$.

The K-Banhatti indices draw inspiration from the foundation of renowned degree-based indices such as the Zagreb indices and the Randi ́ index. The K-Banhatti indices merge both degree and distance metrics, yielding a comprehensive perspective on the topology of graphs. Their innovation aims to improve the connection between molecular structures and their physicochemical properties, offering enhanced insights into the behavior of substances at a molecular level. The first and second K-Banhatti indices were introduced by Kulli

[20], [21], who not only envisioned these indices but also proposed a variety of innovative degree-based topological indices that contribute to the rich tapestry of graph theory. Denoted and defined as below

$$B_1(G) = \sum_{ue \in G}[d(u) + d(e)]$$

and

$$B_2(G) = \sum_{ue \in G} d(u).d(e)$$

where $ue \in G$ means that the vertex u and an edge e These are incidents in the graph G.
In [22 - 24], Kulli proposed various novel degree-based TIs of a graph G such as the First K hyper-Banhatti index ($HB_1(G)$), Second K hyper-Banhatti index ($HB_2(G)$), Modified first K-Banhatti index (${}^{m}B_1(G)$), and Modified second K-Banhatti index (${}^{m}B_2(G)$). The K-Banhatti indices represent an important aspect of chemical graph theory, focusing on the relationship between vertex connectivity and the overall topology of molecular structures. These indices facilitate a more comprehensive analysis in fields such as QSAR/QSPR analyses. By examining how vertex and edge degrees interact, the K-Banhatti indices effectively categorize different molecular graphs. The modified first K-Banhatti index enhances the original version by incorporating the inverse of the sum of vertex degrees. This adjustment highlights the importance of edges that connect vertices of lower degree, which is particularly useful in assessing network vulnerabilities, identifying key chemical structures, and the refinement of modeling approaches in QSAR/QSPR studies. In addition, the modified second K-Banhatti index builds on the foundational Second K-Banhatti index, which improve its responsiveness to branching and connectivity within molecular structures and also fosters a deeper understanding of molecular interactions and properties. Denoted and defined as

$$HB_1(G) = \sum_{ue \in G}[d(u) + d(e)]^2 \quad (1)$$

$$HB_2(G) = \sum_{ue \in G}[d(u).d(e)]^2 \quad (2)$$

$${}^{m}B_1(G) = \sum_{ue \in G}\frac{1}{d(u)+d(e)} \quad (3)$$

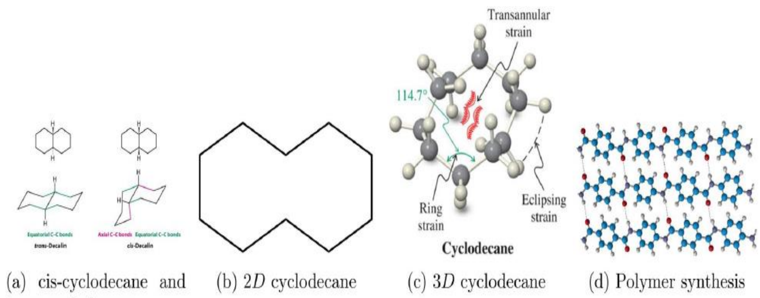
$${}^{m}B_2(G) = \sum_{ue \in G}\frac{1}{d(u).d(e)} \quad (4)$$

Kulli calculated the K-Banhatti indices for various chemical networks, including silicate networks, chain silicates, oxides, and honeycomb networks [25]. Furthermore, the analyses of the first and second K-Banhatti indices, as well as the first and second K-hyper Banhatti indices of windmill graphs [24], have also been analyzed. These indices comprise a range of computationally efficient methods specifically designed for examining continuous data structures. These indices achieve a perfect balance between local and global structural features, making them particularly effective when other indices fail to distinctly characterize molecular graphs. They have demonstrated robust correlations with physicochemical characteristics in QSAR/QSPR studies. Additionally, they often prove more effective in differentiating non-isomorphic graphs that share identical Wiener or Zagreb indices.
The nodes exhibiting maximum K-Banhatti index values, characterized by elevated centrality and reduced distances, are likely to signify hub or driver genes that play significant roles in tumor progression. Unlike traditional indices focused solely on distance or degree, the unique capability of the K-Banhatti index captures both node influence and accessibility, making it particularly relevant for complex cancer networks. For a number of years, they have proven instrumental in various biological contexts, illuminating the complexities of horizontal evolution, multifaceted diseases, cancer genomics, disease transmission, chromatin folding, and gene expression. In the context of a breast cancer protein-protein interaction (PPI) network, K-Banhatti indices can illuminate central signaling proteins, such as TP53 and BRCA1, thereby informing the development of targeted therapeutic interventions.

2. Materials and methods

Cyclodecane is a ten-carbon ring compound, classified as a cycloalkane, with the chemical formula $C_{10}H_{20}$. It possesses two isomers: cis-cyclodecane and trans-cyclodecane. The two-dimensional chemical structure, referred to as the skeletal formula, is the standard representation for organic molecules. In contrast, the three-dimensional representation employs a ball-and-stick model to effectively illustrate the positions of the atoms and the bonds between them. Both the two-dimensional and three-dimensional models of cyclodecane [26] are displayed in Figure 1. At room temperature, cyclodecane appears as a waxy solid, a testament to its versatility. It is commonly utilized as a solvent and significantly plays an essential role in the creation of various polymers, such as polyesters, nylon 12, and synthetic lubricating oils.
Polymer synthesis is an inspiring field that involves the development of synthetic polymers that can emulate the incredible capacity of DNA and RNA to store and process genetic information. These innovative molecules, known as XNAs (xenonucleic acids), provide a diverse range of functionalities and possess significant potential for revolutionizing biotechnology and nanotechnology. XNAs are set to transform targeted gene therapy, drug delivery systems, and the formulation of diagnostic tools, paving the way for scientific exploration and advancement.
Moreover, it possesses distinctive characteristics- Melting Point 10.0 °C, Boiling Point 202.0 °C, Molecular Weight 140.27 g/mol, Potential Health Risks 0.33 mg/L, Vapour Pressure 0.56 mmHg, and Water Solubility 25 °C. The structure of the cyclodecane chain highlights significance in both chemistry and industry, inspiring further exploration and innovation.
Cyclodecane is a highly valuable saturated cyclic hydrocarbon that plays an essential role in chemistry as both a precursor for numerous materials and a temporary binding medium. Researchers are increasingly concentrated on hydrocarbons and their derivatives due to their fundamental structure consisting solely of carbon and hydrogen, which provides a foundation for diverse applications [27], [28]. Notably, plants contain considerable amounts of valuable hydrocarbons, and certain properties of these compounds are vital for the production of chemical raw materials as well as fuels. In terms of applications, cyclodecanes are indispensable as organic solvents in drug synthesis, the petroleum industry, and the perfume manufacturing sector, in addition to being employed in the synthesis of diverse organic compounds [29]. Moreover, they have extensive applications in areas such as motor fuels, natural gas, diesel, kerosene, and numerous heavy oils. The

versatility and significance of cyclodecanes in these industries are essential for various industrial processes and technological advancements [30], [31].



(a) cis-cyclodecane and trans-cyclodecane (b) $2D$ cyclodecane (c) $3D$ cyclodecane (d) Polymer synthesis

Fig. 1: 2D and 3D model of cyclodecanes.

In the field of medicinal inorganic chemistry, recent advancements illustrate the substantial potential for employing metal complexes as therapeutic agents, thereby expanding the scope of this domain. Studies have shown that larger aromatic ring systems are associated with enhancing DNA affinity, leading to remarkable antitumor and photocleaning activities. Moreover, groove-binding molecules, composed of a series of heterocyclic or aromatic hydrocarbon rings with rotational flexibility, are capable of fitting into the minor or major grooves of DNA, which effectively displaces water and facilitates beneficial interactions.

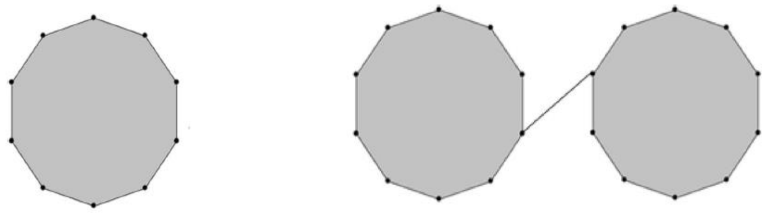
Cyclic molecules, especially cyclodecane derivatives, are currently the focus of research regarding their applications as synthetic transcription modulators and DNA-binding agents. The distinct characteristics of random cyclodecane chains allow for the simulation and screening of a wide range of conformations, enabling the identification of promising candidates that may significantly influence gene expression and function. Through the meticulous analysis of various cyclodecane configurations, researchers can design molecules that may either mimic or inhibit the activity of natural gene regulators.

