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Original Study

Remarks on bipolar cubic fuzzy graphs and its chemical applications

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Abstract

In theoretical chemistry, fuzzy molecular graphs can be used to model chemical molecular structures with uncertainty information, where the vertex membership function and edge membership function describe the uncertainty of atoms and chemical bonds respectively. This paper studies chemical topological index of bipolar cubic fuzzy graphs. The new concepts and theorems are given in terms of graph theory and fuzzy set theory approaches and several theoretical conclusions on bipolar Wiener index of bipolar cubic fuzzy graphs are determined. Furthermore, we apply it in chemical science and calculate the bipolar Wiener index of dimethyltryptamine and hallucinogen which are modelled by bipolar cubic fuzzy graphs.

Keywords: Graph, fuzzy graph, bipolar cubic fuzzy graph, bipolar Wiener index
AMS 2020 codes: 05C72; 05C92.

1 Introduction

An important challenge of the database is how to characterize the previous interrelationships of the data. Graph and hypergraph models are important tasks for the description of data relationships. However, in practical applications, there are a large number of scenarios that make data and the relationship between data uncertain and these uncertainties cannot be collapsed. Therefore, to describe this kind of non-collapsible uncertainty, the conventional probability and statistics trick cannot be used, but the membership function (MF) of vertices and edges should be employed to characterize it (Gao et al. [1], Perumal [2], Ullah et al. [3], Gayathri et al. [4], Nie et al. [5] and Binu et al. [6] for more details on fuzzy graph and its applications).

Chemical graph theory is a key branch of theoretical chemistry, whose main task is to estimate the performance of compounds by means of the calculation of topological parameter of molecular structures, where the atoms and chemical bonds of compounds are represented by vertices and edges respectively. The results

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obtained from chemical graph theory are consistent with experiments, which makes this method popular in chemistry, materials science, pharmacy and other related fields (Gao et al. [7] and Lu et al. [8]).

As the earliest chemical topological index, Wiener index is used to predict the melting and boiling points of compounds. In the past decades, researches have witnessed the emergence of various variants of Wiener index and its polar graph and extreme value problems have also been fully studied. Czabarka et al. [9] determined the extreme Wiener index of 3-connected quadrangulations and 5-connected triangulations. Kathiresan and Parameswaran [10] yielded the Wiener index of the generalized odd complete graphs. Asir and Rabikka [11] computed the Wiener index of zero-divisor graph of Z_n. Asir et al. [12] studied the Wiener and hyper Wiener index of unit graph associated with a commutative ring. Pandey and Patra [13] characterized the extreme Wiener index of graphs with n vertices and k pendant vertices. More related contributions in Wiener index can be referred to Zhang et al. [14] and Dobrynin [15]. More engineering applications can be referred to Umar et al. [16], Ayub et al. [17], Sabir et al. [18], Ayub et al. [19], Shah et al. [20], Shah et al. [21], Sabir et al. [22], Sabir and Ben Said [23] and Sabir [24].

Recently, Shi et al. [25] studied the Wiener index of cubic fuzzy graphs and applied it in chemical science. Inspired by this work, we studied the bipolar Wiener index (BWI) of bipolar cubic fuzzy graphs (BCFGs). The originality of this work is reflected in the following aspects:

1. We extended the Wiener index in BCFG setting and derived the theoretical analysis from a mathematical perspective.
2. We applied the new concept to chemical engineering and specifically computed the bipolar Wiener index of DMT and hallucinogen.

2 Extended concepts

For two bipolar interval-valued fuzzy numbers (BIVFNs) $A = ([p_1^P, q_1^P], [p_1^N, q_1^N])$ and $B = ([p_2^P, q_2^P], [p_2^N, q_2^N])$ where $0 \le p_i^P \le q_i^P \le 1$ and $-1 \le p_i^N \le q_i^N \le 0$ for $i \in \{1,2\}$, we have

$$A \cup B = ([p_1^P \vee p_2^P, q_1^P \vee q_2^P], [p_1^N \wedge p_2^N, q_1^N \wedge q_2^N]),$$

$$A \cap B = ([p_1^P \wedge p_2^P, q_1^P \wedge q_2^P], [p_1^N \vee p_2^N, q_1^N \vee q_2^N]).$$

