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Novel Fuzzy Topological Descriptors for Characterizing Aromatic Hydrocarbons

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Abstract

Fuzzy graphs have gained significant attention in diverse scientific fields, including mathematics and chemistry, owing to their superior accuracy and adaptability compared to conventional models. This study delves into a theoretical exploration of the fuzzy graph representation of aromatic hydrocarbons, focusing on the computation of several fuzzy-based degree topological indices. Novel definitions are introduced for the first Zagreb fuzzy index, Forgotten index, and Y-index, alongside a generalized formula for fuzzy topological indices of linear and cyclic aromatic hydrocarbons, incorporating edge degrees. Moreover, a comprehensive formula is derived to calculate specific topological indices of hydrocarbons based on the number of benzene rings. This methodology empowers researchers to predict and estimate compounds' physical and chemical properties by leveraging topological indices and precise calculations of bond lengths and atomic masses facilitated by computational software.

Keywords: Fuzzy graph, Topological indices, Zagreb index, Randic index, Aromatic hydrocarbons
2020 MSC: 05C72, 05C09, 05C31

1 Introduction

Graph theory, a branch of mathematics, has found significant applications in various scientific disciplines, including physics, chemistry, and engineering [5, 13, 43]. A particular application, chemical graph theory, merges the principles of chemistry and graph theory to represent chemical structures as mathematical models. By employing mathematical theorems and chemical methodologies, this discipline enables the resolution of complex chemical problems. In molecular graphs, atoms and bonds are abstractly represented as vertices and edges, respectively. Graph theory's utility in chemistry extends to tasks such as isomer enumeration and molecular structure generation. Pioneering figures in the field of chemical graph theory include Alexander Balaban, Ante Graovac, Ivan Gutman, Haruo Hosoya, Milan Randi, and Nenad Trinajsti [10, 33, 39].

In many real-world systems, it is often challenging to precisely define the relationships between entities. To address this limitation, fuzzy graph theory offers a flexible framework for representing uncertainty and imprecision in graph structures. By allowing vertices and edges to have degrees of membership, fuzzy graphs enable a more nuanced and realistic modeling of complex systems. Fuzzy graph theory has found wide-ranging applications across diverse fields,

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including neural networks, artificial intelligence, computer networks, engineering sciences, transportation network design, and electrical circuits. In particular, fuzzy graph theory has been instrumental in analyzing the structure of communication networks and circuits where design ambiguity exists [26]. 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.

Topological indices are numerical representations of molecular structures that can predict chemical properties without the need for experimentation. Topological indices, numerical representations of molecular structures, have found widespread applications in theoretical chemistry for predicting physical and chemical properties. Furthermore, they leveraged topological indices and MATLAB programming to predict the physicochemical properties of drugs designed to combat Parkinson's disease [17]. Extending their research in 2024, they analyzed the quantitative structure-property relationship (QSPR) of certain drugs used to treat heart calcium channel-blocking cardiac drugs and beta-blockers diseases [15, 16]. Additionally, they employed entropy graphs weighted by topological indices and MATLAB programming to investigate the QSPR of pyelonephritis drugs [18].

Topological indices, numerical descriptors derived from the graph-theoretical representation of molecules, have been instrumental in quantitative structure-activity relationship (QSAR) studies. This brief overview traces the evolution of key topological indices, from their inception for crisp graphs to their extension to fuzzy graphs. Wiener, in 1947, introduced the Wiener index to characterize alkanes [44]. The concept of fuzzy sets, introduced by Zadeh in 1965, paved the way for the development of fuzzy graph theory [46]. J. Xu's seminal work in 1997 marked a significant milestone by highlighting the initial application of fuzzy graph theory to the field of chemistry [45]. In the realm of crisp graphs, the Zagreb indices and the Forgotten index emerged in the early 1970s [12, 8, 40]. The extension of topological indices to fuzzy graphs began in the 21st century. Researchers have investigated various indices, including the Wiener index, F-index, and connectivity indices, for fuzzy graphs [2, 26]. Additionally, studies have explored these indices for bipolar fuzzy graphs and their applications in various fields, such as chemistry and materials science [35, 37, 21, 22, 23, 24]. In 2022, Shi et al. investigated the dominant energies within the visual phase diagram and their practical uses [41].Simultaneously, Morderson and Peng provided an overview of the potential applications of fuzzy graph theory, highlighting its utility in various domains, including chemistry [27].
Carbon nanotubes, discovered by S. Iijima in 1991 [34], are cylindrical carbon nanostructures with exceptional mechanical properties [20, 42]. Their unique structures, resembling planar hexagonal networks, have implications in the chemistry of benzenoid hydrocarbons [11]. Additionally, acenes, a class of polycyclic aromatic hydrocarbons, have potential applications in optoelectronics. Recent research has explored these indices for various compounds, including nanotubes, fuzzy graphs, and linear and multi-acyclic hydrocarbons. In 2024, Faraz et al. determined the entropy of silicon nanotubes using degree-based topological descriptors [7].
Inspired by previous studies [19, 26, 31], this research aims to investigate several topological indices for a series of aromatic hydrocarbons, including Naphthalene, Anthracene, Tetrasene, Pentacene, Hexacene, Heptacene, Octacene, Nanocene, Decacene, and Undecacene. The primary objectives are to derive new formulas for the first fuzzy Zagreb index, Forgotten index, and Y-index, considering edge degrees, and to develop a general formula for fuzzy topological indices of aromatic hydrocarbons. 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 topology indices.

