

Computing some fuzzy topological indices of linear and multi-cyclic tetracene hydrocarbon

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Abstract

This study focuses on the theoretical study of the fuzzy graph of an aromatic hydrocarbon called tetracene hydrocarbon and calculates several degree topological indices based on fuzzy logic, including the first and second Zagreb index, Randic index, Harmonic index, Forgotten index, and Y-index. The research introduces new definitions for the first Zagreb fuzzy index, forgotten index, and Y-index, and provides a general formula for fuzzy topology indices of hydrocarbons by considering the degree of each edge. Furthermore, a general formula is presented to determine the topological indices of tetracene hydrocarbon based on the number of rows and columns. In continuation, the topological indices of linear tetracene were compared, and among them, the Harmonic and Randic indices had the highest values respectively, while the values of other indices were very close to each other. Additionally, the surface of the Y-index of multi-cyclic tetracene was plotted to determine the effect of row and column parameters on the index, and it was concluded that when the number of parameters is equal, the Y-index has the highest value.

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1. Introduction

1.1 Background

As a thriving branch of mathematics, graph theory has proven invaluable in fields as varied as physics, chemistry, and engineering [5, 9, 29]. Chemical graph theory combines chemistry and graph theory to represent chemical structures as mathematical models. It uses mathematical theorems and chemical methods to solve chemistry problems. In molecular graphs, atoms and bonds are represented as vertices and edges. Chemical graph theory is used to count isomers and generate molecular structures. Many scientists and researchers conduct research in chemical graph theory [7, 21]. Fuzzy graphs, which have practical applications in mathematics, are used in areas such as neural networks, artificial intelligence, computer networks, engineering sciences, transportation network design, and electrical circuits. Fuzzy graph theory is also used to study the structure of communication networks or circuits when there is ambiguity in their design [18].

Fuzzy graph theory allows for membership degrees in the interval $[0,1]$, unlike binary evaluation in traditional sets. A. Rosenfeld introduced the theory, with Zadeh introducing fuzzy sets in graph theory in 1965 [32]. In 1975, Rosenfeld introduced the fuzzy graph [26]. The first usage in chemistry was mentioned by Xu in 1997 [30], while Bhattacharya used fuzzy graphs to create fuzzy groups [3] and discussed automorphisms [4]. Recent years have witnessed a surge of interest in extending graph-theoretic concepts to fuzzy and bipolar fuzzy domains. In 2020, significant strides were made in this direction. Binu, Mathew, and Mordeson [2] introduced the Wiener index, a fundamental topological index, to the realm of fuzzy graphs. Concurrently, Kalathian et al. [18] delved into the computation of various topological indices for fuzzy graphs. Poulik and Ghorai [22] further expanded this research by introducing a novel index for bipolar fuzzy graphs. Building upon these foundations, 2021 saw the introduction of new indices, including the Wiener absolute index and the Randic index, specifically tailored for bipolar fuzzy graphs [23, 24].

Carbon nanotubes are cylindrical nanostructures that belong to the family of carbon allotropes and have unique properties and potential uses in various fields such as medicine, sensing devices, and nanotechnology. They were discovered by S. Iijima in 1991 and have exceptional mechanical properties, being one of the most elastic and hardest substances [16, 27]. The structures formed by connecting regular hexagons in the plane are of great interest in the chemistry of benzenoid hydrocarbons. Benzenoid hydrocarbons are of great interest in chemistry, and acenes, a type of polycyclic aromatic hydrocarbons, have applications in optoelectronics and are actively researched in chemistry and electrical engineering. In the graphical representation of tetracene, hexagons and squares

are connected in a way that each square is between four hexagons. In the tetracene nanotube, the first row consists of a sequence of C_6 , C_6 , C_6 , C_6 , C_4 , C_6 , C_6 , C_6 , C_6 , C_4 , ..., while the second row consists of a sequence of C_6 , C_6 , C_6 , C_8 , C_6 , C_6 , C_6 , C_8 , ..., [31] as shown in Figure 5. Topological indices provide computational measures of graph structure that can be correlated with the properties of chemical compounds, thereby eliminating the need for physical experimentation. These indices are used in various fields such as mathematics, biology, and bioinformatics, but their primary use is in quantitative structure property relationship QSPR [15, 25]. Table 1 presents several topological indices based on degree. In 2023, Hasani and Ghods investigated M-polynomials and topological indices of porphyrin-cored dendrimers in crisp graphs [10]. They also analyzed the quantitative structure-property relationship (QSPR) of certain drugs used to treat heart diseases [11]. Additionally, in the same year, they employed topological indices and MATLAB programming to predict the physicochemical properties of drugs used for Parkinson's disease [12]. In 2024, they continued their work on QSPR, this time focusing on drugs used to treat heart calcium channel-blocking cardiac drug disease [13].

1.2 Motivation

Topological indices are used to analyze the properties of compounds without costly experiments. Previous studies have explored these indices on various compounds, such as nanotube Naphthalene, fuzzy graphs and linear and multi-acyclic hydrocarbons, and we are motivated to investigate several indices on Tetrasene hydrocarbon. In 2015, S. Hayat and M. Imran computed topological indices for nanotube Naphthalene based on vertex degree [14]. In 2020, Kalatgian et al. explored various topological indices within the framework of fuzzy graphs [18]. In 2022, Z. S. Mofti et al. studied the first and second fuzzy Zagreb topological indices on linear hydrocarbon and multi-acyclic Benzene [19]. This research aims to investigate topological indices on Tetrasene hydrocarbon, presenting new formulas for the first fuzzy Zagreb topological index, Forgotten index, and Y -index by considering the degree of each edge. A general formula for fuzzy topological indices of Tetrasene hydrocarbon is also developed based on the number of rows and columns. This method can aid researchers in predicting physical and chemical properties of compounds using software and precise calculations of bond lengths and atomic mass with the help of topological indices.