Cyclodecane derivatives, along with other similar cyclic compounds, can function as ligands- small molecules that specifically bind to proteins or gene regulatory elements. These interactions play a pivotal role in the field of pharmacogenomics, where the structural design of a compound, such as a cyclodecane chain, directly affects its interactions with gene products, including enzymes and receptors. This research holds substantial promise for advancing our understanding of genetic mechanisms and therapeutic applications.

When an edge is utilized to convert two or more decagons, this configuration is referred to as a cyclodecane chain. A random cyclodecane of length k is defined as a chain composed of k decagons that are randomly connected. We denote this intriguing formation as $\mathbb{CDC}_k$. For $k = 1, 2$, figure 2 [26] presents the unique cyclodecane $\mathbb{CDC}_k$. In examining the connections, there are five distinct remarkable ways by which each terminal decagon can link to the preceding cyclodecane chain $\mathbb{CDC}_{k-1}$, each associated with a specific probability p_1, p_2, p_3, p_4, and $p_5 = 1 - p_1 - p_2 - p_3 - p_4$, respectively. At each stage in this process, a random selection is made among these five possibilities, with m Taking on the values $3, 4, 5, \dots, k$.

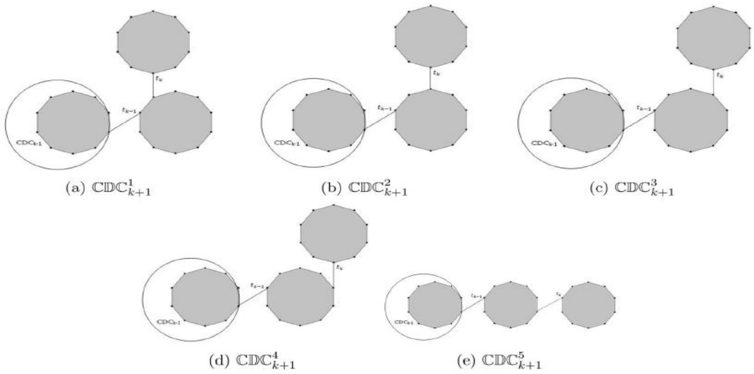
1) $\mathbb{CDC}_{m-1} \rightarrow \mathbb{CDC}_m^1$ with probability p_1.
2) $\mathbb{CDC}_{m-1} \rightarrow \mathbb{CDC}_m^2$ with probability p_2.
3) $\mathbb{CDC}_{m-1} \rightarrow \mathbb{CDC}_m^3$ with probability p_3.
4) $\mathbb{CDC}_{m-1} \rightarrow \mathbb{CDC}_m^4$ with probability p_4.
5) $\mathbb{CDC}_{m-1} \rightarrow \mathbb{CDC}_m^5$ with probability $p_5 = 1 - p_1 - p_2 - p_3 - p_4$.

For $k \geq 3$, the terminal decagon can be attached by local arrangements in five random ways which are described as $\mathbb{CDC}_{k+1}^1$, $\mathbb{CDC}_{k+1}^2$, $\mathbb{CDC}_{k+1}^3$, $\mathbb{CDC}_{k+1}^4$, and $\mathbb{CDC}_{k+1}^5$ as shown in Figure 3 [26].



(a) $\mathbb{CDC}_1$ (b) $\mathbb{CDC}_2$

Fig. 2: Cyclodecane chains for $k = 1$ and $k = 2$.



(a) $\mathbb{CDC}_{k+1}^1$ (b) $\mathbb{CDC}_{k+1}^2$ (c) $\mathbb{CDC}_{k+1}^3$ (d) $\mathbb{CDC}_{k+1}^4$ (e) $\mathbb{CDC}_{k+1}^5$

Fig. 3: Five types of local arrangements in cyclodecane chains for $k \geq 3$.

Consider $\mathbb{CDC}_k$ to be the cyclodecane chain formed from $\mathbb{CDC}_{k-1}$, as shown in Figure 3 [26]. We represent the number of edges of $\mathbb{CDC}_k$ with vertex degree i and j by x_{ij} . From the structure of $\mathbb{CDC}_k$, we see that only $(2,2)$, $(2,3)$, and $(3,3)$ are the types of edges. Therefore, we need to determine $x_{22}(\mathbb{CDC}_k), x_{23}(\mathbb{CDC}_k)$ and $x_{33}(\mathbb{CDC}_k)$ to calculate these indices. Hence, from equations (1), (2), (3), and (4), we have

$$HB_1(\mathbb{CDC}_k) = 16x_{22}(\mathbb{CDC}_k) + 25x_{23}(\mathbb{CDC}_k) + 49x_{33}(\mathbb{CDC}_k) \quad (5)$$

$$HB_2(\mathbb{CDC}_k) = 16x_{22}(\mathbb{CDC}_k) + 36x_{23}(\mathbb{CDC}_k) + 144x_{33}(\mathbb{CDC}_k) \quad (6)$$

$$^mB_1(\mathbb{CDC}_k) = \frac{1}{4}x_{22}(\mathbb{CDC}_k) + \frac{1}{5}x_{23}(\mathbb{CDC}_k) + \frac{1}{7}x_{33}(\mathbb{CDC}_k) \quad (7)$$

$$^mB_2(\mathbb{CDC}_k) = \frac{1}{4}x_{22}(\mathbb{CDC}_k) + \frac{1}{6}x_{23}(\mathbb{CDC}_k) + \frac{1}{12}x_{33}(\mathbb{CDC}_k) \quad (8)$$

3. Results

Recall that $\mathbb{CDC}_k$ is random cyclodecane chain of length k. Therefore, $HB_1(\mathbb{CDC}_k)$, $HB_2(\mathbb{CDC}_k)$, $^mB_1(\mathbb{CDC}_k)$ and $^mB_2(\mathbb{CDC}_k)$ are the random variables for random cyclodecane. Denote the expected values of these indices of random cyclodecane chain by $E^{HB_1}(\mathbb{CDC}_k) = E[HB_1(\mathbb{CDC}_k)]$, $E^{HB_2}(\mathbb{CDC}_k) = E[HB_2(\mathbb{CDC}_k)]$, $E^{^mB_1}(\mathbb{CDC}_k) = E[^mB_1(\mathbb{CDC}_k)]$, and $E^{^mB_2}(\mathbb{CDC}_k) = E[^mB_2(\mathbb{CDC}_k)]$, respectively. Analyzing the expected values of topological indices in cyclodecane chains, allows researchers to investigate the properties and applications of these molecules, as well as in developing and evaluating new chemical structures and theories. The expected value acts as a probabilistic average that quantifies the molecular property of the chains. These also enable the researchers to predict vital properties such as bioactivity, toxicity, and solubility.
Now, we will calculate the expected values of their indices in $\mathbb{CDC}_k$.

