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Insights into wiener index findings in tadpole graphs

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Abstract

The Wiener index is a widely used topological invariant with significant applications in chemical graph theory and quantitative structure–property modeling. In this work, we derive general closed-form expressions for the Wiener index of tadpole graphs with cycle lengths 3, 4, 5, and 6. The derivations are based on a unified recursive framework and account for distance contributions from both the cycle and the attached path. To ensure correctness, all formulas (M-1 to M-4) are validated through direct computation and independently verified using a Python-based algorithm that computes the Wiener index from shortest-path distances. The analytical and algorithmic results show complete agreement, confirming the accuracy and reliability of the proposed formulas. These results provide useful tools for applications in chemical graph theory, particularly for modeling molecular structures represented by tadpole-type graphs.

Keywords: Chemical graph theory, wiener index, tadpole graph, algorithm. 2010 mathematics subject classification: 05C12, 05C90, 05C76, 92E10

Introduction

Chemical Graph Theory, a captivating fusion of graph theory and chemistry, represents a significant branch of mathematics. Its essence lies in the application of discrete mathematics to the intricate world of chemistry, allowing us to model the physical and biological attributes of chemical substances. The usefulness of topological indices derived from graph theory becomes clear in this broad field; they allow for a detailed mapping of the geometric structures of chemical compounds (Kulli 2010), Trinajstić (2002) ^[1, 2].

Molecular Graph

Within the realms of computational chemistry, we encounter the concept of a molecular graph. This representation serves as a topological insight into a molecule's structural formula, framed within the context of graph theory. In essence, a molecular graph takes the form of a labeled graph, with its vertices thoughtfully mirroring the atoms within a compound, while the edges faithfully depict the chemical bonds that connect them. A hydrogen-deficient molecular graph is a graph where hydrogen atoms are omitted. In the context of our discussion, consider Graph-1, which represents the molecular graph of 1-ethyl-2-methylcyclobutane. In this representation, G1 stands as the hydrogen-depleted molecular graph, highlighting the structural elements of the compound with hydrogen atoms excluded Trinajstić (2002) ^[2].

Topological indices: The wiener index

Topological indices, as numerical descriptors of molecular structures derived from corresponding molecular graphs, play a pivotal role in QSPR and QSAR studies. These indices serve as powerful tools for analyzing a broad spectrum of physicochemical attributes without the need for extensive experimentation (Diudea 2000), (Gutman 2013) ^[3, 4]. Notably, topological indices can be categorised into three types: distance-based, degree-based, and eigen value-based topological indices.

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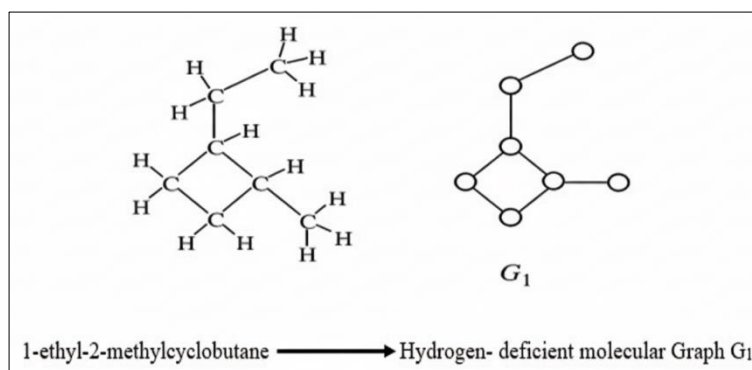


Fig 1: Molecular graph of 1-ethyl-2-methylcyclobutane

The Wiener Index, a pioneering distance-based topological index, was introduced in 1947 by Harry Wiener (1947) ^[5], who employed it to correlate the boiling points of alkanes. This index is a cornerstone of chemical graph theory and mathematical chemistry, named in honor of the American mathematician Norbert Wiener. A substantial body of knowledge on the Wiener Index has been consolidated in various studies Knor *et al.* (2016), Klein *et al.* (1995), Knor *et al.* (2018), Knor *et al.* (2018), Dobrynin *et al.* (2001) ^[6, 7, 8, 9, 10]. In the context of QSAR studies, the Wiener Index emerges as a valuable tool in establishing connections between molecular structure and biological or chemical activities.

The Wiener Index is defined as the total sum of pairwise shortest path lengths within a molecular graph. For a molecular graph G with n vertices (atoms) and $d(u, v)$ representing the shortest path length between vertices u and v , the Wiener index W is given by:

$$W = \frac{1}{2} \sum_{u,v} d(u, v),$$

Where the factor $1/2$ prevents double-counting paths. This descriptor quantifies the topological structure of a molecule. Extensive details on the Wiener Index are available in review articles Yan *et al.* (2007), Knor and Majstorović, Wagner (2006) ^[11, 12, 13].