1.3 Framework of the article

The structure of the article is as follows: Some basic definitions in fuzzy graphs and topology indices that are necessary for the development of our main results are presented as related work in section 2. Additionally, new definitions for the first Zagreb fuzzy index, Forgotten index, and Y -index are provided. In section 3, we investigate the fuzzy topology indices of linear tetracene

theoretically rather than experimentally and obtain a general formula for their extension. Section 4, presents fuzzy topological indices of cyclic tetracene and their general formula for the extension. Finally, section 5, discusses the conclusion and application of the studied indices.

2. Preliminaries

In this section, some basic definitions necessary for the development of our results are presented [14, 20].

Definition 1: Suppose X is a finite set. The graph fuzzy G with vertices set $V(G)$ and edges set $E(G) = \{uv | \mu(u, v) > 0\}$, is a triplet, $G = (V, \sigma, \mu)$, where V is a nonempty finite subset of X with a pair of functions σ and μ such that

$$\begin{aligned}\sigma: V &\rightarrow [0,1] \\ \mu: V \times V &\rightarrow [0,1] \forall u, v \in V(G)\end{aligned}$$

satisfying

$$\mu(u, v) \leq \sigma(u) \wedge \sigma(v),$$

where $\wedge$ represents the minimum.

Table 1
Description of degree-based topological indices

Topological index	Mathematical Formula
First Zagreb index: [8]	$Z_1(G) = \sum_{i=1}^n [d(u_i)]^2 = \sum_{(u_i u_j) \in E(G)} [d(u_i) + d(u_j)]$
Second Zagreb index: [8]	$Z_2(G) = \sum_{(u_i u_j) \in E(G)} d(u_i) d(u_j)$
Forgotten index: [6]	$F(G) = \sum_{i=1}^n [d(u_i)]^3 = \sum_{(u_i u_j) \in E(G)} [d(u_i)^2 + d(u_j)^2]$
Y-index: [1]	$Y(G) = \sum_{i=1}^n [d(u_i)]^4 = \sum_{(u_i u_j) \in E(G)} [d(u_i)^3 + d(u_j)^3]$
Randic index: [28]	$\mathfrak{R}(G) = \sum_{(u_i u_j) \in E(G)} \frac{1}{\sqrt{d(u_i) \times d(u_j)}}$
Harmonic index: [28]	$H(G) = \sum_{(u_i u_j) \in E(G)} \frac{2}{[d(u_i) + d(u_j)]}$

Table 2
Description of degree-based topological indices for fuzzy graphs

Topological index	Mathematical Formula
First Zagreb index: [18]	$Z_{1f}(G) = \sum_{i=1}^n \sigma(u_i) [d(u_i)]^2$

Contd...

Second Zagreb index: [18]	$Z_{2f}(G) = \frac{1}{2} \sum_{(u_i, u_j) \in E(G)} \sigma(u_i)d(u_i)\sigma(u_j)d(u_j) \forall i \neq j$
Forgotten index: [18]	$F_f(G) = \sum_{i=1}^n \sigma(u_i)[d(u_i)]^3$
Y-index: [17]	$Y_f(G) = \sum_{i=1}^n \sigma(u_i)[d(u_i)]^4$
Randic index: [19]	$\mathfrak{R}_f(G) = \frac{1}{2} \sum_{(u_i, u_j) \in E(G)} [(\sigma(u_i)d(u_i)\sigma(u_j)d(u_j))]^{\frac{-1}{2}} \forall i \neq j$
Harmonic index: [19]	$H_f(G) = \frac{1}{2} \sum_{(u_i, u_j) \in E(G)} [\sigma(u_i)d(u_i) + \sigma(u_j)d(u_j)]^{-1} \forall i \neq j$

We define the first Zagreb index, F-index, and Y-index for fuzzy graphs as follows:

Definition 2: Assume G is the fuzzy graph. Then the first Zagreb index for fuzzy graphs is indicated by $Z_\mu(G)$ and is defined by:

$$Z_\mu(G) = \sum_{(u_i, u_j) \in E(G)} \mu(u_i, u_j) [\sigma(u_i)d(u_i) + \sigma(u_j)d(u_j)]$$

Definition 3: Assume G is the fuzzy graph. Then the F-index for fuzzy graphs is indicated by $F_\mu(G)$ and is defined by:

$$F_\mu(G) = \sum_{(u_i, u_j) \in E(G)} \mu(u_i, u_j) [\sigma(u_i)d(u_i)^2 + \sigma(u_j)d(u_j)^2]$$

Definition 4: Assume G is the fuzzy graph. Then the Y-index for fuzzy graphs is indicated by $Y_\mu(G)$ and is defined as follows:

$$Y_\mu(G) = \sum_{(u_i, u_j) \in E(G)} \mu(u_i, u_j) [\sigma(u_i)d(u_i)^3 + \sigma(u_j)d(u_j)^3]$$

It is simple to show that $Z_\mu(G) = Z_f(G)$, $F_\mu(G) = F_f(G)$, and $Y_\mu(G) = Y_f(G)$.