2 Framework of the article

This paper is structured as follows: Section 1 provides a comprehensive literature review, outlining our research motivation and objectives. Section 3 presents essential definitions and concepts related to fuzzy graphs and topological indices, as well as introduces new definitions for the first Zagreb fuzzy index, Forgotten index, and Y-index. In Section 4, we delve into a theoretical investigation of fuzzy topological indices for linear aromatic hydrocarbons, deriving a general formula for their extension. Section 5 focuses on cyclic aromatic hydrocarbons, presenting their fuzzy topological indices and a general formula for extension. Finally, Section 6 concludes the paper by discussing the implications and potential applications of the studied indices.

3 Preliminaries

In this section, some basic definitions necessary for the development of our results are presented [19, 32].

Definition 3.1. Suppose X is a finite set. The graph fuzzy G with vertices set $V(G)$ and edges set $E(G) = \{uv \mid \mu(uv) > 0, \forall u, v \in V(G)\}$, 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

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

satisfying

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

where $\wedge$ represents the minimum.

Definition 3.2. 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

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

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

$$Size(G) = \sum_{uv \in E(G)} \mu(uv)$$

where $\mu(uv) = \mu(u,v)$.

Definition 3.3. [12] Suppose G is a crisp graph. Then the first Zagreb index is shown by $M_1(G)$ and defined as follows:

$$M_1(G) = \sum_{i=1}^{n} [d(u_i)]^2 = \sum_{u_i u_j \in E(G)} [d(u_i) + d(u_j)]$$

Definition 3.4. [12] Suppose G is a crisp graph. Then the second Zagreb index is shown by $M_2(G)$ and defined as follows:

$$M_2(G) = \sum_{u_i u_j \in E(G)} d(u_i) d(u_j)$$

Definition 3.5. [6] Suppose G is a crisp graph. Then the Forgotten index (F-index) is denoted by $F(G)$ and defined as follows:

$$F(G) = \sum_{i=1}^{n} [d(u_i)]^3 = \sum_{u_i u_j \in E(G)} \left[d(u_i)^2 + d(u_j)^2\right]$$

Definition 3.6. [1] Let G be a crisp graph. Then the Y-index is denoted by $Y(G)$ and defined as follows:

$$Y(G) = \sum_{i=1}^{n} [d(u_i)]^4 = \sum_{u_i u_j \in E(G)} \left[d(u_i)^3 + d(u_j)^3\right]$$

Definition 3.7. [26] Assume G is the fuzzy graph. Then the first Zagreb index for fuzzy graphs is denoted by $M(G)$ and is defined as follows:

$$M_1^*(G) = \sum_{i=1}^{n} \sigma(u_i) [d(u_i]^2$$

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

Definition 3.8. Assume G is the fuzzy graph. Then the first Zagreb index for fuzzy graphs is indicated by $Z_\mu(G)$ and is defined by:

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

It is simply proved that Definitions 3.7 and 3.8 are equal.

Definition 3.9. [26] Assume G is the fuzzy graph. Then the second Zagreb index is shown by $M^*(G)$ and is defined by:

$$M_2^*(G) = \frac{1}{2} \sum_{u_iu_j \in E(G)} \sigma(u_i)d(u_i)\sigma(u_j)d(u_j) \qquad \forall i \neq j$$

.

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

Definition 3.10. Assume G is the fuzzy graph. Then the F-index for fuzzy graphs is shown $F^*(G)$ and is introduced as follows:

$$F^*(G) = \sum_{i=1}^{n} \sigma(u_i) \left[d(u_i\right]^3$$

Definition 3.11. Assume G is the fuzzy graph. Then the F-index for fuzzy graphs is indicated by $F_\mu(G)$ and is defined by:

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

It is easy to prove that definitions 3.10 and 3.11 are equivalent.

We have provided another definition of the Y-index in fuzzy graphs.

Definition 3.12. [25] Suppose G is a fuzzy graph. Then the Y-index is denoted by $Y*(G)$ and is introduced by:

$$Y^*(G) = \sum_{i=1}^{n} \sigma(u_i)[d(u_i]^4$$

Definition 3.13. Assume G is the fuzzy graph. Then the Y-index for fuzzy graphs is indicated by $Y_\mu(G)$ and is defined as follows:

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

It is simple to show that definitions 3.12 and 3.13 are equivalent.

Definition 3.14. [31] Suppose G is a fuzzy graph. The Randić index is shown by $\Re^*(G)$ and is defined as

$$\Re^*(G) = \frac{1}{2} \sum_{u_iu_j \in E(G)} [(\sigma(u_i)d(u_i)\sigma(u_j)d(u_j))]^{\frac{-1}{2}} \qquad \forall i \neq j$$

Definition 3.15. [31] Let G be a fuzzy graph. The Harmonic index is shown by $H^*(G)$ and is defined by:

$$H^*(G) = \frac{1}{2} \sum_{u_iu_j \in E(G)} [\sigma(u_i)d(u_i) + \sigma(u_j)d(u_j)]^{-1} \qquad \forall i \neq j$$

Table 1: The topological indices for fuzzy graphs

Index	Abbreviations
The first zagreb index	M_1^*, Z_μ
The second Zagreb index	M_2^*
The Forgotten index	F^*, F_μ
The Y- index	Y^*, Y_μ
The Harmonic index	H^*, H_μ
The Randic index	$\Re^*$

Abbreviations

4 Topological indices of fuzzy graphs of linear hydrocarbons

In this section, some topological indices of linear hydrocarbons in fuzzy graphs are examined, and a general formula based on the number of Benzene rings (K) 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 hydrocarbons, the total number of vertices is $4kn+2n$ and the total number of edges is $5kn+3n-2$, 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 $kn+n$, the vertex set with weight 0.3 has a total number of $2kn$, and the vertex set with weight 0.4 has a total number of $kn+n$.

