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Investigating Fuzzy Topological indices of Linear and Cyclic Anthracene Hydrocarbon

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A B S T R A C T

This research focuses on the theoretical examination of the fuzzy graph of aromatic hydrocarbon of Anthracene and computes several fuzzy-based degree topological indices. 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 Anthracene hydrocarbon by considering the degree of each edge. Moreover, a general formula is presented to determine the specific topology index of a hydrocarbon-based on the number of rows and columns. We compared the topological indices of linear Anthracene and found that the Randic and harmonic indices had the highest values. Continuing with the drawing of the Randic index surface, we concluded that when the number of parameters in the rows and columns of the Anthracene hydrocarbon is equal, the Randic index has the highest value. This approach can help researchers predict and estimate compounds' physical and chemical properties using topology indices and precise bond lengths and atomic mass calculations through software.

1. Introduction

1.1 Background

Carbon nanotubes are a fascinating area of research with unique properties and potential uses in various fields such as medicine, sensing devices, and nanotechnology. They are cylindrical nanostructures and belong to the family of carbon allotropes. In 1991, S. Iijima discovered carbon nanotubes which are long and thin carbon cylinders at the molecular scale. These macromolecules have unique shapes, sizes, and physical properties [41]. Carbon nanotubes have exceptional mechanical properties and are known to be one of the most elastic and hardest substances [23, 47]. The structures formed by connecting regular hexagons in the plane are of great interest in the chemistry of benzenoid hydrocarbons. These structures are in perfect agreement with the curled

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structures in the computation of the molecular energies affiliated with certain benzenoid hydrocarbon molecules. Acenes, a type of polycyclic aromatic hydrocarbons, are organic compounds composed of fused Benzene rings. They have applications in optoelectronics and are actively researched in chemistry and electrical engineering.

Graph theory is a type of mathematics that plays a significant role in fields such as physics, chemistry, and engineering [10], [13], [50]. It is often impossible to fully implement a system, so vertices and edges in a graph can be defined as fuzzy. Fuzzy graphs have many practical applications in mathematics and are used in areas such as neural networks, artificial intelligence, computer networks, engineering sciences, transportation network design, and electrical circuits. Also, fuzzy graph theory is used to study the structure of communication networks or circuits when there is ambiguity in their design [29]. The concept of membership in a set is based on the binary evaluation of connection or non-connection. However, in fuzzy sets, elements have membership degrees in the interval [0,1]. Membership values of vertices and edges are not certain in fuzzy graph theory, which differs from a crisp approach.

Rosenfeld first introduced the theory of fuzzy graphs, and L. A. Zadeh introduced fuzzy sets in graph theory in 1965 [55]. In 1997, J. Xu mentioned the first usage of fuzzy graphs in chemistry [54]. Bhattacharya introduced the idea of using fuzzy graphs to create fuzzy groups [6]. Bhutani discussed automorphisms in fuzzy graphs [7], while Ghani and Lata described the concept of irregularity in such graphs [38]. Ghani and Ahmed also investigated the size and degree of fuzzy graphs [11].

Chemical graph theory is a branch of chemical mathematical topology that combines chemistry and graph theory to represent chemical structures as mathematical models. This theory uses mathematical theorems and chemical methods to solve chemistry problems. In molecular graphs, atoms and bonds are represented as vertices and edges. Graph theory is used in chemistry to count isomers and generate molecular structures. Alexander Balaban, Ante Gravac, Ivan Gutman, Haro Hosoya, Milan Randic, and Nenad Trinasty C are some of the pioneers of chemical graph theory [12, 39, 44].

In the graphical representation of Anthracene, hexagons and squares are connected in a way that each square is between four hexagons. In the Anthracene nanotube, the first row consists of a sequence of C_6, C_6, C_6, C_4, C_6, C_6, C_6, C_4, ..., while the second row consists of a sequence of C_6, C_6, C_8, C_6, C_6, C_8, ..., (Xavier et al., [53]).

Topological indices are used to create crisp graphs and have numerous real-life applications. In theoretical chemistry, they are used to estimate and predict the physical and chemical properties of compounds without the need for expensive laboratory experiments. These indices are used in various fields such as mathematics, biology, and bioinformatics, but their primary use is in quantitative structure–property relationship QSPR [22, 40]. The Randic index is an effective index used in QSPR that relies on the structural properties of atoms [31]. The first and second Zagreb indices help measure the total p-electron energy of molecules [15], while the SDD index determines the total surface area of polychlorobiphenyls [14]). The augmented Zagreb index provides the best approximation of the heat of the foundation of alkanes [9]. The Harmonic index is another type of Randic index introduced by Fajtlowicz.

