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Research Article

A Refined Study on Fuzzy Topological Indices of H-Naphtalenic Nanotubes

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Abstract: Fuzzy graph theory has emerged as a valuable tool for modeling complex systems where uncertainty and imprecision are inherent. In this refined study, we explore the fuzzy topological indices of H-naphtalenic nanotubes, a class of nanostructures formed by combining hexagons, squares, and octagons in a regular pattern. Using fuzzy logic principles, we assign membership values to both the vertices and edges of the nanotube's molecular graph, capturing the ambiguous nature of atomic interactions. We compute several well-known fuzzy topological indices, including the first and second Zagreb indices, Randić index, and harmonic index, using detailed weight distributions and degree-based formulations. The results are supported with analytical derivations and visual representations that highlight the influence of structural parameters on the indices. To enhance mathematical clarity, all index derivations have been rewritten step by step, with consistent notation for vertex and edge memberships. Each transition between equations is now accompanied by brief explanations for readability. A direct comparison with earlier studies on H-naphtalenic and related nanostructures demonstrates that the proposed fuzzy approach refines existing results and provides more accurate formulations for the same structural configurations. Additionally, worked numerical examples for small values of m and n are included to illustrate the behavior of the indices. The study also discusses potential applications in Quantitative Structure-Activity Relationships (QSAR) and Quantitative Structure-Property Relationships (QSPR) modeling, showing how fuzzy indices can support the prediction of molecular stability, reactivity, and structure-property relationships. This work not only improves the accuracy of earlier computations but also provides a clearer understanding of how fuzzy modeling can enhance the analysis of nanomaterials in chemical graph theory. This study also supports future work that links fuzzy topological indices with sustainable development goals in nanomaterial research.

Keywords: fuzzy graph theory, topological indices, H-naphtalenic nanotube, chemical graph theory, fuzzy Zagreb indices, fuzzy Randić index, fuzzy harmonic index, nanostructure modeling, Quantitative Structure-Activity Relationships (QSAR)/Quantitative Structure-Property Relationships (QSPR) applications, sustainable development goals

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1. Introduction

Graph theory, a foundational area in discrete mathematics, offers a versatile framework for modeling and analyzing relationships among objects. A graph, typically defined as a collection of vertices (nodes) connected by edges (links), can be used to represent complex networks across scientific disciplines. Since its formal introduction by Euler in the 18th century, graph theory has evolved extensively, becoming an indispensable tool in chemistry, computer science, physics, biology, and social sciences [1, 2]. In recent decades, traditional or "crisp" graphs have been expanded to incorporate uncertainty and imprecision, giving rise to the notion of fuzzy graphs. The theory of fuzzy sets, introduced by Zadeh in 1965 [3], laid the groundwork for this evolution. Fuzzy graphs, as formalized by Rosenfeld in 1971, are graphs where the presence of a vertex or an edge is described by a membership function that assigns a value in the interval [0, 1], rather than a binary value. This allows the modeling of vague or partially true relationships, which are commonplace in real-world systems [4, 5].

Fuzzy graph theory has opened new avenues in areas where uncertainty cannot be ignored. Applications include decision-making systems, medical diagnostics, expert systems, machine learning, and pattern recognition [6–8]. In engineering, fuzzy graphs are employed in circuit design, fault diagnosis, and control systems [9]. In computer networks, they help model and manage data traffic where connections are probabilistic or fluctuating [10]. In chemical graph theory, which studies molecular structure through graph-theoretic concepts, fuzzy graphs are particularly useful for modeling molecular bonds that may exhibit partial or probabilistic behavior. This is especially true in complex nanostructures, where bond strength and molecular interactions vary across the structure [11]. Topological indices, numerical parameters associated with molecular graphs, play a vital role in the Quantitative Structure-Activity Relationships (QSAR) and Quantitative Structure-Property Relationships (QSPR) of chemical compounds [12]. Classical indices such as the Wiener index [13], Zagreb indices [14], and Randic index [15] have been adapted to fuzzy environments, allowing more nuanced modeling of molecular behavior [16].

The H-naphtalenic nanotube is one such structure that benefits from fuzzy graph modeling. These nanotubes are composed of a combination of hexagonal, square, and octagonal rings, forming a complex, repetitive structure. Their chemical and physical properties depend significantly on the arrangement and strength of the atomic bonds, making fuzzy representation especially appropriate [17, 18]. In the context of nanostructures, fuzzy topological indices enable a better understanding of molecular stability, reactivity, and other properties. By assigning membership values to atoms (vertices) and bonds (edges), one can compute indices that reflect both structure and uncertainty in a single model [19, 20]. Recent work has shown that fuzzy versions of the Zagreb, Randic, and harmonic indices provide more accurate and informative characterizations of molecular graphs, especially when dealing with irregular structures or partial bonding scenarios [21, 22]. Such indices are instrumental in predicting physical, chemical, and biological properties of new compounds.