The bipolar cubic fuzzy set (BCFS) is denoted by $X = ([p^P, q^P], [p^N, q^N]), (r^P, r^N)$ where $0 \le p^P \le q^P \le 1, -1 \le p^N \le q^N \le 0$, $0 \le r^P \le 1$ and $-1 \le r^N \le 0$. X is called the interval if $r^P \in [p^P, q^P]$ and $r^N \in [p^N, q^N]$; and X is called external if $r^P \notin [p^P, q^P]$ and $r^N \notin [p^N, q^N]$. For two positive intervals $[p_1^P, q_1^P]$ and $[p_2^P, q_2^P]$, we have

$$[p_1^P, q_1^P] \le [p_2^P, q_2^P] \Leftrightarrow p_1^P \le p_2^P, q_1^P \le q_2^P.$$

For two negative intervals $[p_1^N, q_1^N]$ and $[p_2^N, q_2^N]$, we have

$$[p_1^N, q_1^N] \le [p_2^N, q_2^N] \Leftrightarrow p_1^N \le p_2^N, q_1^N \le q_2^N.$$

Suppose V is a vertex set, $A = \{([\alpha_A^P(v), \beta_A^P(v)], [\alpha_A^N(v), \beta_A^N(v)], (\gamma_A^P(v), \gamma_A^N(v))) : v \in V\}$ is a BCFS defined on V and $B = \{([\alpha_B^P(v,v'), \beta_B^P(v,v')], [\alpha_B^N(v,v'), \beta_B^N(v,v')], (\gamma_B^P(v,v'), \gamma_B^N(v,v'))) : (v,v') \in V^2\}$ is a BCFS defined

on V^2. $G=(V,A,B)$ is a bipolar cubic fuzzy graph (BCFG), where

$$[\alpha_B^P(v,v'),\beta_B^P(v,v')]\leq \min\{[\alpha_A^P(v),\beta_A^P(v)],[\alpha_A^P(v'),\beta_A^P(v')]\},$$

$$[\alpha_B^N(v,v'),\beta_B^N(v,v')]\geq \max\{[\alpha_A^N(v),\beta_A^N(v)],[\alpha_A^N(v'),\beta_A^N(v')]\},$$

$$\gamma_B^P(v,v')\leq \min\{\gamma_A^P(v),\gamma_A^P(v')\},$$

$$\gamma_B^N(v,v')\geq \max\{\gamma_A^N(v),\gamma_A^N(v')\}.$$

If $vv'\notin E(G)$, then $[\alpha_B^P(v,v'),\beta_B^P(v,v')]=[\alpha_B^N(v,v'),\beta_B^N(v,v')]=[0,0]$ and $\gamma_B^P(v,v')=\gamma_B^N(v,v')=0$. We say G is a complete BCFG if for arbitrary $v,v'\in V(G)$, we have

$$[\alpha_B^P(v,v'),\beta_B^P(v,v')]=\min\{[\alpha_A^P(v),\beta_A^P(v)],[\alpha_A^P(v'),\beta_A^P(v')]\},$$

$$[\alpha_B^N(v,v'),\beta_B^N(v,v')]=\max\{[\alpha_A^N(v),\beta_A^N(v)],[\alpha_A^N(v'),\beta_A^N(v')]\},$$

$$\gamma_B^P(v,v')=\min\{\gamma_A^P(v),\gamma_A^P(v')\},$$

$$\gamma_B^N(v,v')=\max\{\gamma_A^N(v),\gamma_A^N(v')\}.$$

A path in BCFG is a sequence of $v_1,v_2,\cdots,v_k$ such that $\alpha_B^P(v_{i-1},v_i)>0$, $\beta_B^P(v_{i-1},v_i)>0$, $\gamma_B^P(v_{i-1},v_i)>0$, $\alpha_B^N(v_{i-1},v_i)<0$, $\beta_B^N(v_{i-1},v_i)<0$ and $\gamma_B^N(v_{i-1},v_i)<0$ for $i\in\{2,\cdots,k\}$. The strength of path P is denoted by $(S^P(P),S^N(P))$, where $S^P(P)$ and $S^N(P)$ are positive strength and negative strength of P respectively, such that

$$S^P(P)=((\wedge_{i=2}^k\alpha_B^P(v_{i-1},v_i),\wedge_{i=2}^k\beta_B^P(v_{i-1},v_i))),\wedge_{i=2}^k\gamma_B^P(v_{i-1},v_i),$$

$$S^P(N)=((\vee_{i=2}^k\alpha_B^N(v_{i-1},v_i),\vee_{i=2}^k\beta_B^N(v_{i-1},v_i))),\vee_{i=2}^k\gamma_B^N(v_{i-1},v_i).$$

