Wiener Index of Families of Bicyclic Graphs Obtained from a Tree

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***Abstract*—The Wiener index $W(G)$ of a graph G is a widely used topological invariant, which is defined as the sum of the shortest path distances between all pairs of vertices in G. It has significant applications in chemistry, network theory, and combinatorial optimization, where distance-based graph measures play a crucial role in understanding structural properties. For a family $\mathcal{Y}$ of connected graphs, its Wiener index is defined as the sum of the Wiener indices of its members, i.e., $W(\mathcal{Y})$=$\sum_{G\in\mathcal{Y}} W(G)$.**

This study investigates a family of bicyclic graphs U_e, each constructed by replacing an edge e of a tree T with two fixed cycles, each containing at least three vertices and sharing at least one common vertex. We establish a fundamental relationship between the Wiener indices of the family $\{U_e|e \in E(T)\}$ and the original tree T. To achieve this, analytical expressions for the Wiener index of these transformed graphs are derived based on the structural properties of T. Then, we analyze how such modifications affect the overall distance metric and provide theoretical insights into the impact of local transformations on global graph invariants.

Our results extend existing knowledge on Wiener indices of bicyclic graphs and offer a systematic approach for studying similar graph modifications.

***Index Terms*—Wiener index; bicyclic graph; tree; graph invariant.**

I. Introduction

ALL graphs in this paper are assumed to be undirected, connected, and simple, which means that they have neither loops nor multiple edges. A graph G is defined by its vertex set $V(G)$ and edge set $E(G)$. The order of G, denoted by n_G, is the number of vertices in $V(G)$. The *distance* $d_G(u,v)$ between two vertices u and v in G is defined as the number of edges in the shortest path that connects them. The total distance of a vertex v, also known as its transmission, is the sum of its distances to all other vertices in G, given by $d_G(v) = \sum_{u\in V(G)} d_G(u,v)$. The Wiener index is an invariant based on the distances between all the vertices of a graph G, and it can also be applied to acyclic organic molecules [19].

$$W(G) = \sum_{u,v\in V(G)} d(v_i,v_j) = \frac{1}{2}\sum_{v\in V(G)} d_G(v)$$

The Wiener index has notable applications in a variety of fields, such as mathematical chemistry where it serves as an important descriptor for molecular structure analysis. Specifically, in the study of acyclic organic molecules, it can be used to predict physicochemical properties like boiling points and stability [1, 9, 12, 13, 17, 18] [2, 8, 14–16]

This article investigates the families of graphs in terms of their Wiener index, which may give rise to various distinct structures. As a fundamental topological descriptor, the Wiener index can be used to study various graph families with distinct structural characteristics.

One notable transformation that affects the Wiener index is bicyclic construction, where an edge in a graph is replaced by two cycles, resulting in a bicyclic graph family. Such transformations help reveal how structural modifications impact graph distance metrics, which is particularly useful in applications related to network theory and chemical graph analysis.

Specifically, for a family of connected graphs $\mathcal{G}$=$\{G_1, G_2, \ldots, G_r\}$, its Wiener index is defined as the sum of the Wiener indices of its individual members as follows:

$$W(\mathcal{G}) = W(G_1) + W(G_2) + \ldots + W(G_r).$$

In this context, the structural characteristics of different graphs influence the value of the Wiener index $W(G)$. These characteristics play a crucial role in determining the value for each specific graph. When every graph in the family G is isomorphic to either a simple path or a complete graph of order n, then $W(G)$ obtains extremal values among all the families of the n-vertex graphs with the cardinality of r. The properties of the Wiener index for certain families of acyclic structures and benzenoid graphs have been rigorously examined in prior research [4–7, 10, 19].

