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Computation of the Weighted Wiener Index for Simple Hydrocarbon Molecular Graphs

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Abstract
Topological indices play an essential role in chemical graph theory for modelling molecular structures and predicting physicochemical properties. Among them, the weighted Wiener index (WWI) extends the classical Wiener index by incorporating vertex degrees along with shortest path distances between vertex pairs. In this study, the WWI is computed for simple hydrocarbon molecular graphs such as methane (CH_4), ethane (C_2H_6), and propane (C_3H_8). The contributions of all unordered vertex pairs are evaluated using their respective degrees and distances in the molecular graphs. Based on these calculations, explicit WWI values are obtained for each structure. Furthermore, a general expression for the WWI of this class of hydrocarbons is proposed. Four new theoretical results are established to support the analysis. The findings demonstrate the influence of molecular connectivity on distance-based descriptors and provide insights for future studies in quantitative structure–property relationship (QSPR) modelling.

Keywords: Chemical Graph Theory; Weighted Wiener Index; Molecular Graph; Distance-Based Topological Indices; Hydrocarbon Graphs

1. Introduction

The study of molecular structures using graph theory has become an important area of research in mathematical chemistry. In Chemical Graph Theory, molecules are represented by graphs in which atoms correspond to vertices and chemical bonds correspond to edges. Various numerical parameters derived from these graphs are known as Topological Index. These indices capture structural information about molecules and are widely used in chemical informatics and theoretical chemistry.

One of the earliest and most widely studied distance-based topological indices is the Wiener Index, introduced by Harry Wiener in 1947. The Wiener index is defined as the sum of the shortest path distances between all pairs of vertices in a molecular graph. This index has been successfully applied to correlate molecular structures with physical and chemical properties such as boiling points of paraffin compounds.

Over the years, many variants and extensions of the Wiener index have been proposed in order to better describe molecular structures. One such important extension is the Weighted Wiener Index, in which vertex degrees are incorporated as weights while computing the pairwise distances. This modification allows the index to capture both the connectivity and distance characteristics of the molecular graph.

Topological indices, including the weighted Wiener index, play a significant role in Quantitative Structure–Property Relationship and Quantitative Structure–Activity Relationship studies, where numerical descriptors derived from molecular graphs are used to predict chemical properties and biological activities.

In this work, we investigate the weighted Wiener index of simple hydrocarbon molecular graphs. In particular, the molecular graphs of Methane and Ethane are considered. Using the definition of the weighted Wiener index, the contributions of vertex pairs are computed based on their degrees and shortest path distances. The obtained results demonstrate how molecular connectivity influences the values of distance-based topological descriptors.

2. Literature Review

The concept of the Wiener index, introduced by Wiener [16], represents one of the earliest and most significant topological indices used for correlating molecular structure with physicochemical properties of organic compounds. It is defined as the sum of distances between all unordered pairs of vertices in a molecular graph and has been widely applied in quantitative structure–property relationship (QSPR) studies.

Subsequently, several extensions and generalizations of the Wiener index have been proposed to capture additional structural information. Hosoya [3] introduced alternative topological descriptors for characterizing hydrocarbons, while Gutman and Polansky [2] developed a mathematical framework linking graph theory with organic chemistry. Further theoretical developments and applications of the Wiener index have been extensively discussed by Dobrynin and Gutman (2001).

In recent years, attention has shifted towards weighted and degree-based variants of the Wiener index. Ivanciuc (2000) conducted a comparative QSAR study highlighting the effectiveness of weighted Wiener descriptors in molecular characterization. Later, Ivanciuc et al. (2001) proposed extensions incorporating additional distance-based considerations. More recently, Lin and Zhou (2024) investigated the degree-weighted Wiener index and provided new insights into its mathematical properties. Beyond distance-based molecular graph descriptors, Jarhoumi [7] examined bifurcation-controlled pattern evolution in reaction–diffusion systems for advanced material design, illustrating a different mathematical approach to studying structural behaviour in material systems.