The positive strength (resp. negative strength) of connectivity between v and v' is formulated by $C^{P,\infty}(v,v')$ (resp. $C^{N,\infty}(v,v')$). They are defined by

$$C^{P,\infty}(v,v')=([C_\alpha^{P,\infty}(v,v'),C_\beta^{P,\infty}(v,v')],C_\gamma^{P,\infty}(v,v')),$$

$$C^{N,\infty}(v,v')=([C_\alpha^{N,\infty}(v,v'),C_\beta^{N,\infty}(v,v')],C_\gamma^{N,\infty}(v,v')),$$

where

$$C_\alpha^{P,\infty}(v,v')=\max_k\{\wedge_{i=2}^k\alpha_B^P(v_{i-1},v_i)\},$$

$$C_\beta^{P,\infty}(v,v')=\max_k\{\wedge_{i=2}^k\beta_B^P(v_{i-1},v_i)\},$$

$$C_\gamma^{P,\infty}(v,v')=\max_k\{\wedge_{i=2}^k\gamma_B^P(v_{i-1},v_i)\},$$

$$C_\alpha^{N,\infty}(v,v')=\min_k\{\vee_{i=2}^k\alpha_B^N(v_{i-1},v_i)\},$$

$$C_\beta^{N,\infty}(v,v')=\min_k\{\vee_{i=2}^k\beta_B^N(v_{i-1},v_i)\},$$

$$C_\gamma^{N,\infty}(v,v')=\min_k\{\vee_{i=2}^k\gamma_B^N(v_{i-1},v_i)\}.$$

Edge vv' in BCFG is positive strong (PS) if $\alpha_B^P(v,v') \geq C_\alpha^{P,\infty}(v,v')$, $\beta_B^P(v,v') \geq C_\beta^{P,\infty}(v,v')$ and $\gamma_B^P(v,v') \geq C_\gamma^{P,\infty}(v,v')$; vv' in BCFG is negative strong (NS) if $\alpha_B^N(v,v') \leq C_\alpha^{N,\infty}(v,v')$, $\beta_B^N(v,v') \leq C_\beta^{N,\infty}(v,v')$ and $\gamma_B^N(v,v') \leq C_\gamma^{N,\infty}(v,v')$; furthermore, vv' in BCFG is bipolar strong (BS) if it is both PS and NS.

More specifically, edge vv' in BCFG is positive α-strong (α-PS) if $\alpha_B^P(v,v') > C_\alpha^{P,\infty}(v,v')$, $\beta_B^P(v,v') > C_\beta^{P,\infty}(v,v')$ and $\gamma_B^P(v,v') > C_\gamma^{P,\infty}(v,v')$; edge vv' in BCFG is positive β-strong (β-PS) if $\alpha_B^P(v,v') = C_\alpha^{P,\infty}(v,v')$, $\beta_B^P(v,v') = C_\beta^{P,\infty}(v,v')$ and $\gamma_B^P(v,v') = C_\gamma^{P,\infty}(v,v')$; edge vv' in BCFG is positive δ-edge (δ-PE) if $\alpha_B^P(v,v') < C_\alpha^{P,\infty}(v,v')$, $\beta_B^P(v,v') < C_\beta^{P,\infty}(v,v')$ and $\gamma_B^P(v,v') < C_\gamma^{P,\infty}(v,v')$; edge vv' in BCFG is negaive α-strong (α-NS) if $\alpha_B^N(v,v') < C_\alpha^{N,\infty}(v,v')$, $\beta_B^N(v,v') < C_\beta^{N,\infty}(v,v')$ and $\gamma_B^N(v,v') < C_\gamma^{N,\infty}(v,v')$; edge vv' in BCFG is negative β-strong (β-NS) if $\alpha_B^N(v,v') = C_\alpha^{N,\infty}(v,v')$, $\beta_B^N(v,v') = C_\beta^{N,\infty}(v,v')$ and $\gamma_B^N(v,v') = C_\gamma^{N,\infty}(v,v')$; edge vv' in BCFG is negative δ-edge (δ-NE) if $\alpha_B^N(v,v') > C_\alpha^{N,\infty}(v,v')$, $\beta_B^N(v,v') > C_\beta^{N,\infty}(v,v')$ and $\gamma_B^N(v,v') > C_\gamma^{N,\infty}(v,v')$; edge vv' in BCFG is α-strong (α-S) if it is both positive α-strong and negative α-strong; edge vv' in BCFG is β-strong if it is both positive β-strong and negative β-strong; edge vv' in BCFG is δ-edge if it is both positive δ-edge and negative δ-edge. BCFG is called a