1.2 Previous works

In 1947, Wiener introduced the Wiener index for crisp graphs [52]. The Wiener index is used to check the properties of alkanes. In 1972, Gutman and Trinajstic introduced the Zagreb index for crisp graphs [15]. In the same year, the Forgotten index was introduced by Gutman et al and later reinvestigated by Gutman and Furtula [14]. In 1975, Rosenfeld introduced the fuzzy graph [46]. In 2015, Fortula and Gutman introduced the F-index for crisp graphs [10]). In 2016, Rashmanlou et al. studied vague graphs [46]. In 2017, Abdo et al. found maximal trees with respect to the F-index for a crisp graph [1]. In the same year, Akhtar et al. found a maximal unicyclic graph with respect to the F-index for a crisp graph [2]. In 2018, Amin et al. studied the F-index and F-coindex of line graphs of subdivision graphs [4]. In 2019, Binu et al. introduced the connectivity index for fuzzy graphs [8]. In the same year, Mondal et al. introduced some neighborhood degree-based topological indices for crisp graphs [33, 34]. In 2020, Shao et al. studied fuzzy graph concepts for medical diagnostics [48]. Maji and Ghorai studied F-index for kth generalized transformation graphs (crisp) [32]. Poulik et al. introduced the Wiener absolute index and the Randic index for bipolar fuzzy graphs in 2021 and 2022 [42, 43]. Mondal et al. studied the neighborhood Zagreb index for product graphs [35], while Islam and Pal analyzed the first Zagreb index [25], F-index [24], hyper-Wiener index [26], and hyper-connectivity index in the context of fuzzy graphs [27]. In 2022, Shi et al. investigated the primary energies of the image phase diagram and its applications [49]. In 2023, Zeeshan Saleem Mufti et al. studied the fuzzy topological features of the qCn graph using fuzzy topological indices [36]. In 2024, Kosari et al. investigated topological indicators in fuzzy graphs, applying them to decision-making problems [30]. In 2024, Mohammad Azim et al. researched the topological numbers of fuzzy soft graphs and explored their [5]. In 2024, Asad Ullah et al. examined the computational aspects of two significant biochemical networks using novel molecular descriptors [51]. In 2023, Hasani and Ghods investigated M-polynomials and topological indices of porphyrin-cored dendrimers in crisp graphs [20]. In 2023, they analyzed the quantitative structure-property relationship (QSPR) of certain drugs used to treat heart diseases [18]. Additionally, during the same year, they utilized topological indices and MATLAB programming to make predictions about the physicochemical characteristics of drugs used for Parkinson's disease [17]. In 2024, they analyzed the quantitative structure-property relationship (QSPR) of certain drugs used to treat heart calcium channel-blocking cardiac drug disease [19]. In 2024, they conducted QSPR analysis of pyelonephritis drugs using entropy graphs weighted by topological indices and MATLAB programming [16].

1.3 Motivation

Topological indices, numerical quantities affiliated with a graph, can predict the features of chemical compounds without performing experiments. Previous studies have investigated topological indices on various compounds, including nanotube Naphthalene, fuzzy graphs, and linear and multi-acyclic hydrocarbons. In 2015, S. Hayat and M. Imran calculated topology indices based on the degree of nanotube Naphthalene [21]. In 2020, S. Kalatgian et al. investigated some topological indices in fuzzy graphs [29]. In 2022, Z. S. Mofti et al. studied the first and second fuzzy Zagreb topological indices on linear hydrocarbon and multi-acyclic Benzene [37]. This research aims to investigate topological indices on Anthracene hydrocarbon and 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 Anthracene hydrocarbon is also developed based on the number of rows and columns. Our method can help researchers predict and estimate the physical and chemical properties of chemical compounds using software and precise calculations of bond lengths and atomic mass with the help of topological indices.

1.4 Organazation of the paper

The the reminder of the paper is organazied 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 aromatic hydrocarbons theoretically rather than experimentally and obtain a general formula for their extension. Section 4, presents fuzzy topology indices of cyclic aromatic hydrocarbons and their general formula for the extension. Finally, Section 5, discusses the conclusion and application of the studied indices.

2. Preliminaries

Definition 1. Suppose X is a finite set. The graph fuzzy G with vertices set $V(G)$ and edges set $E\ G = \ u,v \ \mid \mu\ u,v \ > 0$, 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

$$\sigma : \mathrm{V} \to [0,1]$$

$$\mu : V \times V \to [0,1] \forall u,v \in V(G)$$

satisfying

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

where $\wedge$ represents the minimum.

Definition 2. Suppose $u \in V$, and $N(u)$ denotes the set of neighbors of u, then the degree of u in a fuzzy graph is defined by

$$d_G(u) = \sum_{v \in N(u)} \mu(u,v)$$

Also, Order of G in a fuzzy graph is defined by

$$Order(G) = \sum_{u_i \in V(G)} \sigma(u_i)$$

and Size of G in a fuzzy graph is denoted by

$$Size(\mathrm{G}) = \sum_{(u,v) \in E(G)} \mu(u,v)$$

Definition 3. [15] Suppose G is a crisp graph. Then the first Zagreb index is shown by $Z_1(G)$ and defined as follows:

$$Z_1(\mathrm{G}) = \sum_{u_i \in V(G)} [d(u_i)]^2 = \sum_{(u_i,u_j) \in E(G)} [d(u_i) + d(u_j)]$$

Definition 4. [15] Suppose G is a crisp graph. Then the second Zagreb index is shown by $Z_2(G)$ and defined as follows:

$$Z_2(\mathrm{G}) = \sum_{(u_i,u_j) \in E(G)} d(u_i) d(u_j)$$

Definition 5. [10] Suppose G is a crisp graph. Then the forgotten index is denoted by $F(G)$ and defined as follows:

$$F(\mathrm{G}) = \sum_{u_i \in V(G)} [d(u_i)]^3 = \sum_{(u_i,u_j) \in E(G)} [d(u_i)^2 + d(u_j)^2]$$

Definition 6. [3] Let G be a crisp graph. Then the Y -index is denoted by $Y(G)$ and defined as follows:

$$Y(G)=\sum_{u_i\in V(G)}[d(u_i)]^4=\sum_{(u_i,u_j)\in E(G)}[d(u_i)^3+d(u_j)^3]$$

Definition 7. [29] Assume G is the fuzzy graph. Then the first Zagreb index for fuzzy graphs is denoted by $Z_1^*(G)$ and is defined as follows:

$$Z_1^*(\mathrm{G})=\sum_{u_i\in V(G)}\sigma(u_i)[d(u_i)]^2$$

We define the first Zagreb index for fuzzy graphs as follows:

Definition 8. Assume G is the fuzzy graph. Then the first Zagreb index for fuzzy graphs is indicated b $Z_\mu(G)$ and is defined by:

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

It is simply proved that Definitions 7 and 8 are equal.