Table 2: Naming hydrocarbons based on the number of Benzene rings connected

K	Hydrocarbon	Molecular formula
1	Benzene	C_6H_6
2	Naphthalene	$C_{10}H_8$
3	Anthracene	$C_{14}H_{10}$
4	Tetracene	$C_{18}H_{12}$
5	Pantacene	$C_{22}H_{14}$
6	Hexacene	$C_{26}H_{16}$
7	Heptacene	$C_{30}H_{18}$
8	Octacene	$C_{34}H_{20}$
9	Nanocene	$C_{38}H_{22}$
10	Decacene	$C_{42}H_{24}$
11	Undecacene	$C_{46}H_{26}$

Note: K is the number of Benzene rings.

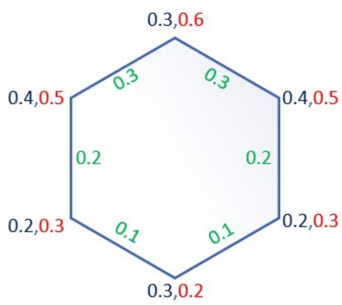

Figure 1: (1,1) unit of fuzzy graph of Benzene

Theorem 4.1. Suppose H_l is a linear hydrocarbon fuzzy graph and K is the number of Benzene rings. Then the first Zagreb index of H_l is
$Z_\mu(H_l) = 0.408kn + 0.064n - 0.116$

Proof .

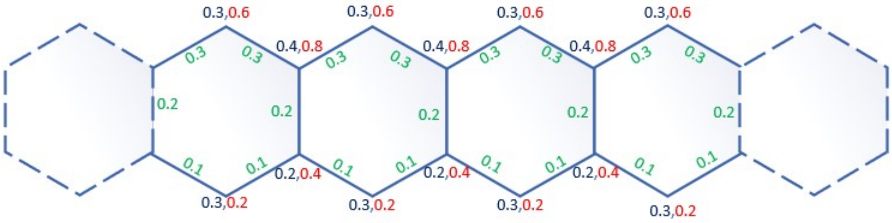

Figure 2: (1,1) unit of the fuzzy graph of linear Hydrocarbon

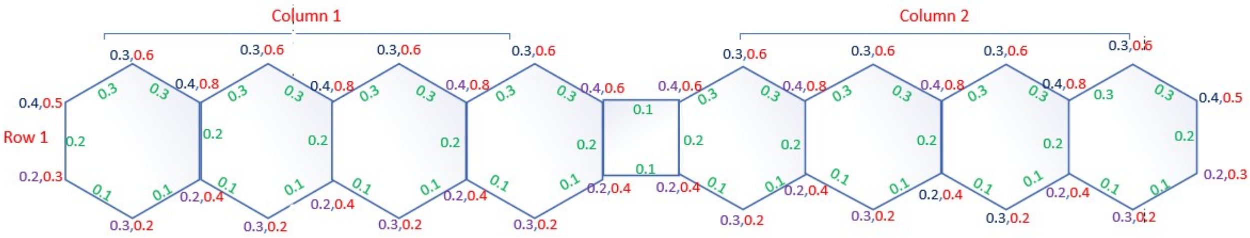

Figure 3: (1,2) unit of the fuzzy graph of linear Tetracene hydrocarbon (K=4)

According to Figure 3, and using Table 4 and Definition 3.8, we have

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

$$= 2(0.3)\left[(0.3)(0.6) + (0.4)(0.5)\right] + (2kn - 2n)(0.3)\left[(0.3)(0.6) + (0.4)(0.8)\right]$$

$$+(2n - 2)(0.3)\left[(0.3)(0.6) + (0.4)(0.6)\right] + 2(0.1)\left[(0.3)(0.2) + (0.2)(0.3)\right]$$

$$+(2kn - 2)(0.1)\left[(0.3)(0.2) + (0.2)(0.4)\right] + 2(0.2)\left[(0.2)(0.3) + (0.4)(0.5)\right]$$

$$+(kn - n)(0.2)\left[(0.2)(0.4) + (0.4)(0.8)\right] + (2n - 2)(0.2)\left[(0.2)(0.4) + (0.4)(0.6)\right]$$

$$+(n - 1)(0.1)\left[(0.4)(0.6) + (0.4)(0.6)\right] + (n - 1)(0.1)\left[(0.2)(0.4) + (0.2)(0.4)\right]$$

$$= 0.408kn + 0.064n - 0.116$$

□

Theorem 4.2. Let H_l be a fuzzy graph of linear Hydrocarbon. Then the second fuzzy Zagreb index of H_l is $M_2^*(H_l) = 0.0752kn + 0.024n - 0.0476$

Proof .

