Electronic Journal of Mathematics
www.shahindp.com/locate/ejm

Electron. J. Math. **9** (2025) 11–22
DOI: 10.47443/ejm.2024.072

Research Article

The minimum Wiener index of Halin graphs with characteristic trees of diameter 4

Hedi Wang, Kexiang Xu*

School of Mathematics, Nanjing University of Aeronautics & Astronautics, Nanjing, Jiangsu 210016, PR China

(Received: 18 December 2024. Received in revised form: 14 January 2025. Accepted: 18 January 2025. Published online: 21 January 2025.)

Abstract

The Wiener index of a connected graph G is defined as the sum of distances between all unordered pairs of vertices of G. A Halin graph is a plane graph consisting of a plane embedding of a tree T of order at least 4 containing no vertex of degree 2, and a cycle connecting all leaves of T. The tree T is called the characteristic tree of the Halin graph. Denote by $\mathbb{H}_{n,4}$ the set of all Halin graphs of order n with characteristic trees of diameter 4. In this paper, we determine the minimum Wiener index of the graphs in $\mathbb{H}_{n,4}$. We also find the corresponding extremal graphs.

Keywords: Wiener index; Halin graph; diameter.

2020 Mathematics Subject Classification: 05C09, 05C12.

1. Introduction

All graphs considered in this paper are finite, undirected, connected, and simple. Let $G = (V(G), E(G))$ be a graph. As usual, denote by $V(G)$, $E(G)$, $|V(G)|$, and $|E(G)|$ the vertex set, edge set, number of vertices, and the number of edges of G, respectively. For any $v \in V(G)$, let $N_G(v)$ be the set of neighbors of v and $d_G(v) = |N_G(v)|$ be the degree of v. The *distance* $d_G(u, v)$ of two vertices $u,\ v \in V(G)$ is the length of a shortest $u - v$ path in G. The greatest distance between any two vertices in G is the *diameter* of G, which is denoted by $diam(G)$. The *eccentricity* of $v \in V(G)$ is denoted by $\varepsilon(v)$ and is defined as

$$\varepsilon(v) = \max_{u \in V(G)} d_G(v, u).$$

The Wiener index, proposed by Wiener [14] in 1947, is one of the most studied topological indices in chemical graph theory. The *Wiener index* of a connected graph G can be defined as

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d(u, v).$$

Klavžar and Nadjafi-Arani [8] gave lower bounds on the difference between the Szeged index and Wiener index; afterward, they improved lower bounds in [10]. Xu, Li, and Luo [16] established some comparative results between the number of nonempty subtrees and the Wiener index of a graph. Das [4] presented upper bounds on the Wiener index of a graph with certain given parameters. Božović et al. [2] presented extremum values of the Wiener index of trees with given parameters and characterized the extremal trees. More results on the Wiener index can be found in [3, 5, 9, 11–13, 15, 17].

A *Halin graph* G is a plane graph consisting of a plane embedding of a tree T of order at least 4 containing no vertex of degree 2, and a cycle C connecting all leaves of T. The tree T (or $T(G)$) and the cycle C (or $C(G)$) are called the characteristic tree and the adjoint cycle of G, respectively. Halin graphs were first introduced by Halin [6], and later they were studied considerably in the mathematical literature [1, 7]. Denote by $\mathbb{H}_{n,4}$ the set of Halin graphs of order n with characteristic trees of diameter 4. In this paper, we determine the minimum Wiener index of graphs in $\mathbb{H}_{n,4}$ and find the corresponding extremal graphs.

Let $G \in \mathbb{H}_{n,4}$, we use $T(G)$ and $C(G)$ to denote the characteristic tree and the adjoint cycle of G throughout this section. Note that G has only one vertex o of eccentricity 2. For a vertex $v \in N_G(o)$, if $v \in C(G)$ then v is called a *hanging vertex*, otherwise v is called a *support vertex*. We use $[n]$ to denote $\{1, 2, \ldots, n\}$. Suppose that G has m support vertices $v_1, v_2, \ldots, v_m$ and $N_G(v_i) \cap C(G) = \{v_i^1, v_i^2, \ldots, v_i^{k_i}\}$, where $i \in [m]$ and $k_i \geq 2$. Let $\mathbb{H}'_{n,4}$ be the set of all those graphs of $\mathbb{H}_{n,4}$ that contain no hanging vertex. Denote by $\mathbb{H}^*_{n,4}$ the set of all those graphs of $\mathbb{H}_{n,4}$ that contain at least one hanging vertex. Also, we

*Corresponding author (kexxu1221@126.com).

denote by $\mathbb{H}^{*1}_{n,4}$ (respectively, $\mathbb{H}^{*2}_{n,4}$) the set of all those graphs of $\mathbb{H}^{*}_{n,4}$ that contain at least 3 (respectively, only 2) support vertices. Let $\gamma_G(i)$ be the numbers of those pairs of vertices of G that have distance i for $i \in [4]$. Then

$$W(G) = \gamma_G(1) + 2\gamma_G(2) + 3\gamma_G(3) + 4\gamma_G(4). \tag{1}$$

In Sections 2, 3, and 4, we give the minimum value of the Wiener index of the graphs belonging to the sets $\mathbb{H}'_{n,4}$, $\mathbb{H}^{*1}_{n,4}$, and $\mathbb{H}^{*2}_{n,4}$, respectively. Section 5 presents the main result of this paper, which not only gives the minimum Wiener index of the graphs in $\mathbb{H}_{n,4}$ but also provides the corresponding extremal graphs.

2. Graphs in $\mathbb{H}'_{n,4}$

Since a graph $G \in \mathbb{H}'_{n,4}$ with m support vertices contains no hanging vertex and any vertex of degree 2, we have $m \geq 3$ and $n \geq 10$. The characteristic tree $T(G)$ is shown in Figure 2.1. Let $E(C(G)) = \{v_i^j v_i^{j+1} : i \in [m], j \in [k_i - 1]\} \cup \{v_i^{k_i} v_{i+1}^1 : i \in [m]\}$. Suppose that the number of k_i with $k_i = 2$ for $i \in [m]$ is ℓ. By the relationship between the support vertices and their neighbors, we have

$$|G| = n = m + 1 + \sum_{i=1}^{m} k_i. \tag{2}$$

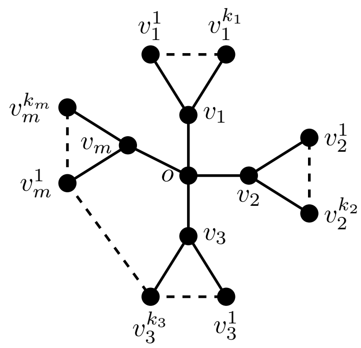

Figure 2.1: The characteristic tree $T(G)$ of $G \in \mathbb{H}'_{n,4}$.