3. Topological indices of fuzzy graphs of linear tetracene ($C_{18}H_{12}$)

In this section, some topological indices of linear tetracene hydrocarbon in fuzzy graphs are examined, and a general formula based on the number of columns is presented for its extension. In Table 2, aromatic hydrocarbons are introduced based on the number of Benzene rings. According to Figures 1, 2 and 3, and based on the structure of linear tetracene, the total number of vertices and edges are $18n$ and $23n - 2$, respectively. The set of all vertices and edges is divided into weight categories, as shown in Tables 3 and 4. Using Table 3, the vertex set with weight 0.2 has a total number of $5n$, the vertex set with weight 0.3 has a total number of $8n$ and the vertex set with weight 0.4 has a total number of $5n$.

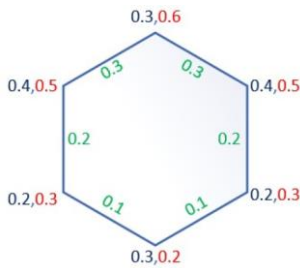


Figure 1
(1,1) unit of graph of Benzene

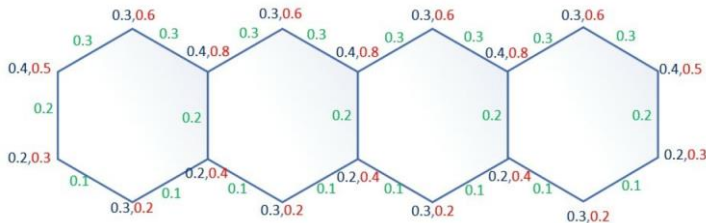


Figure 2
(1,1) unit of graph of linear tetracene

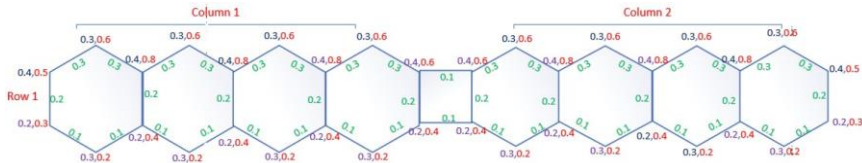


Figure 3
(1,2) unit of graph of linear tetracene hydrocarbon (K=4)

Table 3
Partition of vertices for fuzzy graph of linear tetracene

Weight	Degree	The total number of vertices
(0.2)	(0.3)	2
	(0.4)	$5n - 2$
(0.3)	(0.2)	$4n$
	(0.6)	$4n$
(0.4)	(0.5)	2
	(0.6)	$2n - 2$
	(0.8)	$3n$
		18n

Table 4
Partition of edges for fuzzy graph of linear tetracene

Weight	Degree	The total number of edges
(0.3,0.4)	(0.6,0.5)	2
	(0.6,0.8)	$6n$
	(0.6,0.6)	$2n - 2$
(0.3,0.2)	(0.2,0.3)	2
	(0.2,0.4)	$8n - 2$
(0.2,0.4)	(0.3,0.5)	2
	(0.4,0.8)	$3n$
	(0.4,0.6)	$2n - 2$
(0.4,0.4)	(0.6,0.6)	$n - 1$
(0.2,0.2)	(0.4,0.4)	$n - 1$
		$23n - 2$

Theorem 1: Suppose T_l is a linear tetracene hydrocarbon fuzzy graph and n is the number of columns of linear tetracene. Then the first Zagreb index of T_l is

$$Z_\mu(T_l) = 1.696n - 0.116.$$

Proof: According to Figure 3 and using Table 4 and Definition 3, we have

$$\begin{aligned}
 Z_\mu(T_l) &= \sum_{(u_i u_j) \in E(G)} \mu(u_i, u_j) [\sigma(u_i)d(u_i) + \sigma(u_j)d(u_j)] \\
 &= 2(0.3)[(0.3)(0.6) + (0.4)(0.5)] + (6n)(0.3)[(0.3)(0.6) + (0.4)(0.8)] \\
 &\quad + (2n - 2)(0.3)[(0.3)(0.6) + (0.4)(0.6)] + 2(0.1)[(0.3)(0.2) + (0.2)(0.3)] \\
 &\quad + (8n - 2)(0.1)[(0.3)(0.2) + (0.2)(0.4)] + 2(0.2)[(0.2)(0.3) + (0.4)(0.5)] \\
 &\quad + (3n)(0.2)[(0.2)(0.4) + (0.4)(0.8)] + (2n - 2)(0.2)[(0.2)(0.4) + (0.4)(0.6)] \\
 &\quad + (n - 1)(0.1)[(0.4)(0.6) + (0.4)(0.6)] + (n - 1)(0.1)[(0.2)(0.4) + (0.2)(0.4)] \\
 &= 1.696n - 0.116.
 \end{aligned}$$

Theorem 2: Consider a fuzzy graph T_l that represents linear tetracene with n columns. Then the second fuzzy Zagreb index of T_l is $Z_{2f}(T_l) = 0.3248n - 0.0476$.