The simple path and the simple cycle of order n can be denoted by P_n and C_n, respectively. Since the sum of distances from a particular vertex in the path P_n to the remaining vertices forms the sum of two arithmetic progressions, it follows that the distance $d_{p_n}(v_m) = m^2 - (n+1)m + (n^2+n)/2$. Moreover, the Wiener index of P_n is given by $W(P_n) = n(n^2-1)/6$; where the distance $d_{C_n}(v) = n^2/4$ and the Wiener index of C_n is $W(C_n) = n^3/8$ for even n, and the distance $d_{C_n}(v) = (n-1)^2/4$ and the Wiener index of C_n is $W(C_n) = n(n^2-1)/8$ for odd n [20]. The graph G_e, which is the edge k-subdivision of an edge $e \in E(G)$, is obtained by replacing e in the graph G with a path P_{k+2}=$(v_1, v_2, \ldots, v_k)$. Vertices v_i,$i = 1, 2, \ldots, k$, are called the $subdivision vertices$ of e [7].

Let U_e be a bicyclic graph formed by replacing an edge in the tree T with a bicycle. In general, computing the Wiener index involves calculating the distance between points u and v in the tree T. The varying structures of the cycles yield diverse graphical outcomes. Let U_c represent the collection of replaced cycles; let $U_c = \{U_e|e \in E(T)\}$, which also

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facilitates the determination of the average value of the Wiener index.

II. Main result

Let $T_{e,k}$ and $T_{e,m}$ respectively represent the trees obtained by performing a k- and an m-subdivision of an edge e of tree T. That is, the corresponding vertices in the tree are defined as subdivision vertices. The process of replacing an edge e with a double loop C_{k+m+2} can be viewed as the addition of $T_{e,k}$ and $T_{e,m}$, with a dividing line l that separates them. The vertex connected to $T_{e,m}$ by the dividing line l is denoted as u_p, and the point connected to $T_{e,k}$ is denoted as v_q. In this scenario, the large loop C_{k+m+2} will be divided into two smaller loops.

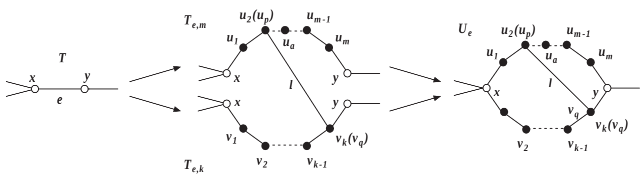

Fig. 1. The edge e of a tree T is replaced with a bicyclic C_{k+m+2}.

The following two lemmas play a crucial role in calculating the Wiener index of families of trees that are obtained through edge subdivisions [7].

Lemma 1: For k-subdivision T_{e_1},T_{e_1},...,$T_{e_{n-1}}$ of edges e_1,e_2,...,e_{n-1} of a tree T of order n,

$$W(T_{e_1}) + W(T_{e_2}) + \ldots + W(T_{e_{n-1}}) = (3k+n+1)W(T) + (n-1)\binom{k+1}{3} + 2\binom{k}{2}\binom{n}{2}.$$

It should be noted that $\binom{k+1}{3}$ represents the Wiener index of path P_k. Throughout the analysis, we use a consistent numbering of subdivision vertices across all the edges. The total sum of distances between vertices from T in the newly trees can also be expressed in terms of the Wiener index of T. This index serves as a key metric in graph theory for quantifying vertex pair distances. The following lemma demonstrates that the Wiener index can also be utilized to express the distances between all the vertices in a graph.

Lemma 2: For an n-vertex tree T, with edges e_1,e_2,...,e_{n-1}, the subdivision vertices v_1,v_2,...,v_k are obtained by subdividing these edges as follows:

$$\sum_{i=1}^{n-1}(d_{T_{e_i}}(v_1) + d_{T_{e_i}}(v_2) + \ldots + d_{T_{e_i}}(v_k)) = 2kW(T) + \frac{1}{6}k(k-1)(n-1)(2k+3n+2).$$

The family $\mathcal{Y}_{k+m+2}$ denotes a graph obtained through the process described above; then, there exists a relationship between $W(T)$ concerning the determination of bi-cycles.