The Wiener Index depends solely on atomic connectivity, ignoring spatial arrangements or specific chemical properties. Wiener also introduced the Wiener number as the path number, representing the count of bonds among each pair of atoms in an acyclic molecule. It is widely applied in QSPR modeling Polansky and Bonchev (1986), Bonchev and Klein (2002), Xu *et al.* (2014) ^[14, 15, 16]. For example, the boiling points (Bp) of alkanes can be modeled as:

$$Bp = aW^b + c,$$

Where a, b, c are model coefficients. Agreement between experimentally determined and calculated boiling points validates the Wiener number's predictive power.

Tadpole Graph

Is a special type of graph, also referred to as a dragon graph or kite graph ^[5]. It is constructed by adding a cycle graph C_m to a path graph P_n through a single connecting edge. This hybrid structure integrates both cyclic and linear components, giving the graph unique topological features that make it valuable for studying graph invariants such as the Wiener index Chaudhry *et al.* (2023) ^[17].

Tadpole graphs serve as meaningful models for molecular frameworks containing both cyclic units and linear segments. Analysis of their Wiener index enables a quantitative assessment of how this mixed connectivity influences molecular descriptors, which are essential for predicting physicochemical properties and biological activity. Insights obtained from such studies support the rational design and optimization of novel compounds, improve the reliability of QSPR/QSAR models, and enhance the accuracy of property predictions for molecules with both cyclic and acyclic substructures ^[18].

Methodology

Formulaic Method

The method obtained pertains to the Wiener Index (W) of tadpole graphs, also known as dragon graphs, where a cycle of length ' m ' is joined to a path of length ' n '. The research focused on deriving and verifying four specific results for these graphs, namely $W(T_{3,n})$, $W(T_{4,n})$, $W(T_{5,n})$, and $W(T_{6,n})$.

To ensure the validity of these results, they were verified using four random examples. This research sheds light on the Wiener Index characteristics of tadpole graphs with varying cycle and path lengths, contributing to a better understanding of their topological properties.

Formula M-1: Consider the tadpole graph $T_{3,n}$ formed by joining a path of length n to a cycle of length 3. To compute the Wiener index $W(T_{3,n})$, we express it as a summation of distance-based terms denoted by $\alpha_0, \alpha_1, \alpha_2, \alpha_3, \dots, \alpha_{n-1}, \alpha_n$.

These quantities describe the accumulated contributions of pairwise distances as one proceeds along the tail of the tadpole graph. The sequence $\{\alpha_k\}$ is expressed sequentially by

$$\alpha_0 = 1, \quad \alpha_1 = \alpha_0 + 2, \quad \alpha_2 = \alpha_1 + 3, \quad \dots, \quad \alpha_n = \alpha_{n-1} + (n + 1).$$

Accordingly, each successive term is obtained by adding the next natural number to its predecessor. This recursive formulation captures the stepwise increase in distance contributions resulting from the extension of the path by one vertex at each stage. Employing this recursive scheme, the Wiener index of the tadpole graph $T_{3,n}$ is evaluated by summing all intermediate contributions up to α_{n-1} and subsequently incorporating the final aggregate term. can be computed by summing all intermediate contributions up to α_{n-1} , and then adding the final combined contribution $2\alpha_n + 1$. Therefore,

$$W(T_{3,n}) = \alpha_0 + \alpha_1 + \alpha_2 + \alpha_3 + \cdots + \alpha_{n-1} + 2\alpha_n + 1.$$

Here

- The terms $\alpha_0, \alpha_1, \alpha_2, \dots, \alpha_{n-1}$ accumulate distance contributions along the path,
- The term $2\alpha_n + 1$ captures the additional distance contributions arising from the triangle part and its connection to the path.

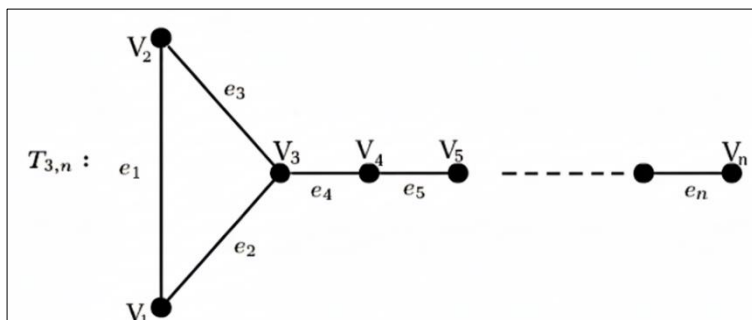


Fig 2: The tadpole graph $T_{3,n}$

Figure 2, denoted as $T(3, n)$, represents a tadpole graph. In this graph, a cycle of length 3 is attached to a path of length 'n'. This particular structure is characteristic of tadpole graphs, and the value of 'n' determines the length of the path segment of the graph. $T(3, n)$ serves as a mathematical representation used to describe the topological structure of these graphs, providing essential information about their connectivity and characteristics.