Proof: By using Tables 2 and 4, we have

$$\begin{aligned}
 Z_{2f}(T_l) &= \frac{1}{2} \sum_{(u_i u_j) \in E(G)} \sigma(u_i)d(u_i)\sigma(u_j)d(u_j) \\
 &= \frac{1}{2} [2(0.3)(0.6)(0.4)(0.5) + (6n)(0.3)(0.6)(0.4)(0.8) + \\
 &\quad (2n - 2)(0.3)(0.6)(0.4)(0.6)] \\
 &\quad + \frac{1}{2} [2(0.3)(0.2)(0.2)(0.3) + (8n - 2)(0.3)(0.2)(0.2)(0.4)]
 \end{aligned}$$

$$\begin{aligned}
& + \frac{1}{2}[2(0.2)(0.3)(0.4)(0.5) + (3n)(0.2)(0.4)(0.4)(0.8) \\
& + (2n - 2)(0.2)(0.4)(0.4)(0.6)] \\
& + \frac{1}{2}[(n - 1)(0.4)(0.6)(0.4)(0.6) + (n - 1)(0.2)(0.4)(0.2)(0.4)] \\
& = 0.3248n - 0.0476.
\end{aligned}$$

Theorem 3: Suppose T_l is a linear tetracene fuzzy graph and n is the number of its columns. Then the Forgotten index of T_l is $F_\mu(T_l) = 1.12n - 0.0876$

Proof: By using Table 4 and Definition 4, we have

$$\begin{aligned}
F_\mu(T_l) &= \sum_{(u_i, u_j) \in E(G)} \mu(u_i, u_j) [\sigma(u_i)d(u_i)^2 + \sigma(u_j)d(u_j)^2] \\
&= 2(0.3)[(0.3)(0.6)^2 + (0.4)(0.5)^2] + (6n)(0.3)[(0.3)(0.6)^2 + (0.4)(0.8)^2] \\
&+ (2n - 2)(0.3)[(0.3)(0.6)^2 + (0.4)(0.6)^2] \\
&+ 2(0.1)[(0.3)(0.2)^2 + (0.2)(0.3)^2] \\
&+ (8n - 2)(0.1)[(0.3)(0.2)^2 + (0.2)(0.4)^2] \\
&+ 2(0.2)[(0.2)(0.3)^2 + (0.4)(0.5)^2] \\
&+ (3n)(0.2)[(0.2)(0.4)^2 + (0.4)(0.8)^2] \\
&+ (2n - 2)(0.2)[(0.2)(0.4)^2 + (0.4)(0.6)^2] \\
&+ (n - 1)(0.1)[(0.4)(0.6)^2 + (0.4)(0.6)^2] \\
&+ (n - 1)(0.1)[(0.2)(0.4)^2 + (0.2)(0.4)^2] \\
&= 1.12n - 0.0876
\end{aligned}$$

Theorem 4: Let T_l be a linear tetracene hydrocarbon fuzzy graph and n is the number of its columns. Then the Y-index of T_l is $Y_\mu(T_l) = 0.7778n - 0.0606$

Proof: By using Table 4 and Definition 5, we have

$$\begin{aligned}
Y_\mu(T_l) &= \sum_{(u_i, u_j) \in E(G)} \mu(u_i, u_j) [\sigma(u_i)d(u_i)^3 + \sigma(u_j)d(u_j)^3] \\
&= 2(0.3)[(0.3)(0.6)^3 + (0.4)(0.5)^3] \\
&+ (6n)(0.3)[(0.3)(0.6)^3 + (0.4)(0.8)^3] \\
&+ (2n - 2)(0.3)[(0.3)(0.6)^3 + (0.4)(0.6)^3] \\
&+ 2(0.1)[(0.3)(0.2)^3 + (0.2)(0.3)^3] \\
&+ (8n - 2)(0.1)[(0.3)(0.2)^3 + (0.2)(0.4)^3] \\
&+ 2(0.2)[(0.2)(0.3)^3 + (0.4)(0.5)^3] \\
&+ (3n)(0.2)[(0.2)(0.4)^3 + (0.4)(0.8)^3] \\
&+ (2n - 2)(0.2)[(0.2)(0.4)^3 + (0.4)(0.6)^3] \\
&+ (n - 1)(0.1)[(0.4)(0.6)^3 + (0.4)(0.6)^3] \\
&+ (n - 1)(0.1)[(0.2)(0.4)^3 + (0.2)(0.4)^3] \\
&= 0.7778n - 0.0606
\end{aligned}$$

Theorem 5: Suppose T_l is a linear tetracene hydrocarbon fuzzy graph and n is the number of its columns. Then the Randic index of T_l is $\mathfrak{R}_f(T_l) = 99.9709n - 3.7293$.

Proof: By using Tables 2 and 4, we have

$$\begin{aligned}\mathfrak{R}_f(T_l) &= \frac{1}{2} \sum_{(u_i u_j) \in E(G)} [(\sigma(u_i)d(u_i)\sigma(u_j)d(u_j))]^{\frac{-1}{2}} \\ &= \frac{1}{2} (2)[(0.3)(0.6)(0.4)(0.5)]^{\frac{-1}{2}} + \frac{1}{2} (6n)[(0.3)(0.6)(0.4)(0.8)]^{\frac{-1}{2}} \\ &\quad + \frac{1}{2} (2n-2)[(0.3)(0.6)(0.4)(0.6)]^{\frac{-1}{2}} + \frac{1}{2} (2)[(0.3)(0.2)(0.2)(0.3)]^{\frac{-1}{2}} \\ &\quad + \frac{1}{2} (8n-2)[(0.3)(0.2)(0.2)(0.4)]^{\frac{-1}{2}} + \frac{1}{2} (2)[(0.2)(0.3)(0.4)(0.5)]^{\frac{-1}{2}} \\ &\quad + \frac{1}{2} (3n)[(0.2)(0.4)(0.4)(0.8)]^{\frac{-1}{2}} + \frac{1}{2} (2n-2)[(0.2)(0.4)(0.4)(0.6)]^{\frac{-1}{2}} \\ &\quad + \frac{1}{2} (n-1)[(0.4)(0.6)(0.4)(0.6)]^{\frac{-1}{2}} + \frac{1}{2} (n-1)[(0.2)(0.4)(0.2)(0.4)]^{\frac{-1}{2}} \\ &= 99.9709n - 3.7293.\end{aligned}$$