Theorem 1: Regarding the Wiener index of the family $\mathcal{Y}_{k+m+2}$,

$$\begin{aligned} W(\mathcal{Y}) = &(3k+n+2m-1)W(T) \\ &+ \frac{n-1}{6}[(k^2-2k)(2k-2) - (m^2+2m)(2m+2) \\ &+ 3mp(m-p+2) + 3pk(k+p-2q+2) \\ &+ 3kq(k-q+2m-2a+4) \\ &+ 3mq(m-q-2a+4)] - m + kn(k-1) \\ &+ (n-1)[\frac{n_1^3 - 2n_1^2 + n_2^3 - 2n_2^2}{8} + q^2 + ma \\ &+ p(2-p-q+a-aq) + aq(q+a-1) \\ &- km + 2q^2 - a^2 - m - 3k - 1] \end{aligned}$$

Proof. Let T be an arbitrary tree of order n. For an edge $e = (x, y)$ of T, let U_e be a bicyclic graph obtained by replacing e with cycle C_{k+m+2}, where $k \geq 0$ and $m \geq k$. Therefore, the definition of graph U_e is as follows: First, by employing k- and m- subdivision vertices, the edge e of tree T is partitioned into two segments. Second, the corresponding vertices in graph T are identified (Figure 1), where one edge is subdivided into $T_{e,m}$ and $T_{e,k}$. Third, the dividing line between the two circular diagrams is designated as l, which connects $T_{e,m}$ at point u_p and connects $T_{e,k}$ at v_q, as depicted in Figure 1. Additionally, it is essential to compare the lengths of paths $(u_1, u_2, \ldots, u_p)$ and $(v_q, v_{q+1}, \ldots, v_k)$ when calculating the Wiener index of U_e. For computational purposes, let the length of path $(u_1, u_2, \ldots, u_p)$ be less than that of path $(u_1, u_2, \ldots, u_m)$, and let the length of path $(v_q, v_{q+1}, \ldots, v_k)$ be less than that of path $(v_q, v_{q+1}, \ldots, v_k)$. Subsequently, the shortest path from $v \in \{u_1, u_2, \ldots, u_p\}$ to $v \in \{v_q, v_{q+1}, \ldots, v_k\}$ is through the path $(u_1, u_2, \ldots, u_p, v_q, v_{q+1}, \ldots, v_k)$. However, two distinct scenarios emerge when tracing from $v \in \{u_p, u_{p+1}, \ldots, u_m\}$ to $v \in \{v_1, v_2, \ldots, v_q\}$. It can be observed that within the path$(u_p, u_{p+1}, \ldots, u_m)$, there exists a vertex u_a such that including the subdivisions on its left reach the shortest path to $v \in \{v_1, v_2, \ldots, v_q\}$ through path $(u_a, u_{a-1}, \ldots, u_p, v_q)$, whereas those on its right traverse path $(u_a, u_{a+1}, \ldots, u_m, y, v_k, v_{k-1}, \ldots, v_q)$ to reach $v \in \{v_1, v_2, \ldots, v_q\}$. Through the equation $(m-a)+2+(k-q) = (a-p)+1$, tis process allows us to determine this vertex u_a. Finally, since $m \geq k$, it is evident that for all $v \in \{u_1, u_2, \ldots, u_m\}$,$d_{U_e}(v)$=$d_{T_{e,k}}(v)$. Then,

$$\begin{aligned} &W(U_e) \\ &= W(T_{e,k}) + \sum_{i=1}^{m} d_{U_e}(u_i) - W(P_m) + \sum_{i=1}^{m}\sum_{j=1}^{k} d_{U_e}(u_i, v_j) \\ &= W(T_{e,k}) + \sum_{i=1}^{m} d_{T_{e,m}}(u_i) - W(P_m) + \sum_{i=1}^{m}\sum_{j=1}^{k} d_{U_e}(u_i, v_j). \end{aligned}$$