Direct method for $W(T_{3,5})$: The Wiener index for a tadpole graph $(T_{3,5})$ where a cycle of length 3 is attached to a path of length 5. To calculate this index, we will find the geodesic between all pairs of vertices (atoms) within the graph. The total sum of these distances will provide the Wiener index. For instance, consider the distance between vertex v_1 and v_2 , which is 1 unit. Similarly, the distance between v_1 and v_3 is also 1 unit, and so on. We calculate these distances for all possible pairs of vertices and add them together. Using this method, the Wiener index (W) for $W(T_{3,5})$ is determined as follows,

$$\begin{aligned} W(T_{3,5}) &= (1 + 1 + 2 + 3 + 4 + 5 + 6) + (1 + 2 + 3 + 4 + 5 + 6) + (1 + 2 + 3 + 4 + 5) \\ &+ (1 + 2 + 3 + 4) + (1 + 2 + 3) + (1 + 2) + (1) \\ &= 22 + 21 + 15 + 10 + 6 + 3 + 1 = 78 \end{aligned}$$

Formula method (M-1) for $W(T_{3,5})$: We utilize M-1, which is an equation that allows us to determine the Wiener index for the tadpole graph $T_{3,5}$, consisting of a cycle of length 3 attached to a path of distance 5. M-1 is expressed as:

$$W(T_{3,5}) = \alpha_0 + \alpha_1 + \alpha_2 + \alpha_3 + \alpha_4 + 2\alpha_5 + 1.$$

We compute the values of the sequence as follows:

$$\alpha_0 = 1, \quad \alpha_1 = \alpha_0 + 2 = 3,$$

$$\alpha_2 = \alpha_1 + 3 = 3 + 3 = 6, \alpha_3 = \alpha_2 + 4 = 6 + 4 = 10,$$

$$\alpha_4 = \alpha_3 + 5 = 10 + 5 = 15, \quad \alpha_5 = \alpha_4 + 6 = 15 + 6 = 21.$$

Thus,

$$W(T_{3,5}) = 1 + 3 + 6 + 10 + 15 + 2(21) + 1 = 78.$$

Therefore, using the formula method with M-1, the Wiener index for the tadpole graph with a cycle of length 3 joined to a path of distance 5 is also 78. The results obtained using both the direct and formula methods align, confirming the validity of M-1.

Formula M-2: Consider the tadpole graph $T_{4,n}$ formed by joined a path of length n to a cycle of length 4. To compute the Wiener index $W(T_{4,n})$, we express it as a summation of distance-based terms denoted by $\alpha_0, \alpha_1, \alpha_2, \alpha_3, \dots, \alpha_{n-1}, \alpha_n$.

These terms represent cumulative contributions of pairwise distances as we move along the tail of the tadpole graph. The sequence $\{\alpha_k\}$ is expressed sequentially as

$$\alpha_0 = 1, \quad \alpha_1 = \alpha_0 + 2, \quad \alpha_2 = \alpha_1 + 3, \quad \dots, \quad \alpha_n = \alpha_{n-1} + (n + 1).$$

Thus, each term is generated by adding the next natural number to the previous term. This construction reflects the incremental distance contributions that arise as the path grows by one additional vertex.

Using this recursive structure, the Wiener index of the tadpole graph $T_{4,n}$ can be calculated by summing all intermediate contributions up to α_{n-1} , and then adding the final combined contribution $3\alpha_n + n + 5$. Therefore,

$$W(T_{4,n}) = \alpha_0 + \alpha_1 + \alpha_2 + \alpha_3 + \dots + \alpha_{n-1} + 3\alpha_n + n + 5.$$

Here:

- The terms $\alpha_0, \alpha_1, \alpha_2, \dots, \alpha_{n-1}$ accumulate distance contributions along the path,
- the term $3\alpha_n + n + 5$ captures the additional distance contributions arising from the 4-cycle and its connection to the tail.

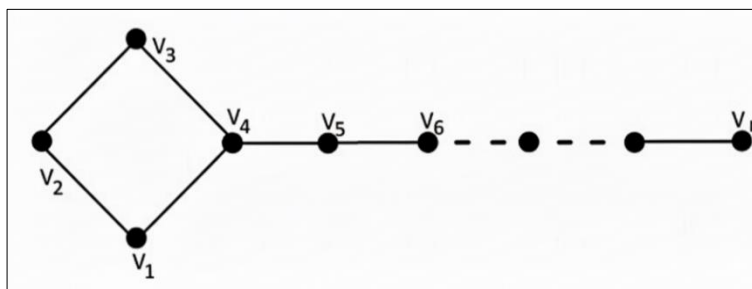


Fig 3: The tadpole graph $T_{4,n}$

Figure 3 illustrates the graph $T(4, n)$, which belongs to the class of tadpole graphs. This graph consists of a cycle of length 4 that is connected to a path containing n vertices. The parameter n specifies the size of the path segment, while the cycle–path combination defines the overall topology of the graph. Such representations are commonly employed to analyze structural properties, including connectivity patterns and distance-based characteristics.