- positive α-saturated (PαS) if every vertex incidents at least one α-PS edge;
- positive β-saturated (PβS) if every vertex incidents at least one β-PS edge;
- positive saturated (PS) if it is both PαS and PβS;
- negative α-saturated (NαS) if every vertex incidents at least one α-NS edge;
- negative β-saturated (NβS) if every vertex incidents at least one β-NS edge;
- negative saturated (NS) if it is both NαS and NβS.

The bipolar Wiener index of a BCFG $G = (V,A,B)$ is formulated by

$$W(G) = (([W_\alpha^P(G), W_\beta^P(G)], [W_\alpha^N(G), W_\beta^N(G)]), (W_\gamma^P(G), W_\gamma^N(G))),$$

where

$$\begin{aligned}
W_\alpha^P(G) &= \sum_{v,v' \in V} \alpha_A^P(v)\alpha_A^P(v')d_\alpha^P(v,v'),\\
W_\beta^P(G) &= \sum_{v,v' \in V} \beta_A^P(v)\beta_A^P(v')d_\beta^P(v,v'),\\
W_\gamma^P(G) &= \sum_{v,v' \in V} \gamma_A^P(v)\gamma_A^P(v')d_\gamma^P(v,v'),\\
W_\alpha^N(G) &= \sum_{v,v' \in V} \alpha_A^N(v)\alpha_A^N(v')d_\alpha^N(v,v'),\\
W_\beta^N(G) &= \sum_{v,v' \in V} \beta_A^N(v)\beta_A^N(v')d_\beta^N(v,v'),\\
W_\gamma^N(G) &= \sum_{v,v' \in V} \gamma_A^N(v)\gamma_A^N(v')d_\gamma^N(v,v').
\end{aligned}$$

Furthermore, the connectivity index of BCFG G is denoted by

$$CI(G) = (([CI_\alpha^P(G), CI_\beta^P(G)], [CI_\alpha^N(G), CI_\beta^N(G)]), (CI_\gamma^P(G), CI_\gamma^N(G))),$$

where

$$CI_\alpha^P(G) = \sum_{v,v' \in V} \alpha_A^P(v)\alpha_A^P(v')C_\alpha^{P,\infty}(v,v'),$$

$$CI_{\beta}^{P}(G) = \sum_{v,v' \in V} \beta_{A}^{P}(v)\beta_{A}^{P}(v')C_{\beta}^{P,\infty}(v,v'),$$

$$CI_{\gamma}^{P}(G) = \sum_{v,v' \in V} \gamma_{A}^{P}(v)\gamma_{A}^{P}(v')C_{\gamma}^{P,\infty}(v,v'),$$

$$CI_{\alpha}^{N}(G) = \sum_{v,v' \in V} \alpha_{A}^{N}(v)\alpha_{A}^{N}(v')C_{\alpha}^{N,\infty}(v,v'),$$

$$CI_{\beta}^{N}(G) = \sum_{v,v' \in V} \beta_{A}^{N}(v)\beta_{A}^{N}(v')C_{\beta}^{N,\infty}(v,v'),$$

$$CI_{\gamma}^{N}(G) = \sum_{v,v' \in V} \gamma_{A}^{N}(v)\gamma_{A}^{N}(v')C_{\gamma}^{N,\infty}(v,v').$$

3 Theoretical conclusions

This section aims to extend the conclusions in Shi et al. [25] and we skip the detailed proofs since they follow the tricks in [25]. The solution methodology is based on graph theory and fuzzy set theory, where the structure analysis is the key approach to get the desired conclusion when it comes to the special graph setting.