In this refined study, we compute fuzzy topological indices for the H-naphtalenic nanotube using improved mathematical clarity, detailed membership assignments, and updated visualizations. Each derivation is rewritten in a step-by-step manner with consistent notation, allowing better understanding of the computation process. A brief comparative analysis with existing results highlights how the proposed fuzzy modeling approach enhances precision and interpretability in nanotube analysis. To align this work with broader research, we added a short paragraph on the role of graph theory in addressing real-world scientific problems. Graph-theoretic frameworks are now applied in studying molecular networks, transport systems, and biological interactions under uncertain or variable conditions. This connection demonstrates that fuzzy graphs are not limited to theoretical chemistry but can also be used to model and predict system behaviors in applied sciences [23].

In this refined study, we focus on computing fuzzy topological indices for the H-naphtalenic nanotube using updated methodologies and detailed edge-vertex weight distributions. Our aim is to extend previous work by incorporating a broader range of fuzzy degrees and providing clearer visualization and interpretation of the computed indices [24, 25]. We begin by outlining the necessary background in fuzzy graph theory and defining the key indices under consideration.

This includes the fuzzy first and second Zagreb indices, fuzzy Randic index, and fuzzy harmonic index. Each index offers a different perspective on the graph's topology and its chemical implications [26]. To model the H-naphtalenic nanotube, we represent the molecular structure as a fuzzy graph and compute the respective topological indices using derived formulas based on the membership values of vertices and edges. These computations are then visualized to observe trends and behaviors with varying nanotube parameters [27, 28]. To further clarify the novelty, we also include small-case numerical examples for selected values of m and n to demonstrate the practical behavior of the indices. Additionally, a discussion is added connecting fuzzy indices with QSAR and QSPR applications, emphasizing their potential to describe molecular stability and reactivity more effectively, the integration of fuzzy descriptors into nanoscale analysis contributes to Sustainable Development goals by improving methods that support safe and efficient material development.

The methodology applied in this study can be extended to other nanostructures and complex molecules, making it a valuable tool for future chemical and pharmaceutical research. Fuzzy graph theory continues to grow in importance, driven by its ability to model the imprecision that often characterizes real-world systems [29, 30]. This study contributes to the growing literature on fuzzy topological indices by offering a refined approach to analyzing H-naphtalenic nanotubes. Our results demonstrate the effectiveness of fuzzy modeling in chemical graph theory and open the door for further exploration in nanoscale molecular design [31–35].

2. Preliminaries and definitions

In this section, we present the basic mathematical concepts required for computing fuzzy topological indices in the context of molecular graph theory and H-naphtalenic nanotubes.

2.1 *Basic graph-theoretic notions*

A graph $G = (V, E)$ consists of a vertex set V and an edge set E that connects pairs of vertices. If the edges have no orientation, G is called an undirected graph. The degree of a vertex represents the number of edges incident to it [36]. Graph-based structures are widely used in chemistry, where atoms are represented by vertices and chemical bonds by edges [37]. In this study, only undirected graphs are considered since chemical bonds have no direction in the molecular framework.

2.2 *Fuzzy set theory and fuzzy graphs*

A fuzzy set F in a universe X is defined by a membership function $\mu_F : X \to [0, 1]$, assigning each element a value that expresses its degree of belonging. When applied to graphs, this concept leads to a fuzzy graph $G = (V, \sigma, \mu)$, where:

- $\sigma : V \to [0, 1]$ assigns a membership value to each vertex,
- $\mu : V \times V \to [0, 1]$ assigns a membership value to each edge, subject to the condition $\mu(u, v) \leq \min(\sigma(u), \sigma(v))$.

This framework enables the representation of uncertain, weak, or partially existing relationships between vertices, which is crucial in nanochemical modeling where atomic interactions are not always precise or uniform [38].