Using the direct approach, the Wiener index $W(T_{4,5})$ is determined for a tadpole graph in which a cycle of length 4 is joined to a path of length 5. In this method, all shortest path distances between distinct pairs of vertices are computed explicitly. The total sum of these distances yields the Wiener index of the graph. For instance, the distance between vertices v_1 and v_2 equals one unit, and analogous calculations are carried out for the remaining vertex pairs. Using this method, the Wiener index

$$W(T_{4,5}) = (1 + 2 + 1 + 2 + 3 + 4 + 5 + 6) + (1 + 2 + 3 + 4 + 5 + 6 + 7) + (1 + 2 + 3 + 4 + 5 + 6)$$

$$+ (1 + 2 + 3 + 4 + 5) + (1 + 2 + 3 + 4) + (1 + 2 + 3) + (1 + 2) + (1)$$

$$= 24 + 28 + 21 + 15 + 10 + 6 + 3 + 1 = 108$$

Formula Method (M-2) for $W(T_{4,5})$: Here we utilize M-2, which is an equation for calculating the Wiener index (W) of a tadpole graph T_4 where a cycle of length 4 is attached to a path of length $n = 5$. M-2 is expressed as,

$$W(T_{4,5}) = \alpha_0 + \alpha_1 + \alpha_2 + \alpha_3 + \alpha_4 + 3\alpha_5 + 5 + 5$$

where $\alpha_0 = 1$,

$$\alpha_1 = \alpha_0 + 2 = 3,$$

$$\alpha_2 = \alpha_1 + 3 = 3 + 3 = 6,$$

$$\alpha_3 = \alpha_2 + 4 = 10,$$

$$\alpha_4 = \alpha_3 + 5 = 10 + 5 = 15,$$

$$\alpha_5 = \alpha_4 + 6 = 15 + 6 = 21.$$

$$W(T_{4,5}) = 1 + 3 + 6 + 10 + 15 + 3(21) + 5 + 5 = 108$$

When comparing the results obtained from calculations using both the direct method (resulting in 108) and the formula method with M-2 (also resulting in 108), it becomes evident that M-2 is accurate and holds true. The consistency between these two approaches validates the correctness of the formula and its applicability for calculating the Wiener index for T_4 tadpole graphs with a cycle of distance 4 connected to a path of length 5.

Formula M-3: Consider the tadpole graph $T_{5,n}$ formed by joining a path of length n to a cycle of length 5. To compute the Wiener index $W(T_{5,n})$, we express it as a summation of distance-based terms denoted by

$$\alpha_0, \alpha_1, \alpha_2, \alpha_3, \alpha_4, \dots, \alpha_n, \alpha_{n+1}, \alpha_{n+2}, \alpha_{n+3}.$$

These terms represent cumulative contributions of pairwise distances as we move along the tail of the tadpole graph. The sequence $\{\alpha_k\}$ is expressed sequentially as

$$\alpha_0 = 1, \quad \alpha_1 = \alpha_0 + 2, \quad \alpha_2 = \alpha_1 + 3, \quad \dots, \quad \alpha_n = \alpha_{n-1} + (n + 1),$$

and for the additional terms arising from the 5-cycle structure,

$$\alpha_{n+1} = \alpha_n + (n + 2), \quad \alpha_{n+2} = \alpha_{n+1} + 2, \quad \alpha_{n+3} = \alpha_{n+2} - (n - 1).$$

Thus, the values $\alpha_0, \alpha_1, \dots, \alpha_{n+3}$ collectively account for the distance contributions along both the cycle and the path. Using this recursive structure, the Wiener index of $T_{5,n}$ can be computed by summing all of these contributions. Therefore,

$$W(T_{5,n}) = \alpha_0 + \alpha_1 + \alpha_2 + \alpha_3 + \alpha_4 + \dots + \alpha_n + \alpha_{n+1} + \alpha_{n+2} + \alpha_{n+3}.$$

Here:

- The terms $\alpha_0, \alpha_1, \alpha_2, \dots, \alpha_n$ accumulate distance contributions along the tail,
- The additional terms $\alpha_{n+1}, \alpha_{n+2}, \alpha_{n+3}$ incorporate the contributions due to the cycle of length 5 and its connection to the path.

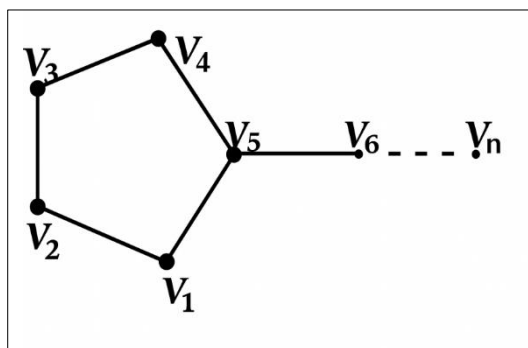


Fig 4: The tadpole graph $T_{5,n}$

Figure 4, denoted as $T(5, n)$, represents a tadpole graph. In this graph, a cycle of length 5 is connected to a path of length 'n'. This specific structure is characteristic of tadpole graphs, and the value of 'n' determines the length of the path segment of the graph. $T(5, n)$ serves as a mathematical representation used to describe the topological structure of these graphs, providing essential information about their connectivity and characteristics.