Theorem 3.1: *Let $k \geq 2$, then the expected value of the First K hyper-Banhatti index of $\mathbb{CDC}_k$ is*

$$E^{HB_1}(\mathbb{CDC}_k) = k(15p_1 + 245) - 30p_1 - 85.$$

Proof: For $k = 2$, we get $E^{HB_1}(\mathbb{CDC}_2) = 405$ which is correct. Let $k \geq 3$, then there are five possibilities.

a) If $\mathbb{CDC}_{k-1} \to \mathbb{CDC}_k^1$, then $x_{22}(\mathbb{CDC}_k^1) = x_{22}(\mathbb{CDC}_{k-1}) + 7$, $x_{23}(\mathbb{CDC}_k^1) = x_{23}(\mathbb{CDC}_{k-1}) + 2$ and $x_{33}(\mathbb{CDC}_k^1) = x_{33}(\mathbb{CDC}_{k-1}) + 2$. Using these values in Eq. (5), we get

$$HB_1(\mathbb{CDC}_k^1) = 16(x_{22}(\mathbb{CDC}_{k-1}) + 7) + 25(x_{23}(\mathbb{CDC}_{k-1}) + 2) + 49(x_{33}(\mathbb{CDC}_{k-1}) + 2)$$

$$HB_1(\mathbb{CDC}_k^1) = HB_1(\mathbb{CDC}_{k-1}) + 260.$$

b) If $\mathbb{CDC}_{k-1} \to \mathbb{CDC}_k^2$, then $x_{22}(\mathbb{CDC}_k^2) = x_{22}(\mathbb{CDC}_{k-1}) + 6$, $x_{23}(\mathbb{CDC}_k^2) = x_{23}(\mathbb{CDC}_{k-1}) + 4$ and $x_{33}(\mathbb{CDC}_k^2) = x_{33}(\mathbb{CDC}_{k-1}) + 1$. Using these values in Eq. (5), we get

$$HB_1(\mathbb{CDC}_k^2) = 16(x_{22}(\mathbb{CDC}_{k-1}) + 6) + 25(x_{23}(\mathbb{CDC}_{k-1}) + 4) + 49(x_{33}(\mathbb{CDC}_{k-1}) + 1)$$

$$HB_1(\mathbb{CDC}_k^2) = HB_1(\mathbb{CDC}_{k-1}) + 245.$$

c) If $\mathbb{CDC}_{k-1} \to \mathbb{CDC}_k^3$, then $x_{22}(\mathbb{CDC}_k^3) = x_{22}(\mathbb{CDC}_{k-1}) + 6$, $x_{23}(\mathbb{CDC}_k^3) = x_{23}(\mathbb{CDC}_{k-1}) + 4$ and $x_{33}(\mathbb{CDC}_k^3) = x_{33}(\mathbb{CDC}_{k-1}) + 1$. Using these values in Eq. (5), we get

$$HB_1(\mathbb{CDC}_k^3) = 16(x_{22}(\mathbb{CDC}_{k-1}) + 6) + 25(x_{23}(\mathbb{CDC}_{k-1}) + 4) + 49(x_{33}(\mathbb{CDC}_{k-1}) + 1)$$

$$HB_1(\mathbb{CDC}_k^3) = HB_1(\mathbb{CDC}_{k-1}) + 245.$$

d) If $\mathbb{CDC}_{k-1} \to \mathbb{CDC}_k^4$, then $x_{22}(\mathbb{CDC}_k^4) = x_{22}(\mathbb{CDC}_{k-1}) + 6$, $x_{23}(\mathbb{CDC}_k^4) = x_{23}(\mathbb{CDC}_{k-1}) + 4$ and $x_{33}(\mathbb{CDC}_k^4) = x_{33}(\mathbb{CDC}_{k-1}) + 1$. Using these values in Eq. (5), we get

$$HB_1(\mathbb{CDC}_k^4) = 16(x_{22}(\mathbb{CDC}_{k-1}) + 6) + 25(x_{23}(\mathbb{CDC}_{k-1}) + 4) + 49(x_{33}(\mathbb{CDC}_{k-1}) + 1)$$

$$HB_1(\mathbb{CDC}_k^4) = HB_1(\mathbb{CDC}_{k-1}) + 245.$$

e) If $\mathbb{CDC}_{k-1} \to \mathbb{CDC}_k^5$, then $x_{22}(\mathbb{CDC}_k^5) = x_{22}(\mathbb{CDC}_{k-1}) + 6$, $x_{23}(\mathbb{CDC}_k^5) = x_{23}(\mathbb{CDC}_{k-1}) + 4$ and $x_{33}(\mathbb{CDC}_k^5) = x_{33}(\mathbb{CDC}_{k-1}) + 1$. Using these values in Eq. (5), we get

$$HB_1(\mathbb{CDC}_k^5) = 16(x_{22}(\mathbb{CDC}_{k-1}) + 6) + 25(x_{23}(\mathbb{CDC}_{k-1}) + 4) + 49(x_{33}(\mathbb{CDC}_{k-1}) + 1)$$

$$HB_1(\mathbb{CDC}_k^5) = HB_1(\mathbb{CDC}_{k-1}) + 245.$$

Thus, we have

$E^{HB_1}(\mathbb{CDC}_k) = p_1 HB_1(\mathbb{CDC}_k^1) + p_2 HB_1(\mathbb{CDC}_k^2) + p_3 HB_1(\mathbb{CDC}_k^3) + p_4 HB_1(\mathbb{CDC}_k^4) + (1 - p_1 - p_2 - p_3 - p_4) HB_1(\mathbb{CDC}_k^5)$

$= HB_1(\mathbb{CDC}_{k-1}) + 15p_1 + 245.$

Since $E[E^{HB_1}(\mathbb{CDC}_k)] = E^{HB_1}(\mathbb{CDC}_k)$, it follows that

$E^{HB_1}(\mathbb{CDC}_k) = E^{HB_1}(\mathbb{CDC}_{k-1}) + 15p_1 + 245.$

On solving the recurrence relation by using the initial condition $E(\mathbb{CDC}_2) = 405$, we get

$E^{HB_1}(\mathbb{CDC}_k) - E^{HB_1}(\mathbb{CDC}_2) = (k-2)(15p_1 + 245)$

$E^{HB_1}(\mathbb{CDC}_k) = (k-2)(15p_1 + 245) + E^{HB_1}(\mathbb{CDC}_2)$

$E^{HB_1}(\mathbb{CDC}_k) = k(15p_1 + 245) - 30p_1 - 85.$

Theorem 3.2: *Let $k \geq 2$, then the expected value of the Second K hyper-Banhatti index of $\mathbb{CDC}_k$ is*

$E^{HB_2}(\mathbb{CDC}_k) = k(88p_1 + 384) - 176p_1 - 224.$

Proof: For $k = 2$, we get $E^{HB_2}(\mathbb{CDC}_2) = 544$ which is correct. Let $k \geq 3$, then there are five possibilities.

a) If $\mathbb{CDC}_{k-1} \rightarrow \mathbb{CDC}_k^1$, then $x_{22}(\mathbb{CDC}_k^1) = x_{22}(\mathbb{CDC}_{k-1}) + 7$, $x_{23}(\mathbb{CDC}_k^1) = x_{23}(\mathbb{CDC}_{k-1}) + 2$ and $x_{33}(\mathbb{CDC}_k^1) = x_{33}(\mathbb{CDC}_{k-1}) + 2$. Using these values in Eq. (6), we get

$HB_2(\mathbb{CDC}_k^1) = 16(x_{22}(\mathbb{CDC}_{k-1}) + 7) + 36(x_{23}(\mathbb{CDC}_{k-1}) + 2) + 144(x_{33}(\mathbb{CDC}_{k-1}) + 2)$

$HB_2(\mathbb{CDC}_k^1) = HB_2(\mathbb{CDC}_{k-1}) + 472.$

b) If $\mathbb{CDC}_{k-1} \rightarrow \mathbb{CDC}_k^2$, then $x_{22}(\mathbb{CDC}_k^2) = x_{22}(\mathbb{CDC}_{k-1}) + 6$, $x_{23}(\mathbb{CDC}_k^2) = x_{23}(\mathbb{CDC}_{k-1}) + 4$ and $x_{33}(\mathbb{CDC}_k^2) = x_{33}(\mathbb{CDC}_{k-1}) + 1$. Using these values in Eq. (6), we get

$HB_2(\mathbb{CDC}_k^2) = 16(x_{22}(\mathbb{CDC}_{k-1}) + 6) + 36(x_{23}(\mathbb{CDC}_{k-1}) + 4) + 144(x_{33}(\mathbb{CDC}_{k-1}) + 1)$

$HB_2(\mathbb{CDC}_k^2) = HB_2(\mathbb{CDC}_{k-1}) + 384.$

c) If $\mathbb{CDC}_{k-1} \rightarrow \mathbb{CDC}_k^3$, then $x_{22}(\mathbb{CDC}_k^3) = x_{22}(\mathbb{CDC}_{k-1}) + 6$, $x_{23}(\mathbb{CDC}_k^3) = x_{23}(\mathbb{CDC}_{k-1}) + 4$ and $x_{33}(\mathbb{CDC}_k^3) = x_{33}(\mathbb{CDC}_{k-1}) + 1$. Using these values in Eq. (6), we get

$HB_2(\mathbb{CDC}_k^3) = 16(x_{22}(\mathbb{CDC}_{k-1}) + 6) + 36(x_{23}(\mathbb{CDC}_{k-1}) + 4) + 144(x_{33}(\mathbb{CDC}_{k-1}) + 1)$

