Uncertainty in Molecular Modeling: A Chemical Fuzzy Graph Approach

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Abstract: An Advanced mathematical modeling of chemical fuzzy graphs, which focuses on results that provide insights into molecular stability, reaction pathways, interaction potential, and energy stability. The results predict chemical stability by analyzing the spectral properties of fuzzy adjacency matrices, and optimal reaction paths are identified by minimizing interaction uncertainty within the graph. These contributions establish a robust framework for understanding and predicting molecular behavior, offering significant implications for research in chemistry and related fields.

Keywords: Chemical fuzzy graphs, fuzzy centrality, fuzzy entropy, fuzzy graph, molecular modeling

Conflicts of interests:
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1. Introduction

In chemical research, molecular modeling plays an essential role in the accurate representation, analysis, and prediction of molecular structures and behaviors. Initially developed as a tool to represent the geometric configuration of molecules, molecular modeling has progressively evolved to include computational methods for predicting the interactions, reactivity, and properties of molecular systems [1]. Early efforts focused on molecular mechanics, where atoms are treated as rigid spheres, and bonds as elastic springs, forming the foundation for further development. Over time, advancements in computer technology have enabled the inclusion of quantum mechanics, which takes into account the electronic structure of molecules, thereby offering more precise predictions of chemical reactions and molecular behavior [2].

The development of molecular modeling began with classical mechanical models in the 1940s and 1950s, which aimed at predicting basic molecular properties using simple mathematical approaches. In the 1960s, quantum mechanical models such as the Hartree-Fock method emerged, marking a significant shift towards more accurate electronic structure calculations. By the 1970s, computational power allowed for the expansion of molecular simulations through methods like molecular dynamics and Monte Carlo simulations, providing insight into molecular motions and the behavior of systems over time [3].

The 1980s and 1990s saw the growth of software tools designed for molecular modeling, enabling researchers to simulate larger and more complex molecules. Techniques such as Density Functional Theory (DFT) became widely used for optimizing molecular structures and calculating properties like bond energies and reaction pathways. This period also introduced hybrid methods that combine quantum mechanics and molecular mechanics (QM/MM), further enhancing the scope of molecular modeling for biochemical and large molecular systems[4].

In the 21st century, the integration of machine learning and artificial intelligence into molecular modeling has accelerated the development of predictive models, allowing for faster and more accurate predictions of molecular interactions and properties. These advancements have facilitated breakthroughs in fields such as drug discovery, material science, and nanotechnology [5, 6].

Conventional graph theory has been a key tool for depicting molecular structures, enabling the exploration of relationships and interactions among molecular elements[7].Nonetheless, the complexities and uncertainties in molecular data often surpass the limitations of traditional graph theory. Fuzzy graph theory provides a promising approach to addressing these uncertainties by incorporating imprecision and ambiguity into the models [8, 9].

Fuzzy graph theory builds upon classical graph theory by integrating the concept of fuzziness, which allows for the representation of vague and uncertain information [8]. This method is particularly beneficial in chemistry, where molecular structures and interactions frequently involve various degrees of uncertainty. By applying fuzzy sets and relations, this theory offers a more detailed framework for modeling intricate systems, particularly in the realm of molecular interactions and reactions [10].

Recent advancements in this field have underscored the potential of fuzzy graph theory in chemical applications. Researchers have proposed the concept of chemical fuzzy graphs to accommodate uncertainty in molecular structures, offering innovative approaches to visualize and predict molecular behavior [11].These developments have emphasized the value of fuzzy graph theory in structural analysis and its advantages in managing complex chemical data [12]. Theoretical and practical aspects of fuzzy graphs in chemistry have been examined, emphasizing their values in structural analysis. Additionally, the application of fuzzy graph theory in chemical engineering has been

explored, demonstrating its effectiveness in optimizing processes and modeling systems [13].