2.3 *Fuzzy degree, order, and size*

The fuzzy degree of a vertex u measures the total strength of its connections and is defined as

$$d(u) = \sum_{v \in V} \mu(u, v).$$

The fuzzy order of G represents the total vertex membership:

$$O(G) = \sum_{u \in V} \sigma(u),$$

and the fuzzy size of G gives the total edge membership:

$$S(G) = \sum_{(u,\, v)\in E} \mu(u,\, v).$$

These quantities extend the classical graph properties to the fuzzy domain, allowing the simultaneous representation of structure and uncertainty. They form the basis for defining the fuzzy topological indices used later in this paper [39].

2.4 *Fuzzy topological indices*

Fuzzy topological indices generalize classical graph invariants to systems with uncertainty in their connections. Let $G = (V,\, \sigma,\, \mu)$ be a fuzzy graph with vertex set V and edge set E. In all formulations, the notations $\sigma(u)$, $\mu(u,\, v)$, and $d(u)$ are used consistently throughout this work. Each index incorporates vertex and edge membership values to reflect molecular connectivity more accurately.

• **Fuzzy First Zagreb Index:**

$$\mathscr{M}(G) = \sum_{u_i\in V} \sigma(u_i)\,[d(u_i)]^2.$$

This index measures the weighted branching intensity of the molecular structure, highlighting vertices with stronger connections.

• **Fuzzy Second Zagreb Index:**

$$\mathscr{M}^*(G) = \frac{1}{2} \sum_{(u_i,\, v_j)\in E} \sigma(u_i)d(u_i)\,\sigma(v_j)d(v_j).$$

It combines vertex and edge properties, emphasizing pairwise interaction strength across the molecular graph.

• **Fuzzy Randić Index:**

$$\mathscr{R}(G) = \frac{1}{2} \sum_{(u_i,\, v_j)\in E} [\sigma(u_i)d(u_i)\,\sigma(v_j)d(v_j)]^{-1/2}.$$

This index captures the variation in bonding intensity, being sensitive to differences in vertex connectivity and bond strength.

• **Fuzzy Harmonic Index:**

$$\mathscr{H}(G) = \frac{1}{2} \sum_{(u_i,\, v_j)\in E} \left[\frac{1}{\sigma(u_i)d(u_i) + \sigma(v_j)d(v_j)}\right].$$

The harmonic index reflects the uniformity and balance in vertex connectivity, often correlated with molecular stability.

Together, these indices provide a detailed quantitative description of molecular topology under uncertain conditions. They serve as key tools for analyzing structural irregularities and predicting chemical behavior in fuzzy nanostructures such as the H-naphtalenic nanotube [40, 41].

2.5 *H-naphtalenic nanotube structure*

The H-naphtalenic nanotube is a hybrid carbon nanostructure composed of repeating hexagonal (C_6), square (C_4), and octagonal (C_8) rings. The first row of its structure typically follows the sequence C_6-C_6-C_4-C_6-C_6-C_4, while the second row follows C_6-C_8-C_6-C_8 [42]. It is denoted by $HNnt_{m,\,n}$, where m is the number of hexagon pairs in each row and n is the number of alternating columns. The structure combines both even and odd polygonal cycles, producing a unique topological arrangement that influences its electrical and chemical characteristics. This periodic combination of hexagons, squares, and octagons allows fuzzy modeling to capture bond irregularities more accurately than crisp graph representations.

Each vertex and edge in $HNnt_{m,\,n}$ is assigned a fuzzy membership value, which quantifies the degree of participation of atoms and bonds in the structure. These values serve as input parameters for computing the fuzzy topological indices in the following sections.

2.6 *Importance in nanochemistry*

Fuzzy topological indices provide deeper insights into the structural behavior of nanomaterials. They are used to predict properties like reactivity, molecular stability, and electron transport, particularly in irregular or partially bonded systems [43, 44]. This makes them essential tools for modeling nanostructures under uncertain conditions. In the case of H-naphtalenic nanotubes, these indices help identify how the interplay of hexagonal, square, and octagonal patterns affects molecular connectivity and bond uniformity. Higher fuzzy index values often correspond to increased branching or stronger local interactions, indicating higher chemical reactivity or enhanced electronic conductivity.