$HB_2(\mathbb{CDC}_k^3) = HB_2(\mathbb{CDC}_{k-1}) + 384.$

d) If $\mathbb{CDC}_{k-1} \rightarrow \mathbb{CDC}_k^4$, then $x_{22}(\mathbb{CDC}_k^4) = x_{22}(\mathbb{CDC}_{k-1}) + 6$, $x_{23}(\mathbb{CDC}_k^4) = x_{23}(\mathbb{CDC}_{k-1}) + 4$

And $x_{33}(\mathbb{CDC}_k^4) = x_{33}(\mathbb{CDC}_{k-1}) + 1$. Using these values in Eq. (6), we get

$HB_2(\mathbb{CDC}_k^4) = 16(x_{22}(\mathbb{CDC}_{k-1}) + 6) + 36(x_{23}(\mathbb{CDC}_{k-1}) + 4) + 144(x_{33}(\mathbb{CDC}_{k-1}) + 1)$

$HB_2(\mathbb{CDC}_k^4) = HB_2(\mathbb{CDC}_{k-1}) + 384.$

e) If $\mathbb{CDC}_{k-1} \rightarrow \mathbb{CDC}_k^5$, then $x_{22}(\mathbb{CDC}_k^5) = x_{22}(\mathbb{CDC}_{k-1}) + 6$, $x_{23}(\mathbb{CDC}_k^5) = x_{23}(\mathbb{CDC}_{k-1}) + 4$ and $x_{33}(\mathbb{CDC}_k^5) = x_{33}(\mathbb{CDC}_{k-1}) + 1$. Using these values in Eq. (6), we get

$HB_2(\mathbb{CDC}_k^5) = 16(x_{22}(\mathbb{CDC}_{k-1}) + 6) + 36(x_{23}(\mathbb{CDC}_{k-1}) + 4) + 144(x_{33}(\mathbb{CDC}_{k-1}) + 1)$

$HB_2(\mathbb{CDC}_k^5) = HB_2(\mathbb{CDC}_{k-1}) + 384.$

Thus, we have

$E^{HB_2}(\mathbb{CDC}_k) = p_1 HB_2(\mathbb{CDC}_k^1) + p_2 HB_2(\mathbb{CDC}_k^2) + p_3 HB_2(\mathbb{CDC}_k^3) + p_4 HB_2(\mathbb{CDC}_k^4) + (1 - p_1 - p_2 - p_3 - p_4) HB_2(\mathbb{CDC}_k^5)$

$= HB_2(\mathbb{CDC}_{k-1}) + 88p_1 + 384.$

Since $E[E^{HB_2}(\mathbb{CDC}_k)] = E^{HB_2}(\mathbb{CDC}_k)$, it follows that

$E^{HB_2}(\mathbb{CDC}_k) = E^{HB_2}(\mathbb{CDC}_{k-1}) + 88p_1 + 384.$

On solving the recurrence relation by using the initial condition $E(\mathbb{CDC}_2) = 544$, we get

$$E^{HB_2}(\mathbb{CDC}_k) - E^{HB_2}(\mathbb{CDC}_2) = (k-2)(88p_1 + 384)$$

$$E^{HB_2}(\mathbb{CDC}_k) = (k-2)(88p_1 + 384) + E^{HB_2}(\mathbb{CDC}_2)$$

$$E^{HB_2}(\mathbb{CDC}_k) = k(88p_1 + 384) - 176p_1 - 224.$$

Theorem 3.3: *Let* $k \geq 2$*, then the expected value of the Modified first K-Banhatti index of* $\mathbb{CDC}_k$ *is*

$$E^{^mB_1}(\mathbb{CDC}_k) = k\left(\frac{342}{140} - \frac{1}{140}p_1\right) - \frac{1}{70}p_1 + \frac{4}{70}.$$

Proof: For $k = 2$, we get $E^{^mB_1}(\mathbb{CDC}_2) = \frac{173}{35}$ which is correct. Let $k \geq 3$, then there are five possibilities.

a) If $\mathbb{CDC}_{k-1} \to \mathbb{CDC}_k^1$, then $x_{22}(\mathbb{CDC}_k^1) = x_{22}(\mathbb{CDC}_{k-1}) + 7$, $x_{23}(\mathbb{CDC}_k^1) = x_{23}(\mathbb{CDC}_{k-1}) + 2$ and $x_{33}(\mathbb{CDC}_k^1) = x_{33}(\mathbb{CDC}_{k-1}) + 2$. Using these values in Eq. (7), we get

$$^mB_1(\mathbb{CDC}_k^1) = \frac{1}{4}(x_{22}(\mathbb{CDC}_{k-1}) + 7) + \frac{1}{5}(x_{23}(\mathbb{CDC}_{k-1}) + 2) + \frac{1}{7}(x_{33}(\mathbb{CDC}_{k-1}) + 2)$$

$$^mB_1(\mathbb{CDC}_k^1) = {}^mB_1(\mathbb{CDC}_{k-1}) + \frac{341}{140}.$$

b) If $\mathbb{CDC}_{k-1} \to \mathbb{CDC}_k^2$, then $x_{22}(\mathbb{CDC}_k^2) = x_{22}(\mathbb{CDC}_{k-1}) + 6$, $x_{23}(\mathbb{CDC}_k^2) = x_{23}(\mathbb{CDC}_{k-1}) + 4$ and $x_{33}(\mathbb{CDC}_k^2) = x_{33}(\mathbb{CDC}_{k-1}) + 1$. Using these values in Eq. (7), we get

$$^mB_1(\mathbb{CDC}_k^2) = \frac{1}{4}(x_{22}(\mathbb{CDC}_{k-1}) + 6) + \frac{1}{5}(x_{23}(\mathbb{CDC}_{k-1}) + 4) + \frac{1}{7}(x_{33}(\mathbb{CDC}_{k-1}) + 1)$$

$$^mB_1(\mathbb{CDC}_k^2) = {}^mB_1(\mathbb{CDC}_{k-1}) + \frac{342}{140}.$$

c) If $\mathbb{CDC}_{k-1} \to \mathbb{CDC}_k^3$, then $x_{22}(\mathbb{CDC}_k^3) = x_{22}(\mathbb{CDC}_{k-1}) + 6$, $x_{23}(\mathbb{CDC}_k^3) = x_{23}(\mathbb{CDC}_{k-1}) + 4$ and $x_{33}(\mathbb{CDC}_k^3) = x_{33}(\mathbb{CDC}_{k-1}) + 1$. Using these values in Eq. (7), we get

$$^mB_1(\mathbb{CDC}_k^3) = \frac{1}{4}(x_{22}(\mathbb{CDC}_{k-1}) + 6) + \frac{1}{5}(x_{23}(\mathbb{CDC}_{k-1}) + 4) + \frac{1}{7}(x_{33}(\mathbb{CDC}_{k-1}) + 1)$$

$$^mB_1(\mathbb{CDC}_k^3) = {}^mB_1(\mathbb{CDC}_{k-1}) + \frac{342}{140}.$$

d) If $\mathbb{CDC}_{k-1} \to \mathbb{CDC}_k^4$, then $x_{22}(\mathbb{CDC}_k^4) = x_{22}(\mathbb{CDC}_{k-1}) + 6$, $x_{23}(\mathbb{CDC}_k^4) = x_{23}(\mathbb{CDC}_{k-1}) + 4$ and $x_{33}(\mathbb{CDC}_k^4) = x_{33}(\mathbb{CDC}_{k-1}) + 1$. Using these values in Eq. (7), we get

$$^mB_1(\mathbb{CDC}_k^4) = \frac{1}{4}(x_{22}(\mathbb{CDC}_{k-1}) + 6) + \frac{1}{5}(x_{23}(\mathbb{CDC}_{k-1}) + 4) + \frac{1}{7}(x_{33}(\mathbb{CDC}_{k-1}) + 1)$$

$$^mB_1(\mathbb{CDC}_k^4) = {}^mB_1(\mathbb{CDC}_{k-1}) + \frac{342}{140}.$$

e) If $\mathbb{CDC}_{k-1} \to \mathbb{CDC}_k^5$, then $x_{22}(\mathbb{CDC}_k^5) = x_{22}(\mathbb{CDC}_{k-1}) + 6$, $x_{23}(\mathbb{CDC}_k^5) = x_{23}(\mathbb{CDC}_{k-1}) + 4$ and $x_{33}(\mathbb{CDC}_k^5) = x_{33}(\mathbb{CDC}_{k-1}) + 1$. Using these values in Eq. (7), we get