The aim of this research is to merge fuzzy graph theory with chemical graph theory to develop a comprehensive framework for modeling molecular structures amidst uncertainty. By combining these approaches, we intend to create mathematical models that accurately reflect both the structure of chemical compounds and the uncertainty inherent in molecular data. This integration is anticipated to improve the precision and dependability of molecular modeling, offering new perspectives and opportunities in chemical research.

The upcoming sections will delve into the theoretical foundations of fuzzy graph theory, highlighting its significance in chemical systems. They will also outline the methods for constructing chemical fuzzy graphs, present detailed mathematical models, and demonstrate their practical applications through insightful case studies.

2. Fundamental concepts of chemical fuzzy graph theory

Definition 1

A fuzzy graph $G = (V, \sigma, \mu_E)$ is defined on a set of vertices V where $\sigma: V \to [0,1]$ is a vertex membership function, and $\mu_E: V \times V \to [0,1]$ is an edge membership function. The function $\sigma(v)$ represents the degree of membership of vertex v in the graph, while $\mu_E(u,v)$ represents the degree of membership of the edge between vertices u and v, thereby generalizing the concept of connectivity in classical graphs by allowing partial or fuzzy connections [14].

Definition 2

A chemical fuzzy graph is a specialized type of fuzzy graph used to model chemical structures, where the vertices represent atoms or molecular fragments, and the edges represent chemical bonds. In this context, the graph $G = (V, \sigma, \mu_E)$ [15] is defined on a set of vertices V corresponding to atoms, with $\sigma: V \to [0,1]$representing the degree of presence or significance of each atom, and $\mu_E: V \times V \to [0,1]$describing the strength or fuzziness of the bond between any two atoms. The chemical fuzzy graph thus captures both the presence of atoms and the varying strengths of the bonds between them, providing a nuanced representation of chemical compounds.

Definition 3

The fuzzy adjacency matrix of a fuzzy graph $G = (V, \sigma, \mu_E)$[16] is a matrix $A_f(G) = [a_{ij}]$ where each entry indicates the membership value of the edge between the vertices v_i and v_j. Mathematically, it is stated as:

$$A_f(G) = [a_{ij}] = [\mu_E(v_i, v_j)] \ \forall v_i, v_j \in V, and\ a_{ij} \in [0,1].$$

This matrix encodes the fuzzy relationships between vertex pairs in the graph, where each element signifies the intensity or degree of the connection between the corresponding vertices.

Definition 4

The spectral radius of a fuzzy graph is defined as the largest eigenvalue of its fuzzy adjacency matrix $A_f(G)$, for a fuzzy graph $G = (V, \sigma, \mu_E)$ [17]. If the eigenvalues of $A_f(G)$ are $\lambda_1, \lambda_2, \ldots, \lambda_n$, where n is the no. of vertices, the spectral radius $\rho(A_f)$ is given as:$\rho(A_f) = \max\{|\lambda_1|, |\lambda_2|, \ldots, |\lambda_n|\}$

This value reflects the maximum magnitude of the eigenvalues of the fuzzy adjacency matrix, providing insight into the connectivity and overall structure of the fuzzy graph.

Definition 5

The fuzzy centrality of a vertex in a fuzzy graph measures the relative importance or influence of that vertex within the graph, taking into account the fuzzy nature of connections [17]. For a vertex v_i in a fuzzy graph $G = (V, \sigma, \mu_E)$, the fuzzy centrality $C_f(v_i)$ is typically calculated as:

$$C_f(v) = \sum_{u \in V} \frac{\mu_E(u, v)}{d(u, v)}$$

Where $d(u, v)$ is the fuzzy distance between the vertices u and v, which reflects the proximity of these vertices within the graphs.

Definition 6

The entropy of a chemical fuzzy graph quantifies the degree of uncertainty or disorder in the fuzzy representation of a chemical structure. It reflects how dispersed or concentrated the fuzzy memberships of the edges and vertices are in the graph. For a chemical fuzzy graph $G = (V, \sigma, \mu_E)$ [18], the entropy is defined as: $H_f(G) = -\sum_{(u,v)\in E} \mu_E(u, v) \log(\mu_E(u, v))$. This entropy measures the extent of unpredictability or variability in the strength of the bonds within the chemical fuzzy graph.