Proposition 2.1. *If $G \in \mathbb{H}'_{n,4}$ has $m \geq 3$ support vertices, then*

$$W(G) = n^2 + (m-6)n + 2\sum_{1 \leq i < j \leq m} k_i k_j - (m+2)m + 5 - \ell, \tag{3}$$

with $n \geq 10$ and $k_i = |N_G(v_i) \cap C(G)| \geq 2$ for $i \in [m]$.

Proof. We consider the pairs of vertices at distance i and calculate the values of $\gamma_G(i)$ for every $i \in [4]$. By Equation (2), we have

$$\gamma_G(1) = |E(G)| = m + 2\sum_{i=1}^{m} k_i = 2n - m - 2. \tag{4}$$

In the following discussion, we assume that k_i, v_i, and v_i^j have subscripts modulo m for $i \in [m]$. There are three cases for the pairs of vertices at distance 2.

Case A1. Pairs of vertices contain o: $\{(o, v_i^1), (o, v_i^2) \ldots, (o, v_i^{k_i}) : i \in [m]\}$. By Equation (2), the number of these pairs is

$$\sum_{i=1}^{m} k_i = n - m - 1.$$

Case A2. Pairs of vertices contain support vertices v_i for $i \in [m]$: $\{(v_i, v_j) : i, j \in [m], i \neq j\}$ and $\{(v_i, v_{i+1}^1), (v_{i+1}, v_i^{k_i}) : i \in [m]\}$. The number of these pairs is $\frac{1}{2}m(m+3)$.

Case A3. Pairs of vertices whose both vertices are in $C(G)$: $\{(u, v) : i \in [m], d_G(u, v) = 2, u, v \in N_G(v_i) \cap C(G)\}$ and $\{(v_i^{k_i}, v_{i+1}^2), (v_i^{k_i - 1}, v_{i+1}^1) : i \in [m]\}$. By Equation (2), the number of such pairs is

$$\frac{1}{2}\sum_{i=1}^{m}(k_i)^2 - \frac{3}{2}\sum_{i=1}^{m} k_i + 3m = \frac{1}{2}n^2 - (m + \frac{5}{2})n - \sum_{1 \leq i < j \leq m} k_i k_j + \frac{1}{2}m^2 + \frac{11}{2}m + 2.$$

Hence, by Cases A1, A2, and A3, we have

$$\gamma_G(2) = \frac{1}{2}n^2 - (m + \frac{3}{2})n - \sum_{1\le i<j\le m} k_i k_j + m^2 + 6m + 1. \tag{5}$$

For the pairs of vertices at distance 3, there are two cases.

Case B1. Pairs of vertices contain support vertices: $\{(v_j, v) : v \in \bigcup_{i\in[m]\setminus\{j\}}\{v_i^1, v_i^2, \ldots, v_i^{k_i}\} \setminus \{v_{j+1}^1, v_{j-1}^{k_{j-1}}\}, j \in [m]\}$ (if $j = 1$, then we assume that $v_{j-1}^{k_{j-1}}$ is $v_m^{k_m}$). By Equation (2), the number of these pairs is

$$(m-1)\sum_{i=1}^{m} k_i - 2m = (m-1)n - m^2 - 2m + 1.$$

Case B2. Pairs of vertices whose both vertices are in $C(G)$.

Subcase B2.1. $\{(v_i^{k_i-1}, v_{i+1}^2) : i \in [m]\}$. The number of these pairs is m.

Subcase B2.2. First, we consider the case when $k_i \ge 3$ for $i \in [m]$. Then, we list such pairs of vertices as follows: $\{(v_j^{k_j}, v_{j+1}^h) : h \in [k_{j+1}] \setminus \{1, 2\}, j \in [m]\}$ and $\{(v_{j+1}^1, v_j^h) : h \in [k_j] \setminus \{k_j - 1, k_j\}, j \in [m]\}$. By Equation (2), the number of such pairs of vertices is

$$2\sum_{i=1}^{m} k_i - 4m = 2n - 6m - 2.$$

However, if $k_p = 2,\ p \in [m]$, and the rest $k_i \ge 3$, then we note that a new pair of vertices $\{(v_{p-1}^{k_{p-1}}, v_{p+1}^1)\}$ with distance 3 has emerged, due to $k_p = 2$ (if $p = 1$, then this pair of vertices is $\{(v_m^{k_m}, v_2^1)\}$). Obviously, all other situations still satisfy our previous discussion. Recall that the number of k_i whose value is 2 for $i \in [m]$ is ℓ. Thus, the number of these pairs is $2n - 6m - 2 + \ell$.

Hence, by Cases B1 and B2, we have

$$\gamma_G(3) = (m+1)n - m^2 - 7m - 1 + \ell. \tag{6}$$

Finally, we consider the case when there are pairs of vertices at distance 4: $\{(u, v) : u, v \in C(G), d_G(u, v) = 4\}$. Then, the number of these pairs is

$$\gamma_G(4) = \sum_{1\le i<j\le m} k_i k_j - 2n + 2m + 2 - \ell. \tag{7}$$

Now, from Equations (1), (4), (5), (6), and (7), the required result follows. □

Lemma 2.1. *Let $x_n \ge x_{n-1} \ge \cdots \ge x_2 \ge x_1 \ge 2$ be n positive integers with $\sum_{i=1}^{n} x_i = M$. Define*

$$f(x_1, x_2, \ldots, x_n) = \sum_{1\le i<j\le n} x_i x_j,$$

where $i, j \in [n]$. Then $f(x_1, x_2, \ldots, x_n)$ attains the minimum value if and only if there exists $l \in [n]$ such that $x_l = M - 2(n-1)$ and $x_i = 2$ for $i \in [n] \setminus \{l\}$.