Using Table 4 and Definition 3.9, we have

$$M_2^*(H_l) = \frac{1}{2} \sum_{u_iu_j \in E(G)} \sigma(u_i)d(u_i)\sigma(u_j)d(u_j)$$

$$= \frac{1}{2}\left[2(0.3)(0.6)(0.4)(0.5) + (2kn - 2n)(0.3)(0.6)(0.4)(0.8) + (2n - 2)(0.3)(0.6)(0.4)(0.6)\right]$$

$$+\frac{1}{2}\left[2(0.3)(0.2)(0.2)(0.3) + (2kn - 2)(0.3)(0.2)(0.2)(0.4)\right]$$

Table 3: Partition of vertices for fuzzy graphs of linear hydrocarbons

Weight	**Degree**	**The total number of vertices**
(0.2)	(0.3)	2
	(0.4)	$kn + n - 2$
(0.3)	(0.2)	kn
	(0.6)	kn
(0.4)	(0.5)	2
	(0.6)	$2n - 2$
	(0.8)	$kn - n$

Table 4: Partitionof edges for fuzzy graphs of linear hydrocarbons

Weight	**Degree**	**The total number of edges**
(0.3,0.4)	(0.6,0.5)	2
	(0.6,0.8)	$2kn - 2n$
	(0.6,0.6)	$2n - 2$
(0.3,0.2)	(0.2,0.3)	2
	(0.2,0.4)	$2kn - 2$
(0.2,0.4)	(0.3,0.5)	2
	(0.4,0.8)	$kn - n$
	(0.4,0.6)	$2n - 2$
(0.4,0.4)	(0.6,0.6)	$n - 1$
(0.2,0.2)	(0.4,0.4)	$n - 1$

$$+\frac{1}{2}\left[2(0.2)(0.3)(0.4)(0.5) + (kn-n)(0.2)(0.4)(0.4)(0.8) + (2n-2)(0.2)(0.4)(0.4)(0.6)\right]$$

$$+\frac{1}{2}\left[(n-1)(0.4)(0.6)(0.4)(0.6) + (n-1)(0.2)(0.4)(0.2)(0.4)\right]$$

$$= 0.0752kn + 0.024n - 0.0476$$

□

Theorem 4.3. Suppose H_l is a linear hydrocarbon fuzzy graph. Then the Forgotten index of H_l is $F_\mu(H_l) = 0.2848kn - 0.0192n - 0.0876$

Proof . Using Table 4 and Definition 3.11, we have

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

$$= 2(0.3)\left[(0.3)(0.6)^2 + (0.4)(0.5)^2\right] + (2kn-2n)(0.3)\left[(0.3)(0.6)^2 + (0.4)(0.8)^2\right]$$

$$+(2n-2)(0.3)\left[(0.3)(0.6)^2 + (0.4)(0.6)^2\right] + 2(0.1)\left[(0.3)(0.2)^2 + (0.2)(0.3)^2\right]$$

$$+(2kn-2)(0.1)\left[(0.3)(0.2)^2 + (0.2)(0.4)^2\right] + 2(0.2)\left[(0.2)(0.3)^2 + (0.4)(0.5)^2\right]$$

$$+(kn-n)(0.2)\left[(0.2)(0.4)^2 + (0.4)(0.8)^2\right] + (2n-2)(0.2)\left[(0.2)(0.4)^2 + (0.4)(0.6)^2\right]$$

$$+(n-1)(0.1)\left[(0.4)(0.6)^2 + (0.4)(0.6)^2\right] + (n-1)(0.1)\left[(0.2)(0.4)^2 + (0.2)(0.4)^2\right]$$

$$= 0.2848kn - 0.0192n - 0.0876$$

□

Theorem 4.4. Let H_l be a linear hydrocarbon fuzzy graph. Then the Y-index of H_l is $Y_\mu(H_l) = 0.2082kn - 0.055n - 0.0606$

Proof .

Using Table 4 and Definition 3.13, we have

$$Y_\mu(H_l) = \sum_{u_iu_j \in E(G)} \mu(u_iu_j)\left[\sigma(u_i)d(u_i)^3 + \sigma(u_j)d(u_j)^2\right]$$
$$= 2(0.3)\left[(0.3)(0.6)^3 + (0.4)(0.5)^3\right] + (2kn-2n)(0.3)\left[(0.3)(0.6)^3 + (0.4)(0.8)^3\right]$$
$$+(2n-2)(0.3)\left[(0.3)(0.6)^3 + (0.4)(0.6)^3\right] + 2(0.1)\left[(0.3)(0.2)^3 + (0.2)(0.3)^3\right]$$
$$+(2kn-2)(0.1)\left[(0.3)(0.2)^3 + (0.2)(0.4)^3\right] + 2(0.2)\left[(0.2)(0.3)^3 + (0.4)(0.5)^3\right]$$
$$+(kn-n)(0.2)\left[(0.2)(0.4)^3 + (0.4)(0.8)^3\right]$$
$$+(2n-2)(0.2)\left[(0.2)(0.4)^3 + (0.4)(0.6)^3\right]$$
$$+(n-1)(0.1)\left[(0.4)(0.6)^3 + (0.4)(0.6)^3\right] + (n-1)(0.1)\left[(0.2)(0.4)^3 + (0.2)(0.4)^3\right]$$
$$= 0.2082kn - 0.055n - 0.0606$$

□

Theorem 4.5. Suppose H_l is a linear hydrocarbon fuzzy graph. Then the Randić index of H_l is $\Re^*(H_l) = 21.7253kn + 13.0697 - 3.7293$

Proof .