By calculating the Wiener index of the cycle C_{k+m+2}, the last term of equation (1) can be expanded as given below.

$$
\begin{aligned}
&\sum_{i=1}^{m}\sum_{j=1}^{k} d_{U_e}(u_i, v_j) \\
&= W_{C_{(x,u_p,v_q)}} - d_{C_{(x,u_p,v_q)}}(x) \\
&- \sum_{1\le i<j}^{p} d_P(u_i,u_j) - \sum_{1\le i<j}^{q} d_P(v_i,v_j) \\
&+ W_{C_{(y,u_p,v_q)}} - d_{C_{(y,u_p,v_q)}}(y) \\
&- \sum_{p\le i<j}^{m} d_P(u_i,u_j) - \sum_{q\le i<j}^{k} d_P(v_i,v_j) \\
&- d(u_p,v_q) + W_P(u_1,u_2,\ldots,u_p,v_q,\ldots,v_k) \\
&- W_P(k-q+2) + d(u_p,v_q) - W_P(p+1) \\
&+ W_P(u_a,u_{a-1},\ldots,u_p,v_q,v_{q-1},\ldots,v_1) - W_P(a-p+2) \\
&+ W_P(q+1) + d(u_p,v_q) - W_P(k+1) \\
&+ W_P(u_{a+1},u_{a+2},\ldots,u_m,y,v_k,v_{k-1},\ldots,v_1) \\
&- W_P(k-q+m-a+2) + W_P(k-q+2)
\end{aligned}
$$

Given $d_{(u_p,v_q)} = 1$, the above equation can be deduced to the following.

$$
\begin{aligned}
&\sum_{i=1}^{m}\sum_{j=1}^{k} d_{U_e}(u_i, v_j) \\
&= W_{C_{(x,u_p,v_q)}} - d_{C_{(x,u_p,v_q)}}(x) - W_P(u_1,u_p) - W_P(v_1,v_q) \\
&+ W_{C_{(y,u_p,v_q)}} - d_{C_{(y,u_p,v_q)}}(y) \\
&- W_P(p+1) - W_P(q+1) - 1 \\
&+ W_P(u_1,u_2,\ldots,u_p,v_q,\ldots,v_k) \\
&- W_P(p+1) - W_P(q+1) + 1 \\
&+ W_P(u_a,u_{a-1},\ldots,u_p,v_q,v_{q-1},\ldots,v_1) - W_P(a-p+2) \\
&+ W_P(q+1) + 1 \\
&+ W_P(u_{a+1},u_{a+2},\ldots,u_m,y,v_k,v_{k-1},\ldots,v_1) \\
&- W_P(k+1) - W_P(k-q+m-a+2) + W_P(k-q+2)
\end{aligned} \tag{1}
$$

Then, Equation (2) can be summed for all the edges $e \in E(T)$.

$$
\begin{aligned}
W(\mathcal{Y}_{k+m+2}) &= \sum_{e\in E(T)} W(U_e) \\
&= \sum_{e\in E(T)} W(T_{e,k}) + \sum_{e\in E(T)} \sum_{i=1}^{m} d_{T_{e,m}}(u_i) \\
&- (n-1)W(P_m) + (n-1)\sum_{i=1}^{m}\sum_{j=1}^{k} d_{U_e}(u_i,v_j)
\end{aligned}
$$

By substituting the results from Equation (2), Lemma 1, and Lemma 2 into this expression, the proof is thereby concluded.

When both m and k are small, the Wiener index of the family can be correlated through organic chemistry. Similar graphs are given below.

Let $W_a(\mathcal{Y})$ be the average Wiener index of family $\mathcal{Y}.W_a(\mathcal{Y}) = W(\mathcal{Y})/|\mathcal{Y}|$. From Theorem 1, it can be inferred that $W_a(\mathcal{Y})$ is determined by the structure of the graph and the specified cycles, with its value possibly being fractional.