Theorem 6: Suppose T_l be a linear tetracene hydrocarbon fuzzy graph. Then the Harmonic index of T_l is $H_f(T_l) = 47.9937n - 4.6359$.

Proof: By using Tables 2 and 4, we have

$$\begin{aligned}H_f(T_l) &= \frac{1}{2} \sum_{u_i u_j \in E(G)} [\sigma(u_i)d(u_i) + \sigma(u_j)d(u_j)]^{-1} \\ &= \frac{1}{2} \left[\frac{2}{(0.3)(0.6)+(0.4)(0.5)} \right] + \frac{1}{2} \left[\frac{6n}{(0.3)(0.6)+(0.4)(0.8)} \right] \\ &\quad + \frac{1}{2} \left[\frac{2n-2}{(0.3)(0.6)+(0.4)(0.6)} \right] + \frac{1}{2} \left[\frac{2}{(0.3)(0.2)+(0.2)(0.3)} \right] \\ &\quad + \frac{1}{2} \left[\frac{8n-2}{(0.3)(0.2)+(0.2)(0.4)} \right] + \frac{1}{2} \left[\frac{2}{(0.2)(0.3)+(0.4)(0.5)} \right] \\ &\quad + \frac{1}{2} \left[\frac{3n}{(0.2)(0.4)+(0.4)(0.8)} \right] + \frac{1}{2} \left[\frac{2n-2}{(0.2)(0.4)+(0.4)(0.6)} \right] \\ &\quad + \frac{1}{2} \left[\frac{n-1}{(0.4)(0.6)+(0.4)(0.6)} \right] + \frac{1}{2} \left[\frac{n-1}{(0.2)(0.4)+(0.2)(0.4)} \right] \\ &= 47.9937n - 4.6359\end{aligned}$$

The topological indices of linear tetracene are compared in Figure 4.

4. Topological indices of fuzzy graph of multi-cyclic tetracene

In this section, some topological indices of multi-cyclic tetracene in fuzzy graphs are computed, and a general formula based on the number of their rows and columns is presented for its extension. According to Figures 3 and 5, and based on the structure of multi-cyclic tetracene with m rows and n columns, the total number of vertices and edges are $18mn$ and $27mn - 2m - 4n$, respectively. The set of all vertices and edges is divided into weight categories, as shown in Tables 5 and 6. Using Table 5, the vertex set with weight 0.2 has a total

number of $5mn$, the vertex set with weight 0.3 has a total number of $8mn$ and the vertex set with weight 0.4 has a total number of $5mn$.

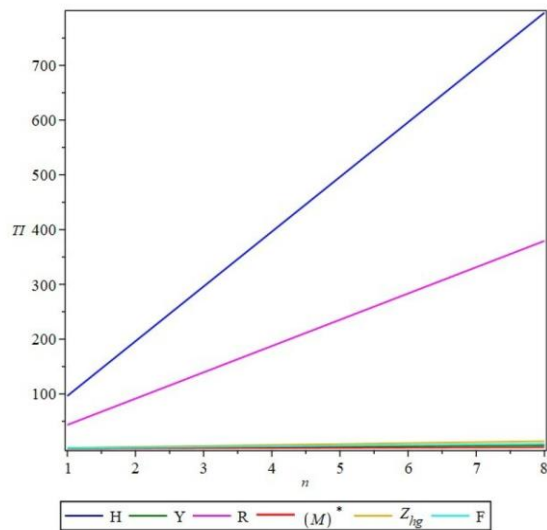


Figure 4
Comparison of topological indices of linear tetraene

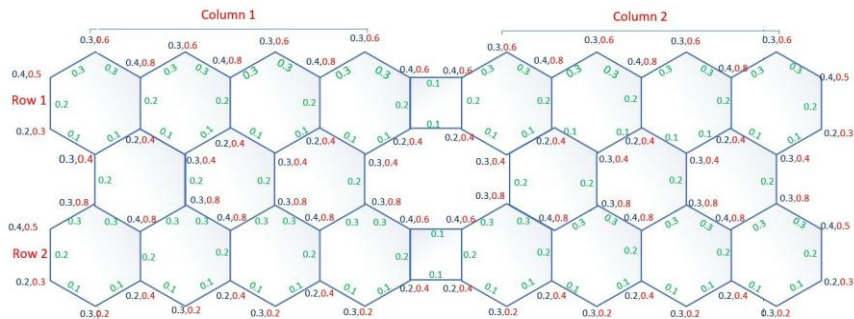


Figure 5
(2,2) unit of fuzzy graphs of tetraene hydrocarbon (K=4)

Table 5
Partition of vertices in fuzzy graphs of multi-cyclic tetraene

Weight	Degree	The total number of vertices
(0.2)	(0.3)	$2m$
	(0.4)	$m(5n - 2)$
(0.3)	(0.2)	$4n$

Contd...