Using Table 4 and Definition 3.14, we have

$$\Re^*(H_l) = \frac{1}{2}\sum_{u_iu_j \in E(G)} [(\sigma(u_i)d(u_i)\sigma(u_j)d(u_j)]^{\frac{-1}{2}}$$
$$= \frac{1}{2}(2)\left[(0.3)(0.6)(0.4)(0.5)\right]^{\frac{-1}{2}} + \frac{1}{2}(2kn-2n)\left[(0.3)(0.6)(0.4)(0.8)\right]^{\frac{-1}{2}}$$
$$+\frac{1}{2}(2n-2)\left[(0.3)(0.6)(0.4)(0.6)\right]^{\frac{-1}{2}} + \frac{1}{2}(2)\left[(0.3)(0.2)(0.2)(0.3)\right]^{\frac{-1}{2}}$$
$$+\frac{1}{2}(2kn-2)\left[(0.3)(0.2)(0.2)(0.4)\right]^{\frac{-1}{2}} + \frac{1}{2}(2)\left[(0.2)(0.3)(0.4)(0.5)\right]^{\frac{-1}{2}}$$
$$+\frac{1}{2}(kn-n)\left[(0.2)(0.4)(0.4)(0.8)\right]^{\frac{-1}{2}} + \frac{1}{2}(2n-2)\left[(0.2)(0.4)(0.4)(0.6)\right]^{\frac{-1}{2}}$$
$$+\frac{1}{2}(n-1)\left[(0.4)(0.6)(0.4)(0.6)\right]^{\frac{-1}{2}} + \frac{1}{2}(n-1)\left[(0.2)(0.4)(0.2)(0.4)\right]^{\frac{-1}{2}}$$
$$= 21.7253kn + 13.0697 - 3.7293$$

□

Theorem 4.6. Let H_l be a linear hydrocarbon fuzzy graph. Then the Harmonic index of H_l is $H^*(H_l) = 10.3928kn + 6.4225n - 4.6359$

Proof .

Using Table 4 and Definition 3.15, we have

$$H^*(H_l) = \frac{1}{2}\sum_{u_iu_j\in E(G)} [\sigma(u_i)d(u_i) + \sigma(u_j)d(u_j)]^{-1}$$
$$= \frac{1}{2}\left[\frac{2}{(0.3)(0.6)+(0.4)(0.5)}\right] + \frac{1}{2}\left[\frac{2kn-2n}{(0.3)(0.6)+(0.4)(0.8)}\right]$$
$$+\frac{1}{2}\left[\frac{2n-2}{(0.3)(0.6)+(0.4)(0.6)}\right] + \frac{1}{2}\left[\frac{2}{(0.3)(0.2)+(0.2)(0.3)}\right]$$
$$+\frac{1}{2}\left[\frac{2kn-2}{(0.3)(0.2)+(0.2)(0.4)}\right] + \frac{1}{2}\left[\frac{2}{(0.2)(0.3)+(0.4)(0.5)}\right]$$
$$+\frac{1}{2}\left[\frac{kn-n}{(0.2)(0.4)+(0.4)(0.8)}\right] + \frac{1}{2}\left[\frac{2n-2}{(0.2)(0.4)+(0.4)(0.6)}\right]$$
$$+\frac{1}{2}\left[\frac{n-1}{(0.4)(0.6)+(0.4)(0.6)}\right] + \frac{1}{2}\left[\frac{n-1}{(0.2)(0.4)+(0.2)(0.4)}\right]$$
$$= 10.3928kn + 6.4225n - 4.6359$$

□

5 Topological indices of fuzzy graphs of multi-hydrocarbon

In this section, some topological indices of multi-hydrocarbons in fuzzy graphs are computed, and a general formula based on the number of Benzene rings (K) is presented for it's extension. According to Figures 4 and 5, and based on the structure of multi-hydrocarbons, the total number of vertices is $4kmn + 2mn$ and the total number of edges is $6kmn + 3mn - 2m - kn$, 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 $(k + 1)mn$, the vertex set with weight 0.3 has a total number of $2kmn$, and the vertex set with weight 0.4 has a total number of $(k + 1)mn$.

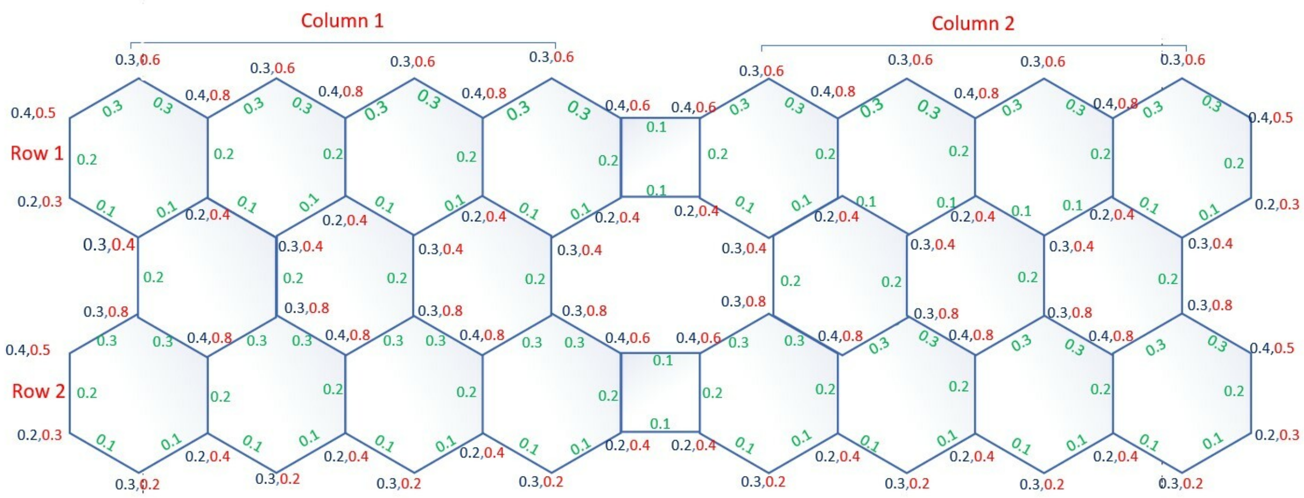

Figure 4: (2,2) unit of the fuzzy graph of Tetracene Hydrocarbon (K=4)

Theorem 5.1. Suppose H_m is a multi-hydrocarbon fuzzy graph and K is the number of Benzene rings. Then the first Zagreb index of H_m is

$$Z_\mu(H_m) = 0.528kmn - 0.12kn - 0.116m + 0.064mn$$

Proof .