Definition 9. [29] Assume G is the fuzzy graph. Then the second Zagreb index is shown by $Z_2^*(G)$ and is defined as follows:

$$Z_2^*(\mathrm{G})=\frac{1}{2}\sum_{(u_i,u_j)\in E(G)}\sigma(u_i)d(u_i)\sigma(u_j)d(u_j),\ \forall i\neq j \qquad \forall i\neq j$$

We have provided another definition of the F -index in fuzzy graphs as follows:

Definition 10. Assume G is the fuzzy graph. Then the F -index for fuzzy graphs is shown $F^*(G)$ and is introduced as follows:

$$F^*(\mathrm{G})=\sum_{u_i\in V(G)}\sigma(u_i)[d(u_i)]^3$$

Definition 11. Assume G is the fuzzy graph. Then the F -index for fuzzy graphs is indicated by $F_\mu(G)$ and is defined by:

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

It is easy to prove that Definitions 10 and 11 are equivalent. We have provided another definition of the Y -index in fuzzy graphs.

Definition 12. [28] Suppose G is a fuzzy graph. Then the Y -index is denoted by $Y^*(G)$ and is introduced by:

$$Y^*(\mathrm{G})=\sum_{u_i\in V(G)}\sigma(u_i)[d(u_i)]^4$$

Definition 13. Assume G is the fuzzy graph. Then the Y -index for fuzzy graphs is indicated by $Y_{\mu}(G)$ and is defined as follows:

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

It is simple to show that definitions 12 and 13 are equivalent.

Definition 14. [29] Suppose G is a fuzzy graph. The Randic index is shown by $R^*(G)$ and is defined as follows:

$$R^*(\mathrm{G}) = \frac{1}{2} \sum_{(u_i,u_j)\in E(G)} [\sigma(u_i)d(u_i)\sigma(u_j)d(u_j)]^{\frac{-1}{2}}$$

Definition 15. [29] Let G be a fuzzy graph. The Harmonic index is shown by $H^*(G)$ and is defined by:

$$H^*(\mathrm{G}) = \frac{1}{2} \sum_{(u_i,u_j)\in E(G)} [\sigma(u_i)d(u_i) + \sigma(u_j)d(u_j)]^{-1}$$

3. Topological indices of fuzzy graphs of linear Anthracene

In this section, some topological indices of linear Anthracene in fuzzy graphs are examined, and a general formula based on the number of rows and columns is presented for its extension. Table 1, introduces the abbreviations of some topological indices of fuzzy graphs. According to Figures 1, 2, and 3, and based on the structure of linear Anthracene, the total number of vertices is 14n and the total number of edges is 18n − 2, respectively. The set of all vertices and edges is divided into weight categories, as shown in Tables 2 and 3. Using Table 2, the vertex set with weight 0.2 has a total number of 4n, the vertex set with weight 0.3 has a total number of 6n, and the vertex set with weight 0.4 has a total number of 4n.

3.1 Abbreviations

Table 1. The topological indices for fuzzy graphs

Index	Abbreviations
The first zagreb index	$Z_1^*(G), Z_{\mu}(G)$
The second Zagreb index	$Z_2^*(G)$
The Forgotten index	$F^*(G), F_{\mu}(G)$
The Y- index	$Y^*(G), \mathrm{Y}_{\mu}(G)$
The Harmonic index	$H^*(G)$
The Randic index	$R^*(G)$

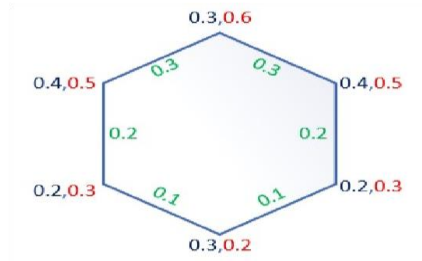


Figure 1: (1,1) unit of fuzzy graph of Benzene

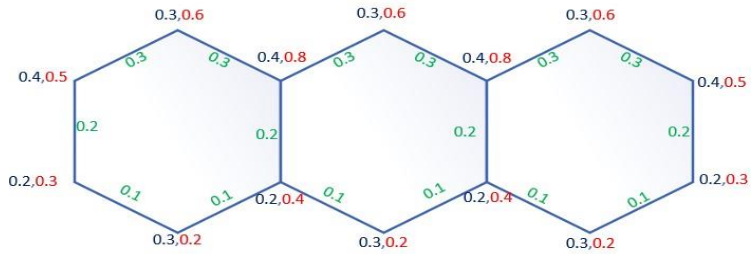


Figure 2: (1,1) unit of the fuzzy graph of linear Anthracene

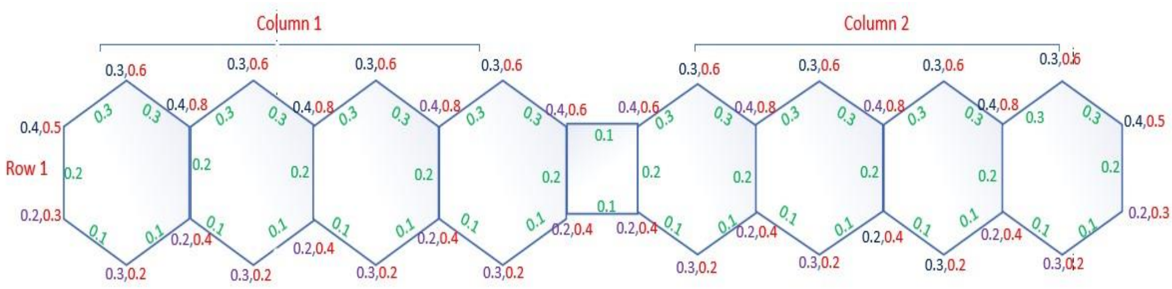


Figure 3: (1,2) unit of the fuzzy graph of linear Anthracene hydrocarbon

Table 2. Partition of vertices for fuzzy graphs of linear Anthracene

Weight	Degree	The total number of vertices
0.2	0.3 0.4	2 4n-2
0.3	0.2 0.6	3n 3n
0.4	0.5 0.6 0.8	2 2n-2 2n