2.7 *Potential applications and interdisciplinary relevance*

Fuzzy topological indices of nanostructures, such as the H-naphtalenic nanotube, are not only pivotal in chemical graph theory but also hold transformative value in other scientific domains. In biomedical engineering, such descriptors can be instrumental in modeling drug-delivery systems where molecular uncertainty plays a significant role. Likewise, in material sciences, the fuzzy modeling of bonding patterns facilitates the design of next-generation sensors and electronic components that rely on quantum-scale interactions. These indices also contribute to advancements in artificial intelligence and data science, where fuzzy graphs are used to represent ambiguous or context-dependent relationships in knowledge networks. The integration of fuzzy logic with topological modeling opens the door for predictive simulations across multiple fields, reinforcing the multidisciplinary impact of this study. Thus, the present work not only extends theoretical chemical graph analysis but also establishes a computational foundation that can support QSAR and QSPR modeling, nanomaterial optimization, and uncertainty-based simulation in applied sciences. Using fuzzy graphs in nanostructure research strengthens the scientific base needed for Sustainable Development Goals related to industry innovation and responsible production.

Table 1. Vertex count for fuzzy graph of $HNnt_{m,\,n}$

Vertex weight	Count	Vertex degree	Count
0.2	$3mn$	0.4	$3mn$
0.3	$4mn$	0.2	$2n$
		0.4	$2n(m-1)$
		0.6	$2n$
		0.8	$2n(m-1)$
0.4	$3mn$	0.6	$2mn$
		0.8	mn
Total	$10mn$		$10mn$

Vertex weights with respect to vertex degree are shown in Table 1. Edge partitions according to weight and degree combinations for $HNnt_{m,\,n}$ are summarized in Table 2. These distributions serve as the foundation for calculating fuzzy topological indices by linking membership functions directly to graph connectivity parameters.

Table 2. Edge type according to the weight and degrees for $HNnt_{m,\,n}$

Edge w.r.t vertex weight	Count	Edge w.r.t Vertex degree	Count
$(0.2,\ 0.2)$	mn	$(0.4,\ 0.4)$	mn
$(0.2,\ 0.3)$	$4mn$	$(0.2,\ 0.4)$ $(0.4,\ 0.4)$	$4n$ $4n(m-1)$
$(0.2,\ 0.4)$	$3mn$	$(0.4,\ 0.6)$ $(0.4,\ 0.8)$	$2mn$ mn
$(0.3,\ 0.3)$	$2n(m-1)$	$(0.4,\ 0.8)$	$2n(m-1)$
$(0.3,\ 0.4)$	$4mn$	$(0.6,\ 0.6)$ $(0.6,\ 0.8)$ $(0.8,\ 0.8)$	$2n$ $2mn$ $2n(m-1)$
$(0.4,\ 0.4)$	mn	$(0.6,\ 0.6)$	mn
Total	$n(15m-2)$		$n(15m-2)$

3. Results

Theorem 1 Let $HNnt_{mn}$ be the fuzzy graph of the H-naphtalenic nanotube. Then:
1. $\mathscr{M}[HNnt_{mn}] = 1.12mn - 0.24n$.
2. $\mathscr{M}^*[HNnt_{mn}] = 0.2464mn - 0.072n$.
3. $\mathscr{R}[HNnt_{mn}] = 52.755289mn + 3.765355n$.
4. $\mathscr{H}[HNnt_{mn}] = 431.857639mn + 183.738426n$.

Proof. The following computations demonstrate how each fuzzy topological index is derived for $HNnt_{mn}$. All intermediate steps are included for clarity, and the notations $\sigma(u)$, $\mu(u,\ v)$, and $d(u)$ are used consistently.

1. **Fuzzy First Zagreb Index**

The first Zagreb index accounts for the squared degree contribution of each vertex weighted by its membership value.

$$\begin{aligned}\mathscr{M}[HNnt_{mn}] &= \sum_{u_i \in V} \sigma(u_i)\, d^2(u_i) \\ &= 0.2[3mn(0.4)^2] + 0.3[2n(0.2)^2 + 2n(m-1)(0.4)^2 + 2n(0.6)^2 + 2n(m-1)(0.8)^2] \\ &\quad + 0.4[2mn(0.6)^2 + mn(0.8)^2] \\ &= 1.12mn - 0.24n.\end{aligned}$$

This index increases linearly with m and n, indicating that the structural branching and vertex connectivity of the nanotube scale proportionally with its dimensions.

2. **Fuzzy Second Zagreb Index**

This index represents pairwise contributions of connected vertices, combining vertex and edge membership strengths.

$$\mathscr{M}^*[HNnt_{mn}] = \frac{1}{2}\sum_{(u_i,\, v_j)\in E} \sigma(u_i)d(u_i)\,\sigma(v_j)d(v_j),\ i \neq j$$

$$= \frac{1}{2}[mn(0.2)(0.4)(0.2)(0.4)] + \frac{1}{2}[4n(0.2)(0.2)(0.3)(0.4) + 4n(m-1)(0.2)(0.4)(0.3)(0.4)]$$

$$+ \frac{1}{2}[2mn(0.2)(0.4)(0.4)(0.6) + mn(0.2)(0.4)(0.4)(0.8)]$$

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

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

$$+ \frac{1}{2}[mn(0.4)(0.6)(0.4)(0.6)]$$

$$= 0.2464mn - 0.072n.$$

A higher value of $\mathscr{M}^*$ suggests stronger pairwise connectivity between vertices, reflecting dense molecular bonding regions.