Proof. Suppose to the contrary that there exist two positive integers $x_i \ge x_j \ge 3$ for $i, j \in [n]$. We replace x_i and x_j with $x_i + 1$ and $x_j + 1$, respectively. Then

$$f(x_1, \ldots, x_j - 1, \ldots, x_i + 1, \ldots, x_n) - f(x_1, x_2, \ldots, x_n) = x_j - x_i - 1 < 0,$$

which is a contraction. Therefore, at most one $x_i, i \in [n]$, is greater than 2. □

Let $G_{1,m} \in \mathbb{H}'_{n,4}$ be a graph with $m \ge 3$ support vertices. Also, let

$$k_m = \sum_{i=1}^{m} k_i - 2(m-1) = n - 3m + 1$$

and $k_i = 2$ for $i \in [m-1]$. For an example, The characteristic tree $T(G_{1,3})$ of $G_{1,3}$ is shown in Figure 2.2.

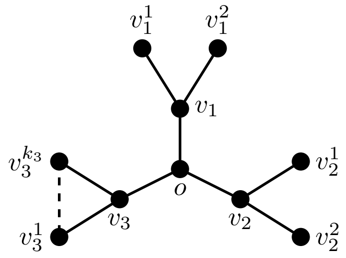

Figure 2.2: The characteristic tree $T(G_{1,3})$ of $G_{1,3}$.

By Proposition 2.1,

$$W(G_{1,m}) = \begin{cases} -9m^2 + (5n+1)m + n^2 - 10n + 10, & \text{if } k_m \geq 3, \\ -9m^2 + (5n+1)m + n^2 - 10n + 9, & \text{if } k_m = 2. \end{cases} \tag{8}$$

In the following, we give the graphs with the minimum Wiener index in $\mathbb{H}'_{n,4}$.

Theorem 2.1. *For any graph $G \in \mathbb{H}'_{n,4}$, we have $W(G) \geq F_1(n)$ and*

$$F_1(n) = \begin{cases} 81, & \text{if } n = 10, \\ n^2 + 5n - 68, & \text{if } n \geq 11, \end{cases} \tag{9}$$

where the equality $W(G) = F_1(n)$ holds if and only if $G \cong G_{1,3}$.

Proof. Suppose that $G \in \mathbb{H}'_{n,4}$ has m support vertices and attains the minimum Wiener index. By Proposition 2.1,

$$W(G) = n^2 + (m-6)n + 2 \sum_{1 \leq i < j \leq m} k_i k_j - (m+2)m + 5 - \ell,$$

with $n \geq 10$, where $k_i = |N_G(v_i) \cap C(G)| \geq 2$ for $i \in [m]$ and ℓ is the number of k_i with $k_i = 2$ for $i \in [m]$. Without loss of generality, by Lemma 2.1, $k_m = \sum_{i=1}^{m} k_i - 2(m-1) = n - 3m + 1$ and $k_i = 2$ for $i \in [m-1]$ in G. Note that $G \cong G_{1,m}$.

By Equation (8), we define the function

$$f_1(x) = -9x^2 + (5n+1)x \ \text{ for } x \in \left[3, \left\lfloor \frac{n-1}{3} \right\rfloor\right] \text{ with } n \in N^* \text{ and } n \geq 10.$$

Note that $f_1(x)$ attains the minimum value if and only if $x = 3$. Hence, we conclude that $W(G_{1,m})$ takes the minimum value if and only if $m = 3$. Thus, $G \cong G_{1,3}$. By taking $m = 3$ in Equation (8), we have $W(G_{1,3}) = F_1(n)$. □

3. Graphs in $\mathbb{H}^{*1}_{n,4}$

For a graph $G \in \mathbb{H}^*_{n,4}$ with m support vertices, we now define some terms related to hanging vertices in G. In Figure 3.1, there is a hanging vertex z_1 between the vertices $v_{l_1}^{k_{l_1}}$ and $v_{l_1+1}^1$; we call such a vertex the *single hanging vertex* in the region l_1. There are also at least 2 hanging vertices $y_1^1, \ldots, y_1^{p_1}$ between the vertices $v_{r_1}^{k_{r_1}}$ and $v_{r_1+1}^1$; we call such vertices the *multiple hanging vertices* in the region r_1.

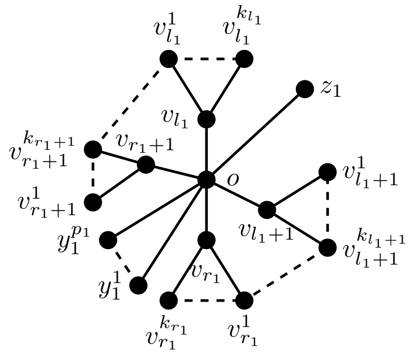

Figure 3.1: The characteristic tree $T(G)$ of $G \in \mathbb{H}^*_{n,4}$.

Suppose that $G \in \mathbb{H}^{*1}_{n,4}$ has $m \geq 3$ support vertices. Recall that if v_i is a support vertex, then $k_i = |N_G(v_i) \cap C(G)| \geq 2$ for $i \in [m]$. Let t be the number of regions with a single hanging vertex and s be the number of regions with multiple hanging vertices. Without loss of generality, suppose that there are t single hanging vertices $z_1, z_2, \ldots, z_t$ in the regions $l_1, l_2, \ldots, l_t \in [m]$ in G, respectively. Let $\{y_1^1, y_1^2, \ldots, y_1^{p_1}\}, \{y_2^1, y_2^2, \ldots, y_1^{p_2}\}, \ldots, \{y_s^1, y_s^2, \ldots, y_s^{p_s}\}$ be the sets of $p_1, p_2, \ldots, p_s$ multiple hanging vertices in the regions $r_1, r_2, \ldots, r_s \in [m]$, respectively. Note that $p_i \geq 2$ for $i \in [s]$. Let ε be the number of p_i with $p_i = 2$ for $i \in [s]$. Let σ be the set of all hanging vertices and $x = \sum_{i=1}^{s} p_i + t$ be the number of hanging vertices. Also, let $\Phi = \{l_1, l_2, \ldots, l_t, r_1, r_2, \ldots, r_s\}$ denote the set of regions with hanging vertices in G and $\Psi = \Phi \cup \{l_1+1, \ldots, l_t+1, r_1+1, \ldots, r_s+1\}$. Let λ be the number of k_i with $k_i = 2$ for $i \in [m] \setminus \Psi$. Let

$$\begin{aligned} E(C(G)) =& \{v_i^j v_i^{j+1} : i \in [m], j \in [k_i - 1]\} \cup \{v_i^{k_i} v_{i+1}^1 : i \in [m] \setminus \Phi\} \cup \{v_{l_i}^{k_{l_i}} z_i, z_i v_{l_i+1}^1 : i \in [t]\} \\ & \cup \{v_{r_i}^{k_{r_i}} y_i^1, y_i^j y_i^{j+1}, y_i^{p_i} v_{r_i+1}^1 : i \in [s], j \in [p_i - 1]\}. \end{aligned} \tag{10}$$