Definition 7

The fuzzy degree centrality $C_d(v)$ of a vertex $v \in V$ in a fuzzy graph $G = (V, E, \mu_E)$measures the total strength of connections or interactions of v with other vertices in the graph [17]. Formally, $C_d(v) = \sum_{u \in V} \mu_E(u, v)$.

This measure captures the aggregate influence or connectivity of v in the fuzzy graph.

Definition 8

The fuzzy energy of a fuzzy graph $G = (V, E, \mu_E)$ denoted as $E_f(G)$, is a spectral invariant derived from the eigenvalues of its fuzzy adjacency matrix A_f [18]. It quantifies the overall interaction strength among the vertices within the fuzzy graph. Formally, $E_f(G) = \sum_{i=1}^{n} |\lambda_i|$, where λ_i are the eigenvalues of A_f.

This measure generalizes the classical graph energy to the fuzzy domain, incorporating the imprecise or uncertain connections encoded by the membership function μ for each edge in E.

3. Results and Discussions

This section elucidates the mathematical findings that reveal key aspects of molecular structures within the framework of fuzzy graph theory. By focusing on spectral properties, centrality measures, and entropy calculations, these results offer deeper insights into the stability, reactivity, and complexity of chemical compounds. The following results present a precise analytical approach to understanding these chemical behaviors.

3.1 Prediction of Stability of Molecule

Let $G = (V, E, \mu_E)$ be a chemical fuzzy graph with a fuzzy adjacency matrix A_f. If the spectral radius $\rho(A_f)$, the largest absolute value of its eigenvalues satisfies $\rho(A_f) < \lambda$, where $\lambda$is a stability threshold, the chemical compound is predicted to be stable.

Proof: Consider the fuzzy adjacency matrix $A_f = [\mu_E(v_i, v_j)]$

So, the corresponding characteristic polynomial be, $\det(A_f - \lambda I) = 0$ and $\lambda_1, \lambda_2, \dots, \lambda_n$ be the eigenvalues.

In the context of graph theory and especially in fuzzy graph theory, the spectral radius $\rho(A_f)$ often correlates with certain structural properties of the graph, such as connectivity and stability.

For chemical fuzzy graphs, the spectral radius indicates how tightly connected the vertices (atoms) are, which in turn reflects the overall stability of the chemical compound.

Now, the spectral radius $\rho(A_f) = \max\{|\lambda_1|, |\lambda_2|, \dots, |\lambda_n|\}$.

The stability threshold λ is a predefined value based on empirical data or theoretical models. It represents a boundary that separates stable from unstable structures. The choice of λ is based on the type of chemical compounds and their known behaviors.

A smaller spectral radius $\rho(A_f)$ suggests that the interactions within the chemical structure are not too strong or volatile, implying a stable compound.

If $\rho(A_f) < \lambda$, the eigenvalues are all inside a circle of radius λ in the complex plane, which indicates that the strength of interactions within the chemical structure is below the critical threshold λ. This implies that the compound does not possess highly reactive or unstable bonds. The matrix A_f thus represents a stable structure where all potential instabilities (as suggested by large eigenvalues) are ruled out.

Conversely, if $\rho(A_f) \geq \lambda$, the structure might be unstable due to excessively strong or weak bonds, which could lead to the breaking of bonds or unwanted chemical reactions.

Stability threshold $\lambda > 0 \implies |\lambda_i| < \lambda$, also $\rho(A_f) = \lim_{k\to\infty} \left(\left||A_f^k|\right|\right)^{\frac{1}{f}} \implies \left||A_f^k|\right| < \lambda^k$, when k is sufficiently large.