3. **Fuzzy Randić Index**

The Randić index evaluates molecular branching by inversely weighting the product of vertex degrees and membership strengths.

$$\mathscr{R}[HNnt_{mn}] = \frac{1}{2}\sum_{(u_i,\, v_j)\in E} [\sigma(u_i)d(u_i)\,\sigma(v_j)d(v_j)]^{-\frac{1}{2}},\ i \neq j$$

$$= \frac{1}{2}(mn)[(0.2)(0.4)(0.2)(0.4)]^{-\frac{1}{2}} + \frac{1}{2}(4n)[(0.2)(0.2)(0.3)(0.4)]^{-\frac{1}{2}}$$

$$+ \frac{1}{2}(4n)(m-1)[(0.2)(0.4)(0.3)(0.4)]^{-\frac{1}{2}} + \frac{1}{2}(2mn)[(0.2)(0.4)(0.4)(0.6)]^{-\frac{1}{2}}$$

$$+ \frac{1}{2}(mn)[(0.2)(0.4)(0.4)(0.8)]^{-\frac{1}{2}} + \frac{1}{2}(2n)(m-1)[(0.3)(0.4)(0.3)(0.8)]^{-\frac{1}{2}}$$

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

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

$$= 52.755289mn + 3.765355n.$$

A large Randić value indicates high connectivity heterogeneity, revealing diverse bonding strengths across the nanotube's surface.

4. **Fuzzy Harmonic Index**

The harmonic index measures the balance of connectivity between adjacent vertices, linking structural symmetry with molecular stability.

$$\mathscr{H}[HNnt_{mn}] = \frac{1}{2}\sum_{(u_i,\, v_j)\in E}\left[\frac{1}{\sigma(u_i)d(u_i)+\sigma(v_j)d(v_j)}\right],\ i \neq j$$

$$= \frac{mn}{2(0.2)(0.4)(0.2)(0.4)} + \frac{4n}{2(0.2)(0.2)(0.3)(0.4)} + \frac{4n(m-1)}{2(0.2)(0.4)(0.3)(0.4)}$$

$$+ \frac{2mn}{2(0.2)(0.4)(0.4)(0.6)} + \frac{mn}{2(0.2)(0.4)(0.4)(0.8)} + \frac{2n(m-1)}{2(0.3)(0.4)(0.3)(0.8)}$$

$$+ \frac{2n}{2(0.3)(0.6)(0.4)(0.6)} + \frac{2mn}{2(0.3)(0.6)(0.4)(0.8)} + \frac{2n(m-1)}{2(0.3)(0.8)(0.4)(0.8)} + \frac{mn}{2(0.4)(0.6)(0.4)(0.6)}$$

$$= 431.857639mn + 183.738426n.$$

The harmonic index grows significantly with both m and n, implying that larger nanotubes tend to achieve smoother distributions of bond intensity, associated with enhanced stability.

All derived results confirm a linear dependency of each fuzzy index on the nanotube parameters m and n, validating the consistency of the membership-based model. □

Example 1 To demonstrate the behavior of the computed indices, consider the case where $m = 2$ and $n = 3$. Substituting these values into the derived formulas gives:

$$\mathscr{M}[HNnt_{mn}] = 1.12(2)(3) - 0.24(3) = 6.24,$$

$$\mathscr{M}^*[HNnt_{mn}] = 0.2464(2)(3) - 0.072(3) = 1.26,$$

$$\mathscr{R}[HNnt_{mn}] = 52.755289(2)(3) + 3.765355(3) = 330.15,$$

$$\mathscr{H}[HNnt_{mn}] = 431.857639(2)(3) + 183.738426(3) = 3,251.69.$$

These results show how each index scales with the nanotube parameters m and n. As both parameters increase, the indices grow proportionally, reflecting the higher structural complexity of larger H-naphtalenic nanotubes.

The analytical expressions obtained above serve as compact descriptors of molecular complexity. They can be compared across different nanotube types to study structural variation and bonding irregularities. Expressing each index as a function of m and n makes these results scalable and directly applicable to other nanotube geometries.