Table 5: Partition of vertices in fuzzy graphs of multi-hydrocarbons

Weight	**Degree**	**The total number of vertices**
(0.2)	(0.3)	$2m$
	(0.4)	$m(kn+n-2)$
(0.3)	(0.2)	kn
	(0.4)	$kn(m-1)$
	(0.6)	kn
	(0.8)	$kn(m-1)$
(0.4)	(0.5)	$2m$
	(0.6)	$2m(n-1)$
	(0.8)	$(k-1)mn$

Table 6: Partition of edges in fuzzy graphs of multi-hydrocarbons

Weight	**Degree**	**The total number of edges**
(0.3,0.4)	(0.6,0.5)	2
	(0.6,0.8)	$2kn-2n$
	(0.6,0.6)	$2n-2$
	(0.8,0.5)	$2m-2$
	(0.8,0.8)	$(2kn-2n)(m-1)$
	(0.8,0.6)	$(m-1)(2n-2)$
(04,0.2)	(0.5,0.3)	$2m$
	(0.8,0.4)	$(k-1)mn$
	(0.6,0.4)	$2m(n-1)$
(0.2,0.3)	(0.3,0.4)	$2m-2$
	(0.4,0.4)	$(m-1)(2kn-2)$
	(0.3,0.2)	2
	(0.4,0.2)	$2kn-2$
(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)	$kn(m-1)$

Using Table 6 and Definition 3.8, we have

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

$$= 2(0.3)\left[(0.3)(0.6)+(0.4)(0.5)\right] + (2kn-2n)(0.3)\left[(0.3)(0.6)+(0.4)(0.8)\right]$$

$$+(2n-2)(0.3)\left[(0.3)(0.6)+(0.4)(0.6)\right] + (2m-2)(0.3)\left[(0.3)(0.8)+(0.4)(0.5)\right]$$

$$+(2kn-2n)(m-1)(0.3)\left[(0.3)(0.8)+(0.4)(0.8)\right] + (m-1)(2n-2)(0.3)\left[(0.3)(0.8)+(0.4)(0.6)\right]$$

$$+(2m)(0.2)\left[(0.4)(0.5)+(0.2)(0.3)\right] + (k-1)mn(0.2)\left[(0.4)(0.8)+(0.2)(0.4)\right]$$

$$+(0.2)(2m)(n-1)\left[(0.4)(0.6)+(0.2)(0.4)\right] + (2m-2)(0.1)\left[(0.2)(0.3)+(0.3)(0.4)\right]$$

$$+(0.1)(m-1)(2kn-2)\left[(0.2)(0.4)+(0.3)(0.4)\right] + 2(0.1)\left[(0.2)(0.3)+(0.3)(0.2)\right]$$

$$+(0.1)(2kn-2)\left[(0.2)(0.4)+(0.3)(0.2)\right] + (0.1)m(n-1)\left[(0.4)(0.6)+(0.4)(0.6)\right]$$

$$+(0.1)m(n-1)\left[(0.2)(0.4)+(0.2)(0.4)\right] + (0.2)kn(m-1)\left[(0.3)(0.4)+(0.3)(0.8)\right]$$

$= 0.528kmn - 0.12kn - 0.116m + 0.064mn$

□

Theorem 5.2. Let H_m be a fuzzy graph of multi-hydrocarbon. Then the second fuzzy Zagreb index of multi-hydrocarbons is

$$M_2^*(H_m) = 0.1136kmn + 0.0192mn - 0.0384kn - 0.0944m + 0.0048n + 0.468$$

Proof .

Using Table 6 and Definition 3.9, we have

$$M_2^*(H_m) = \frac{1}{2}\sum_{u_iu_j\in E(G)} \sigma(u_i)d(u_i)\sigma(u_j)d(u_j)$$

$$= \frac{1}{2}[2(0.3)(0.6)(0.4)(0.5) + (2kn - 2n)(0.3)(0.6)(0.4)(0.8)$$

$$+(2n - 2)(0.3)(0.6)(0.4)(0.6) + (2m - 2)(0.3)(0.8)(0.4)(0.5)$$

$$+(2kn - 2n)(m - 1)(0.3)(0.8)(0.4)(0.8) + (m - 1)(2n - 2)(0.3)(0.8)(0.4)(0.6)$$

$$+(2m)(0.4)(0.5)(0.2)(0.3) + (k - 1)mn(0.4)(0.8)(0.2)(0.4)$$

$$+2m(n - 1)(0.4)(0.6)(0.2)(0.4) + (2m - 2)(0.2)(0.3)(0.3)(0.4)$$

$$+(m - 1)(2kn - 2)(0.2)(0.4)(0.3)(0.4) + 2(0.2)(0.3)(0.3)(0.2)$$

$$+(2kn - 2)(0.2)(0.4)(0.3)(0.2) + m(n - 1)(0.4)(0.6)(0.4)(0.6)$$

$$+m(n - 1)(0.2)(0.4)(0.2)(0.4) + kn(m - 1)(0.3)(0.4)(0.3)(0.8)]$$

$$= 0.1136kmn + 0.0192mn - 0.0384kn - 0.0944m + 0.0048n + 0.468$$

□

Theorem 5.3. Suppose H_m is a fuzzy graph of multi-hydrocarbon. Then the Randić index of multi-hydrocarbons is

$$\Re * (H_m) = 19.8858kmn - 8.1605kn + 12.9783mn - 4.5704m + 0.0914n + 10.8411$$

Proof .