By the relationship between the support vertices and their neighbors, we have

$$|V(G)| = n = m + 1 + \sum_{i=1}^{m} k_i + \sum_{i=1}^{s} p_i + t = m + 1 + \sum_{i=1}^{m} k_i + x. \tag{11}$$

Proposition 3.1. *If $G \in \mathbb{H}^{*1}_{n,4}$, then keeping in mind the concepts defined before this proposition, we have*

$$\begin{aligned} W(G) =& n^2 + (m-6)n + 2 \sum_{1 \leq i < j \leq m} k_i k_j - (m+2)m + 5 - \lambda \\ & + x(\sum_{i=1}^{m} k_i - m + 3) - s - 3t + \sum_{i \in \Phi} (k_i + k_{i+1}) - \varepsilon, \end{aligned} \tag{12}$$

with $n \geq 11$ and $m \geq 3$.

Proof. We consider the pairs of vertices at distance i and calculate the values of $\gamma_G(i)$ for every $i \in [4]$. By Equation (11), we have

$$\gamma_G(1) = |E(G)| = m + 2\sum_{i=1}^{m} k_i + 2t + 2\sum_{i=1}^{s} p_i = 2n - m - 2. \tag{13}$$

In the following discussion, we assume that k_i, v_i, and v_i^j have subscripts modulo m for $i \in [m]$. For the pairs of vertices at distance 2, there are four cases.

Case A1. Pairs of vertices contain o: $\{(o, v_i^1), (o, v_i^2), \ldots, (o, v_i^{k_i}) : i \in [m]\}$. By Equation (11), the number of these pairs is

$$\sum_{i=1}^{m} k_i = n - m - 1 - x.$$

Case A2. Pairs of vertices contain support vertices and no hanging vertex:

$$\{(v_i, v_j) : i, j \in [m], i \neq j\} \quad \text{and} \quad \{(v_i, v_{i+1}^1), (v_{i+1}, v_i^{k_i}) : i \in [m] \setminus \Phi\}.$$

The number of these pairs is

$$\frac{m(m+3)}{2} - 2(t+s).$$

Case A3. Pairs of vertices with no hanging vertices and whose both vertices are in $C(G)$.

Subcase A3.1. $\{(u, v) : i \in [m], d_G(u, v) = 2, u, v \in N_G(v_i) \cap C(G)\}$. By Equation (11), the number of these pairs is

$$\frac{1}{2}\sum_{i=1}^{m}(k_i)^2 - \frac{3}{2}\sum_{i=1}^{m} k_i + m = \frac{1}{2}n^2 - \left(m + \frac{5}{2}\right)n - \sum_{1 \leq i < j \leq m} k_i k_j + \frac{1}{2}m^2 + \frac{7}{2}m + 2 - nx + \frac{1}{2}x^2 + \left(m + \frac{5}{2}\right)x.$$

Subcase A3.2. $\{(v_i^{k_i}, v_{i+1}^2), (v_i^{k_i - 1}, v_{i+1}^1) : i \in [m] \setminus \Phi\}$ and $\{(v_i^{k_i}, v_{i+1}^1) : i \in \{l_1, l_2, \ldots, l_t\}\}$. The number of these pairs is $2m - 2s - t$.

Case A4. Pairs of vertices contain hanging vertices.

Subcase A4.1. Pairs of vertices contain hanging vertices and support vertices:

$$\{(z_i, v_k) : i \in [t], k \in [m]\} \quad \text{and} \quad \{(y_i^1, v_k), (y_i^2, v_k), \ldots, (y_i^{p_i}, v_k) : i \in [s], k \in [m]\}.$$

The number of these pairs is mx.

Subcase A4.2. Pairs of vertices contain only hanging vertices: $\{(u,v) : u, v \in \sigma, d_G(u,v) = 2\}$. The number of these pairs is

$$\frac{1}{2}x^2 - \frac{1}{2}x - \sum_{i=1}^{s} p_i + s.$$

Subcase A4.3. Pairs of vertices contain both hanging vertices and the vertices in $C(G)$:

$$\{(y_i^1, v_{r_i}^{k_{r_i}-1}), (y_i^2, v_{r_i}^{k_{r_i}}), (y_i^{p_i-1}, v_{r_i+1}^1), (y_i^{p_i}, v_{r_i+1}^2) : i \in [s]\} \quad \text{and} \quad \{(z_i, v_{l_i}^{k_{l_i}-1}), (z_i, v_{l_i+1}^2) : i \in [t]\}.$$

The number of these pairs is $4s + 2t$.

Hence, by Cases A1, A2, A3, and A4, we have

$$\gamma_G(2) = \frac{1}{2}n^2 - (m + \frac{3}{2})n - \sum_{1 \le i < j \le m} k_i k_j + m^2 + 6m + 1 + x^2 + (2m - n)x + s. \tag{14}$$

There are four cases for the pairs of vertices at distance 3.

Case B1. Pairs of vertices contain support vertices.

Subcase B1.1. $\{(v_j, v) : v \in \bigcup_{i \in [m] \setminus \{j\}} \{v_i^1, v_i^2, \ldots, v_i^{k_i}\} \setminus \{v_{j+1}^1, v_{j-1}^{k_{j-1}}\}, j \in [m]\}$ (if $j = 1$, then we assume that $v_{j-1}^{k_{j-1}}$ is $v_m^{k_m}$). By Equation (11), the number of these pairs is

$$(m-1)\sum_{i=1}^{m} k_i - 2m = (m-1)n - m^2 - 2m + 1 + (1-m)x.$$

Subcase B1.2. $\{(v_j, v_{j+1}^1), (v_{j+1}, v_j^{k_j}) : j \in \Phi\}$. The number of such pairs is $2(s+t)$.

Case B2. Pairs of vertices with no hanging vertices and whose both vertices are in $C(G)$.

Subcase B2.1. $\{(v_i^{k_i-1}, v_{i+1}^2) : i \in [m] \setminus \Phi\}$. The number of these pairs is $m - s - t$.