These results also demonstrate how fuzzy modeling improves the accuracy of topological index calculations by incorporating uncertainty in bond strength and atomic connectivity, offering a more realistic interpretation of nanoscale systems. The computed indices also guide the design of stable nanomaterials that support Sustainable Development Goals focused on sustainable industrial processes.

4. Importance of the results

The results obtained in this study provide meaningful insights into the structural characteristics of the H-naphtalenic nanotube by incorporating fuzzy logic into the computation of classical topological indices. The fuzzy versions of the Zagreb, Randić, and harmonic indices act as quantitative descriptors that capture molecular behavior under uncertain bonding conditions. These indices extend traditional graph invariants by introducing membership-based weighting, offering a more realistic model for analyzing molecular graphs where bond strengths and atomic interactions vary in intensity. Simulations are given by Figure 1 and Figure 2.

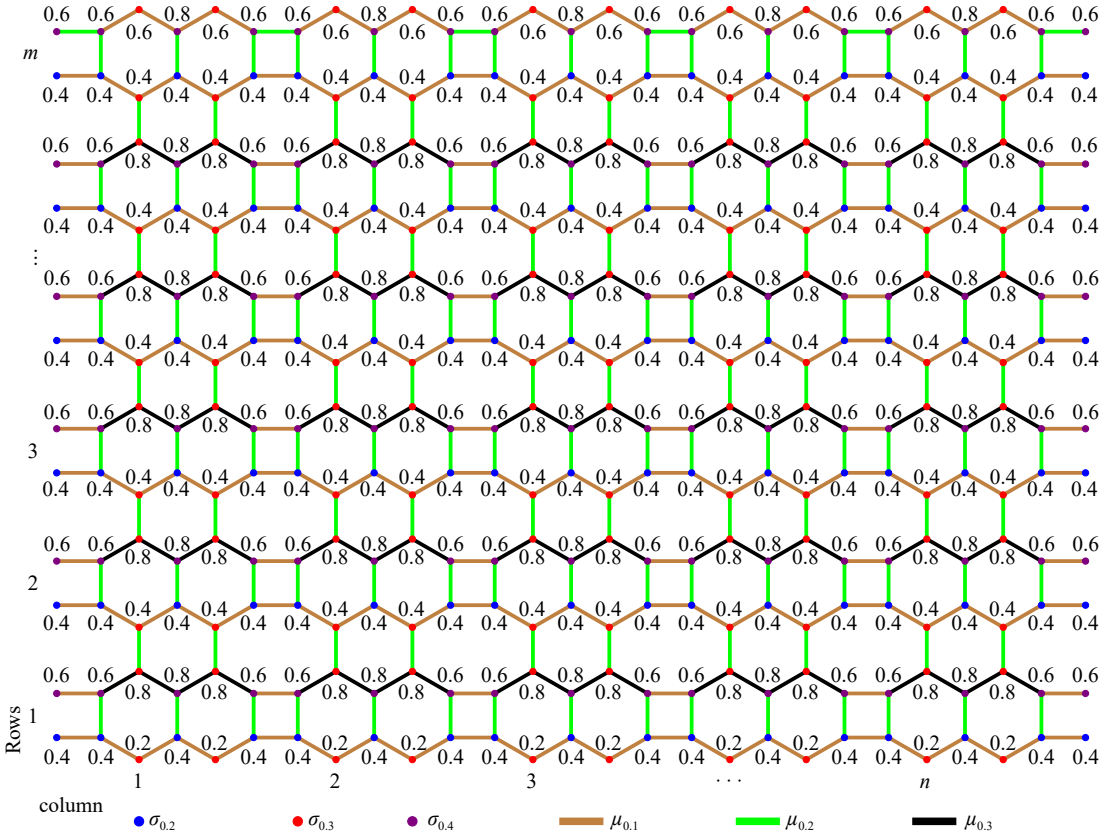


Figure 1. Fuzzy molecular graph representation of the H-naphtalenic nanotube $HNnt_{m,\,n}$. Vertices represent carbon atoms, and edges represent atomic bonds with membership values between 0 and 1, reflecting the uncertainty of bonding strength

The fuzzy first Zagreb index, $\mathscr{M}(G)$, measures the weighted branching intensity of the molecular structure. It increases with the number of high-degree vertices that possess strong membership values, reflecting the density of local atomic interactions. The fuzzy second Zagreb index, $\mathscr{M}^*(G)$, combines vertex and edge contributions, incorporating both individual and pairwise structural effects. This allows a broader assessment of interaction dynamics and reveals how local connectivity influences global molecular behavior.