III. For two odd cycles

If an edge of the tree is replaced by two odd cycles (n_1, n_2 are odd), then $k = m$. This particular insertion method can be easily implemented for composition.

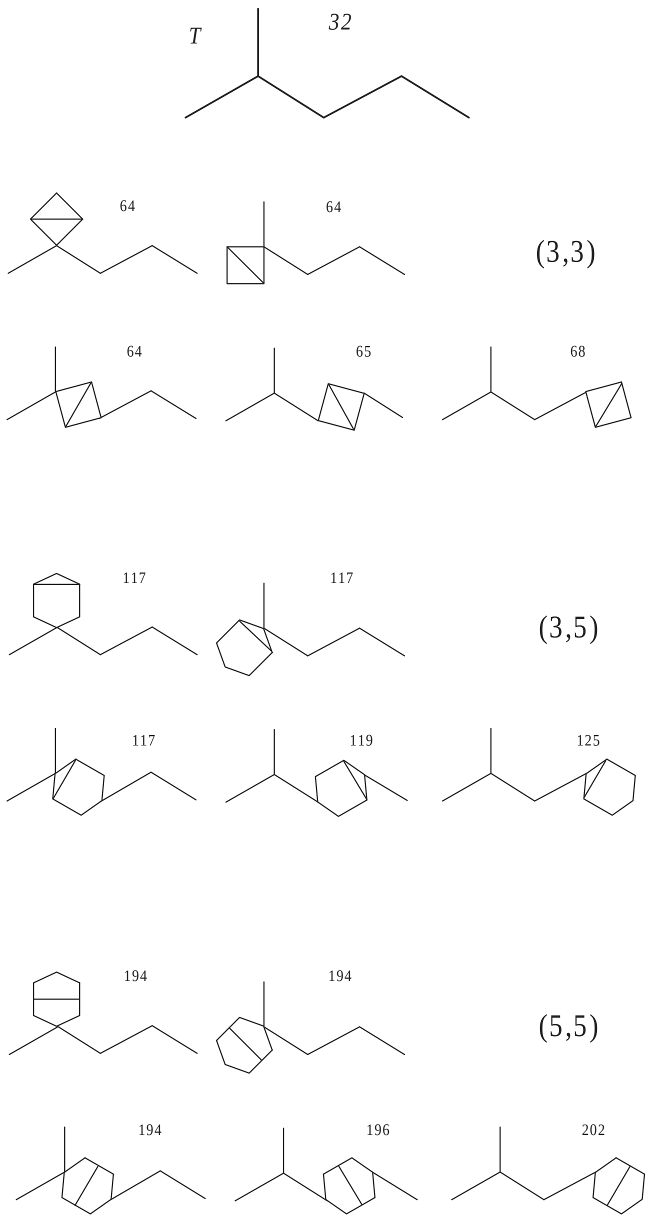

Fig. 2. Families of graphs with combinations of (3,3), (3,5), and (5,5).

Corollary 1: Consider a family of bicyclic graphs $\mathcal{Y}_{2k+3}$ that is derived from a tree T of order n by substituting its edges with two odd cycles C_{2k+2},$k \ge 0$,$m = k$. Then,

$$
\begin{aligned}
&W(\mathcal{Y}_{2k+2}) \\
&= (5k+n+1)W(T) + \frac{n-1}{6}[(k^2-2k)(2k-2) \\
&- (k^2+2k)(2k+2) + 3kp(k-p+2) \\
&+ 3pk(k+p-2q+2) + 3kq(3k-q-2a+4) \\
&+ 3kq(k-q-2a+4)] \\
&+ (n-1)[\frac{n_1(n_1^2-1) - 2(n_1^2-1) + n_2(n_2^2-1) - 2n_2^2}{8} \\
&- k + kn(k-1) + p(2-p-q+a-aq) \\
&+ aq(q+a-1) + q^2 + ka - k^2 + 2q^2 - a^2 - 4k - 1],
\end{aligned}
$$