Table 3. Partition of edges for fuzzy graphs of linear hydrocarbons

Weight	Degree	The total number of edges

(0.3, 0.4)	(0.6, 0.5) (0.6, 0.8) (0.6, 0.6)	2 4n 2n-2
(0.3, 0.2)	(0.2, 0.3) (0.2, 0.4)	2 6n-2
(0.2, 0.4)	(0.3, 0.5) (0.4, 0.8) (0.4, 0.6)	2 2n 2n-2
(04, 0.4)	(0.6, 0.6)	n-1
(0.2, 0.2)	(0.4, 0.4)	n-1

Theorem 1: Suppose A_l is a linear Anthracene fuzzy graph. Then the first Zagreb index of A_l is

$$Z_\mu(A_l) = 1.288n - 0.116$$

Proof: According to Figure 3, and using Table 3 and Definition 8, we have

$$Z_\mu(\mathrm{A}_l) = \sum_{(u_i,u_j)\in E(A_l)} \mu(u_i, u_j)[\sigma(u_i)d(u_i) + \sigma(u_j)d(u_j)]$$
$$= 2(0.3)[(0.3)(0.6) + (0.4)(0.5)] + (4\mathrm{n})(0.3)[(0.3)(0.6) + (0.4)(0.8)]$$
$$+(2\mathrm{n} - 2)(0.3)[(0.3)(0.6) + (0.4)(0.6)] + 2(0.1)[(0.3)(0.2) + (0.2)(0.3)]$$
$$+(6\mathrm{n} - 2)(0.1)[(0.3)(0.2) + (0.2)(0.4)] + 2(0.2)[(0.2)(0.3) + (0.4)(0.5)]$$
$$+(2\mathrm{n})(0.2)[(0.2)(0.4) + (0.4)(0.8)] + (2\mathrm{n} - 2)(0.2)[(0.2)(0.4) + (0.4)(0.6)]$$
$$+(\mathrm{n} - 1)(0.1)[(0.4)(0.6) + (0.4)(0.6)] + (\mathrm{n} - 1)(0.1)[(0.2)(0.4) + (0.2)(0.4)]$$
$$= 1.288\mathrm{n} - 0.116$$

Theorem 2: Let A_l be a fuzzy graph of linear Anthracene. Then the second fuzzy Zagreb index of A_l is

$$Z_2^*(A_l) = 0.24964n - 0.0476$$

Proof: Using Table 3 and Definition 9, we have

$$Z_2^*(A_l) = \frac{1}{2}\sum_{(u_i,u_j)\in E(A_l)} \sigma(u_i)d(u_i)\sigma(u_j)d(u_j)$$
$$= \frac{1}{2}[2(0.3)(0.6)(0.4)(0.5) + (4\mathrm{n})(0.3)(0.6)(0.4)(0.8) + (2\mathrm{n} - 2)(0.3)(0.6)(0.4)(0.6)]$$

$$+\frac{1}{2}[2(0.3)(0.2)(0.2)(0.3) + (6\text{n} - 2)(0.3)(0.2)(0.2)(0.4)]$$
$$+\frac{1}{2}[2(0.2)(0.3)(0.4)(0.5) + (2\text{n})(0.2)(0.4)(0.4)(0.8) + (2\text{n} - 2)(0.2)(0.4)(0.4)(0.6)]$$
$$+\frac{1}{2}[(\text{n} - 1)(0.4)(0.6)(0.4)(0.6) + (\text{n} - 1)(0.2)(0.4)(0.2)(0.4)]$$
$$= 0.24964n - 0.0476$$

Theorem 3: Suppose A_l is a linear Anthracene fuzzy graph. Then the Forgotten index of A_l is

$$F_\mu(A_l) = 0.8352n - 0.0876$$

Proof: Using Table 3 and Definition 11, we have

$$F_\mu(A_l) = \sum_{(u_i,u_j)\in E(A_l)} \mu(u_i, u_j)[\sigma(u_i)d(u_i)^2 + \sigma(u_j)d(u_j)^2]$$
$$= 2(0.3)[(0.3)(0.6)^2+(0.4)(0.5)^2]+(4\text{n})(0.3)[(0.3)(0.6)^2+ (0.4)(0.8)^2]$$
$$+(2\text{n} - 2)(0.3)[(0.3)(0.6)^2+(0.4)(0.6)^2]+2(0.1)[(0.3)(0.2)^2+(0.2)(0.3)^2]$$
$$+(6\text{n} - 2)(0.1)[(0.3)(0.2)^2+(0.2)(0.4)^2]+2(0.2)[(0.2)(0.3)^2+(0.4)(0.5)^2]$$
$$+(2\text{n})(0.2)[(0.2)(0.4)^2+(0.4)(0.8)^2]+(2\text{n} - 2)(0.2)[(0.2)(0.4)^2+(0.4)(0.6)^2]$$
$$+(\text{n}-1)(0.1)[(0.4)(0.6)^2+(0.4)(0.6)^2]+(\text{n}-1)(0.1)[(0.2)(0.4)^2+(0.2)(0.4)^2]$$
$$= 0.8352\text{n} - 0.0876$$

Theorem 4: Let A_l be a linear Anthracene fuzzy graph. Then the Y-index of A_l is

$$Y_\mu(A_l) = 0.5696n - 0.0606$$

Proof: Using Table 3 and Definition 13, we have

$$Y_\mu(A_l) = \sum_{(u_i,u_j)\in E(A_l)} \mu(u_i, u_j)[\sigma(u_i)d(u_i)^3 + \sigma(u_j)d(u_j)^3]$$
$$=2(0.3)[(0.3)(0.6)^3+(0.4)(0.5)^3]+(4\text{n})(0.3)[(0.3)(0.6)^3+(0.4)(0.8)^3]$$
$$+(2\text{n} - 2)(0.3)[(0.3)(0.6)^3+(0.4)(0.6)^3]+2(0.1)[(0.3)(0.2)^3+(0.2)(0.3)^3]$$
$$+(6\text{n} - 2)(0.1)[(0.3)(0.2)^3+(0.2)(0.4)^3]+ 2(0.2)[(0.2)(0.3)^3+(0.4)(0.5)^3]$$
$$+(2\text{n})(0.2)[(0.2)(0.4)^3+(0.4)(0.8)^3]+(2\text{n} - 2)(0.2)[(0.2)(0.4)^3+(0.4)(0.6)^3]$$
$$+(\text{n}-1)(0.1)[(0.4)(0.6)^3+(0.4)(0.6)^3]+(\text{n}-1)(0.1)[(0.2)(0.4)^3+(0.2)(0.4)^3]$$
$$= 0.5696\text{n} - 0.0606$$