Subcase B2.2. $\{(v_i^{k_i}, v_{i+1}^2), (v_i^{k_i-1}, v_{i+1}^1) : i \in \{l_1, l_2, \ldots, l_t\}\}$. The number of these pairs is $2t$.

Subcase B2.3. First, we assume that $k_i \ge 3$ for $i \in [m] \setminus \Psi$. Then, we list such pairs of vertices:

$$\{(v_j^{k_j}, v_{j+1}^i) : i \in [k_{j+1}] \setminus \{1, 2\}, j \in [m] \setminus \Phi\} \quad \text{and} \quad \{(v_{j+1}^1, v_j^i) : i \in [k_j] \setminus \{k_j - 1, k_j\}, j \in [m] \setminus \Phi\}.$$

By Equation (11), the number of the pairs of vertices mentioned above is

$$2\sum_{i=1}^{m} k_i - 4(m - s - t) - \sum_{i \in \Phi}(k_i + k_{i+1}) = 2n - 6m - 2 + 4(s+t) - 2x - \sum_{i \in \Phi}(k_i + k_{i+1}).$$

As discussed in Proposition 2.1, the number of those k_i whose value is 2 for $i \in [m] \setminus \Psi$ is λ. Thus, the number of these pairs of vertices is

$$2n - 6m - 2 + \lambda + 4(s+t) - 2x - \sum_{i \in \Phi}(k_i + k_{i+1}).$$

Case B3. Pairs of vertices contain a single hanging vertex. By Equation (11), for any $h \in [t]$, the number of pairs of vertices

$$\{(z_h, v_i^p) : i \in [m] \setminus \{l_h, l_{h+1}\}, p \in [k_i]\} \cup \{(z_h, v_{l_h}^p) : p \in [k_{l_h}] \setminus \{k_{l_h} - 1, k_{l_h}\}\} \cup \{(z_h, v_{l_h+1}^p) : p \in [k_{l_h+1}] \setminus \{1, 2\}\}$$

is

$$\sum_{i=1}^{m} k_i - 4 = n - m - 5 - x.$$

Thus, the total number of such pairs is $t(n - m - 5 - x)$.

Case B4. Pairs of vertices contain multiple hanging vertices. For any $i \in [s]$, we list these pairs of vertices as follows:

$$\{(u, v_j^1), (u, v_j^2), \ldots, (u, v_j^{k_j}) : u \in \{y_i^1, y_i^2, \ldots, y_i^{p_i}\}, j \in [m] \setminus \{r_i, r_i + 1\}\};$$
$$\{(y_i^1, v_{r_i}^h) : h \in [k_{r_i}] \setminus \{k_{r_i} - 1, k_{r_i}\}\} \cup \{(y_i^2, v_{r_i}^h) : h \in [k_{r_i} - 1]\};$$
$$\{(u, v_{r_i}^1), (u, v_{r_i}^2), \ldots, (u, v_{r_i}^{k_{r_i}}) : u \in \{y_i^1, \ldots, y_i^{p_i}\} \setminus \{y_i^1, y_i^2\}\};$$
$$\{(y_i^{p_i}, v_{r_i+1}^h) : h \in [k_{r_i+1}] \setminus \{1, 2\}\} \cup \{(y_i^{p_i-1}, v_{r_i+1}^h) : h \in [k_{r_i+1}] \setminus \{1\}\};$$
$$\{(u, v_{r_i+1}^1), (u, v_{r_i+1}^2), \ldots, (u, v_{r_i+1}^{k_{r_i+1}}) : u \in \{y_i^1, \ldots, y_i^{p_i}\} \setminus \{y_i^{p_i-1}, y_i^{p_i}\}\}.$$

We note that if $p_i = 2$, then there exists a pair of vertices $\left(v_{r_i}^{k_{r_i}}, v_{r_i+1}^1\right)$; otherwise, the pair of vertices does not exist. Thus, for $i \in [s]$, the total number of such pairs is

$$\sum_{j=1}^{s} p_j \sum_{i=1}^{m} k_i - 6s + \varepsilon.$$

Hence, by Cases B1, B2, B3, and B4, we have

$$\gamma_G(3) = (m+1)n - m^2 - 7m - 1 + \lambda + x(\sum_{i=1}^{m} k_i - m - 1) + 3t - s - \sum_{i\in\Phi}(k_i + k_{i+1}) + \varepsilon. \tag{15}$$

For the pairs of vertices at distance 4, there is only one possibility: $\{(u,v) : u, v \in V(C(G)) \setminus \sigma, d_G(u,v) = 4\}$, where σ is the set of all hanging vertices. Hence,

$$\gamma_G(4) = \sum_{1\le i<j\le m} k_i k_j - 2n + 2m + 2 - \lambda + 2x - 3t + \sum_{i\in\Phi}(k_i + k_{i+1}) - \varepsilon. \tag{16}$$

Now, by using Equations (1), (13), (14), (15), and (16), we obtain the required result. □

Now, we consider a graph in $\mathbb{H}_{n,4}^{*1}$ with the minimum Wiener index. For a graph $G \in \mathbb{H}_{n,4}^{*1}$ with $m \ge 3$ support vertices and for any support vertex v_i, recall that $k_i = |N_G(v_i) \cap C(G)| \ge 2$ when $i \in [m]$. Let t be the number of regions with a single hanging vertex, s be the number of regions with multiple hanging vertices, x be the number of hanging vertices, and Φ be the set of regions with hanging vertices in G.

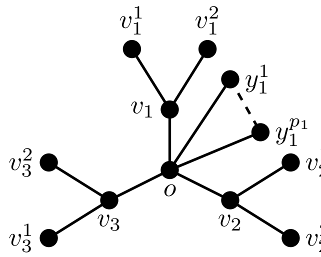

Figure 3.2: The characteristic tree $T(G_{3,3})$ of $G_{3,3}$.

Let $G_{2,m} \in \mathbb{H}_{n,4}^{*1}$ be a graph having m support vertices provided that $k_m = \sum_{i=1}^{m} k_i - 2(m-1)$, $k_i = 2$ for $i \in [m-1]$, and $\Phi = \{1\}$. Let $G_{3,m} \in \mathbb{H}_{n,4}^{*1}$ be a graph with m support vertices such that $k_i = 2$ for $i \in [m]$ and $\Phi = \{1\}$. For an example, $T(G_{3,3})$ is shown in Figure 3.2.