and the average value of the Wiener index for the graphs in the family is

$$\begin{aligned}
&W(\mathcal{Y}_{2k+2})\\
&=(\frac{5k+2}{n-1}+1)W(T)+\frac{1}{6}[(k^2-2k)(2k-2)\\
&-(k^2+2k)(2k+2)+3kp(k-p+2)\\
&+3pk(k+p-2q+2)+3kq(3k-q-2a+4)\\
&+3kq(k-q-2a+4)]\\
&+\frac{n_1(n_1^2-1)-2(n_1^2-1)+n_2(n_2^2-1)-2(n_2^2-1)}{8}\\
&-k+kn(k-1)+p(2-p-q+a-aq)+aq(q+a-1)\\
&+q^2+ka-k^2+2q^2-a^2-4k-1.
\end{aligned}$$

The final expression can be used to approximate the Wiener index of trees that have undergone edge cyclization. In a bicyclic graph, the average value of the Wiener index can be divided by $n-1$. For certain small bicyclic graphs, the familial Wiener index can be directly computed.

For bicomplete graphs, consider the example where the bicomplete graph is (3,3), (3,5), or (5,5), as depicted in Figure 2. The Wiener index is denoted alongside graph diagrams. According to Corollary 3.1, $W(\mathcal{Y}_{3,3})$=$(3+6+2-1)\cdot 32+\frac{5}{6}\cdot(-12)+15=325$ for $k=1$, $m=1$, $p=1$, $q=1$, $a=1$, $W(\mathcal{Y}_{3,5})$=$(6+6+4-1)\cdot 32+\frac{5}{6}\cdot(78)+50=595$ for $k=2$, $m=2$, $p=1$, $q=1$, $a=2$,$W(\mathcal{Y}_{5,5})$=$(6+9+6-1)\cdot 32+\frac{5}{6}\cdot(300)+90=980$ for $k=3$, $m=3$, $p=2$, $q=2$, $a=3$. Here, the value of $W_a(\mathcal{Y}_{3,3})$=65, $W_a(\mathcal{Y}_{3,5})$=119, and $W_a(\mathcal{Y}_{5,5})$=196.

IV. For two even cycles

When the edges of a tree are substituted by two even cycles (where n_1+n_2 is even), then both n_1 and n_2 are either even or odd. Consequently, the two cycles can be inserted at suitable locations.

Corollary 2: Let a family bicyclic graph $\mathcal{Y}_{2k+2}$ be obtained from a tree T of order n by replacing its edges with even cycles C_{2k+2}, $k\geq 0$, $m=k$, or $m=k+2$, and the value of n_1+n_2 is even. Then,

$$\begin{aligned}
&W(\mathcal{Y}_{2k+2})\\
&=(5k+n+1)W(T)+\frac{n-1}{6}[(k^2-2k)(2k-2)\\
&-(k^2+2k)(2k+2)+3kp(k-p+2)\\
&+3pk(k+p-2q+2)+3kq(3k-q-2a+4)\\
&+3kq(k-q-2a+4)]+(n-1)[\frac{n_1^3-2n_1^2+n_2^3-n_2^3)}{8}\\
&-k+kn(k-1)+p(2-p-q+a-aq)+aq(q+a-1)\\
&+q^2+ka-k^2+2q^2-a^2-4k-1],
\end{aligned}$$

and the average Wiener index of the graphs in the family is

$$\begin{aligned}
&W(\mathcal{Y}_{2k+2})\\
&=(\frac{5k+2}{n-1}+1)W(T)+\frac{1}{6}[(k^2-2k)(2k-2)-\\
&(k^2+2k)(2k+2)+3kp(k-p+2)+3pk(k+p-2q+2)\\
&+3kq(3k-q-2a+4)+3kq(k-q-2a+4)]\\
&+\frac{n_1^3-2n_1^2+n_2^3-n_2^3-1)}{8}-k+kn(k-1)\\
&+kn(k-1)+p(2-p-q+a-aq)+aq(q+a-1)\\
&+q^2+ka-k^2+2q^2-a^2-4k-1.
\end{aligned}$$