Theorem 1. *Let G be a BCFG with $\alpha_{A}^{P}(v) = \beta_{A}^{P}(v) = \gamma_{A}^{P}(v) = 1$ and $\alpha_{A}^{N}(v) = \beta_{A}^{N}(v) = \gamma_{A}^{N}(v) = -1$ for each $v \in V(G)$. Assume $n = |V(G)|$ and $m = |E(G)|$. Set*

$$p^{P} = \min\{\alpha_{B}^{P}(v,v') : \alpha_{B}^{P}(v,v') \geq C_{\alpha}^{P,\infty}(v,v')\},$$

$$q^{P} = \min\{\beta_{B}^{P}(v,v') : \beta_{B}^{P}(v,v') \geq C_{\beta}^{P,\infty}(v,v')\},$$

$$r^{P} = \min\{\gamma_{B}^{P}(v,v') : \gamma_{B}^{P}(v,v') \geq C_{\gamma}^{P,\infty}(v,v')\},$$

$$p^{N} = \max\{\alpha_{B}^{N}(v,v') : \alpha_{B}^{N}(v,v') \leq C_{\alpha}^{N,\infty}(v,v')\},$$

$$q^{N} = \max\{\beta_{B}^{N}(v,v') : \beta_{B}^{N}(v,v') \leq C_{\beta}^{N,\infty}(v,v')\},$$

$$r^{N} = \max\{\gamma_{B}^{N}(v,v') : \gamma_{B}^{N}(v,v') \leq C_{\gamma}^{N,\infty}(v,v')\}.$$

Then, we have

$$W_{\alpha}^{P}(G) \geq p^{P}[n(n-1) - m],$$

$$W_{\beta}^{P}(G) \geq q^{P}[n(n-1) - m],$$

$$W_{\gamma}^{P}(G) \geq r^{P}[n(n-1) - m],$$

$$W_{\alpha}^{N}(G) \leq p^{N}[n(n-1) - m],$$

$$W_{\beta}^{N}(G) \leq q^{N}[n(n-1) - m],$$

$$W_{\gamma}^{N}(G) \leq r^{N}[n(n-1) - m].$$

Theorem 2. *Suppose G and G' are two BCFGs. If $G \cong G'$, then $W(G) = W(G')$.*

Theorem 3. *If a BCFG G is complete, then $W(G) = CI(G)$.*

Theorem 4. *Suppose G is a complete BCFG with n vertices. Set* $\alpha_A^P(v) = p_i^P$, $\beta_A^P(v) = q_i^P$, $\gamma_A^P(v) = r_i^P$, $\alpha_A^N(v) = p_i^N$, $\beta_A^N(v) = q_i^N$ *and* $\gamma_A^N(v) = r_i^N$ *for* $i \in \{1, \cdots, n\}$ *such that* $p_1^P \leq p_2^P \leq \cdots \leq p_n^P$, $q_1^P \leq q_2^P \leq \cdots \leq q_n^P$, $r_1^P \leq r_2^P \leq \cdots \leq r_n^P$, $p_1^N \geq p_2^P \geq \cdots \geq p_n^N$, $q_1^N \geq q_2^N \geq \cdots \geq q_n^N$, $r_1^N \geq r_2^N \geq \cdots \geq r_n^N$. *Then*