Theorem 3.1. *For any graph $G \in \mathbb{H}_{n,4}^{*1}$, we have $W(G) \ge F_2(n)$ and*

$$F_2(n) = \begin{cases} 106, & \text{if } n = 11, \\ 133, & \text{if } n = 12, \\ n^2 + 3n - 46, & \text{if } n \ge 13, \end{cases} \tag{17}$$

where the equality $W(G) = F_2(n)$ holds if and only if $G \cong G_{3,3}$.

Proof. Let $G \in \mathbb{H}_{n,4}^{*1}$ be a graph attaining the minimum Wiener index. Suppose that G has $m \ge 3$ support vertices. By Proposition 3.1, we have

$$W(G) = n^2 + (m-6)n + 2\sum_{1\le i<j\le m} k_i k_j - (m+2)m + 5 - \lambda + x(\sum_{i=1}^{m} k_i - m + 3) - s - 3t + \sum_{i\in\Phi}(k_i + k_{i+1}) - \varepsilon.$$

Since to $k_i \ge 2$ for $i \in [m]$, all the hanging vertices of G should be in the same region provided that

$$\sum_{i\in\Phi}(k_i + k_{i+1}) = min(k_h + k_{h+1})$$

for $h \in [m]$. Without loss of generality, by Lemma 2.1, we have $k_m = \sum_{i=1}^{m} k_i - 2(m-1)$, $k_i = 2$ for $i \in [m-1]$, and $\Phi = \{1\}$ in G. Note that $G \cong G_{2,m}$. By Proposition 3.1, we have the values of $W(G_{2,m})$, and $W(G_{3,m})$. Note that $W(G_{2,m}) \ge W(G_{3,m})$, where the equality holds if and only if $G_{2,m} \cong G_{3,m}$. Next, we show that $W(G_{3,m}) \ge W(G_{3,3})$. For the graph $G_{3,m}$, we have three cases.

Case 1. $x \geq 3$.
By Proposition 3.1, we have $n = 1 + 3m + x \geq 13$ and $W(G_{3,m}) = (2n - 17)m + n^2 - 3n + 5$. Consequently, we have $W(G_{3,m}) \geq W(G_{3,3})$ and

$$W(G_{3,3}) = n^2 + 3n - 46. \tag{18}$$

Case 2. $x = 2$.
By Proposition 3.1, we have $n = 3 + 3m \geq 12$ and

$$W(G_{3,m}) = \frac{5}{3}n^2 - \frac{32}{3}n + 21.$$

If $n = 12$, then $m = 3$ and $W(G_{3,3}) = 133$. However, if $n = 3m + 3 \geq 15$, then we have

$$\frac{5}{3}n^2 - \frac{32}{3}n + 21 > n^2 + 3n - 46.$$

Case 3. $x = 1$.
By Proposition 3.1, we have $n = 2 + 3m \geq 11$ and

$$W(G_{3,m}) = \frac{5}{3}n^2 - 10n + \frac{43}{3}.$$

If $n = 11$, then $m = 3$ and $W(G_{3,3}) = 106$. However, if $n = 3m + 2 \geq 14$, we have

$$\frac{5}{3}n^2 - 10n + \frac{43}{3} > n^2 + 3n - 46.$$

Therefore, $G \cong G_{3,3}$ and we can obtain Equation (17). □

4. Graphs in $\mathbb{H}^{*2}_{n,4}$

Since every graph $G \in \mathbb{H}^{*2}_{n,4}$ has only 2 support vertices, we have $\Phi(G) \subseteq [2]$, where $\Phi(G)$ is the set of regions with hanging vertices in G. Let $\mathbb{G}_{t1}$ denote the set of all those graphs of $\mathbb{H}^{*2}_{n,4}$ that contain multiple hanging vertices only in one region and no single hanging vertex. Also, denote by $\mathbb{G}_{t2}$ the set of all those graphs of $\mathbb{H}^{*2}_{n,4}$ that contain multiple hanging vertices in two regions. Furthermore, we denote by $\mathbb{G}_{t3}$ the set of all those graphs of $\mathbb{H}^{*2}_{n,4}$ that contain single hanging vertices in two regions. Moreover, let $\mathbb{G}_{t4}$ be the set of all those graphs of $\mathbb{H}^{*2}_{n,4}$ that contain a single hanging vertex only in one region and no multiple hanging vertices. Finally, we denote by $\mathbb{G}_{t5}$ the set of all those graphs of $\mathbb{H}^{*2}_{n,4}$ that contain both multiple hanging vertices and single hanging vertices. By the properties of the isomorphism, the set $\mathbb{H}^{*2}_{n,4}$ can be divided into $\mathbb{G}_{t1}$, $\mathbb{G}_{t2}$, $\mathbb{G}_{t3}$, $\mathbb{G}_{t4}$, and $\mathbb{G}_{t5}$. The $E(C(G))$ for $G \in \mathbb{H}^{*2}_{n,4}$ is similar to Equation (10). Since the proofs of the following propositions are similar to that of Proposition 3.1, we omit them.

Proposition 4.1. *If $G \in \mathbb{G}_{t1}$ has two support vertices, then*

$$W(G) = \begin{cases} 63, & \text{if } n = 9, \\ n^2 - 3n - 7 + p_1(k_1 + k_2) + 2k_1k_2 - \varepsilon, & \text{if } n \geq 10, \end{cases} \tag{19}$$

with $k_1, k_2, p_1 \geq 2$ and $n \geq 9$, where ε is the number of p_i with $p_i = 2$ for $i \in \{1\}$ and $T(G)$ is shown in Figure 4.1.

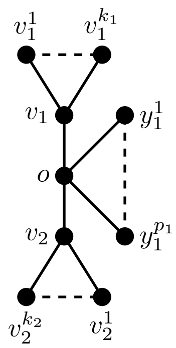

Figure 4.1: The characteristic tree $T(G)$ of $G \in \mathbb{G}_{t1}$.

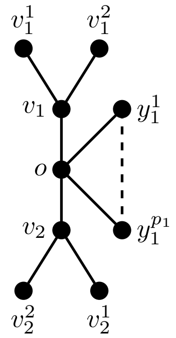

Figure 4.2: The characteristic tree $T(G'_{t1})$ of G'_{t1}.