Theorem 5: Suppose A_l is a linear Anthracene fuzzy graph. Then the Randic index of A_l is

$$R^*(A_l) = 78.2456n - 3.7293$$

Proof: Using Table 3 and Definition 14, we have

$$R^*(A_l) = \frac{1}{2}\sum_{(u_i,u_j)\in E(A_l)} [\sigma(u_i)d(u_i)\sigma(u_j)d(u_j)]^{\frac{-1}{2}}$$
$$= \frac{1}{2}(2)[(0.3)(0.6)(0.4)(0.5)]^{\frac{-1}{2}} + \frac{1}{2}(4\text{n})[(0.3)(0.6)(0.4)(0.8)]^{\frac{-1}{2}}$$
$$+\frac{1}{2}(2\text{n - }2)[(0.3)(0.6)(0.4)(0.6)]^{\frac{-1}{2}} + \frac{1}{2}(2)[(0.3)(0.2)(0.2)(0.3)]^{\frac{-1}{2}}$$
$$+\frac{1}{2}(6\text{n - }2)[(0.3)(0.2)(0.2)(0.4)]^{\frac{-1}{2}} + \frac{1}{2}(2)[(0.2)(0.3)(0.4)(0.5)]^{\frac{-1}{2}}$$
$$+\frac{1}{2}(2\text{n})[(0.2)(0.4)(0.4)(0.8)]^{\frac{-1}{2}} + \frac{1}{2}(2\text{n - }2)[(0.2)(0.4)(0.4)(0.6)]^{\frac{-1}{2}}$$
$$+\frac{1}{2}(\text{n - }1)[(0.4)(0.6)(0.4)(0.6)]^{\frac{-1}{2}} + \frac{1}{2}(\text{n - }1)[(0.2)(0.4)(0.2)(0.4)]^{\frac{-1}{2}}$$
$$= 78.2456\text{n - }3.7293$$

Theorem 6: Let A_l be a linear hydrocarbon fuzzy graph. Then the Harmonic index of A_l is

$$H^*(A_l) = 37.6009n - 4.6359$$

Proof: Using Table 3 and Definition 15, we have

$$H^*(A_l) = \frac{1}{2}\sum_{(u_i,u_j)\in E(A_l)} [\sigma(u_i)d(u_i) + \sigma(u_j)d(u_j)]^{-1}$$
$$= \frac{1}{2}[\frac{2}{(0.3)(0.6) + (0.4)(0.5)}] + \frac{1}{2}[\frac{4\text{n}}{(0.3)(0.6) + (0.4)(0.8)}]$$
$$+\frac{1}{2}[\frac{2\text{n - }2}{(0.3)(0.6) + (0.4)(0.6)}] + \frac{1}{2}[\frac{2}{(0.3)(0.2) + (0.2)(0.3)}]$$
$$+\frac{1}{2}[\frac{6\text{n - }2}{(0.3)(0.2) + (0.2)(0.4)}] + \frac{1}{2}[\frac{2}{(0.2)(0.3) + (0.4)(0.5)}]$$
$$+\frac{1}{2}[\frac{2\text{n}}{(0.2)(0.4) + (0.4)(0.8)}] + \frac{1}{2}[\frac{2\text{n - }2}{(0.2)(0.4) + (0.4)(0.6)}]$$
$$+\frac{1}{2}[\frac{\text{n - }1}{(0.4)(0.6) + (0.4)(0.6)}] + \frac{1}{2}[\frac{\text{n - }1}{(0.2)(0.4) + (0.2)(0.4)}]$$
$$=37.6009\text{n - }4.6359$$

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

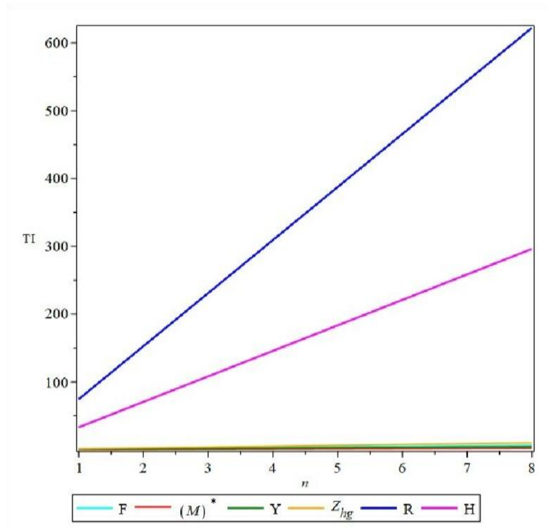


Figure 4: Comparison of topological indices of linear Anthracene

4. Topological indices of fuzzy graphs of multi-cyclic Anthracene

In this section, some topological indices of multi-cyclic Anthracene in fuzzy graphs are computed, and a general formula based on the number of rows and columns is presented for it's extension. According to Figures 5 and 6, and based on the structure of multi-cyclic Anthracene, the total number of vertices is 14mn and the total number of edges is 21mn−2m−kn, respectively. The set of all vertices and edges is divided into weight categories, as shown in Tables 4 and 5. Using Table 4, the vertex set with weight 0.2 has a total number of 4mn, the vertex set with weight 0.3 has a total number of 6mn, and the vertex set with weight 0.4 has a total number of 4mn.