$$W_\alpha^P(G) = \sum_{i=1}^{n-1} (p_i^P)^2 \sum_{j=i+1}^{n} p_j^P,$$

$$W_\beta^P(G) = \sum_{i=1}^{n-1} (q_i^P)^2 \sum_{j=i+1}^{n} q_j^P,$$

$$W_\gamma^P(G) = \sum_{i=1}^{n-1} (r_i^P)^2 \sum_{j=i+1}^{n} r_j^P,$$

$$W_\alpha^N(G) = \sum_{i=1}^{n-1} (p_i^N)^2 \sum_{j=i+1}^{n} p_j^N,$$

$$W_\beta^N(G) = \sum_{i=1}^{n-1} (q_i^N)^2 \sum_{j=i+1}^{n} q_j^N,$$

$$W_\gamma^N(G) = \sum_{i=1}^{n-1} (r_i^N)^2 \sum_{j=i+1}^{n} r_j^N.$$

Theorem 5. *Suppose a BCFG G is a tree with at least three vertices. Then*

$$CI_\alpha^P(G) \leq W_\alpha^P(G),$$

$$CI_\beta^P(G) \leq W_\beta^P(G),$$

$$CI_\gamma^P(G) \leq W_\gamma^P(G),$$

$$CI_\alpha^N(G) \geq W_\alpha^N(G),$$

$$CI_\beta^N(G) \geq W_\beta^N(G),$$

$$CI_\gamma^N(G) \geq W_\gamma^N(G).$$

Theorem 6. *Let G be a BCFG. For* $v, v' \in V(G)$, *let* $P^P(v,v')$ *be the path between v and* v' *with minimum sum of positive MF values among the shortest paths and* $P^N(v,v')$ *be the path between v and* v' *with maximum sum of negative MF values among the shortest paths.*

(1) If $st \in E(G)$ *is a positive strong edge in G such that* $\{s,t\} \neq \{v,v'\}$ *and st is not a part in* $P^P(v,v')$, *then* $W^P(G-st) \neq W^P(G)$.

(2) If st is not a PS edge, then $W^P(G-st) = W^P(G)$.

(3) If $st \in E(G)$ *is a negative strong edge in G such that* $\{s,t\} \neq \{v,v'\}$ *and st is not a part in* $P^N(v,v')$, *then* $W^N(G-st) \neq W^N(G)$.

(4) If st is not a NS edge, then $W^N(G-st) = W^N(G)$.

Theorem 7. *Suppose a BCFG G is a cycle. Then,*

(1) G is positive satisfied if and only if $n \equiv 0 (mod 2)$ *and* α*-PS edge and* β*-PS edge appear consecutively.*

(2) G is negative satisfied if and only if $n \equiv 0 (mod 2)$ *and* α*-NS edge and* β*-NS edge appear consecutively.*

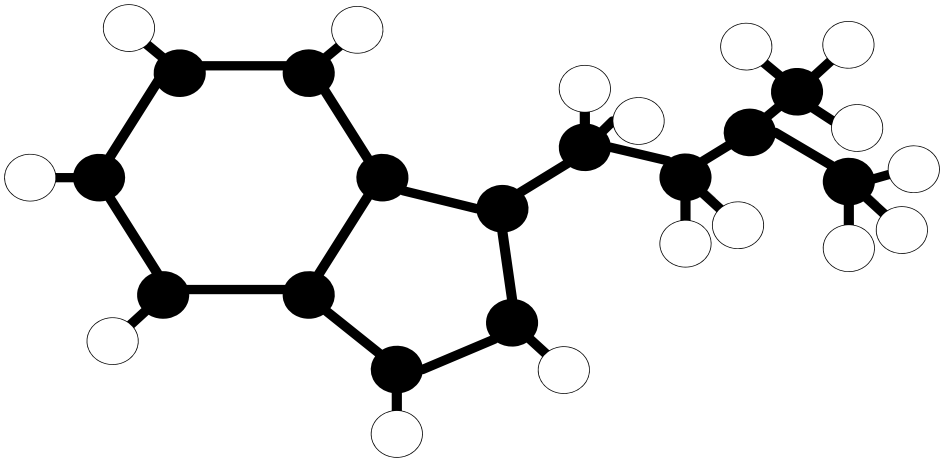


Fig. 1 The Structure of DMT.