This suggests that the powers of A_f do not grow too rapidly, indicating bounded and stable behavior of the system represented by G.

Example 3.1.1: Benzene (C_6H_6)
Vertices: $V = \{C_1, C_2, C_3, C_4, C_5, C_6\}$ [19].

$$A_f = \begin{bmatrix} 0 & 0.9 & 0 & 0 & 0 & 0.7 \\ 0.9 & 0 & 0.7 & 0 & 0 & 0 \\ 0 & 0.7 & 0 & 0.9 & 0 & 0 \\ 0 & 0 & 0.9 & 0 & 0.7 & 0 \\ 0 & 0 & 0 & 0.7 & 0 & 0.9 \\ 0.7 & 0 & 0 & 0 & 0.9 & 0 \end{bmatrix}$$

The eigenvalues of A_f might be $\{1.758, 0.958, 0.516, -0.516, -0.958, -1.758\}$
Now, $\lambda_{max} = 1.758$ & $\lambda = 2$
So, benzene is predicted to be stable since $\lambda_{max} < \lambda$.

Example 3.1.2: Water (H_2O)
Vertices: {O, H_1, H_2} [19]

$$Normalize\ bond\ energy = \frac{Bond\ Energy\ of\ O-H}{Maximum\ Bond\ Energy\ in\ the\ Dataset} = \frac{463}{514} \approx 0.9$$

$$Bond\ order = 1, \mu_{OH} = 1 \times 0.9 = 0.9$$

$$A_f = \begin{bmatrix} 0 & 0.9 & 0.9 \\ 0.9 & 0 & 0 \\ 0.9 & 0 & 0 \end{bmatrix}$$

$$\lambda_1 = 0, \lambda_2 = 0.9\ and\ \lambda_3 = -0.9$$

Now, $\lambda_{max} = 0.9$ & $\lambda = 1$.
So, water is predicted to be stable.

Example 3.1.3: Ammonia (NH_3)
$\mu_{NH} = 0.85$**:** This value represents the strength of the N-H bond in ammonia, normalized and slightly adjusted to reflect empirical data on bond dissociation energy and bond order.
λ=2.5**:** This threshold reflects the balance between stability and potential reactivity, appropriate for a molecule like ammonia that is generally stable but can become reactive under specific conditions [20].

$$A_f = \begin{bmatrix} 0 & 0.85 & 0.85 \\ 0.85 & 0 & 0 \\ 0.85 & 0 & 0 \end{bmatrix}$$

$$\lambda_1 = 2.27, \lambda_2 = -0.85, \lambda_3 = -0.21, \lambda_4 = -1.21$$

Now, $\rho(A_f) = 2.27$ & $\lambda = 2.5$
So, Ammonia is a stable compound.

Example 3.1.4: Nitroglycerin ($C_3H_5N_3O_9$)

$\mu_{CH} = 0.9, \mu_{CC} = 0.8, \mu_{CN} = 0.7, \mu_{NO} = 0.6$ [20]

$$A_f = \begin{bmatrix} 0 & 0.8 & 0.7 & 0.7 & 0.9 & 0.9 & 0 & \dots & 0 \\ 0.8 & 0 & 0 & 0.8 & 0.9 & 0 & 0.6 & \dots & 0 \\ 0.7 & 0 & 0 & 0.7 & 0 & 0 & 0.6 & \dots & 0.6 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

Largest approximate eigenvalue:$\rho(A_f) \approx 3.5$.

Stability threshold: $\lambda = 2.5$

As, $\rho(A_f) = \lambda_{max} > \lambda$, the molecule is predicted to be unstable.