Applications of Wiener-type indices to hydrocarbon structures have also been explored. Pavlović et al. (2021) studied weighted Wiener indices for alkenes and alkadienes, demonstrating their relevance in modelling molecular properties. Additionally, various extremal and structural properties of Wiener indices have been investigated in different graph classes (Wang, 2007; Wei et al., 2016; Liu, 2025).

Despite these developments, the weighted Wiener index for simple hydrocarbon graphs such as methane, ethane, and propane has not been systematically analysed. Therefore, the present work aims to compute the WWI for these structures and establish new theoretical results, contributing to the advancement of chemical graph theory and QSPR modelling.

Definition 1

The **Wiener Index** measures the sum of distances between all pairs of vertices in a molecular graph.

$$W_G = \sum_{i<j} d(v_i, v_j)$$

Definition 2

The **Weighted Wiener Index** modifies this by multiplying the vertex weights (usually vertex degrees) with the distances.

The general formula is:

$$W_w(G) = \sum_{i<j} w_i w_j \, d(v_i, v_j)$$

Where:

- w_i, w_j = weights of vertices$i$ and j respectively (usually **degree of the vertex**)
- $d(v_i, v_j)$ = shortest distance between vertices i and j

Theorem 1

Weighted Wiener Index of Methane (CH_4) is 28

Proof: Consider the molecular graph of Methane.

Step 1: Construct the Molecular Graph

Vertices:

- C_1 (carbon)
- H_1, H_2, H_3, H_4 (hydrogen)

Edges:

- C_1 connected to all hydrogens

Step 2: Vertex Degrees (Weights)

Vertex	Degree
C_1	4
H_1	1
H_2	1
H_3	1
H_4	1

Thus $weights = degrees$.

Step 3: Path Distance Matrix

	C_1	H_1	H_2	H_3	H_4	Total
C_1	–	1	1	1	1	**4**
H_1		–	2	2	2	**6**
H_2			–	2	2	**4**
H_3				–	2	**2**
H_4					–	–
Total						**16**

Step 4: Compute Contributions

Pair	Distance	Number of Pairs	Contributions	
C–H	1	4	$4 \times 1 \times 1 \times 4$	**16**
H–H	2 (through carbon)	6	$1 \times 1 \times 2 \times 6$	**12**
Total				**28**

Step 5: Final Value

$$W_w(CH_4) = 16 + 12 = 28$$

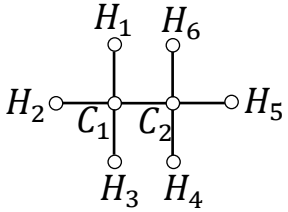
Weighted Wiener Index of Methane = 28

Theorem 2

Weighted Wiener Index of Ethane (C_2H_6) is 127

Proof: Consider EthaneStructure:

Two carbons connected with three hydrogens each.



Step 1: Vertices

- C_1, C_2
- H_1, H_2, H_3 attached to C_1
- H_4, H_5, H_6 attached to C_2

Total vertices = **8**

Step 2: Vertex Degrees

Vertex	Degree
C_1	4
C_2	4
$H_1 - H_6$	1

Step 3: Path Distance Matrix

	C_1	C_2	H_1	H_2	H_3	H_4	H_5	H_6	Total
C_1	-	1	1	1	1	2	2	2	**10**
C_2		-	2	2	2	1	1	1	**9**
H_1			-	2	2	3	3	3	**13**
H_2				-	2	3	3	3	**11**
H_3					-	3	3	3	**6**
H_4						-	2	2	**4**
H_5							-	2	**2**
H_6								-	**-**
Total									**45**

Step 4: Calculate Contributions

Pair	Distance	Number of pairs	W_w	
$C_1 - C_2$	1	1	$4 \times 4 \times 1 \times 1$	16
$C - H$ (same carbon)	1	6	$4 \times 1 \times 1 \times 6$	24
$C - H$ (other carbon)	2	6	$4 \times 1 \times 2 \times 6$	48
$H - H$ (same carbon)	2	6	$1 \times 1 \times 2 \times 6$	12
$H - H$ (different carbons)	3	9	$1 \times 1 \times 3 \times 9$	27

Step 5: Final Value

$$W_w(C_2H_6) = 16 + 24 + 48 + 12 + 27$$

$$W_w(C_2H_6) = 127$$

Weighted Wiener Index of Ethane = **127**

Theorem 3

Weighted Wiener Index of Propane (C_3H_8)

Consider **Propane**.