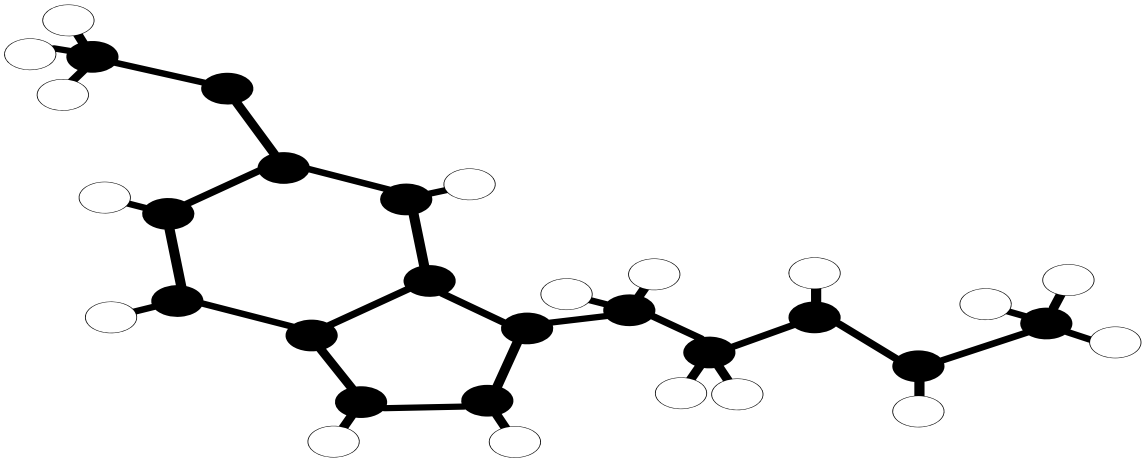


Fig. 2 The Structure of hallucinogen.

4 Chemical application

Dimethyltryptamine (in short, DMT) is an organic compound with the chemical formula $C_{12}H_{16}N_2$. It is the first class of psychotropic drugs and belongs to tryptamine hallucinogens. It exists both in plants and human body in trace amounts. It is catalyzed by tryptamine-N-methyltransferase, but its specific function is unknown. It is structurally similar to neurotransmitters, serotonin and other tryptamine-like hallucinogens 5-methoxydimethyltryptamine, bufotryptamine and dephosphorylated psilocybin.

DMT, like melatonin, is a hallucinogen that can cause hallucinations after injection. Its molecular structure is shown in the figure below. It should be noted that the figures given in Figure 1 and Figure 2 are the general structures of the two compounds and their real structures are much more complicated. However, we target at more specific complex structures in our actual calculations.

A key issue in modelling is how to determine the membership functions of atoms and chemical bonds. According to the suggestions of domain experts, we describe the value of the vertex membership function from

the following angles: (1) Types of atoms; (2) The offset angle of atoms; (3) Spin type; (4) Orbital stability. Regarding the membership function of the edge, we describe it from the following perspectives: (1) the type of atomic bond; (2) the strength of the connection; (3) the energy state of the chemical bond. Specifically, we first give the membership function of each aspect separately and then the domain experts give the weights of each aspect and finally we weight the membership function obtained by each sub-item. For the four types of membership functions of vertices, the weight coefficients are 0.5, 0.2, 0.2, 0.1. For the three types of membership functions of edges, the weight coefficients are 0.4, 0.3 and 0.3. It is worth noting that after the membership function of the edge is weighted, it needs to be compared with the membership function values of the vertices at both ends. The positive part takes the smallest value while the negative part takes the largest value. Finally, the program runs in Matlab and gets the corresponding results.

As a result, DMT has bipolar Winer index (([0.81,0.89],[-0.68,-0.32]),(0.31,-0.43)) and hallucinogen has bipolar Winer index (([0.69,0.82],[-0.83,-0.66]),(0.41,-0.83)).

5 Conclusions

In this remark, we propose the new concept of bipolar cubic fuzzy graph and define several new related concepts. The results on cubic fuzzy graph presented in Shi et al. [25] are extended. Finally, we applied the new concept in chemical science, where the bipolar Wiener index of DMT and hallucinogen are calculated. These theoretical theorems have potential practical utilization for the prediction of relevant compound characteristics.

The following topics can be used for future research:

• As there are the various kinds of fuzzy sets on vertex sets and edge sets, bipolar fuzzy graphs have different definitions in different fuzzy set settings. In this paper, we only describe the theoretical properties of the bipolar Wiener index in one class of bipolar fuzzy graphs, while the bipolar Wiener index of bipolar fuzzy graphs in more settings needs to be defined and analyzed.

• For very special graph classes, such as planar graphs, cubic graphs, etc., can the bipolar Wiener index show special theoretical characteristics?

6 Declarations

6.1 Conflict of interest:

The authors hereby declare that there is no conflict of interests regarding the publication of this paper.

6.2 Funding:

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6.3 Authors Contribution:

J.J. L. - Writing original draft; L.L. Z.- Writing review editing; W. G.- Writing review editing.

6.4 Acknowledgement:

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6.5 Data availability statement:

All data that support the findings of this study are included within the article (and any supplementary files).

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