Let $G'_{t1} \in \mathbb{G}_{t1}$ be a graph with $k_1 = k_2 = 2$. The graph $T(G'_{t1})$ is shown in Figure 4.2.

Lemma 4.1. *For any graph $G \in \mathbb{G}_{t1}$, we have $W(G) \geq F_3(n)$ and*

$$F_3(n) = \begin{cases} 63, & \text{if } n = 9, \\ n^2 + n - 27, & \text{if } n \geq 10, \end{cases} \tag{20}$$

where the equality $W(G) = F_3(n)$ holds if and only if $G \cong G'_{t1}$.

Proof. By Proposition 4.1 we have $W(G'_{t1}) = F_3(n)$. For any graph $G \in \mathbb{G}_{t1}$, by Proposition 4.1 and Lemma 2.1, we conclude that if $n = 9$ then $W(G) = W(G'_{t1}) = 63$, and if $n \geq 10$ then

$$\begin{aligned} W(G) &= n^2 - 3n - 7 + p_1(k_1 + k_2) + 2k_1k_2 - \varepsilon \\ &\geq n^2 - 3n - 7 + p_1(k_1 + k_2) + 4(k_1 + k_2 - 2) - \varepsilon \\ &= n^2 - 3n - 7 + p_1(k_1 + k_2) + 4(n - p_1 - 5) - \varepsilon \\ &= n^2 + n - 27 + p_1(k_1 + k_2 - 4) - \varepsilon \\ &\geq W(G'_{t1}). \end{aligned}$$

□

Proposition 4.2. *If $G \in \mathbb{G}_{t2}$ has two support vertices, then*

$$W(G) = n^2 - 3n - 8 + (p_1 + p_2 + 1)(k_1 + k_2) + 2k_1k_2 - \varepsilon, \tag{21}$$

with $k_1, k_2, p_1, p_2 \geq 2$ and $n \geq 11$, where ε is the number of p_i with $p_i = 2$ for $i \in [2]$ and $T(G)$ is shown in Figure 4.3.

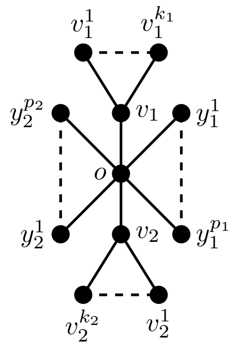

Figure 4.3: The characteristic tree $T(G)$ of $G \in \mathbb{G}_{t2}$.

Lemma 4.2. *For any graph $G \in \mathbb{G}_{t2}$, it holds that $W(G) > W(G'_{t1})$.*

Proof. By Proposition 4.2 and Lemma 2.1, we have

$$\begin{aligned} W(G) &= n^2 - 3n - 8 + (p_1 + p_2 + 1)(k_1 + k_2) + 2k_1k_2 - \varepsilon \\ &\geq n^2 - 3n - 8 + (p_1 + p_2 + 1)(k_1 + k_2) + 4(k_1 + k_2 - 2) - \varepsilon \\ &= n^2 + n - 27 + (p_1 + p_2)(k_1 + k_2 - 4) + (k_1 + k_2) - 1 - \varepsilon \\ &> W(G'_{t1}). \end{aligned}$$

□

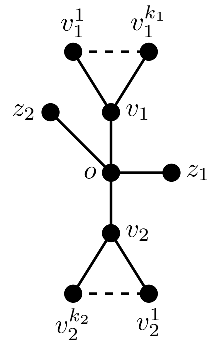

Figure 4.4: The characteristic tree $T(G)$ of $G \in \mathbb{G}_{t3}$.

Proposition 4.3. *If $G \in \mathbb{G}_{t3}$ has two support vertices, then*

$$W(G) = \begin{cases} 64, & \text{if } n = 9, \\ n^2 + 2k_1k_2 - 27, & \text{if } n \geq 10, \end{cases} \tag{22}$$

with $k_1, k_2 \geq 2$ and $n \geq 9$, where $T(G)$ is shown in Figure 4.4.

Lemma 4.3. *For any graph $G \in \mathbb{G}_{t3}$, it holds that $W(G) > W(G'_{t1})$.*

Proof. By Proposition 4.3 and Lemma 2.1, if $n = 9$ then $W(G) > W(G'_{t1})$, and if $n \geq 10$ then

$$\begin{aligned} W(G) &= n^2 + 2k_1k_2 - 27 \\ &\geq n^2 + 4(k_1 + k_2 - 2) - 27 \\ &= n^2 + 4(n - 7) - 27 \\ &> W(G'_{t1}). \end{aligned}$$

□

Proposition 4.4. *If $G \in \mathbb{G}_{t4}$ has two support vertices, then*

$$W(G) = \begin{cases} 46, & \text{if } n = 8, \\ 64, & \text{if } n = 9, \\ n^2 - 2n + 2k_1k_2 - 12, & \text{if } n \geq 10, \quad k_1 = 2 \text{ or } k_2 = 2, \\ n^2 - 2n + 2k_1k_2 - 13, & \text{if } n \geq 10, \quad k_1 \neq 2 \text{ and } k_2 \neq 2, \end{cases} \tag{23}$$

with $k_1, k_2 \geq 2$ and $n \geq 8$, where $T(G)$ is shown in Figure 4.5.

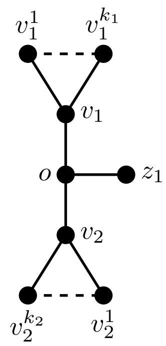

Figure 4.5: The characteristic tree $T(G)$ of $G \in \mathbb{G}_{t4}$.

Let $G'_{t4} \in \mathbb{G}_{t4}$ be the graph with $n = 8$.

Lemma 4.4. *For any graph $G \in \mathbb{G}_{t4}$ with $n \geq 9$, it holds that $W(G) > W(G'_{t1})$.*

Proof. By Proposition 4.4 and Lemma 2.1, if $n = 9$ then $W(G) > W(G'_{t1})$, and if $n \geq 10$ then

$$\begin{aligned} W(G) &\geq n^2 - 2n + 2k_1k_2 - 13 \geq n^2 - 2n + 4(k_1 + k_2 - 2) - 13 \\ &= n^2 - 2n + 4(n-6) - 13 = n^2 + 2n - 37 \\ &> W(G'_{t1}). \end{aligned}$$

Hence, $W(G) > W(G'_{t1})$ for $n \geq 9$. □

Proposition 4.5. *If $G \in \mathbb{G}_{t5}$ has two support vertices, then*

$$W(G) = n^2 - 3n - 10 + (p_1 + 2)(k_1 + k_2) + 2k_1k_2 - \varepsilon, \tag{24}$$

with $k_1, k_2, p_1 \geq 2$ and $n \geq 10$, where ε is the number of p_i with $p_i = 2$ for $i \in \{1\}$ and $T(G)$ is shown in Figure 4.6.