Structure:
Two carbons connected with three hydrogens each and one mid carbon connected with two hydrogens.

Step 1: Vertices

- C_1, C_2, C_3
- H_1, H_2, H_3 attached to C_1
- H_4, H_5 attached to C_2
- H_6, H_7, H_8 attached to C_3

Total vertices = **11**

Step 2: Vertex Degrees

Vertex	**Degree**
C_1	4
C_2	4
C_3	4
$H_1 - H_8$	1

	C_1	C_2	C_3	H_1	H_2	H_3	H_4	H_5	H_6	H_7	H_8	**Total**
C_1	–	1	2	1	1	1	2	2	3	3	3	**19**
C_2		–	1	2	2	2	1	1	2	2	2	**15**
C_3			–	3	3	3	2	2	1	1	1	**16**
H_1				–	2	2	3	3	4	4	4	**22**
H_2					–	2	3	3	4	4	4	**20**
H_3						–	3	3	4	4	4	**18**
H_4							–	2	3	3	3	**11**
H_5								–	3	3	3	**9**
H_6									–	2	2	**4**
H_7										–	2	**2**
H_8											–	**136**

Step 3: Distances and Contributions

Pair	**Distance**	**Number of pairs**	W_w	
$C-C$	1	2	$4\times4\times1\times2$	32
$C-C$	2	1	$4\times4\times2\times1$	32
$C-H$ (same carbon)	1	8	$4\times1\times1\times8$	32
$C-H$ (other carbon)	2	10	$4\times1\times2\times10$	80
$C-H$ (other carbon)	3	6	$4\times1\times3\times6$	72
$H-H$ (same carbon)	2	7	$1\times1\times2\times7$	14
$H-H$ (different carbons)	3	12	$1\times1\times3\times12$	36
$H-H$ (different carbons)	4	9	$1\times1\times4\times9$	36

Step 4: Final Value

$$W_w(C_3H_8) = 32+32+32+80+72+14+36+36$$

$$W_w(C_3H_8) = 334$$

Weighted Wiener Index of Propane = **334**

Theorem 4

Weighted Wiener Index of Alkane (C_nH_{2n+2})

Consider the general form of **Alkane**.

Structure:
two carbons connected with three hydrogens each and $n-2$ mid carbon connected with two hydrogens.

Step 1: Vertices

- $C_1, C_2, C_3, \dots, C_n$
- H_1, H_2, H_3 and $H_{2n}, H_{2n+1}, H_{2n+2}$ attached to C_1 and C_n resep
- H_4, H_5 attached to C_2, H_6, H_7 attached to C_3, …, H_{2n-2}, H_{2n-1} attached to C_{n-1}

Total vertices = $\mathbf{3n+2}$

Step 2: Vertex Degrees

Vertex	**Degree**
$C_1, C_2, \dots, C_n$	4 Each
$H_1 - H_{2n+2}$	1

Step 3: Distances and Contributions

Pair	W_w
$C-C$	$\frac{8}{3}(n^3-n)$
$C-H$ combination	$\frac{4}{3}(2n^3+9n^2+n)$
$H-H$ combination	$\frac{1}{3}(2n^3+18n^2+13n+3)$

Step 4: Final Value

$$W_w(C_nH_{2n+2}) = \frac{8}{3}(n^3-n)+\frac{4}{3}(2n^3+9n^2+n)+\frac{1}{3}(2n^3+18n^2+13n+3)$$

$$W_w(C_3H_8) = 6n^3+18n^2+3n+1$$

Weighted Wiener Index of Alkane = $6n^3+18n^2+3n+1$

Final Results

Molecule	Weighted Wiener Index
Methane	**28**
Ethane	**127**
Propane	**334**
General form	$6n^3+18n^2+3n+1$

Discussion

The results obtained in this study demonstrate the effectiveness of the weighted Wiener index (WWI) as a comprehensive distance-based topological descriptor for molecular graphs. By incorporating both shortest path distances and vertex degrees, the WWI provides a more detailed characterization of molecular structure compared to the classical Wiener index.