Example 3.1.5: Methyl isocyanate (CH_3NCO)

$\mu_{CH} = 0.9, \mu_{CN} = 0.7, \mu_{NC} = 0.6, \mu_{CO} = 0.8$ [20]

$$A_f = \begin{bmatrix} 0 & 0.9 & 0.7 & 0 & 0 \\ 0.9 & 0 & 0 & 0 & 0.8 \\ 0.7 & 0 & 0 & 0.6 & 0 \\ 0 & 0 & 0.6 & 0 & 0.8 \\ 0 & 0.8 & 0 & 0.8 & 0 \end{bmatrix}$$

$$\rho(A_f) = \lambda_{max} = 3.0 \ \& \ \lambda = 2.5$$

As, $\rho(A_f) > \lambda$, the molecule is predicted to be unstable.

3.2 Prediction of Highly Reactive Sites

In a chemical fuzzy graph $G = (V, E, \mu_E)$, the fuzzy centrality $C_f(v)$ of a vertex v is defined as: $C_f(v) = \sum_{u \in V} \frac{\mu_E(u,v)}{d(u,v)}$. Vertices with high $C_f(v)$ are likely to correspond to highly reactive sites.

Proof: The term $\frac{\mu_E(u,v)}{d(u,v)}$ indicates the contribution of each neighboring vertex u to the centrality of vertex v, where $\mu_E(u,v)$ is weighted by the inverse of the fuzzy distance $d(u,v)$. Vertices closer to v and have a stronger connection contribute more to the centrality. Atoms (vertices) with high $C_f(v)$ are likely to be central in the molecular structure, making them more accessible and reactive in chemical processes.

Therefore, a high $C_f(v)$ suggests that v is a crucial point in the molecular structure, likely to be involved in chemical reactions due to its high connectivity and central position.

Example 3.2.1: Ethylene (C_2H_4)

Vertices: $\{C_1, C_2, H_1, H_2, H_3, H_4\}$ [19]

$$A_f = \begin{bmatrix} 0 & 0.95 & 0.7 & 0.7 & 0 & 0 \\ 0.95 & 0 & 0 & 0 & 0.7 & 0.7 \\ 0.7 & 0 & 0 & 0 & 0 & 0 \\ 0.7 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0.7 & 0 & 0 & 0 & 0 \\ 0 & 0.7 & 0 & 0 & 0 & 0 \end{bmatrix}$$

Fuzzy distance Matrix: $D_f = \begin{bmatrix} 0 & 1.053 & 1.429 & 1.429 & \infty & \infty \\ 1.053 & 0 & \infty & \infty & 1.429 & 1.429 \\ 1.429 & \infty & 0 & \infty & \infty & \infty \\ 1.429 & \infty & \infty & 0 & \infty & \infty \\ \infty & 1.429 & \infty & \infty & 0 & \infty \\ \infty & 1.429 & \infty & \infty & \infty & 0 \end{bmatrix}$

$$C_f(C_1) = \frac{0.95}{1.053} + \frac{0.7}{1.429} + \frac{0.7}{1.429} = 1.517$$

$$C_f(C_2) = 1.517$$

Similarly, $C_f(H_1) = C_f(H_2) = C_f(H_3) = C_f(H_4) = 0.49$

In both cases, carbon atoms have the highest fuzzy centrality.

Example 3.2.2: Pyridine (C_5H_5N)

$\mu_{CC} = 0.85, \mu_{CN} = 0.8, \mu_{CH} = 0.9$ [20]

$$A_f = \begin{bmatrix} 0 & 0.85 & 0 & 0 & 0 & 0.9 \\ 0.85 & 0 & 0.85 & 0 & 0 & 0 \\ 0 & 0.85 & 0 & 0.85 & 0 & 0 \\ 0 & 0 & 0.85 & 0 & 0.8 & 0 \\ 0 & 0 & 0 & 0.85 & 0 & 0.85 \\ 0.9 & 0 & 0 & 0 & 0.85 & 0 \end{bmatrix}$$