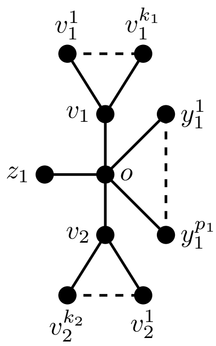

Figure 4.6: The characteristic tree $T(G)$ of $G \in \mathbb{G}_{t5}$.

Let $G'_{t5} \in \mathbb{G}_{t5}$ be a graph of order $n = 10$ in which $k_1 = k_2 = p_1 = 2$.

Lemma 4.5. *For any graph $G \in \mathbb{G}_{t5}$, we have $W(G) \geq W(G'_{t1})$, where equality holds if and only if $G \cong G'_{t5}$.*

Proof. By Proposition 4.5 and Lemma 2.1, we have

$$\begin{aligned} W(G) &= n^2 - 3n - 10 + (p_1 + 2)(k_1 + k_2) + 2k_1k_2 - \varepsilon \\ &\geq n^2 - 3n - 10 + (p_1 + 2)(k_1 + k_2) + 4(k_1 + k_2 - 2) - \varepsilon \\ &= n^2 - 3n - 10 + (p_1 + 2)(k_1 + k_2) + 4(n - p_1 - 6) - \varepsilon \\ &= n^2 + n - 27 + (p_1 + 2)(k_1 + k_2 - 4) + 1 - \varepsilon \\ &\geq W(G'_{t1}), \end{aligned}$$

where the equality $W(G) = W(G'_{t1})$ holds if and only if $k_1 = k_2 = p_1 = 2$, that is, $G \cong G'_{t5}$. □

Theorem 4.1. *Let $G \in \mathbb{H}^{*2}_{n,4}$. If $n = 8$, then $G \cong G'_{t4}$. If $n = 10$, then $W(G) \geq W(G'_{t1})$, where the equality holds if and only if $G \cong G'_{t1}$ or $G \cong G'_{t5}$. If $n = 9$ or $n \geq 11$, then $W(G) \geq W(G'_{t1})$, where the equality holds if and only if $G \cong G'_{t1}$.*

Proof. By Lemmas 4.1, 4.2, 4.3, 4.4, and 4.5, we obtain the desired result. □

5. Main result

This section gives the main theorem of this paper, which is proved by using the results established in the previous three sections.

Theorem 5.1. *Let $G \in \mathbb{H}_{n,4}$ be a graph with the minimum Wiener index. If $n = 8$ then $G \cong G'_{t4}$, if $n = 10$ then $G \cong G_{1,3}$, and if $n = 9$ or $n \geq 11$, then $G \cong G'_{t1}$. Also,*

$$W(G) = \begin{cases} 46, & \text{if } n = 8, \\ 63, & \text{if } n = 9, \\ 81, & \text{if } n = 10, \\ n^2 + n - 27, & \text{if } n \geq 11. \end{cases} \tag{25}$$

Proof. By Theorems 2.1, 3.1, and 4.1, we compare the values of $W(G_{1,3})$, $W(G_{3,3})$, and $W(G'_{t1})$, and then we obtain the required result. □

References

[1] J. A. Bondy, L. Lovász, Lengths of cycles in Halin graphs, *J. Graph Theory* **9** (1985) 397–410.

[2] V. Božović, Ž. K. Vukićević, G. Popivoda, R. Pan, X. Zhang, Extreme Wiener indices of trees with given number of vertices of maximum degree, *Discrete Appl. Math.* **304** (2021) 23–31.

[3] P. Dankelmann, A. Alochukwu, Wiener index in graphs with given minimum degree and maximum degree, *Discrete Math. Theor. Comput. Sci.* **23** (2021) #11.

[4] K. C. Das, M. J. Nadjafi-Arani, On maximum Wiener index of trees and graphs with given radius, *J. Comb. Optim.* **34** (2017) 574–587.

[5] I. Gutman, A property of the Wiener number and its modifications, *Indian J. Chem.* **36A** (1997) 128–132.

[6] R. Halin, Über simpliziale Zerfallungen beliebiger, *Math. Ann.* **156** (1964) 216–225.

[7] S. He, H. Liu, The maximum number of short paths in a Halin graph, *Discrete Optim.* **50** (2023) #100809.

[8] S. Klavžar, M. J. Nadjafi-Arani, On the difference between the revised Szeged index and the Wiener index, *Discrete Math.* **333** (2014) 28–34.

[9] S. Klavžar, M. J. Nadjafi-Arani, Wiener index in weighted graphs via unification of Θ^*-classes, *European J. Combin.* **36** (2014) 71–76.

[10] S. Klavžar, M. J. Nadjafi-Arani, Improved bounds on the difference between the Szeged index and the Wiener index of graphs, *European J. Combin.* **39** (2014) 148–156.

[11] M. Knor, R. Škrekovski, A. Tepeh, Selected topics on Wiener index, *Ars Math. Contemp.* **24** (2024) #P4.07.

[12] L. Li, X. Li, W. Liu, Note on the product of Wiener and Harary indices, *MATCH Commun. Math. Comput. Chem.* **91** (2024) 299–305.

[13] X. Liu, Y. Mao, I. Gutman, The Steiner Wiener index of a graph, *Discuss. Math. Graph Theory* **36** (2016) 455–465.

[14] H. Wiener, Structural determination of paraffin boiling points, *J. Am. Chem. Soc.* **69** (1947) 17–20.

[15] K. Xu, A. Ilić, V. Iršič, S. Klavžar, H. Li, Comparing Wiener complexity with eccentric complexity, *Discrete Appl. Math.* **290** (2021) 7–16.

[16] K. Xu, J. Li, Z. Luo, Comparative results between the number of subtrees and Wiener index of graphs, *RAIRO Oper. Res.* **56** (2022) 2495–2511.

[17] K. Xu, M. Wang, J. Tian, Relations between Merrifield-Simmons and Wiener indices, *MATCH Commun. Math. Comput. Chem.* **85** (2021) 147–160.