	(0.4)	$4n(m-1)$
	(0.6)	$4n$
	(0.8)	$4n(m-1)$
(0.4)	(0.5)	$2m$
	(0.6)	$2m(n-1)$
	(0.8)	$3mn$
		$18mn$

Table 6
Partition of edges in fuzzy graphs of multi-cyclic tetracene

Weight	Degree	The total number of edges
(0.3,0.4)	(0.6,0.5)	2
	(0.6,0.8)	$6n$
	(0.6,0.6)	$2n-2$
	(0.8,0.5)	$2m-2$
	(0.8,0.8)	$6n(m-1)$
	(0.8,0.6)	$(m-1)(2n-2)$
(0.4,0.2)	(0.5,0.3)	$2m$
	(0.8,0.4)	$3mn$
	(0.6,0.4)	$2m(n-1)$
(0.2,0.3)	(0.3,0.4)	$2m-2$
	(0.4,0.4)	$(m-1)(8n-2)$
	(0.3,0.2)	2
	(0.4,0.2)	$8n-2$
(0.4,0.4)	(0.6,0.6)	$m(n-1)$
(0.2,0.2)	(0.4,0.4)	$m(n-1)$
(0.3,0.3)	(0.4,0.8)	$4n(m-1)$
		$27mn-2m-4n$

Theorem 7: Suppose T_m is multi-cyclic tetracene fuzzy graph and K is the number of benzene rings. Then the first Zagreb index of T_m is

$$Z_\mu(T_m) = 2.176mn - 0.48n - 0.116m.$$

Proof: By using Tables 2 and 6, we have

$$\begin{aligned}
 Z_\mu(T_m) &= \sum_{(u_i, u_j) \in E(G)} \mu(u_i, u_j) [\sigma(u_i)d(u_i) + \sigma(u_j)d(u_j)] \\
 &= 2(0.3)[(0.3)(0.6) + (0.4)(0.5)] \\
 &\quad + (6n)(0.3)[(0.3)(0.6) + (0.4)(0.8)] \\
 &\quad + (2n-2)(0.3)[(0.3)(0.6) + (0.4)(0.6)] \\
 &\quad + (2m-2)(0.3)[(0.3)(0.8) + (0.4)(0.5)]
 \end{aligned}$$

$$\begin{aligned}
& + (6n)(m-1)(0.3)[(0.3)(0.8) + (0.4)(0.8)] \\
& + (m-1)(2n-2)(0.3)[(0.3)(0.8) + (0.4)(0.6)] \\
& + (2m)(0.2)[(0.4)(0.5) + (0.2)(0.3)] \\
& + 3mn(0.2)[(0.4)(0.8) + (0.2)(0.4)] \\
& + (0.2)(2m)(n-1)[(0.4)(0.6) + (0.2)(0.4)] \\
& + (2m-2)(0.1)[(0.2)(0.3) + (0.3)(0.4)] \\
& + (0.1)(m-1)(8n-2)[(0.2)(0.4) + (0.3)(0.4)] \\
& + 2(0.1)[(0.2)(0.3) + (0.3)(0.2)] \\
& + (0.1)(8n-2)[(0.2)(0.4) + (0.3)(0.2)] \\
& + (0.1)m(n-1)[(0.4)(0.6) + (0.4)(0.6)] \\
& + (0.1)m(n-1)[(0.2)(0.4) + (0.2)(0.4)] \\
& + (0.2)4n(m-1)[(0.3)(0.4) + (0.3)(0.8)] \\
& = 2.176mn - 0.48n - 0.116m.
\end{aligned}$$

Theorem 8: Consider a fuzzy graph T_m that models a multi-cyclic tetracene with m rows and n hydrocarbon columns. Then the second fuzzy Zagreb index of multi-cyclic tetracene is

$$Z_{2f}(T_m) = 0.4736mn - 0.5952n - 0.0944m + 0.468.$$

Proof: By using Tables 2 and 6, we have

$$\begin{aligned}
Z_{2f}(T_m) &= \frac{1}{2} \sum_{(u_i u_j) \in E(G)} \sigma(u_i) d(u_i) \sigma(u_j) d(u_j) \\
&= \frac{1}{2} [2(0.3)(0.6)(0.4)(0.5) + (6n)(0.3)(0.6)(0.4)(0.8) \\
&\quad + (2n-2)(0.3)(0.6)(0.4)(0.6) \\
&\quad + (2m-2)(0.3)(0.8)(0.4)(0.5) \\
&\quad + (6n)(m-1)(0.3)(0.8)(0.4)(0.8) \\
&\quad + (m-1)(2n-2)(0.3)(0.8)(0.4)(0.6) \\
&\quad + (2m)(0.4)(0.5)(0.2)(0.3) \\
&\quad + 3mn(0.4)(0.8)(0.2)(0.4) \\
&\quad + 2m(n-1)(0.4)(0.6)(0.2)(0.4) \\
&\quad + (2m-2)(0.2)(0.3)(0.3)(0.4) \\
&\quad + (m-1)(8n-2)(0.2)(0.4)(0.3)(0.4) \\
&\quad + 2(0.2)(0.3)(0.3)(0.2) \\
&\quad + (8n-2)(0.2)(0.4)(0.3)(0.2) \\
&\quad + m(n-1)(0.4)(0.6)(0.4)(0.6) \\
&\quad + m(n-1)(0.2)(0.4)(0.2)(0.4) \\
&\quad + 4n(m-1)(0.3)(0.4)(0.3)(0.8)]
\end{aligned}$$