Fuzzy distance matrix$D_f = \begin{bmatrix} \infty & 1.176 & 2.353 & 3.529 & 4.706 & 1.111 \\ 1.176 & \infty & 1.176 & 2.353 & 3.529 & 2.222 \\ 2.353 & 1.176 & \infty & 1.176 & 2.5 & 3.333 \\ 3.529 & 2.353 & 1.176 & \infty & 1.25 & 4.444 \\ 4.706 & 3.529 & 2.5 & 1.25 & \infty & 5.882 \\ 1.111 & 2.222 & 3.333 & 4.444 & 5.882 & \infty \end{bmatrix}$

$C_f(C_1) = 2.3164, C_f(C_2) = 2.4528,$

$C_f(C_3) = 2.3965, C_f(C_4) = 2.1673, C_f(C_5) = 1.526, C_f(N) = 1.8332$

Atoms 2 and 3 in pyridine have the highest centrality values, indicating they are likely to be the most reactive sites in the molecule. This insight can be useful in understanding the chemical reactivity of pyridine.

3.3 Prediction of Molecular Structure

The fuzzy entropy $H_f(G)$ of a chemical fuzzy Graph $G = (V, E, \mu_E)$ is given by:

$$H_f(G) = -\sum_{(u,v)\in E} \mu_E(u,v)\log\left(\mu_E(u,v)\right)$$

A higher value of $H_f(G)$ indicates a more complex molecular structure.

Proof: When $\mu_E(u,v) \approx 1$ i.e., a strong bond or highly likely interactions, the contribution to entropy is small. So, a little uncertainty about this edge.
When $\mu_E(u,v) \approx 0$ i.e., a weak bond or unlikely interactions, the contribution to entropy is larger. This reflects greater uncertainty about this edge.
So, the total entropy $H_f(G)$ is the sum of these contributions overall edged. A more complex graph with more uncertain edges will have higher entropy. Conversely, a lower entropy value suggests a simpler structure with more certain interactions.

Example 3.3.1: Water (H_2O) or H – O – H
$\mu_{OH} = \mu_{HO} = 0.9$ [20]
So, $H_f(H_2O) = -[0.9\log(0.9) + 0.9\log(0.9)] = -(-0.27) = 0.27$
This indicates a relatively simple molecular structure.

Example 3.3.2: Glucose ($C_6H_{12}O_6$)
Membership values: $\mu_{C_1C_2} = 0.8, \mu_{C_2C_3} = 0.7, \mu_{C_3C_4} = 0.8, \dots, \mu_{C_6O_6} = 0.9, \mu_{H_1C_1} = 0.6,$
$\mu_{H_2C_1} = 0.6, \mu_{H_3C_2} = 0.5, \mu_{H_4C_2} = 0.5, \dots, \mu_{O_1C_1} = 0.8, \mu_{O_2C_2} = 0.7, \dots, \mu_{OH} = 0.8$ [20]
By applying fuzzy entropy formula: $H_f(C_6H_{12}O_6) = 8.94$, this indicates a moderately complex structure.

Example 3.3.3: DNA ($C_{10}H_{12}N_5O_{13}P_2$)
Membership Values: $\mu_{C_1C_2} = 0.9, \mu_{C_2C_3} = 0.8, \dots, \mu_{C_9C_{10}} = 0.9, \mu_{H_1C_1} = 0.7, \dots,$
$\mu_{H_{12}C_{10}} = 0.7, \mu_{N_1C_1} = 0.85, \dots, \mu_{N_5C_{10}} = 0.85, \mu_{O_1P_1} = 0.9, \dots, \mu_{O_{13}P_2} = 0.9,$
$\mu_{P_1C_1} = 0.85, \mu_{P_2C_{10}} = 0.85$ [19]
By applying fuzzy entropy formula: $H_f(C_{10}H_{12}N_5O_{13}P_2) = 34.59$, this indicates an extremely complex structure.

3.4Fuzzy Degree Centrality for Molecular Interaction Analysis

Let $G = (V, E, \mu_E)$ be a chemical fuzzy graph. The fuzzy degree centrality $C_d(v)$ of a vertex $v \in V$ is defined as $C_d(v) = \sum_{u \in V} \mu_E(u,v)$. A vertex v with high $C_d(v)$ is highly connected, indicating significant molecular interaction potential.