$$^mB_1(\mathbb{CDC}_k^5) = \frac{1}{4}(x_{22}(\mathbb{CDC}_{k-1}) + 6) + \frac{1}{5}(x_{23}(\mathbb{CDC}_{k-1}) + 4) + \frac{1}{7}(x_{33}(\mathbb{CDC}_{k-1}) + 1)$$

$$^mB_1(\mathbb{CDC}_k^5) = {}^mB_1(\mathbb{CDC}_{k-1}) + \frac{342}{140}.$$

Thus, we have

$$E^{^mB_1}(\mathbb{CDC}_k) = p_1\,{}^mB_1(\mathbb{CDC}_k^1) + p_2\,{}^mB_1(\mathbb{CDC}_k^2) + p_3\,{}^mB_1(\mathbb{CDC}_k^3) + p_4\,{}^mB_1(\mathbb{CDC}_k^4) + (1 - p_1 - p_2 - p_3 - p_4)\,{}^mB_1(\mathbb{CDC}_k^5)$$

$$= {}^mB_1(\mathbb{CDC}_{k-1}) + \frac{342}{140} - \frac{1}{140}p_1.$$

Since $E\left[E^{^mB_1}(\mathbb{CDC}_k)\right] = E^{^mB_1}(\mathbb{CDC}_k)$, it follows that

$$E^{^mB_1}(\mathbb{CDC}_k) = E^{^mB_1}(\mathbb{CDC}_{k-1}) + \frac{342}{140} - \frac{1}{140}p_1.$$

On solving the recurrence relation by using the initial condition $E(\mathbb{CDC}_2) = \frac{173}{35}$, we get

$$E^{^mB_1}(\mathbb{CDC}_k) - E^{^mB_1}(\mathbb{CDC}_2) = (k-2)\left(\frac{342}{140} - \frac{1}{140}p_1\right)$$

$$E^{mB_1}(\mathbb{CDC}_k) = (k-2)\left(\frac{342}{140} - \frac{1}{140}p_1\right) + E^{mB_1}(\mathbb{CDC}_2)$$

$$E^{mB_1}(\mathbb{CDC}_k) = k\left(\frac{342}{140} - \frac{1}{140}p_1\right) - \frac{1}{70}p_1 + \frac{4}{70}.$$

Theorem 3.4: *Let $k \geq 2$, then the expected value of the Modified second K-Banhatti index of $\mathbb{CDC}_k$ is*

$$E^{mB_2}(\mathbb{CDC}_k) = \frac{9k+1}{4}.$$

Proof: For $k = 2$, we get $E^{mB_2}(\mathbb{CDC}_2) = \frac{57}{12}$ which is correct. Let $k \geq 3$, then there are five possibilities.

a) If $\mathbb{CDC}_{k-1} \to \mathbb{CDC}_k^1$, then $x_{22}(\mathbb{CDC}_k^1) = x_{22}(\mathbb{CDC}_{k-1}) + 7$, $x_{23}(\mathbb{CDC}_k^1) = x_{23}(\mathbb{CDC}_{k-1}) + 2$ and $x_{33}(\mathbb{CDC}_k^1) = x_{33}(\mathbb{CDC}_{k-1}) + 2$. Using these values in Eq. (8), we get

$$^{m}B_2(\mathbb{CDC}_k^1) = \frac{1}{4}(x_{22}(\mathbb{CDC}_{k-1}) + 7) + \frac{1}{6}(x_{23}(\mathbb{CDC}_{k-1}) + 2) + \frac{1}{12}(x_{33}(\mathbb{CDC}_{k-1}) + 2)$$

$$^{m}B_2(\mathbb{CDC}_k^1) = {}^{m}B_2(\mathbb{CDC}_{k-1}) + \frac{9}{4}.$$

b) If $\mathbb{CDC}_{k-1} \to \mathbb{CDC}_k^2$, then $x_{22}(\mathbb{CDC}_k^2) = x_{22}(\mathbb{CDC}_{k-1}) + 6$, $x_{23}(\mathbb{CDC}_k^2) = x_{23}(\mathbb{CDC}_{k-1}) + 4$ and $x_{33}(\mathbb{CDC}_k^2) = x_{33}(\mathbb{CDC}_{k-1}) + 1$. Using these values in Eq. (8), we get

$$^{m}B_2(\mathbb{CDC}_k^2) = \frac{1}{4}(x_{22}(\mathbb{CDC}_{k-1}) + 6) + \frac{1}{6}(x_{23}(\mathbb{CDC}_{k-1}) + 4) + \frac{1}{12}(x_{33}(\mathbb{CDC}_{k-1}) + 1)$$

$$^{m}B_2(\mathbb{CDC}_k^2) = {}^{m}B_2(\mathbb{CDC}_{k-1}) + \frac{9}{4}.$$

c) If $\mathbb{CDC}_{k-1} \to \mathbb{CDC}_k^3$, then $x_{22}(\mathbb{CDC}_k^3) = x_{22}(\mathbb{CDC}_{k-1}) + 6$, $x_{23}(\mathbb{CDC}_k^3) = x_{23}(\mathbb{CDC}_{k-1}) + 4$ and $x_{33}(\mathbb{CDC}_k^3) = x_{33}(\mathbb{CDC}_{k-1}) + 1$. Using these values in Eq. (8), we get

$$^{m}B_2(\mathbb{CDC}_k^3) = \frac{1}{4}(x_{22}(\mathbb{CDC}_{k-1}) + 6) + \frac{1}{6}(x_{23}(\mathbb{CDC}_{k-1}) + 4) + \frac{1}{12}(x_{33}(\mathbb{CDC}_{k-1}) + 1)$$

$$^{m}B_2(\mathbb{CDC}_k^3) = {}^{m}B_2(\mathbb{CDC}_{k-1}) + \frac{9}{4}.$$

d) If $\mathbb{CDC}_{k-1} \to \mathbb{CDC}_k^4$, then $x_{22}(\mathbb{CDC}_k^4) = x_{22}(\mathbb{CDC}_{k-1}) + 6$, $x_{23}(\mathbb{CDC}_k^4) = x_{23}(\mathbb{CDC}_{k-1}) + 4$ and $x_{33}(\mathbb{CDC}_k^4) = x_{33}(\mathbb{CDC}_{k-1}) + 1$. Using these values in Eq. (8), we get

$$^{m}B_2(\mathbb{CDC}_k^4) = \frac{1}{4}(x_{22}(\mathbb{CDC}_{k-1}) + 6) + \frac{1}{6}(x_{23}(\mathbb{CDC}_{k-1}) + 4) + \frac{1}{12}(x_{33}(\mathbb{CDC}_{k-1}) + 1)$$

$$^{m}B_2(\mathbb{CDC}_k^4) = {}^{m}B_2(\mathbb{CDC}_{k-1}) + \frac{9}{4}.$$

e) If $\mathbb{CDC}_{k-1} \to \mathbb{CDC}_k^5$, then $x_{22}(\mathbb{CDC}_k^5) = x_{22}(\mathbb{CDC}_{k-1}) + 6$, $x_{23}(\mathbb{CDC}_k^5) = x_{23}(\mathbb{CDC}_{k-1}) + 4$ and $x_{33}(\mathbb{CDC}_k^5) = x_{33}(\mathbb{CDC}_{k-1}) + 1$. Using these values in Eq. (8), we get

$$^{m}B_2(\mathbb{CDC}_k^5) = \frac{1}{4}(x_{22}(\mathbb{CDC}_{k-1}) + 6) + \frac{1}{6}(x_{23}(\mathbb{CDC}_{k-1}) + 4) + \frac{1}{12}(x_{33}(\mathbb{CDC}_{k-1}) + 1)$$

$$^{m}B_2(\mathbb{CDC}_k^5) = {}^{m}B_2(\mathbb{CDC}_{k-1}) + \frac{9}{4}.$$

Thus, we have

$$E^{mB_2}(\mathbb{CDC}_k) = p_1{}^{m}B_2(\mathbb{CDC}_k^1) + p_2{}^{m}B_2(\mathbb{CDC}_k^2) + p_3{}^{m}B_2(\mathbb{CDC}_k^3) + p_4{}^{m}B_2(\mathbb{CDC}_k^4) + (1 - p_1 - p_2 - p_3 - p_4){}^{m}B_2(\mathbb{CDC}_k^5)$$

$$= {}^{m}B_2(\mathbb{CDC}_{k-1}) + \frac{9}{4}.$$

Since $E\left[E^{mB_2}(\mathbb{CDC}_k)\right] = E^{mB_2}(\mathbb{CDC}_k)$, it follows that

$$E^{mB_2}(\mathbb{CDC}_k) = E^{mB_2}(\mathbb{CDC}_{k-1}) + \frac{9}{4}.$$

On solving the recurrence relation by using the initial condition $E(\mathbb{CDC}_2) = \frac{57}{12}$, we get

$$E^{mB_2}(\mathbb{CDC}_k) - E^{mB_2}(\mathbb{CDC}_2) = (k-2)\left(\frac{9}{4}\right)$$

$$E^{mB_2}(\mathbb{CDC}_k) = (k-2)\left(\frac{9}{4}\right) + E^{mB_2}(\mathbb{CDC}_2)$$