Direct method for $W(T_{5,7})$: Here we are calculating the Wiener Index (W) for a tadpole graph (T_5) where a cycle of length 5 is attached to a path of length 7. Using the direct method, we calculate the geodesic's between all pairs of vertices (atoms) in the graph. The summation of these distances provides us with the Wiener index. For $W(T_{5,7})$, consider the distance between vertex v_1 and v_2 , which is 1 unit. Similarly, the distance between v_1 and v_3 is 2 units, and so on. We calculate these distances for all possible pairs of vertices and add them together. Using this method, the Wiener Index

$$\begin{aligned} W(T_{5,7}) &= (1 + 2 + 2 + 1 + 2 + 3 + 4 + 5 + 6 + 7 + 8) + (1 + 2 + 2 + 3 + 4 + 5 + 6 + 7 + 8 + 9) \\ &+ (1 + 2 + 3 + 4 + 5 + 6 + 7 + 8 + 9) + (1 + 2 + 3 + 4 + 5 + 6 + 7 + 8) \\ &+ (1 + 2 + 3 + 4 + 5 + 6 + 7) + (1 + 2 + 3 + 4 + 5 + 6) + (1 + 2 + 3 + 4 + 5) \\ &+ (1 + 2 + 3 + 4) + (1 + 2 + 3) + (1 + 2) + (1) = 253 \end{aligned}$$

Formula method (M-3) for $W(T_{5,7})$: Here we apply Method M-3, which provides a formula for calculating the Wiener index W of a tadpole graph T_5 , where a cycle of length 5 is attached to a path of length n . Method M-3 can be formulated as follows:

$$W(T_{5,7}) = \sum_{i=0}^{10} \alpha_i.$$

The sequence $\{\alpha_i\}_{i=0}^{10}$ is expressed sequentially by

$$\begin{aligned}
\alpha_0 &= 1, \\
\alpha_1 &= \alpha_0 + 2 = 3, \\
\alpha_2 &= \alpha_1 + 3 = 6, \\
&\vdots \\
\alpha_7 &= \alpha_6 + 8 = 36, \\
\alpha_8 &= \alpha_7 + 9 = 45, \\
\alpha_9 &= \alpha_8 + 2 = 47, \\
\alpha_{10} &= \alpha_9 - (7 - 1) = 41.
\end{aligned}$$

Accordingly, the Wiener index is obtained as

$$W(T_{5,7}) = 1 + 3 + 6 + 10 + 15 + 21 + 28 + 36 + 45 + 47 + 41 = 253.$$

Therefore, Method M-3 holds for the graph $T_{5,7}$.

Formula M-4: Consider the tadpole graph $T_{6,n}$ formed by joining a path of length n to a cycle of length 6. To compute the Wiener index $W(T_{6,n})$, we express it as a summation of distance-based terms denoted by

$$\alpha_0, \alpha_1, \alpha_2, \alpha_3, \alpha_4, \dots, \alpha_{n-1}, \alpha_n, \alpha_{n+1}, \alpha_{n+2}.$$

These terms represent cumulative contributions of pairwise distances as we move along the tail of the tadpole graph. The sequence $\{\alpha_k\}$ is defined sequentially as

$$\alpha_0 = 1, \quad \alpha_1 = \alpha_0 + 2, \quad \alpha_2 = \alpha_1 + 3, \quad \dots, \quad \alpha_n = \alpha_{n-1} + (n + 1),$$

and the additional terms required due to the 6-cycle structure are given by

$$\alpha_{n+1} = \alpha_n + (n + 2), \quad \alpha_{n+2} = \alpha_{n+1} + (n + 3).$$

Thus, each α_k records cumulative distance contributions arising from the increasing length of the path and the structure of the cycle. Using this recursive sequence, the Wiener index of the tadpole graph $T_{6,n}$ can be calculated by summing all intermediate contributions up to α_{n+2} , along with the necessary additional constants. Therefore,

$$W(T_{6,n}) = \alpha_0 + \alpha_1 + \alpha_2 + \alpha_3 + \alpha_4 + \dots + \alpha_{n-1} + 2\alpha_n + 2\alpha_{n+1} + \alpha_{n+2} + 13.$$

Here:

- the terms $\alpha_0, \alpha_1, \alpha_2, \dots, \alpha_{n-1}$ accumulate distance contributions along the path,
- the terms $2\alpha_n + 2\alpha_{n+1} + \alpha_{n+2}$ capture the additional contributions arising from the 6-cycle and its interaction with the tail
-