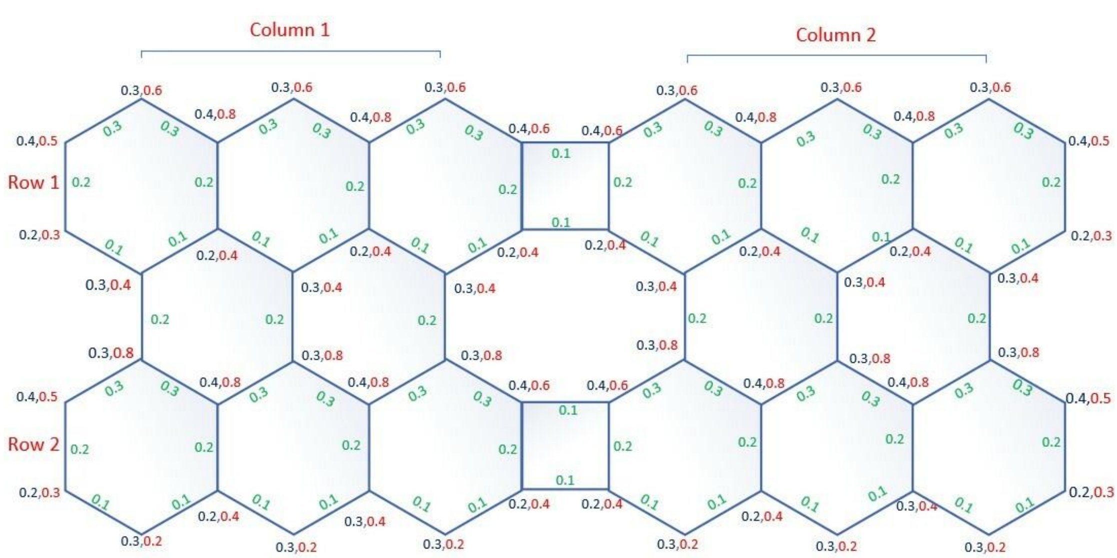


Figure 5: (2,2) unit of the fuzzy graph of multi-cyclic Anthracene

Table 4: Partition of vertices in fuzzy graphs of multi-cyclic Anthracene

Weight	Degree	The total number of vertices
0.2	0.3 0.4	2m m(4n-2)
0.3	0.2 0.4 0.6 0.8	3n 3n(m-1) 3n 3n(m-1)
0.4	0.5 0.6 0.8	2m 2m(n-1) 2mn

Table 5: Partition of edges in fuzzy graphs of multi-cyclic Anthracene

Weight	Degree	The total number of edges
(0.3, 0.4)	(0.6, 0.5) (0.6, 0.8) (0.6, 0.6) (0.8, 0.5) (0.8, 0.8) (0.8, 0.6)	2 4n 2n-2 2m-2 4n(m-1) (m-1)(2n-2)
(0.4, 0.2)	(0.5, 0.3) (0.8, 0.4) (0.6, 0.4)	2m 2mn 2m(n-1)
(0.2, 0.3)	(0.3, 0.4) (0.4, 0.4) (0.3, 0.2) (0.4, 0.2)	2m-2 (m-1)(6n-2) 2 6n-2
(04, 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)	2n(m-1)

Theorem 7: Suppose A_m is a multi-cyclic Anthracene fuzzy graph. Then the first Zagreb index of A_m is

$$Z_\mu(A_m) = 1.648mn - 0.36n - 0.116m$$

Proof: Using Table 5 and Definition 8, we have

$$Z_\mu(\mathrm{A}_m) = \sum_{(u_i,u_j)\in E(\mathrm{A}_m)} \mu(u_i,u_j)[\sigma(u_i)d(u_i)+\sigma(u_j)d(u_j)]$$
$$= 2(0.3)[(0.3)(0.6) + (0.4)(0.5)] + (4n)(0.3)[(0.3)(0.6) + (0.4)(0.8)]$$
$$+(2n - 2)(0.3)[(0.3)(0.6) + (0.4)(0.6)] + (2m - 2)(0.3)[(0.3)(0.8) + (0.4)(0.5)]$$
$$+4n(m - 1)(0.3)[(0.3)(0.8) + (0.4)(0.8)] + (m - 1)(2n - 2)(0.3)[(0.3)(0.8) + (0.4)(0.6)]$$
$$+(2m)(0.2)[(0.4)(0.5) + (0.2)(0.3)] + 2mn(0.2)[(0.4)(0.8) + (0.2)(0.4)]$$
$$+(0.2)(2m)(n-1)[(0.4)(0.6) + (0.2)(0.4)] + (2m-2)(0.1)[(0.2)(0.3) + (0.3)(0.4)]$$
$$+(0.1)(m - 1)(6n - 2)[(0.2)(0.4) + (0.3)(0.4)] + 2(0.1)[(0.2)(0.3) + (0.3)(0.2)]$$
$$+(0.1)(6n - 2)[(0.2)(0.4) + (0.3)(0.2)] + (0.1)m(n - 1)[(0.4)(0.6) + (0.4)(0.6)]$$
$$+(0.1)m(n - 1)[(0.2)(0.4) + (0.2)(0.4)] + (0.2)2n(m - 1)[(0.3)(0.4) + (0.3)(0.8)]$$
$$= 1.648mn - 0.36n - 0.116m$$