Using Table 6 and Definition 3.14, we have

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

$$= \frac{1}{2}(2)\,[(0.3)(0.6)(0.4)(0.5)]^{\frac{-1}{2}} + \frac{1}{2}(2kn - 2n)\,[(0.3)(0.6)(0.4)(0.8)]^{\frac{-1}{2}}$$

$$+\frac{1}{2}(2n - 2)\,[(0.3)(0.6)(0.4)(0.6)]^{\frac{-1}{2}} + \frac{1}{2}(2m - 2)\,[(0.3)(0.8)(0.4)(0.5)]^{\frac{-1}{2}}$$

$$+\frac{1}{2}(2kn-2)(m-1)\left[(0.3)(0.8)(0.4)(0.8)\right]^{\frac{-1}{2}}$$
$$+\frac{1}{2}(m-1)(2n-2)\left[(0.3)(0.8)(0.4)(0.6)\right]^{\frac{-1}{2}}$$
$$+\frac{1}{2}(2m)\left[(0.4)(0.5)(0.2)(0.3)\right]^{\frac{-1}{2}}+\frac{1}{2}(k-1)mn\left[(0.4)(0.8)(0.2)(0.4)\right]^{\frac{-1}{2}}$$
$$+\frac{1}{2}2m(n-1)\left[(0.4)(0.6)(0.2)(0.4)\right]^{\frac{-1}{2}}+\frac{1}{2}(2m-2)\left[(0.2)(0.3)(0.3)(0.4)\right]^{\frac{-1}{2}}$$
$$+\frac{1}{2}(m-1)(2kn-2)\left[(0.2)(0.4)(0.3)(0.4)\right]^{\frac{-1}{2}}+\frac{1}{2}(2)\left[(0.2)(0.3)(0.3)(0.2)\right]^{\frac{-1}{2}}$$
$$+\frac{1}{2}(2kn-2)\left[(0.2)(0.4)(0.3)(0.2)\right]^{\frac{-1}{2}}+\frac{1}{2}m(n-1)\left[(0.4)(0.6)(0.4)(0.6)\right]^{\frac{-1}{2}}$$
$$+\frac{1}{2}m(n-1)\left[(0.2)(0.4)(0.2)(0.4)\right]^{\frac{-1}{2}}+\frac{1}{2}kn(m-1)\left[(0.3)(0.4)(0.3)(0.8)\right]^{\frac{-1}{2}}$$
$$=19.8858kmn-8.1605kn+12.9783mn-4.5704m+0.0914n+10.8411$$

□

Theorem 5.4. Let H_m be a fuzzy graph of multi-hydrocarbon. Then the Harmonic index of multi-hydrocarbons is

$$H^*(H_m)=8.0357kmn-4.7857kn+6.3442mn-2.7056m+0.0783n+7.844$$

Proof .

Using Table 6 and Definition 3.15, we have

$$H^*(G)=\frac{1}{2}\sum_{u_iu_j\in E(G)}\left[\sigma(u_i)d(u_i)+\sigma(u_j)d(u_j)\right]^{-1}$$
$$=\frac{1}{2}\left[\frac{2}{(0.3)(0.6)+(0.4)(0.5)}\right]+\frac{1}{2}\left[\frac{(2kn-2n)}{(0.3)(0.6)+(0.4)(0.8)}\right]$$
$$+\frac{1}{2}\left[\frac{2n-2}{(0.3)(0.6)+(0.4)(0.6)}\right]+\frac{1}{2}\left[\frac{2m-2}{(0.3)(0.8)+(0.4)(0.5)}\right]$$
$$+\frac{1}{2}\left[\frac{(2kn-2n)(m-1)}{(0.3)(0.8)+(0.4)(0.8)}\right]+\frac{1}{2}\left[\frac{(m-1)(2n-2)}{(0.3)(08)+(0.4)(0.6)}\right]$$
$$+\frac{1}{2}\left[\frac{2m}{(0.4)(0.5)+(0.2)(0.3)}\right]+\frac{1}{2}\left[\frac{(k-1)mn}{(0.4)(0.8)+(0.2)(0.4)}\right]$$
$$+\frac{1}{2}\left[\frac{m(2n-2)}{(0.4)(0.6)+(0.2)(0.4)}\right]+\frac{1}{2}\left[\frac{2m-2}{(0.2)(0.3)+(0.3)(0.4)}\right]$$
$$+\frac{1}{2}\left[\frac{(m-1)(2kn-2)}{(0.2)(0.4)+(0.3)(0.4)}\right]+\frac{1}{2}\left[\frac{2}{(0.2)(0.3)+(0.3)(0.2)}\right]$$
$$+\frac{1}{2}\left[\frac{(2kn-2)}{(0.2)(0.4)+(0.3)(0.2)}\right]+\frac{1}{2}\left[\frac{m(n-1)}{(0.4)(0.6)+(0.4)(0.6)}\right]$$
$$+\frac{1}{2}\left[\frac{m(n-1)}{(0.2)(0.4)+(0.2)(0.4)}\right]+\frac{1}{2}\left[\frac{kn(m-1)}{(0.3)(0.4)+(0.3)(0.8)}\right]$$
$$=8.0357kmn-4.7857kn+6.3442mn-2.7056m+0.0783n+7.844$$

□

Theorem 5.5. Suppose H_m is a multi-hydrocarbon fuzzy graph and K is the number of Benzene rings. Then the Y-index of H_m is

$$Y_\mu(H_m) = 0.528kmn + 0.064mn - 0.12kn - 0.116m$$

Proof .