$$= 0.4736mn - 0.5952n - 0.0944m + 0.468.$$

Theorem 9: Suppose T_m is a fuzzy graph representing a multi-cyclic tetracene with m rows and n hydrocarbon columns. Then the Randic index of multi-cyclic tetracene is

$$\mathfrak{R}_f(T_m) = 92.5215mn - 32.5506n - 4.5704m + 10.8411.$$

Proof: By using Tables 2 and 6, we have

$$\begin{aligned}\mathfrak{R}_f(T_m) &= \frac{1}{2} \sum_{(u_i u_j) \in E(G)} [(\sigma(u_i) d(u_i) \sigma(u_j) d(u_j))^{\frac{-1}{2}}] \\ &= \frac{1}{2} (2) [(0.3)(0.6)(0.4)(0.5)]^{\frac{-1}{2}} \\ &\quad + \frac{1}{2} (6n) [(0.3)(0.6)(0.4)(0.8)]^{\frac{-1}{2}} \\ &\quad + \frac{1}{2} (2n - 2) [(0.3)(0.6)(0.4)(0.6)]^{\frac{-1}{2}} \\ &\quad + \frac{1}{2} (2m - 2) [(0.3)(0.8)(0.4)(0.5)]^{\frac{-1}{2}} \\ &\quad + \frac{1}{2} (8n - 2)(m - 1) [(0.3)(0.8)(0.4)(0.8)]^{\frac{-1}{2}} \\ &\quad + \frac{1}{2} (m - 1)(2n - 2) [(0.3)(0.8)(0.4)(0.6)]^{\frac{-1}{2}} \\ &\quad + \frac{1}{2} (2m) [(0.4)(0.5)(0.2)(0.3)]^{\frac{-1}{2}} \\ &\quad + \frac{1}{2} 3mn [(0.4)(0.8)(0.2)(0.4)]^{\frac{-1}{2}} \\ &\quad + \frac{1}{2} 2m(n - 1) [(0.4)(0.6)(0.2)(0.4)]^{\frac{-1}{2}} \\ &\quad + \frac{1}{2} (2m - 2) [(0.2)(0.3)(0.3)(0.4)]^{\frac{-1}{2}} \\ &\quad + \frac{1}{2} (m - 1)(8n - 2) [(0.2)(0.4)(0.3)(0.4)]^{\frac{-1}{2}} \\ &\quad + \frac{1}{2} (2) [(0.2)(0.3)(0.3)(0.2)]^{\frac{-1}{2}} \\ &\quad + \frac{1}{2} (8n - 2) [(0.2)(0.4)(0.3)(0.2)]^{\frac{-1}{2}} \\ &\quad + \frac{1}{2} m(n - 1) [(0.4)(0.6)(0.4)(0.6)]^{\frac{-1}{2}} \\ &\quad + \frac{1}{2} m(n - 1) [(0.2)(0.4)(0.2)(0.4)]^{\frac{-1}{2}} \\ &\quad + \frac{1}{2} 4n(m - 1) [(0.3)(0.4)(0.3)(0.8)]^{\frac{-1}{2}} \\ &= 92.5215mn - 32.5506n - 4.5704m + 10.8411.\end{aligned}$$

The Y -index surface for multi-cyclic tetracene is drawn in Figure 6.

Theorem 10: Let T_m be fuzzy graph of multi-cyclic tetracene with m rows and n columns. Then the Harmonic index of multi-cyclic tetracene is

$$H_f(T_m) = 38.487mn - 19.0645n - 2.7056m + 7.844.$$

Proof: By using Tables 2 and 6, we have

$$\begin{aligned} H_f(T_m) &= \frac{1}{2} \sum_{(u_i u_j) \in E(G)} [\sigma(u_i)d(u_i) + \sigma(u_j)d(u_j)]^{-1} \\ &= \frac{1}{2} \left[\frac{2}{(0.3)(0.6) + (0.4)(0.5)} \right] + \frac{1}{2} \left[\frac{(6n)}{(0.3)(0.6) + (0.4)(0.8)} \right] \\ &\quad + \frac{1}{2} \left[\frac{2n-2}{(0.3)(0.6) + (0.4)(0.6)} \right] + \frac{1}{2} \left[\frac{2m-2}{(0.3)(0.8) + (0.4)(0.5)} \right] \\ &\quad + \frac{1}{2} \left[\frac{(6n)(m-1)}{(0.3)(0.8) + (0.4)(0.8)} \right] + \frac{1}{2} \left[\frac{(m-1)(2n-2)}{(0.3)(0.8) + (0.4)(0.6)} \right] \\ &\quad + \frac{1}{2} \left[\frac{2m}{(0.4)(0.5) + (0.2)(0.3)} \right] + \frac{1}{2} \left[\frac{3mn}{(0.4)(0.8) + (0.2)(0.4)} \right] \\ &\quad + \frac{1}{2} \left[\frac{m(2n-2)}{(0.4)(0.6) + (0.2)(0.4)} \right] + \frac{1}{2} \left[\frac{2m-2}{(0.2)(0.3) + (0.3)(0.4)} \right] \\ &\quad + \frac{1}{2} \left[\frac{(m-1)(8n-2)}{(0.2)(0.4) + (0.3)(0.4)} \right] + \frac{1}{2} \left[\frac{2}{(0.2)(0.3) + (0.3)(0.2)} \right] \\ &\quad + \frac{1}{2} \left[\frac{(8n-2)}{(0.2)(0.4) + (0.3)(0.2)} \right] + \frac{1}{2} \left[\frac{m(n-1)}{(0.4)(0.6) + (0.4)(0.6)} \right] \\ &\quad + \frac{1}{2} \left[\frac{m(n-1)}{(0.2)(0.4) + (0.2)(0.4)} \right] + \frac{1}{2} \left[\frac{4n(m-1)}{(0.3)(0.4) + (0.3)(0.8)} \right] \\ &= 38.487mn - 19.0645n - 2.7056m + 7.844. \end{aligned}$$