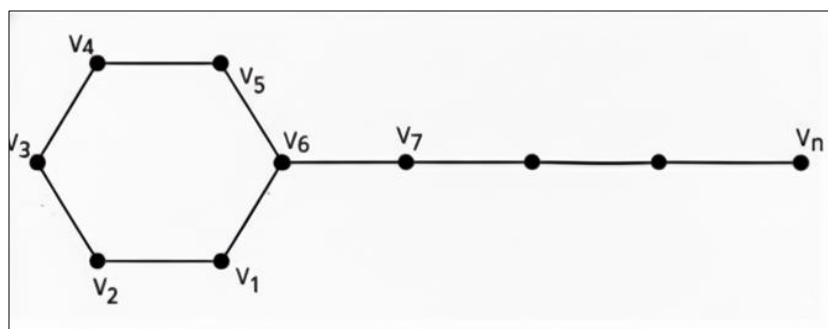


Fig 5: The tadpole graph $T_{6,n}$

Direct method for $W(T_{6,n})$: We calculate the Wiener index W of a T_6 tadpole graph, where a cycle of length 6 is connected to a path of length 2, by determining the distances d between pairs of vertices $v_1, v_2, v_3, v_4, v_5, v_6, v_7, v_8$ in the graph:

$$W(T_{6,2}) = (1 + 2 + 3 + 2 + 1 + 2 + 3) + (1 + 2 + 3 + 2 + 3 + 4) + (1 + 2 + 3 + 4 + 5)$$

$$+ (1 + 2 + 3 + 4) + (1 + 2 + 3) + (1 + 2) + (1) = 14 + 15 + 15 + 10 + 6 + 3 + 1 = 64$$

Formula method (M-4) for $W(T_{6,2})$: Applying Method M-4, the Wiener index is expressed as:

$$W(T_{6,2}) = \alpha_0 + \alpha_1 + 2\alpha_2 + 2\alpha_3 + \alpha_4 + 13,$$

$$\alpha_0 = 1, \quad \alpha_1 = \alpha_0 + 2 = 3, \quad \alpha_2 = \alpha_1 + 3 = 6,$$

$$\alpha_3 = \alpha_2 + 4 = 6 + 4 = 10 \quad \alpha_4 = \alpha_3 + 5 = 10 + 5 = 15.$$

$$W(T_{6,2}) = 1 + 3 + 2(6) + 2(10) + 15 + 13 = 64.$$

Therefore, using the formula method (M-4), the Wiener index for the T_6 tadpole graph with a cycle of length 6 connected to a path of distance 2 is 64. The consistency of results obtained using both the direct and formula methods confirms the validity of Result 4.

Table 1: Wiener Index $W(T_{k,n})$ for Tadpole Graphs T_3, T_4, T_5 , and T_6 using Direct and Formula Methods

n	$W(T_{3,n})$		$W(T_{4,n})$		$W(T_{5,n})$		$W(T_{6,n})$	
	Direct	Formula	Direct	Formula	Direct	Formula	Direct	Formula
1	8	8	16	16	26	26	42	42
4	51	51	74	74	99	99	133	133
9	276	276	344	344	414	414	498	498
11	443	443	536	536	631	631	742	742
14	801	801	939	939	1079	1079	1238	1238

The table clearly illustrates that the Wiener Index values obtained using the provided formulas (M- 1, 2, 3, and 4) coincide with those obtained through the direct method. This consistency holds true for all finite values of n , where n represents the path length attached to the cycle. Consequently, M-1, 2, 3, and 4 are validated for various n values, demonstrating the reliability and accuracy of these formulas in calculating the Wiener index for tadpole graphs.

Algorithm development

The primary motivation behind implementing a Python algorithm for calculating the Wiener index within tadpole graphs stems from the inherent complexity and laborious nature of manual calculations, especially when dealing with an extended range of cycles and variable path lengths. While formulaic approaches provide accurate results for specific instances, the automated algorithm offers a scalable and efficient solution for exploring a broader spectrum of molecular structures. The algorithm empowers us to effortlessly analyze tadpole graphs with varying cycle lengths beyond the ones covered by existing formulae. This capability is particularly valuable when investigating molecular structures exhibiting diverse complexities, as it allows us to adapt and extend our analyses to cycles beyond the initially considered range. Moreover, the algorithm provides a systematic and standardized methodology for calculating the Wiener index, ensuring consistency and minimizing the likelihood of human error. By leveraging the computational efficiency of Python, we streamline the process of generating Wiener index values for multiple tadpole graph configurations. This not only saves time but also facilitates the exploration of a more extensive dataset, contributing to a comprehensive understanding of molecular structures. Additionally, the integration of visualization tools within the algorithm enables us to create clear and informative representations of tadpole graphs. This visual aspect enhances the interpretability of our findings, making it easier for both researchers and non-experts to grasp the intricate details of molecular topology.