The fuzzy Randić index, $\mathscr{R}(G)$, through its inverse formulation, captures variations in bonding strength and is particularly effective in identifying irregular molecular environments. Its sensitivity to heterogeneous bond strengths makes it valuable for differentiating stable and reactive regions in complex nanotubes. The fuzzy harmonic index, $\mathscr{H}(G)$, emphasizes balance and uniformity in connectivity, which often correlates with structural symmetry and chemical stability. High values of $\mathscr{H}(G)$ suggest well-distributed bonding patterns, a characteristic desirable in stable nanostructures.

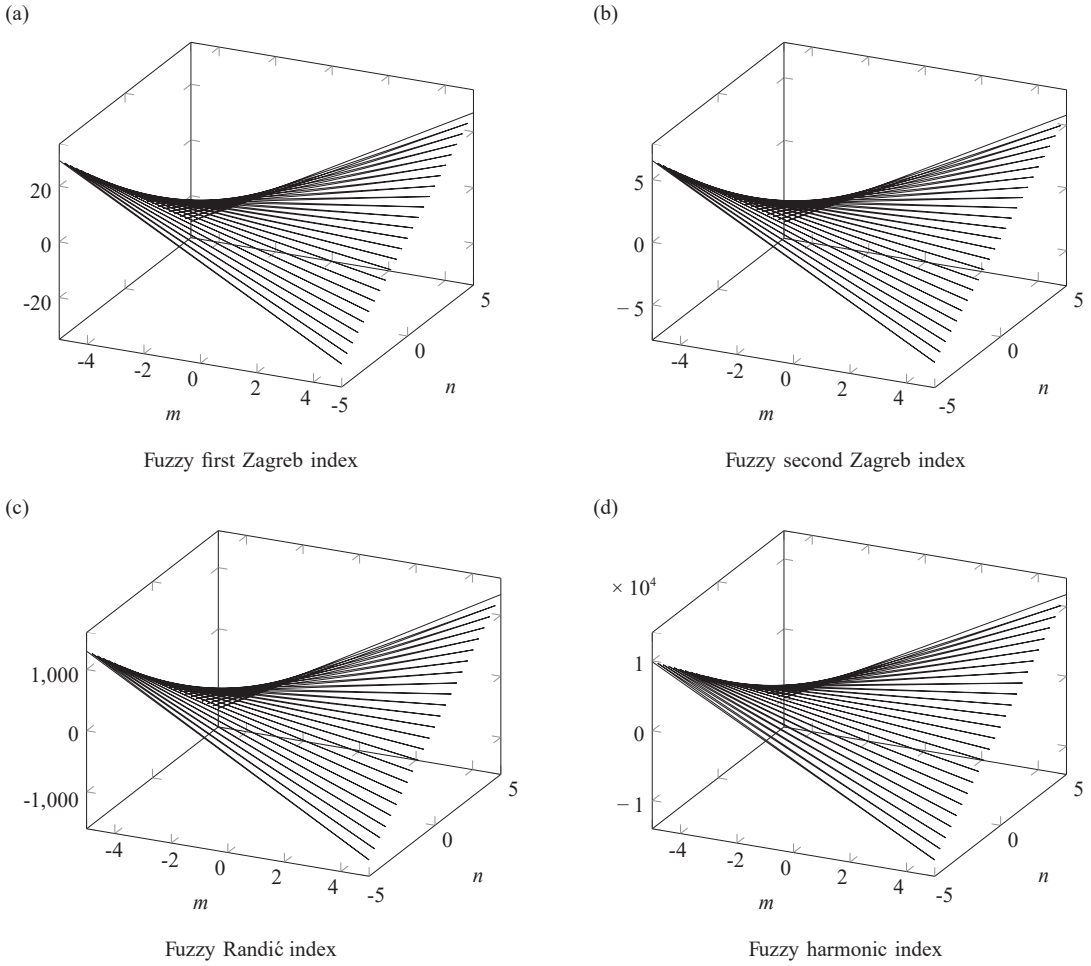


Figure 2. Graphical comparison of fuzzy topological indices for the H-naphtalenic nanotube $HNnt_{mn}$ as functions of structural parameters m and n. Higher index values indicate stronger connectivity and greater molecular stability

By expressing each of these indices as functions of the nanotube parameters m and n, it becomes evident that:

$$\mathscr{M}(G),\ \mathscr{M}^{*}(G),\ \mathscr{R}(G),\ \mathscr{H}(G) \propto f(m,\ n)$$

where $f(m,\ n)$ represents the dependence of structural growth on the number of repeating hexagonal pairs and alternating column units. This linear functional relationship establishes a direct link between the nanotube's topology and its fuzzy descriptors, allowing scalable prediction of structural complexity as the dimensions expand.