Using Table 6 and Definition 3.13, we have

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

$$= 2(0.3)\left[(0.3)(0.6)^3 + (0.4)(0.5)^3\right] + (2kn - 2n)(0.3)\left[(0.3)(0.6)^3 + (0.4)(0.8)^3\right]$$

$$+(2n-2)(0.3)\left[(0.3)(0.6)^3 + (0.4)(0.6)^3\right] + (2m-2)(0.3)\left[(0.3)(0.8)^3 + (0.4)(0.5)^3\right]$$

$$+(2kn-2n)(m-1)(0.3)\left[(0.3)(0.8)^3 + (0.4)(0.8)^3\right] + (m-1)(2n-2)(0.3)\left[(0.3)(0.8)^3 + (0.4)(0.6)^3\right]$$

$$+(2m)(0.2)\left[(0.4)(0.5)^3 + (0.2)(0.3)^3\right] + (k-1)mn(0.2)\left[(0.4)(0.8)^3 + (0.2)(0.4)^3\right]$$

$$+(0.2)(2m)(n-1)\left[(0.4)(0.6)^3 + (0.2)(0.4)^3\right] + (2m-2)(0.1)\left[(0.2)(0.3)^3 + (0.3)(0.4)^3\right]$$

$$+(0.1)(m-1)(2kn-2)\left[(0.2)(0.4)^3 + (0.3)(0.4)^3\right] + 2(0.1)\left[(0.2)(0.3)^3 + (0.3)(0.2)^3\right]$$

$$+(0.1)(2kn-2)\left[(0.2)(0.4)^3 + (0.3)(0.2)^3\right] + (0.1)m(n-1)\left[(0.4)(0.6)^3(0.4)(0.6)^3\right]$$

$$+(0.1)m(n-1)\left[(0.2)(0.4)^3 + (0.2)(0.4)^3\right] + (0.2)kn(m-1)\left[(0.3)(0.4)^3 + (0.3)(0.8)^3\right]$$

$$= 0.528kmn + 0.064mn - 0.12kn - 0.116m$$

□

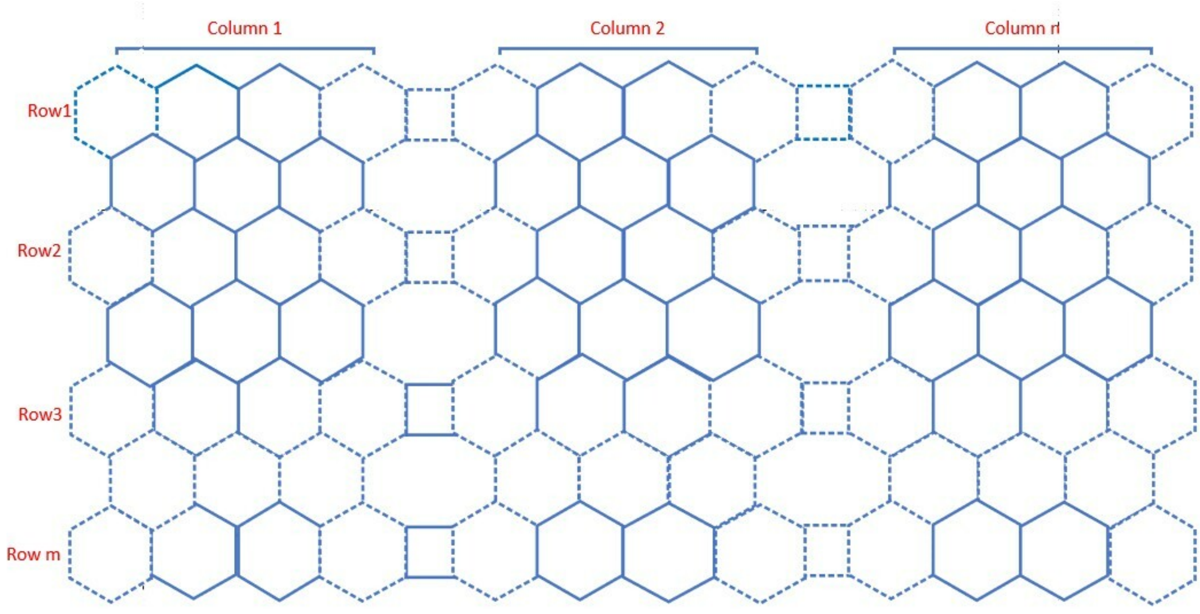

Figure 5: (m,n) unit of fuzzy graphs of multi-Hydrocarbons

6 Conclusion

This study investigated a range of topological indices within the framework of fuzzy graphs, specifically focusing on the first and second Zagreb indices, Randi index, Harmonic index, Forgotten index, and Y-index, as applied to linear and multicyclic aromatic hydrocarbons. Novel definitions were introduced for the first Zagreb index, Forgotten index, and Y-index, alongside generalized formulas based on the number of benzene rings. These formulas systematically calculate topological index values for specific hydrocarbons, enabling comparisons among different compounds. Our findings contribute to the field by offering tools that can assist researchers in predicting and estimating the physicochemical properties of molecules through accurate assessments of bond lengths and atomic masses.

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