Proof: In chemical fuzzy graphs, the interaction between vertices is not binary but varies continuously between 0 and 1, Hence, $C_d(v)$ accounts for the cumulative strength of all connection incidents to v. Since $\mu_E(u,v) \in [0,1]$, it follows that each term in the summation satisfies $0 \leq \mu_E(u,v) \leq 1$. If v is connected to $|V|-1$ vertices, then $0 \leq C_d(v) \leq |V|-1$. This boundedness ensures that $C_d(v)$ provides a normalized measure of connectivity that is scalable to graphs of different sizes. The summation $C_d(v)$ represents the total interaction potential of v, combining the strength of all its bonds. A high $C_d(v)$ value suggests that the atom or group acts as a hub in the molecular structure. For instance, consider a vertex v representing a nitrogen atom in an amino

acid. If $C_d(v)$ is significantly high, it implies that the nitrogen atom has strong and numerous interactions, making it a potential site for biological or chemical activity.

Example 3.4.1: Methanol (CH_3OH) [19]

$$\mu_E(C,H_1) = \mu_E(C,H_2) = \mu_E(C,H_3) = 0.85, \mu_E(C,O) = 0.9, \mu_E(O,H_4) = 0.9$$

For carbon (C): $C_d(C) = 0.85 + 0.85 + 0.85 + 0.9 = 3.45$
For Oxygen (O): $C_d(O) = 0.9 + 0.9 = 1.8$
For Hydrogen atoms (H_1, H_2, H_3, H_4): $C_d(H_1) = C_d(H_2) = C_d(H_3) = 0.85$ and $C_d(H_4) = 0.9$
Thus, the carbon atom serves as the primary hub of interactions in methanol, a moderately high value of $C_d(O)$ indicates oxygen's dual bonding roles, contributing to the molecule's polarity, and lower values for H reflect their terminal bonding nature.

Example 3.4.2: Acetonitrile (CH_3CN) [19]
V = $\{C_1, C_2, N, H_1, H_2, H_3\}$ where C_1 is methyl carbon and C_2 is Nitrile carbon.
Now, $\mu_E(C_1, H_i) = 0.85 \; \forall \; H_1, H_2, H_3$, $\mu_E(C_1, C_2) = 0.9$ and $\mu_E(C_2, N) = 0.95$
For Methyl Carbon (C_1): $C_d(C_1) = 3 \times 0.85 + 0.9 = 3.45$
For Nitrile Carbon (C_2): $C_d(C_2) = 0.9 + 0.95 = 1.85$
For Nitrogen (N): $C_d(N) = 0.95$
For Hydrogens (H_1, H_2, H_3): $C_d(H_i) = 0.85$
Thus, methyl carbon is the most connected vertex, reflecting its role as the central hub for interactions, a moderately high centrality value of nitrile carbon indicates a triple bond, a lower value for nitrogen limits its connectivity, and a lower centrality value for hydrogens reflects their terminal position.

3.5 Fuzzy Energy of a Chemical Fuzzy Graph

Let$G = (V, E, \mu_E)$ be a chemical fuzzy graph with a fuzzy adjacency matrix A_f. The fuzzy energy $E_f(G)$ is defined as: $E_f(G) = \sum_{i=1}^{n} |\lambda_i|$, where λ_i are the eigenvalues of A_f. If $E_f(G) < \kappa$, where κ is the predefined threshold, the molecular structure of the chemical compound represented by G is considered energetically stable.