Theorem 8: Let A_m be a fuzzy graph of multi-cyclic Anthracene. Then the second fuzzy Zagreb index of multi-cyclic Anthracene is

$$Z_2^*(A_m) = 0.36mn - 0.1104n - 0.0944m + 0.468$$

Proof: Using Table 5 and Definition 9, we have

$$Z_2^*(A_m) = \frac{1}{2}\sum_{(u_i,u_j)\in E(A_m)} \sigma(u_i)d(u_i)\sigma(u_j)d(u_j)$$
$$= \frac{1}{2}[2(0.3)(0.6)(0.4)(0.5) + (4n)(0.3)(0.6)(0.4)(0.8) + (2n - 2)(0.3)(0.6)(0.4)(0.6)$$
$$+(2m - 2)(0.3)(0.8)(0.4)(0.5) + 4n(m - 1)(0.3)(0.8)(0.4)(0.8)$$
$$+(m - 1)(2n - 2)(0.3)(0.8)(0.4)(0.6) + (2m)(0.4)(0.5)(0.2)(0.3)$$
$$+2mn(0.4)(0.8)(0.2)(0.4) + 2m(n - 1)(0.4)(0.6)(0.2)(0.4)$$
$$+(2m - 2)(0.2)(0.3)(0.3)(0.4) + (m - 1)(6n - 2)(0.2)(0.4)(0.3)(0.4)$$
$$+2(0.2)(0.3)(0.3)(0.2) + (6n - 2)(0.2)(0.4)(0.3)(0.2) + m(n - 1)(0.4)(0.6)(0.4)(0.6)$$
$$+m(n - 1)(0.2)(0.4)(0.2)(0.4) + 2n(m - 1)(0.3)(0.4)(0.3)(0.8)]$$
$$= 0.36mn - 0.1104n - 0.0944m + 0.468$$

Theorem 9: Suppose A_m is a fuzzy graph of multi-cyclic Anthracene. Then the Randic index of multi-cyclic Anthracene is

$$R^*(A_m) = 72.6357mn - 24.3901n - 4.5704m + 10.8411$$

Proof: Using Table 5 and Definition 14, we have

$$R^*(A_m) = \frac{1}{2}\sum_{(u_i,u_j)\in E(A_m)} [\sigma(u_i)d(u_i)\sigma(u_j)d(u_j)]^{\frac{-1}{2}}$$
$$= \frac{1}{2}(2)[(0.3)(0.6)(0.4)(0.5)]^{\frac{-1}{2}} + \frac{1}{2}(4\text{n})[(0.3)(0.6)(0.4)(0.8)]^{\frac{-1}{2}}$$
$$+\frac{1}{2}2\ (2\text{n - }2)[(0.3)(0.6)(0.4)(0.6)]^{\frac{-1}{2}} + \frac{1}{2}(2\text{m - }2)[(0.3)(0.8)(0.4)(0.5)]^{\frac{-1}{2}}$$
$$+\frac{1}{2}(6\text{n - }2)(\text{m - }1)[(0.3)(0.8)(0.4)(0.8)]^{\frac{-1}{2}} + \frac{1}{2}(\text{m - }1)(2\text{n - }2)[(0.3)(0.8)(0.4)(0.6)]^{\frac{-1}{2}}$$
$$+\frac{1}{2}(2\text{m})[(0.4)(0.5)(0.2)(0.3)]^{\frac{-1}{2}} + \frac{1}{2}2\text{mn}[(0.4)(0.8)(0.2)(0.4)]^{\frac{-1}{2}}$$
$$+\frac{1}{2}2\text{m}(\text{n - }1)[(0.4)(0.6)(0.2)(0.4)]^{\frac{-1}{2}} + \frac{1}{2}(2\text{m - }2)[(0.2)(0.3)(0.3)(0.4)]^{\frac{-1}{2}}$$
$$+\frac{1}{2}(\text{m - }1)(6\text{n - }2)[(0.2)(0.4)(0.3)(0.4)]^{\frac{-1}{2}} + \frac{1}{2}(2)[(0.2)(0.3)(0.3)(0.2)]^{\frac{-1}{2}}$$
$$+\frac{1}{2}(6\text{n - }2)[(0.2)(0.4)(0.3)(0.2)]^{\frac{-1}{2}} + \frac{1}{2}\text{m}(\text{n - }1)[(0.4)(0.6)(0.4)(0.6)]^{\frac{-1}{2}}$$
$$+\frac{1}{2}\ \text{m}(\text{n - }1)[(0.2)(0.4)(0.2)(0.4)]^{\frac{-1}{2}} + \frac{1}{2}2\text{n}(\text{m - }1)[(0.3)(0.4)(0.3)(0.8)]^{\frac{-1}{2}}$$
$$= 72.6357\text{mn - }24.3901\text{n - }4.5704\text{m} + 10.8411$$

Theorem 10: Let A_m be a fuzzy graph of multi-cyclic Anthracene. Then the Harmonic index of multi-cyclic Anthracene is

$$H^*(A_m) = 30.4513\text{mn - }14.2788\text{n - }2.7056\text{m} + 7.844$$

Proof: Using Table 5 and Definition 15, we have

$$H^*(A_m) = \frac{1}{2}\sum_{(u_i,u_j)\in E(A_m)} [\sigma(u_i)d(u_i) + \sigma(u_j)d(u_j)]^{-1}$$
$$= \frac{1}{2}[\frac{2}{(0.3)(0.6)+(0.4)(0.5)}] + \frac{1}{2}[\frac{4\text{n}}{(0.3)(0.6)+(0.4)(0.8)}] + \frac{1}{2}[\frac{2\text{n - }2}{(0.3)(0.6)+(0.4)(0.6)}]$$
$$+\frac{1}{2}[\frac{2\text{m - }2}{(0.3)(0.8)+(0.4)(0.5)}] + \frac{1}{2}[\frac{(4\text{n})(\text{m - }1)}{(0.3)(0.8)+(0.4)(0.8)}] + \frac{1}{2}[\frac{(\text{m - }1)(2\text{n - }2)}{(0.3)(08)+(0.4)(0.6)}]$$
$$+\frac{1}{2}[\frac{2\text{m}}{(0.4)(0.5)+(0.2)(0.3)}] + \frac{1}{2}[\frac{2\text{mn}}{(0.4)(0.8)+(0.2)(0.4)}] + \frac{1}{2}[\frac{\text{m}(2\text{n - }2)}{(0.4)(0.6)+(0.2)(0.4)}]$$