$E^{^mB_2}(\mathbb{CDC}_k) = \frac{9k+1}{4}$.

We now focus on the unique cyclodecane chains $\mathbb{CF}_k$, $\mathbb{CG}_k$, $\mathbb{CH}_k$, $\mathbb{CI}_k$ and $\mathbb{CJ}_k$ as shown in Figure 4 [26], as a special cases by setting $(p_1, p_2, p_3, p_4) = (1,0,0,0), (0,1,0,0), (0,0,1,0), (0,0,0,1)$, and $(0,0,0,0)$ respectively.

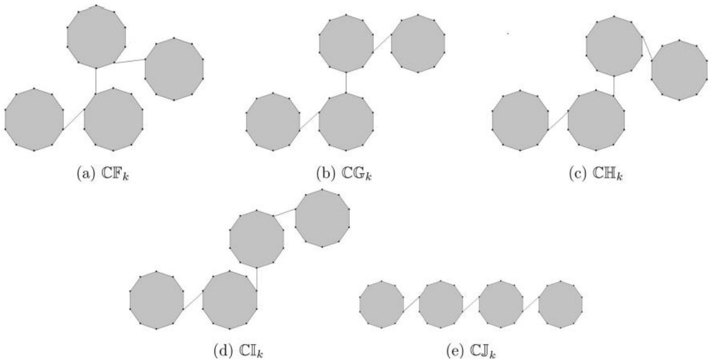


Fig. 4: Cyclodecane chains for $k = 1$ and $k = 2$.

Corollary 3.1. For $k \geq 2$, we have the following:

- $E^{HB_1}(\mathbb{CF}_k) = 260k - 115$.
- $E^{HB_2}(\mathbb{CF}_k) = 472k - 400$.
- $E^{^mB_1}(\mathbb{CF}_k) = \frac{341k+10}{140}$.
- $E^{^mB_2}(\mathbb{CF}_k) = \frac{9k+1}{4}$.
- $E^{HB_1}(\mathbb{CG}_k) = E^{HB_1}(\mathbb{CH}_k) = E^{HB_1}(\mathbb{CI}_k) = E^{HB_1}(\mathbb{CJ}_k) = 245k - 85$.
- $E^{HB_2}(\mathbb{CG}_k) = E^{HB_2}(\mathbb{CH}_k) = E^{HB_2}(\mathbb{CI}_k) = E^{HB_2}(\mathbb{CJ}_k) = 384k - 224$.
- $E^{^mB_1}(\mathbb{CG}_k) = E^{^mB_1}(\mathbb{CH}_k) = E^{^mB_1}(\mathbb{CI}_k) = E^{^mB_1}(\mathbb{CJ}_k) = \frac{171k+4}{70}$.
- $E^{^mB_2}(\mathbb{CG}_k) = E^{^mB_2}(\mathbb{CH}_k) = E^{^mB_2}(\mathbb{CI}_k) = E^{^mB_2}(\mathbb{CJ}_k) = \frac{9k+1}{4}$.

4. Comparisons and graphical representation

In this section, we will lay out an elucidative comparison between the expected values for the describe topological descriptors for a random cyclodecane chains with identical probabilities. The comparison of the expected values of topological indices is crucial as it enable the chemists and researchers to evaluate the diversity and common characteristics of the molecular structures of entire classes. This analysis aids in comprehending the influence of structural differences and can create predictive models for QSAR/QSPR studies. By comparing the topological indices of potential new drug-like compounds, researchers can identify hidden gems in drug discovery. Table 1, 2, 3, and 4 showcases the expected values of indices for various probability $p_1 = 0, \frac{1}{4}, \frac{1}{2}$, and 1, respectively. It is evident that HB_2 is more conspicuous than other three indices, namely the First K hyper-Banhatti index, Modified first K-Banhatti index, and Modified second K-Banhatti index. The graphical comparisons Figure 5, 6, 7, and 8 also illustrate the expected values of four distinct topological indices $E[HB_1], E[HB_2], E[^mB_1]$ and $E[^mB_2]$, as a function of the parameter k, corresponding to various probability values p_1. In this context, probability p_1 denotes the presence of an edge in the aforesaid random graph structure. The orange line $(E[HB_2])$ in all four figures exhibits an upward trend with increasing values of k for each probability p_1. Notably, the slope becomes more sharp as p_1 transitions from 0 and 1, suggesting high sensitivity of the index corresponding to both the parameters k and p_1. This sensitivity reveals that HB_2 profoundly captures the essence of structural growth of the graph and attains greater density. In contrast, while HB_1 also demonstrates sensitivity, it does so to a lesser degree, rendering it moderately effective for structural monitoring purposes. The indices $^mB_1$ and $^mB_2$, however, exhibit relative stability across the analyzed parameters.

Table 1: The expected values of topological indices for $p_1 = 0$

k	E^{HB_1}	E^{HB_2}	$E^{^mB_1}$	$E^{^mB_2}$
4	895	1312	9.8285	9.25
5	1140	1696	12.2714	11.5
6	1385	2080	14.7142	13.75
7	1630	2464	17.1571	16
8	1875	2848	19.6	18.25
9	2120	3232	22.0428	20.5
10	2365	3616	24.4857	22.75
11	2610	4000	26.9285	25
12	2855	4384	29.3714	27.25
13	3100	4768	31.8142	29.5

Table 2: The expected values of topological indices for $p_1 = \frac{1}{4}$

k	E^{HB_1}	E^{HB_2}	E^{mB_1}	E^{mB_2}
4	902.5	1356	9.825	9.25
5	1151.25	1762	12.2660	11.5
6	1400	2168	14.7071	13.75
7	1648.75	2574	17.1482	16
8	1897.5	2980	19.5892	18.25
9	2146.25	3386	22.0303	20.5
10	2395	3792	24.4714	22.75
11	2643.75	4198	26.9125	25
12	2892.5	4604	29.3535	27.25
13	3141.25	5010	31.7946	29.5

Table 3: The expected values of topological indices for $p_1 = \frac{1}{2}$

k	E^{HB_1}	E^{HB_2}	E^{mB_1}	E^{mB_2}
4	910	1400	9.8214	9.25
5	1162.5	1828	12.2607	11.5
6	1415	2256	14.7000	13.75
7	1667.5	2684	17.1392	16
8	1920	3112	19.5785	18.25
9	2172.5	3540	22.0178	20.5
10	2425	3968	24.4571	22.75
11	2677.5	4396	26.8964	25
12	2930	4824	29.3357	27.25
13	3182.5	5252	31.7750	29.5

Table 4: The expected values of topological indices for $p_1 = 1$

k	E^{HB_1}	E^{HB_2}	E^{mB_1}	E^{mB_2}
4	925	1488	9.8142	9.25
5	1185	1960	12.2499	11.5
6	1445	2432	14.6857	13.75
7	1705	2904	17.1214	16
8	1965	3376	19.5571	18.25
9	2225	3848	21.9928	20.5
10	2485	4320	24.4285	22.75
11	2745	4792	26.8642	25
12	3005	5264	29.3	27.25
13	3265	5736	31.7357	29.5

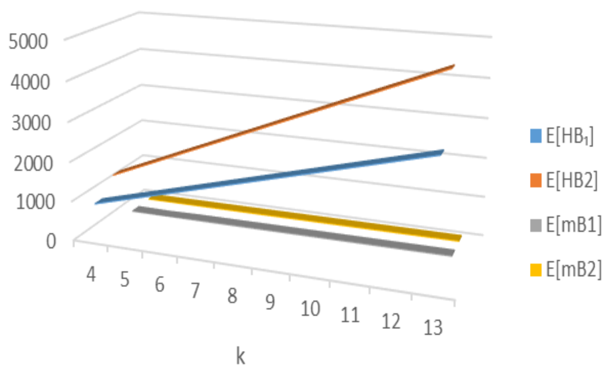


Fig. 5: Plot of expected values of topological indices for $p_1 = 0$.