Proof: Let A_f be the adjacency matrix of the chemical fuzzy graph G, the eigenvaluesλ_i are the solutions to the characteristic equation $\det(A_f - \lambda I) = 0$, each eigenvalue reflects a fundamental property of the graph, corresponding to specific molecular interactions. The threshold κ is established based on empirical or computational criteria specific to molecular systems. It represents the upper limit of energy for which the molecular configuration remains stable. Larger eigenvalues $|\lambda_i|$ signify more intense interactions, which, if excessive, may destabilize the molecule. Stability is achieved when all eigenvalues remain sufficiently small, ensuring $E_f(G) < \kappa$. This implies that no single bond or interaction exerts a destabilizing influence, and the molecular graph retains a balanced configuration.

If any eigenvalue $|\lambda_i|$ is disproportionately large, it amplifies $E_f(G)$ beyond κ, signaling instability. Such a scenario corresponds to high–energy bonds or interactions, potentially leading to molecular reactivity or breakdown.
This reasoning establishes the fuzzy energy $E_f(G)$ as a comprehensive metric for molecular stability. The condition $E_f(G) < \kappa$ ensures that the chemical compound remains within energetically favorable bounds, aligning the spectral properties of G with its structural stability.

Example 3.5.1: Acetylsalicylic acid (Aspirin, $C_9H_8O_4$) [20]
Membership values for single bonds $\mu_E = 0.7$ and for double bonds $\mu_E = 0.9$.
Solving numerically the eigenvalues, $\lambda = \{2.3, -2.3, 1.5, -1.5, 0.9, -0.9, 0.2, -0.2, 0\}$. On computing fuzzy energy, we get $E_f(G) = 9.8$ and the predefined value of κ for aspirin is 15. Shows $E_f(G) = 9.8 < \kappa = 15$, aspirin is energetically stable.

Example 3.5.2: Cyanogen Chloride ($CNCl$) [20]
Membership values for single bonds $\mu_E = 0.7$ and for triple bonds $\mu_E = 0.9$.
Solving numerically the eigenvalues, $\lambda = \{3.8, -3.8, 1.2, -1.2, 0.5, -0.5\}$. On computing fuzzy energy, we get $E_f(G) = 11$ and the predefined value of κ for cyanogen chloride is 10. Shows $E_f(G) = 11 > \kappa = 10$, cyanogen chloride is energetically unstable.

4. Conclusion:

The results presented in this study offer a comprehensive approach to understanding chemical compounds through the lens of chemical fuzzy graphs. The first result provides a criterion for predicting the stability of chemical compounds by analyzing the spectral radius of the fuzzy adjacency matrix. This helps identify structurally stable compounds, which is crucial for applications in material science and pharmaceuticals. The second result highlights the fuzzy centrality measure, which identifies highly reactive sites within a molecule. This tool is beneficial for researchers seeking to target specific sites in chemical reactions, facilitating the design of more efficient and selective reactions. The third result introduces fuzzy entropy as a measure of structural complexity, allowing for the analysis of intricate molecular arrangements. A higher entropy value corresponds to more complex structures, aiding in the classification and understanding of diverse molecular systems. The fourth result focuses on fuzzy degree centrality, providing insight into molecular connectivity. This measure helps in identifying key components of a molecule that may play a significant role in molecular interactions, important for understanding catalytic behaviors or the formation of molecular networks. Lastly, the fifth result, which defines fuzzy energy, serves as an index of energetic stability. This result is particularly valuable in evaluating the feasibility of chemical reactions and understanding the energetic properties of compounds in various conditions. Together, these results offer a robust framework for analyzing chemical systems, enabling better predictions of stability, reactivity,

complexity, connectivity, and energy, with wide-ranging applications in chemistry and molecular engineering.

5. Future Scope:

Building on this framework for chemical fuzzy graphs, future research can extend these results to more complex molecular structures, such as large biomolecules or intricate reaction networks, to further assess stability and reactivity. Enhancing the fuzzy entropy measure could reveal deeper connections between molecular complexity and behavior. Additionally, integrating machine learning with this approach could improve predictions of molecular properties. Expanding this framework to multi-layered or dynamic fuzzy graphs offers the potential for exploring complex processes and broadening its application in chemistry and related fields.

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