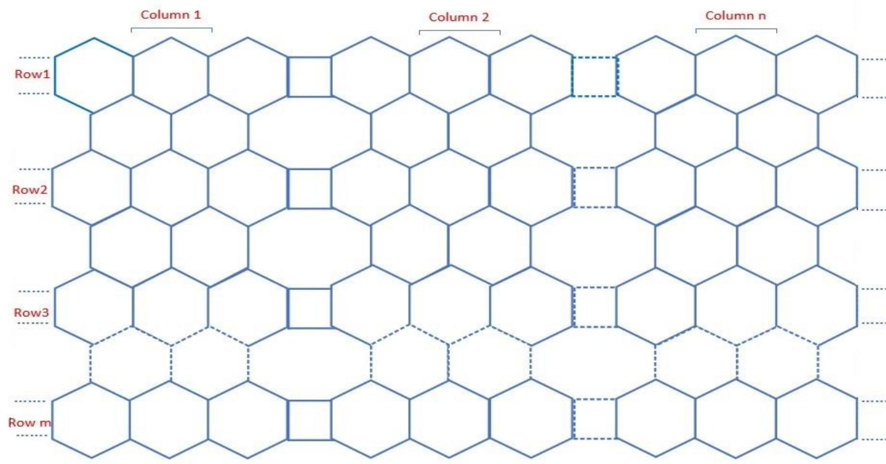
$$+\frac{1}{2}[\frac{2m - 2}{(0.2)(0.3)+(0.3)(0.4)}]+\frac{1}{2}[\frac{(m - 1)(6n - 2)}{(0.2)(0.4)+(0.3)(0.4)}]+\frac{1}{2}[\frac{2}{(0.2)(0.3)+(0.3)(0.2)}]$$
$$+\frac{1}{2}[\frac{(6n - 2)}{(0.2)(0.4)+(0.3)(0.2)}]+\frac{1}{2}[\frac{m(n - 1)}{(0.4)(0.6)+(0.4)(0.6)}]+\frac{1}{2}[\frac{m(n - 1)}{(0.2)(0.4)+(0.2)(0.4)}]$$
$$+\frac{1}{2}[\frac{2n(m - 1)}{(0.3)(0.4)+(0.3)(0.8)}$$
$$= 30.4513mn - 14.2788n - 2.7056m + 7.844$$

Theorem 11: Suppose A_m is a multi-cyclic Anthracene fuzzy graph. Then the Y-index of A_m is

$$Y_\mu(A_m) = 0.3786mn + 0.3674m + 0.1909n + 0.2169$$

Proof: Using Table 5 and Definition 13, we have

$$Y_\mu(A_m) = \sum_{(u_i,u_j)\in E(A_m)} \mu(u_i,u_j)[\sigma(u_i)d(u_i)^3 + \sigma(u_j)d(u_j)^3]$$
$$= 2(0.3)[(0.3)(0.6)^3+(0.4)(0.5)^3]+ (4n)(0.3)[(0.3)(0.6)^3+(0.4)(0.8)^3]$$
$$+(2n - 2)(0.3)[(0.3)(0.6)^3+ (0.4)(0.6)^3]+(2m - 2)(0.3)[(0.3)(0.8)^3+ (0.4)(0.5)^3]$$
$$+(4n)(m - 1)(0.3)[(0.3)(0.8)^3+ (0.4)(0.8)^3]+(m - 1)(2n - 2)(0.3)[(0.3)(0.8)^3+ (0.4)(0.6)^3]$$
$$+(2m)(0.2)[(0.4)(0.5)^3+ (0.2)(0.3)^3]+ 2mn(0.2)[(0.4)(0.8)^3+ (0.2)(0.4)^3]$$
$$+(0.2)(2m)(n - 1)[(0.4)(0.6)^3+ (0.2)(0.4)^3]+(2m - 2)(0.1)[(0.2)(0.3)^3+ (0.3)(0.4)^3]$$
$$+(0.1)(m - 1)(6n - 2)[(0.2)(0.4)^3+ (0.3)(0.4)^3]+2(0.1)[(0.2)(0.3)^3+ (0.3)(0.2)^3]$$
$$+(0.1)(6n - 2)[(0.2)(0.4)^3+ (0.3)(0.2)^3]+(0.1)m(n - 1)[(0.4)(0.6)^3+ (0.4)(0.6)^3]$$
$$+(0.1)m(n - 1)[(0.2)(0.4)^3+ (0.2)(0.4)^3]+(0.2)n(2m - 2)[(0.3)(0.4)^3+ (0.3)(0.8)^3]$$
$$= 0.3786mn + 0.3674m + 0.1909n + 0.2169$$



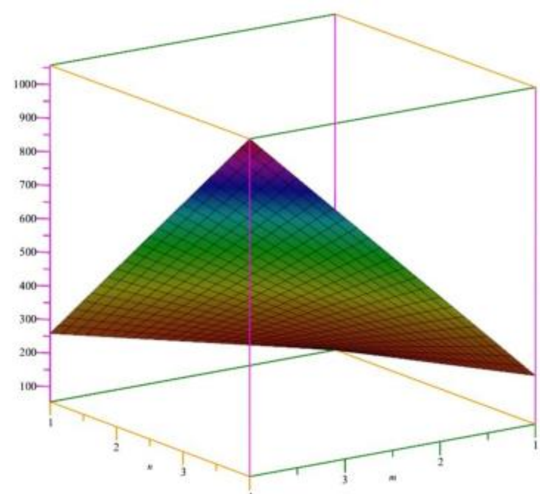


Figure 7: Plot of the Randic index for multi-cyclic Anthracene

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 multi-cyclic Anthracene. We provided new definitions for the first Zagreb index and the Forgotten index and Y −index. We compared the topological indices of linear Anthracene in Figure 4, and found that the Randic and Harmonic indices had the highest values. We also plotted the surface of the Randi´ c index of multi-cyclic Anthracene to determine the effect of row and column parameters on the index. In Figure 7, we concluded that when the number of parameters is equal, the Randic 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. Conducting experimental research to validate this study's results will enhance prediction accuracy. Exploring practical applications in chemistry and materials can lead to new technologies and optimized industrial processes. This research can also serve as a foundation for further exploration in graph topology and its chemistry applications.

Conflict of interest: 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.

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