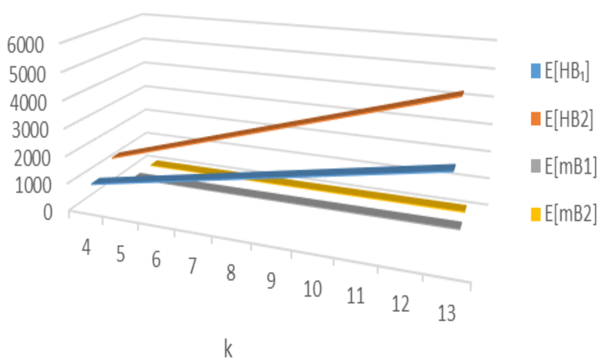


Fig. 6: Plot of expected values of topological indices for $p_1 = \frac{1}{4}$.

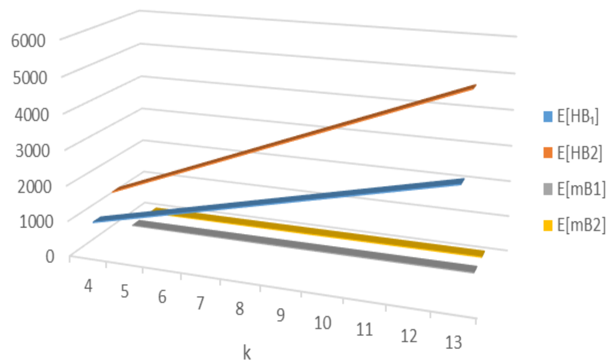


Fig. 7: Plot of expected values of topological indices for $p_1 = \frac{1}{2}$.

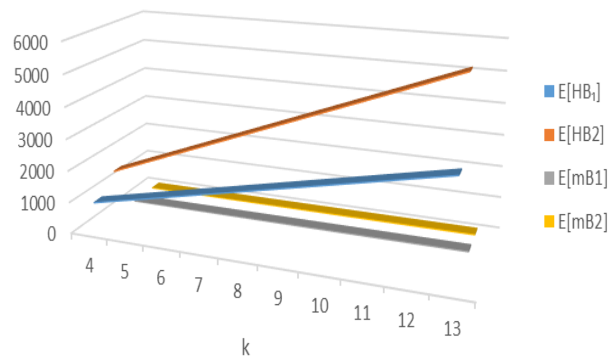


Fig. 8: Plot of expected values of topological indices for $p_1 = 1$.

Theorem 4.1: *If* $k \geq 2$, *then*

$E[HB_2(\mathbb{CDC}_k)] > E[HB_1(\mathbb{CDC}_k)]$.

Proof: Since $E^{HB_2}(\mathbb{CDC}_2) = 544$ and $E^{HB_1}(\mathbb{CDC}_2) = 405$, it is true for $k = 2$.
Now, let us solve it for $k > 2$; by using Theorems 3.1 and 3.2, we have

$$E[HB_2(\mathbb{CDC}_k)] > E[HB_1(\mathbb{CDC}_k)]$$

$$= (k(88p_1 + 384) - 176p_1 - 224) - (k(15p_1 + 245) - 30p_1 - 85)$$

$$= k(88p_1 + 384 - 15p_1 - 245) - 176p_1 - 224 + 30p_1 + 85$$

$$= k(73p_1 + 139) - 146p_1 - 139$$

$$= (k-2)(73p_1 + 139) + 139$$

$$> 0 \qquad \text{as } k > 2 \text{ and } 0 \leq p_1 \leq 1.$$

Theorem 4.2: *If* $k \geq 2$, *then*

$E[HB_1(\mathbb{CDC}_k)] > E[{}^mB_1(\mathbb{CDC}_k)]$.

Proof: Since $E^{HB_1}(\mathbb{CDC}_2) = 405$ and $E^{{}^mB_1}(\mathbb{CDC}_2) = \frac{173}{35}$, it is true for $k = 2$.
Now, let us solve it for $k > 2$; by using Theorems 3.1 and 3.3, we have

$$E[HB_1(\mathbb{CDC}_k)] > E[{}^mB_1(\mathbb{CDC}_k)]$$

$$= (k(15p_1 + 245) - 30p_1 - 85) - \left(k\frac{(342-p_1)}{140} + \frac{1}{70}p_1 + \frac{4}{70}\right)$$

$$= k\left(15p_1 + 245 - \frac{(342-p_1)}{140}\right) - 30p_1 - 85 - \frac{1}{70}p_1 - \frac{4}{70}$$

$$= k\left(\frac{2101}{140}p_1 + \frac{33958}{140}\right) - \frac{2101}{70}p_1 - \frac{5954}{70}$$

$$= (k-2)\left(\frac{2101p_1 + 33958}{140}\right) + \frac{56008}{140}$$

$$> 0 \qquad \text{as } k > 2 \text{ and } 0 \leq p_1 \leq 1.$$

Theorem 4.3: *If* $k \geq 2$, *then*

$E[{}^mB_1(\mathbb{CDC}_k)] > E[{}^mB_2(\mathbb{CDC}_k)]$.

Proof: Since $E^{{}^mB_1}(\mathbb{CDC}_2) = \frac{173}{35}$ and $E^{{}^mB_2}(\mathbb{CDC}_2) = \frac{57}{12}$, it is true for $k = 2$.
Now, let us solve it for $k > 2$; by using Theorems 3.3 and 3.4, we have

$$E[{}^mB_1(\mathbb{CDC}_k)] > E[{}^mB_2(\mathbb{CDC}_k)]$$

$$= \left(k\frac{(342-p_1)}{140} + \frac{1}{70}p_1 + \frac{4}{70}\right) - \frac{(9k+1)}{4}$$

$$= k\left(\frac{(342-p_1)}{140} - \frac{9}{4}\right) + \frac{1}{70}p_1 + \frac{4}{70} - \frac{1}{4}$$

$$= k\left(\frac{27-p_1}{140}\right) + \frac{1}{70}p_1 - \frac{27}{140}$$

$$= (k-2)\left(\frac{27-p_1}{140}\right) + \frac{27}{140}$$

$$> 0 \qquad \text{as } k > 2 \text{ and } 0 \leq p_1 \leq 1.$$

5. Conclusion

The K-Banhatti index family provides enhanced versatility in simulating various molecular properties. The expected value functions as a powerful statistical tool for delineating the intricate behaviors of a random cyclodecane chain, empowering chemists and researchers to compare the probabilistic characteristics of these molecular structures. In this paper, we focus on deriving explicit formulas for the expected values of the First K hyper-Banhatti index, Second K hyper-Banhatti index, Modified first K-Banhatti index, and Modified second K-Banhatti index in random cyclodecane chain. Furthermore, we present compelling analytic proofs of these indices for comparison, both numerically and graphically, with respect to these random chain. The numerical tables and graphical lineaments solidify that the HB_2 is continuously more prominent than the other three indices, especially the First K hyper-Banhatti index, Modified first K-Banhatti index, and Modified second K-Banhatti index , i.e., $E^{HB_2} > E^{HB_1} > E^{{}^mB_1} > E^{{}^mB_2}$. Additionally, the ${}^mB_2$ index is shown to be independent of probability for random cyclodecane chain. The HB_2 index stands out as a highly promising, accurate, and dependable tool, offering consistent and enhanced insights for predicting the chemical and physical properties of molecular structures. Its significance extends far beyond mere analysis; the HB_2 index is essential for fields like materials science, drug design, and pharmaceutical sciences, empowering researchers to thoroughly understand the behavior of entire classes of molecules. This makes it an invaluable asset in the quest for innovative solutions and breakthroughs. For our future endeavors, we can leverage the same technique to determine the anticipated values of diverse topological indices for other random chemical graphs.