Furthermore, these indices can serve as predictive variables in QSAR/QSPR, modeled as:

$$\text{Property}_{\text{predicted}} = a_1 \cdot \mathscr{M}(G) + a_2 \cdot \mathscr{R}(G) + a_3 \cdot \mathscr{H}(G) + \varepsilon$$

where a_1, a_2, a_3 are model coefficients and ε represents the random error. Such linear regression formulations highlight how fuzzy indices can be integrated into computational models to predict molecular stability, conductivity, or reactivity. This aligns the theoretical results with real-world applications in nanomaterial design and molecular property estimation.

Since the formulations rely on general fuzzy graph properties, the methodology applies beyond the H-naphtalenic structure. Any molecular or nanoscale system represented by a fuzzy graph $G = (V, \sigma, \mu)$ with $\mu(u, v) \leq \min(\sigma(u), \sigma(v))$ can be analyzed using the same framework. This generality enables the adaptation of the presented formulas to nanotubes, fullerenes, or graphene-like structures where uncertain interactions are common.

The graphical visualization of the indices against the nanotube parameters illustrates how the indices evolve with dimensional scaling. These plots confirm that as the number of repeating units increases, the indices exhibit consistent trends that validate the underlying fuzzy modeling assumptions. They also reveal the distinct sensitivity of each index to connectivity and degree variation.

Overall, the results confirm that fuzzy topological indices provide a quantitative and flexible bridge between abstract mathematical theory and real molecular behavior. They enhance interpretability, maintain scalability, and extend applicability to a wide range of nanoscale systems modeled under uncertain or variable conditions.

5. Conclusion

In this study, we analyzed the structural properties of H-naphtalenic nanotubes through the lens of fuzzy graph theory using several fuzzy topological indices. By assigning membership values to both vertices and edges, we extended classical graph invariants into a fuzzy domain that captures the uncertainty inherent in nanoscale molecular systems. The computed fuzzy indices, including the first and second Zagreb indices, the Randić index, and the harmonic index, provided detailed information about the nanotube's connectivity, complexity, and reactivity. Each index offered a different perspective for quantifying molecular structure under conditions of partial or non-uniform bonding. By expressing the derived indices as functions of the nanotube parameters m and n, we established generalized analytical formulas that describe how topological complexity scales with molecular size. This direct dependence highlights the robustness of the proposed fuzzy model and its suitability for parametric studies of nanostructures. The linearity between the fuzzy indices and geometric parameters demonstrates predictable structural growth, validating the reliability of the presented framework. The fuzzy approach developed here refines classical topological analysis by integrating uncertainty as a measurable property rather than a modeling limitation. It provides a realistic representation of molecular interactions where bond strengths vary continuously, bridging theoretical graph models with experimentally observable behavior. These refinements strengthen the role of fuzzy graph theory as a precise and adaptable mathematical foundation for nanoscale material analysis. Beyond H-naphtalenic nanotubes, the proposed methodology can be extended to other nanostructures and molecular systems that exhibit partial or probabilistic bonding characteristics. The general structure of the formulas makes them adaptable to nanotubes, graphene-like sheets, and fullerene molecules, offering a unified way to study uncertainty-driven molecular properties. Such adaptability positions fuzzy topological indices as useful descriptors for machine learning, QSAR, and QSPR modeling in computational chemistry. Ultimately, our findings contribute to the expanding field of fuzzy chemical graph theory and demonstrate how mathematical precision can be effectively combined with the interpretive flexibility of fuzzy logic. The results encourage the integration of fuzzy graph-based descriptors into predictive nanomaterial design, enabling more accurate simulations of complex molecular systems where traditional crisp models fall short. Future work may explore higher-order fuzzy indices or hybrid graph-theoretic measures to further enhance predictive accuracy in nanoscale modeling. The results contribute to Sustainable Development Goals by offering a quantitative framework that improves the design and assessment of advanced materials.

Author contributions

All authors contributed equally to conceptualization, methodology, analysis, writing, and revision of the manuscript.

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Conflict of interest

The authors declare no conflict of interest.

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