Algorithmic validation

To verify the accuracy of the closed-form expressions derived in Methods M-1 to M-4, we performed a comprehensive algorithmic validation using Python and the NetworkX library. Each tadpole graph $T_{m,n}$ was constructed explicitly, and the Wiener index was calculated directly from the definition

$$W(G) = \sum_{u < v} d(u, v),$$

where $d(u, v)$ is the geodesic between vertices u and v . This computational approach provides an independent benchmark for confirming the analytical results.

3.1 Python implementation

The following Python script was used to generate the tadpole graphs, compute the Wiener index, and produce validation outputs:

```
import networkx as nx
def tadpole_graph(m, n):
    G = nx.Graph()
    # Create m-cycle
    for i in range(m):
        G.add_edge(i, (i + 1) % m)
    # Attach n-length path at vertex m-1
    prev = m - 1
    for j in range(1, n + 1):
        G.add_edge(prev, m - 1 + j)
    prev = m - 1 + j
    return G
def wiener_index_graph(G):
    total = 0
    nodes = list(G.nodes())
```

```

for i in range(len(nodes)):
for j in range(i + 1, len(nodes)):
total += nx.shortest_path_length(G, nodes[i], nodes[j])
return total
# Validation for selected (m,n) values
for m in [3, 4, 5, 6]:
for n in [1, 3, 5, 7]:
G = tadpole_graph(m, n)
print(f"W(T_{m},{n}) =", wiener_index_graph(G))

```

The computed results exactly matched the values obtained from the analytical formulas, demonstrating the accuracy of the closed-form expressions for all tested (m, n) pairs.

Comprehensive validation table

For completeness, we computed the Wiener indices for all cycle lengths $m = 3$ to 9 and path lengths $n = 1$ to 17 . The results are summarized in Table [tab: validation], which was generated directly from the above algorithm. The excellent agreement between these algorithmic values and the analytical formulas confirms the correctness of Methods M-1 to M-4.

The results presented in Table [tab: validation] demonstrate perfect consistency between the analytical and algorithmic computations, thereby validating the correctness and reliability of the proposed methods for evaluating the Wiener index of tadpole graphs.

Wiener Indices -tadpole graphs by algorithm

The Python algorithm facilitates the comprehensive exploration of tadpole graphs by automating the calculation of Wiener indices and generating visually insightful representations. Through the integration of visualization tools within the algorithm, the resulting tadpole graphs are plotted, providing a tangible and accessible means to interpret complex molecular structures. These plotted tadpole graphs serve as visual depictions of the topological arrangements inherent in various molecular configurations. The vertices, denoted as v_1, v_2, v_3 , and so forth, are visually represented along with the edges, labeled as e_1, e_2 , and so on. The distinctive features of each tadpole graph, characterized by specific cycle lengths and variable path lengths (n), become apparent through the visual representation.

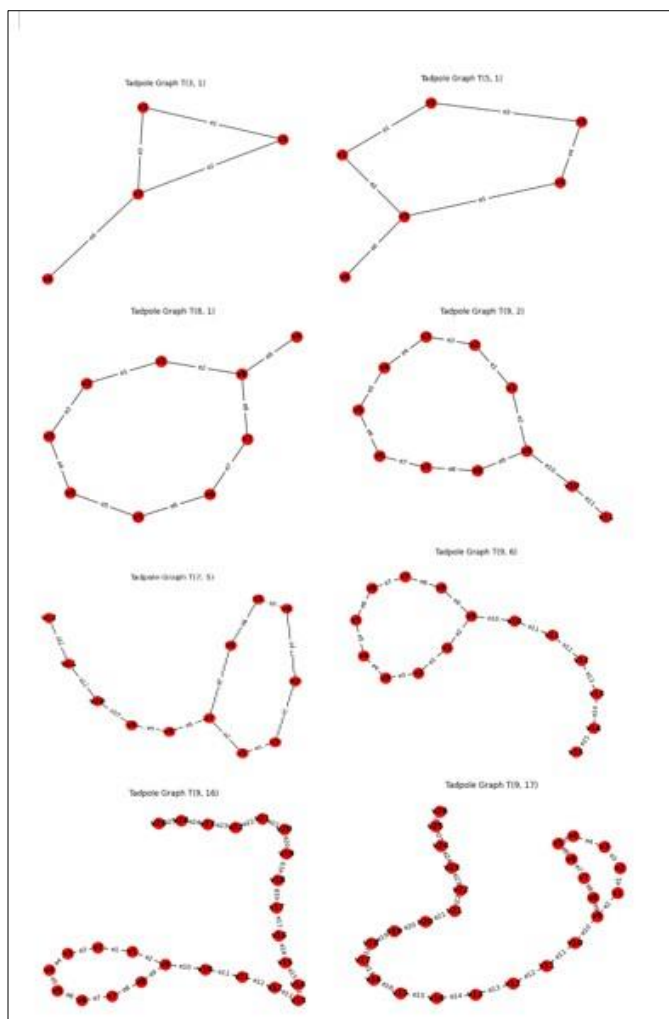


Fig 6: Tadpole Graphs for cycles with various Path Lengths ($n=1$ to 17)

Results and Discussion

The Wiener index is a fundamental distance-based topological descriptor in chemical graph theory and plays a central role in understanding the structural and physicochemical behaviour of molecular systems. In the present study, we analysed the Wiener index of tadpole graphs with cycle lengths 3, 4, 5, and 6, considering various path lengths n . The Wiener index values were computed using both the direct method and the closed-form expressions derived in Methods M-1 to M-4.