If $m=k$ and it is an even cycle, then there might be combinations, such as (4,4), (4,6), and so on. For example, consider a bicomplete graph composed of (4,4) and (4,6), as shown in Figure 3. Based on Corollary 4.1,$W(\mathcal{Y}_{4,4})$=$(6+4+6-1)\cdot 32+\frac{5}{6}\cdot(78)+45=590$ for $k=2$, $m=2$, $p=1$, $q=2$, $a=2$, $W(\mathcal{Y}_{4,6})$=$(6+9+6-1)\cdot 32+\frac{5}{6}\cdot(570)+85=1295$ for $k=3$, $m=3$, $p=1$, $q=2$, $a=3$. Here, the value of $W_a(\mathcal{Y}_{4,4})$=118 and $W_a(\mathcal{Y}_{4,6})$=259.

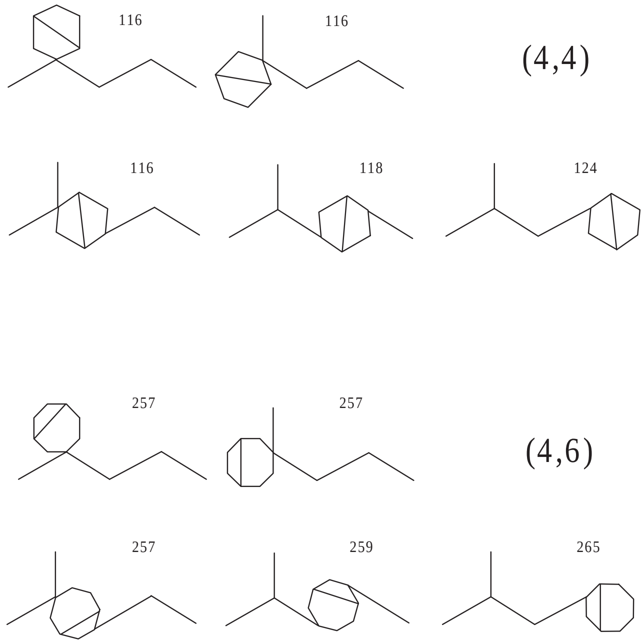

Fig. 3. Families of graphs with combinations of (4,4) and (4,6).

V. For one odd and one even

For a bicomplete graph consisting of one odd and one even cycle, where n_1+n_2 is odd and $k+m$ is also odd: when the cycles are evenly distributed, the bicomplete graph can be appropriately positioned.

Corollary 3: Consider a family of bicyclic graphs $\mathcal{Y}_{2m+3}$ or $\mathcal{Y}_{2m+2}$ constructed from a tree T of order n by substituting its edges with even cycles C_{2k+2}, where $k\geq 0$, $m=k$ or $m=k+2$, and the value of n_1+n_2 is even, then

$$\begin{aligned}
&W(\mathcal{Y}_{2k+2})\\
&=(5k+n+1)W(T)+\frac{n-1}{6}[(k^2-2k)(2k-2)\\
&-(k^2+2k)(2k+2)+3kp(k-p+2)\\
&+3pk(k+p-2q+2)+3kq(3k-q-2a+4)\\
&+3kq(k-q-2a+4)]\\
&+(n-1)[\frac{n_1^3-2n_1^2+n_2(n_2^2-1)-2(n_2^2-1)}{8}-k\\
&+kn(k-1)+p(2-p-q+a-aq)+aq(q+a-1)\\
&+q^2+ka-k^2+2q^2-a^2-4k-1],
\end{aligned}$$