Theorem 11: Suppose T_m is a multi-cyclic tetracene fuzzy graph with m rows and n columns. Then the Y - index of T_m is

$$Y_\mu(T_m) = 2.176mn - 0.48n - 0.116m.$$

Proof: By using Tables 2 and Definition 5, we have

$$\begin{aligned} Y_\mu(T_m) &= \sum_{(u_i u_j) \in E(G)} \mu(u_i, u_j) [\sigma(u_i)d(u_i)^3 + \sigma(u_j)d(u_j)^3] \\ &= 2(0.3)[(0.3)(0.6)^3 + (0.4)(0.5)^3] \\ &\quad + (8n - 2n)(0.3)[(0.3)(0.6)^3 + (0.4)(0.8)^3] \\ &\quad + (2n - 2)(0.3)[(0.3)(0.6)^3 + (0.4)(0.6)^3] \\ &\quad + (2m - 2)(0.3)[(0.3)(0.8)^3 + (0.4)(0.5)^3] \\ &\quad + (8n - 2n)(m - 1)(0.3)[(0.3)(0.8)^3 + (0.4)(0.8)^3] \\ &\quad + (m - 1)(2n - 2)(0.3)[(0.3)(0.8)^3 + (0.4)(0.6)^3] \\ &\quad + (2m)(0.2)[(0.4)(0.5)^3 + (0.2)(0.3)^3] \\ &\quad + 3mn(0.2)[(0.4)(0.8)^3 + (0.2)(0.4)^3] \\ &\quad + (0.2)(2m)(n - 1)[(0.4)(0.6)^3 + (0.2)(0.4)^3] \\ &\quad + (2m - 2)(0.1)[(0.2)(0.3)^3 + (0.3)(0.4)^3] \\ &\quad + (0.1)(m - 1)(8n - 2)[(0.2)(0.4)^3 + (0.3)(0.4)^3] \end{aligned}$$

$$\begin{aligned}
& +2(0.1)[(0.2)(0.3)^3 + (0.3)(0.2)^3] \\
& + (0.1)(8n - 2)[(0.2)(0.4)^3 + (0.3)(0.2)^3] \\
& + (0.1)m(n - 1)[(0.4)(0.6)^3(0.4)(0.6)^3] \\
& + (0.1)m(n - 1)[(0.2)(0.4)^3 + (0.2)(0.4)^3] \\
& + (0.2)4n(m - 1)[(0.3)(0.4)^3 + (0.3)(0.8)^3] \\
& = 2.176mn - 0.48n - 0.116m
\end{aligned}$$

The Y –index surface for multi-cyclic tetracene is drawn in Figure 6.

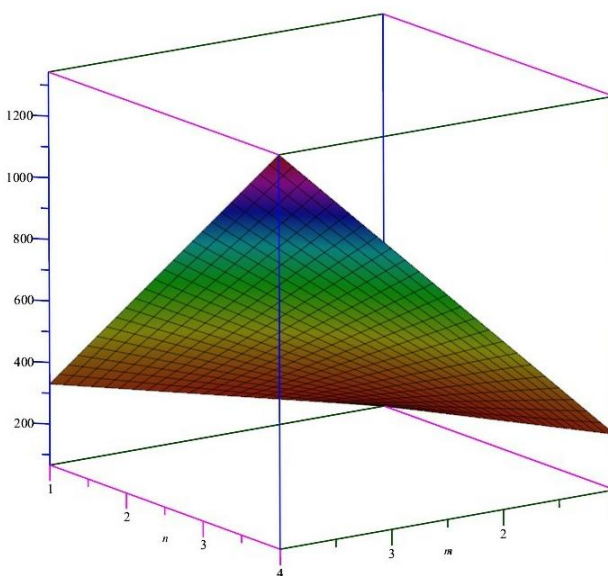


Figure 6
Plot of the Y –index for multi-cyclic tetracene

5. Conclusion

In this study, we investigated various topological indices in fuzzy graphs, including topological indices of the first and second Zagreb, Randic, Harmonic, Forgotten, and Y -index, on linear and multicyclic aromatic hydrocarbons. We provided new definitions for the first Zagreb index and the Forgotten index and Y –index. We compared the topological indices of linear tetracene in Figure 4, and found that the Harmonic and Randic indices had the highest values. We also plotted the surface of the Y – index of multi-cyclic tetracene to determine the effect of row and column parameters on the index. In Figure 6, we concluded that when the number of parameters is equal, the Y –index has the highest value. Our research will aid scientists in predicting or estimating the physicochemical properties of molecules by determining their actual bond length and atomic mass.

Declarations

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- **Authors' contributions**

The contributions of all authors were equal.

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