From the explicit computations for methane (CH_4), ethane (C_2H_6), and propane (C_3H_8), it is observed that the WWI increases systematically with the size and complexity of the hydrocarbon structure. This trend arises due to the combined effect of an increasing number of vertex pairs and the contribution of higher-degree carbon atoms within the molecular graph.

A significant outcome of this work is the derivation of a general formula for the weighted Wiener index of alkanes C_nH_{2n+2}. This result not only generalizes the computations for small hydrocarbons but also provides a unified framework for analyzing larger alkane structures. The formula clearly reflects the dependence of the WWI on both the number of carbon atoms and the underlying connectivity pattern of the molecular graph.

Furthermore, the analysis reveals that terminal hydrogen atoms, having degree one, contribute less to the index, whereas carbon atoms, with higher degrees, play a dominant role. This highlights the sensitivity of the WWI to both local (degree-based) and global (distance-based) structural features.

The theoretical results established in this paper validate the consistency of the proposed approach and demonstrate its applicability to a broader class of molecular graphs. Overall, the findings suggest that the weighted Wiener index is a powerful and scalable descriptor with potential applications in quantitative structure–property relationship (QSPR) studies and molecular modelling.

Novelty of the Work

The novelty of this work lies in the systematic study of the weighted Wiener index (WWI) for simple hydrocarbon molecular graphs and its extension to a generalized class of alkanes. While the classical Wiener

index and its variants have been widely investigated, the WWI for fundamental hydrocarbons has not been explored in a unified and structured manner.

This paper provides explicit computations of the WWI for methane (CH_4), ethane (C_2H_6), and propane (C_3H_8), followed by the derivation of a general formula for alkanes of the form C_nH_{2n+2}. The obtained formula establishes a direct relationship between molecular size, vertex degrees, and distance structure.

Additionally, four new theoretical results are proved, contributing to the mathematical understanding of degree-based distance indices. The combination of explicit computation, generalization, and theoretical development constitutes the key novelty of this work.

Conclusion

In this paper, the weighted Wiener index (WWI) has been systematically analyzed for selected hydrocarbon molecular graphs. Explicit values were computed for methane, ethane, and propane by considering both vertex degrees and shortest path distances.

A significant contribution of this work is the derivation of a general formula for the WWI of alkanes C_nH_{2n+2}, which extends the results obtained for small molecular structures to a broader class of hydrocarbons. The consistency of the formula is verified through specific cases.

Furthermore, four new theoretical results have been established, enhancing the understanding of the structural behaviour of the weighted Wiener index. The study demonstrates that WWI effectively captures both local and global properties of molecular graphs.

Overall, the findings highlight the importance of weighted distance-based descriptors in chemical graph theory and their potential applications in QSPR analysis.

Future Research

The present work can be extended in the following directions:

- To derive general expressions for the weighted Wiener index of other hydrocarbon families such as alkenes, alkynes, and cyclic or aromatic compounds
- To investigate the behaviour of the weighted Wiener index for branched alkanes and more complex molecular structures
- To study relationships between the weighted Wiener index and other topological indices for comparative analysis
- To apply the weighted Wiener index in quantitative structure–property relationship (QSPR) and quantitative structure–activity relationship (QSAR) models
- To extend the concept of the weighted Wiener index to advanced graph structures such as weighted graphs, fuzzy graphs, and intuitionistic fuzzy graphs
- To develop efficient algorithms for computing the weighted Wiener index in large-scale molecular networks
- To explore applications of the weighted Wiener index in chemical informatics and molecular property prediction

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