Funding information

Authors state no funding involved.

Conflict of interest

Authors state no conflict of interest.

Declaration

Not Applicable.

References

[1] H. Wiener, "Structure determination of paraffin boiling points," *Journal of the American Chemical Society*, vol. 69, no. 1, pp. 17-20, 1947, doi: https://doi.org/10.1021/ja01193a005.
[2] H. Y. Deng, "Wiener indices of spiro and polyphenyl hexagonal chains," *Mathematical and Computer Modelling*, vol. 55, no. 3-4, pp. 634-644, 2012, https://doi.org/10.1016/j.mcm.2011.08.037.
[3] M. Randi ć, "Characterization of molecular branching," *Journal of the American Chemical Society*, vol. 97, pp. 6609-6615, 1975, doi: https://doi.org/10.1021/ja00856a001.
[4] I. Gutman, J. W. Kennedy, and L. V. Quintas, "Wiener numbers of random benzenoid chains," *Chemical Physics Letters*, vol. 173, no. 4, pp. 403-408, 1990, https://doi.org/10.1016/0009-2614(90)85292-K.
[5] I. Gutman, and K. Das, "The first Zagreb index 30 years after," *MATCH Communications in Mathematical and in Computer Chemistry*, vol. 50, pp. 83-92, 2004.
[6] J. L. Zhang, X. H. Peng, and H. L. Chen, "The Limiting Behaviours for the Gutman Index, Schultz Index, Multiplicative Degree-Kirchhoff Index and Additive Degree-Kirchhoff Index of a Random Polyphenylene Chain," *Discrete Applied Mathematics*, vol. 299, pp. 62-73, 2021, doi: https://doi.org/10.1016/j.dam.2021.04.016.
[7] L. L. Zhang, Q. S. Li, S. C. Li, and M. J. Zhang, "The expected values for the Schultz Index, Gutman Index, multiplicative degree-Kirchhoff Index and additive degree-Kirchhoff index of a random polyphenylene chain," *Discrete Applied Mathematics*, vol. 282, pp. 243-256, 2020, doi: https://doi.org/10.1016/j.dam.2019.11.007.

[8] D. Bonchev, "Information Theoretic Indices for Characterization of Molecular Structure," Research Studies Press-Wiley, Chichester, 1983.
[9] D. Vukičević, and M. Gašperov, "Bond Additive Modeling 1. Adriatic Indices," *Croatica Chemica Acta*, vol. 83, no. 3, pp. 243-260, 2010.
[10] H. C. Liu, R. W. Wu, and L. H. You, "Three Types of Kirchhoff Indices in the Random Cyclooctane Chains," *Journal of South China Normal University (Natural Science Edition)*, vol. 53, no. 2, pp. 96-103, 2021.
[11] S. L. Wei, X. L. Ke, and G. L. Hao, "Comparing the expected values of atom-bond connectivity and geometric-arithmetic indices in random spiro chains," *Journal of Inequalities and Applications*, vol. 2018, pp. 45, 2018, https://doi.org/10.1186/s13660-018-1628-8.
[12] A. Ali, A. A. Bhatti, and Z. Raza, "Topological study of tree-like polyphenylene systems, spiro hexagonal systems and polyphenylene dendrimer nanostars," *Quantum Matter*, vol. 5, no. 4, pp. 534-538, 2016, https://doi.org/10.1166/qm.2016.1345
[13] A. Ali, Z. Raza, and A. A. Bhatti, "Extremal pentagonal chains with respect to degree-based topological indices," *Canadian Journal of Chemistry*, vol. 94, pp. 870-876, 2016, https://doi.org/10.1139/cjc-2016-0308.
[14] A. Ali, Z. Raza, and A. A. Bhatti, "Some vertex-degree based topological indices of cacti," *Ars Combinatoria*, vol. 144, pp. 195-206, 2019.
[15] A. Jahanbani, "The expected values of the first Zagreb and Randić indices in random polyphenyl chains," *Polycyclic Aromatic Compounds*, vol. 42, no. 4, pp. 1851-1860, 2022, https://doi.org/10.1080/10406638.2020.1809472.
[16] G. Huang, M. Kuang, and H. Deng, "The expected values of Hosoya index and Merrifield-Simmons index in a random polyphenylene chain," *Journal of Combinatorial Optimization*, vol. 32, pp. 550-562, 2016, https://doi.org/10.1007/s10878-015-9882-x
[17] G. Huang, M. Kuang, and H. Deng, "The expected values of Kirchhoff indices in the random polyphenyl and spiro chains," *Ars Mathematica Contemporanea*, vol. 9, no. 2, pp. 207-217, 2015, https://doi.org/10.26493/1855-3974.458.7b0
[18] P. Žigert Pleteršek, "The edge-Wiener index and the edge-hyper-Wiener index of phenylenes," *Discrete Applied Mathematics*, vol. 255, pp. 326-333, 2019, https://doi.org/10.1016/j.dam.2018.07.024.
[19] R. Mojarad, B. Daneshian, and J. Asadpour, "Omega and related polynomials of phenylenes and their hexagonal squeezes," *Optoelectronics and Advanced Materials-Rapid Communications*, vol. 10, no. 1, pp. 113-116, 2016.
[20] V. R. Kulli, "Computing Banhatti indices of networks," *International Journal of Advances in Mathematics*, vol. 2018, no. 1, pp. 31-40, 2018.
[21] V. R. Kulli, "On K Banhatti Indices of Graphs," *Journal of Computer and Mathematical Sciences*, vol. 7, no. 4, pp. 213-218, 2016.
[22] V. R. Kulli, "On K hyper-Banhatti Indices and coindices of graphs," *International Research Journal of Pure Algebra*, vol. 6, no. 5, pp. 300-304, 2016.
[23] V. R. Kulli, "On K Banhatti indices and K hyper-Banhatti indices of V-Phenylenic nanotubes and nanotorus," *Journal of Computer and Mathematical Sciences*, vol. 7, no. 6, pp. 302-307, 2016.
[24] V. R. Kulli, B. Chaluvaraju, and H. S. Baregowda, "K-Banhatti and K hyper-Banhatti indices of windmill graphs," *South East Asian Journal of Mathematics and Mathematical Sciences*, vol. 13, no. 1, pp. 11-18, 2017.
[25] F. Dayan, M. Javaid, M. Zulqarnain, M. T. Ali, and B. Ahmad, "Computing Banhatti indices of hexagonal, honeycomb and derived graphs," *American Journal of Mathematical and Computer Modelling*, vol. 3, no. 2, pp. 38-45, 2018, https://doi.org/10.11648/j.ajmcm.20180302.11.
[26] B. Chunsong, A. Naeem, S. Yousaf, A. Aslam, F. Tchier, and A. Issa, "Exploring expected values of topological indices of random cyclodecane chains for chemical insights," *Scientific* Reports, vol. 14, pp. 10065, 2024, https://doi.org/10.1038/s41598-024-60484-x.
[27] W. Wei, and L. Shuchao, "Extremal phenylene chains with respect to the coefficients sum of the permanental polynomial, the spectral radius, the Hosoya index and the Merrifield-Simmons index," *Discrete Applied Mathematics*, vol. 271, no. 1, pp. 205-217, 2019, https://doi.org/10.1016/j.dam.2019.07.024.
[28] W. Yang, and F. Zhang, "Wiener index in random polyphenyl chains," *MATCH Communications in Mathematical and in Computer Chemistry*, vol. 68, no. 1, pp. 371-376, 2012.
[29] X. L. Chen, B. Zhao, and P. Y. Zhao, "Six-membered ring spiro chains with extremal Merrified-Simmons index and Hosoya index," *MATCH Communications in Mathematical and in Computer Chemistry*, vol. 62, pp. 657-665, 2009.
[30] X. Y. Li, G. P. Wang, H. Bian, and R. W. Hu, "The Hosoya polynomial decomposition for polyphenyl chains," *MATCH Communications in Mathematical and in Computer Chemistry*, vol. 67, pp. 357-368, 2012.
[31] Z. Raza, "The Harmonic and Second Zagreb Indices in Random Polyphenyl and Spiro Chains," *Polycyclic Aromatic Compounds*, vol. 42, no. 3, pp. 671-680, 2022, https://doi.org/10.1080/10406638.2020.1749089.