and the average Wiener index of the graphs in the family is

$$\begin{aligned}
&W(\mathcal{Y}_{2k+2})\\
&=(\frac{5k+2}{n-1}+1)W(T)+\frac{1}{6}[(k^2-2k)(2k-2)\\
&-(k^2+2k)(2k+2)+3kp(k-p+2)\\
&+3pk(k+p-2q+2)+3kq(3k-q-2a+4)\\
&+3kq(k-q-2a+4)]\\
&+\frac{n_1^3-2n_1^2+n_2(n_2^2-1)-2(n_2^2-1)}{8}-k+kn(k-1)\\
&+p(2-p-q+a-aq)+aq(q+a-1)\\
&+q^2+ka-k^2+2q^2-a^2-4k-1.
\end{aligned}$$

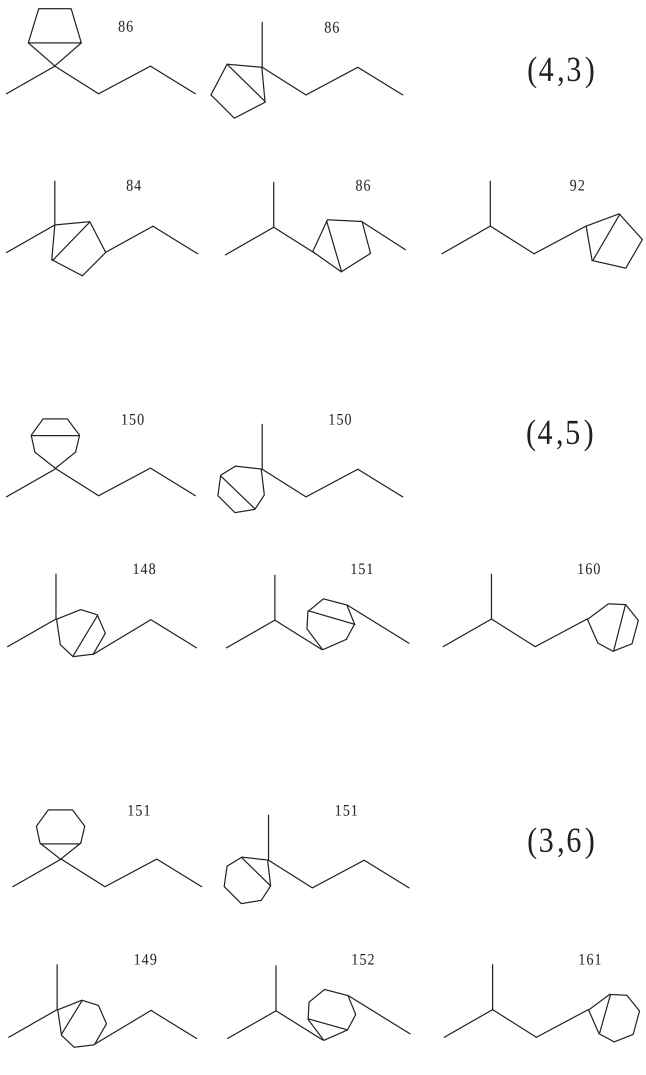

Fig. 4. Families of graphs with combinations of (3,4), (4,5), and (3,6).

In this example, cases such as (4,3), (4,5), (6,3), and so on can be provided. From Corollary 5.1, it follows that $W(\mathcal{Y}_{4,3})$=$(6+6+4-1)\cdot 32+\frac{5}{6}\cdot(24)+30=434$ for $k=1$, $m=2$, $p=1$, $q=1$, $a=2$,$W(\mathcal{Y}_{4,5})$=$(6+6+6-1)\cdot 32+\frac{5}{6}\cdot(174)+70=759$ for $k=2$, $m=3$, $p=1$, $q=1$, $a=2$, $W(\mathcal{Y}_{6,3})$=$(6+6+6-1)\cdot 32+\frac{5}{6}\cdot(144)+100=746$ for $k=2$, $m=3$, $p=1$, $q=1$, $a=3$. All the average values are fractional.

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