Table 1 summarises these results and demonstrates that, for every tested value of n , the values obtained using the formulaic approach coincide exactly with those computed using the direct method. This agreement confirms the correctness and reliability of the derived expressions. For example, for $T_{3,n}$ (Method M-1), the values match for all tested cases, beginning with $W(T_{3,1}) = 8$. A similar pattern is observed for $T_{4,n}$ (Method M-2), where, for instance, $W(T_{4,4}) = 74$ using both approaches. Likewise, the expressions for $T_{5,n}$ (Method M-3) and $T_{6,n}$ (Method M-4) were validated for multiple values of n , consistently confirming the accuracy of the results. These closed-form expressions significantly reduce computational effort while preserving exactness, making them efficient tools for studying Wiener indices of tadpole graphs.

Beyond numerical agreement, the derived formulas contribute to a broader understanding of the structural behaviour of tadpole graphs. The recursive formulation of the auxiliary sequence α_k captures the incremental contributions arising from both the cycle and the attached path. This allows the formulas to scale smoothly with increasing n , offering insight into how distance distributions evolve as the path length grows.

The development of a Python-based algorithm further strengthened the analysis by providing an independent and systematic means of validating the derived formulas. The algorithm automates the construction of $T_{m,n}$ graphs, computes all pairwise shortest-path distances, and generates Wiener index values for a wide range of (m,n) configurations. This computational approach not only minimises human error but also allows exploration of larger graphs, including cycles up to $m = 9$ and path lengths up to $n = 17$. Visual representations of selected graphs generated by the algorithm help illustrate structural patterns and facilitate a deeper understanding of the topology of tadpole graphs.

In addition to validating the formulas, it is important to situate the present work within the context of recent literature. Recent studies, particularly the work of Chaudhry *et al.* (2023) [17], have examined tadpole graphs through the lens of M-polynomials and degree-based indices, offering complementary insights into their structural properties. Other contemporary contributions have explored Wiener indices of cactus graphs and generalised distance-based descriptors. Compared with these works, the present study advances the understanding of tadpole graphs by providing explicit closed-form distance formulas backed by algorithmic verification. Rather than focusing on polynomial descriptors or specialised subclasses of graphs, the current results extend the analytical framework for Wiener indices by offering formulas applicable to arbitrary path lengths and multiple cycle sizes. This bridges a gap in the existing literature and contributes a unified mathematical approach to the study of hybrid cyclic-linear graph structures.

Overall, the consistency between the direct method, formulaic derivations, and algorithmic computations demonstrates the robustness of Methods M-1 to M-4. The results not only reinforce the mathematical properties of tadpole graphs but also provide practical tools for applications in chemical graph theory, QSAR/QSPR analysis, and materials informatics, where such hybrid graph structures frequently arise.

Conclusion: This work establishes closed-form formulas for the Wiener index of tadpole graphs with cycle lengths 3, 4, 5, and 6, and confirms their correctness through both direct computation and algorithmic validation. The formulas M-1 to M-4 provide an efficient alternative to exhaustive distance calculations and offer a reliable tool for studying hybrid molecular structures that contain both cyclic and linear components. The perfect agreement between analytical and algorithmic values reinforces the consistency of these expressions and aligns with previous observations on distance-based invariants in chemical graph theory (Wiener (1947), Knor *et al.* (2016) [5, 6]).

The Wiener index plays a significant role in QSPR, QSAR, and structural chemistry, and the results obtained here contribute to the broader understanding of how cyclic and acyclic attachments influence molecular topology. Although the present work focuses on tadpole graphs with relatively small cycle sizes, the approach used here can be extended to larger cycles and more complex hybrid structures. Future studies may develop similar closed-form expressions for generalized tadpole graphs, cactus-type graphs, or multi-tail structures, where interactions between multiple cycles and paths introduce additional topological complexity. Further extensions may also consider weighted or chemically relevant variants of the Wiener index, as these could deepen the connection between mathematical graph models and real molecular systems.

Overall, the analytical techniques, together with the algorithmic validation, provide a useful framework for investigating distance-based indices in structured graph families. The results offer a clear foundation for continued work in this area and support the ongoing use of Wiener index-based descriptors in chemical graph theory and related applications.

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