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A Survey on Recent Results of Variable Wiener Index *

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Abstract: In this paper, we report some recent results, mainly focusing on the ordering results, of some typical variable Wiener indices, Wiener polarity index or hyper-Wiener index in some given classes of graphs.

1 Introduction

The *distance* $d_G(u, v)$ (or simply $d(u, v)$ when no confusion arise) between the vertices u and v of G is equal to the length of (number of edges in) the shortest path that connects u and v. Let $\gamma(G, k)$ denote the number of unordered vertex pairs of G, the distance of which is equal to k.

As early as in 1947, Wiener [1] used the next formula to calculate the boiling points t_B of the paraffins:

$$t_B = aW(G) + bW_P(G) + c,$$

where a, b, and c are constants for a given isomeric group, $W(G)$ is equal to the sum of distance $d_G(u, v)$ of unordered vertex pairs pertaining to G, and $W_P(G)$ is equal to the

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number of unordered vertex pairs of distance 3. In the sequel, this simple numerical representation of a molecule has shown to be a very useful quantity to use in the quantitative structure-property relationships (QSPR) [2, 3]. Moreover, it also has many applications in communication, facility location, cryptology, etc., that are effectively modeled by a connected graph G satisfying certain restrictions [4]. Thus, $W(G)$ receives much attention and it is called *Wiener index* of G, while $W_P(G)$ is named *Wiener polarity index* of G.

By the definitions of $W_P(G)$ and $W(G)$, it turns out that $W_P(G) = \gamma(G, 3)$ and

$$W(G) = \sum_{\{u,v\}\subseteq V(G)} d(u, v) = \sum_{k\geq 1} k\gamma(G, k). \tag{1.1}$$

Actually, Wiener himself conceived $W(G)$ only for acyclic molecules and he showed that his index can be computed by means of the next formula:

$$W(T) = \sum_{e} n_1(e) \cdot n_2(e) \tag{1.2}$$

where T is a tree, $n_1(e)$ and $n_2(e)$ are the number of vertices on the two sides of the edge e, and where the summation goes over all edges of T. The definition of the Wiener index in term of distances between vertices of a graph, such as in Eq. (1.1), was first given by Hosoya [5]. When G is a tree, Eq. (1.1) is equivalent to Eq. (1.2). For the proof, one can refer to [4]. Moreover, [4] is a comprehensive survey for the Wiener index, and the reader is referred to the paper for further details.

A large number of modifications and extensions of the Wiener index was considered in the chemical literature; an extensive bibliography on this matter can be found in the reviews [6, 7]. Lately, Nikolić, Trinajstić and Randić [8] put forward a *modified Wiener index* ${}^mW$, defined as

$${}^mW(T) = \sum_{e} (n_1(e) \cdot n_2(e))^{-1} \tag{1.3}$$

In the same paper, they illustrated some examples to show that this modification leads to improved QSPR models by comparing with the Wiener index, and they also used this index to establish the structure-boiling point models for octanes. Recently, motivated by the analogy between Eqs. (1.2) and (1.3), Gutman, Vukičević and Žerovnik [9] extended the definitions of $W(T)$ and ${}^mW(T)$ to

$${}^mW_\lambda(T) = \sum_{e} (n_1(e) \cdot n_2(e))^\lambda. \tag{1.4}$$

In [9], the authors called ${}^mW(T)$ the *modified Wiener index* of T, and ${}^mW_\lambda(T)$ the *variable Wiener index* of T. The Wiener index and all kinds of variable Wiener indices have important applications in chemistry, for instance, the optima value of λ which gives the smallest standard error of estimate, in the the structure-boiling point modeling of isomeric octanes was studied in [10], and the relation between variable Wiener indices and internal molecular energy was studied in [11]. Thus, more and more mathematicians and chemists became interested in them and devoted themselves to the study (see e. g. [10–14]). For more results on the mathematical properties and their applications in chemistry of different kinds of variable Wiener indices, one can refer to [10–15] and the references cited therein.

Among these modifications and extensions of Wiener index, the hyper-Wiener index is another important one. The *hyper-Wiener index* $WW(G)$ is introduced by Randić in [16] and is defined as

$$WW(G) = \frac{1}{2}W(G) + \frac{1}{2}\sum_{\{u,v\}\subseteq V(G)} d^2(u,v) = \frac{1}{2}\sum_{k\geq 1} k(k+1)\gamma(G,k). \tag{1.5}$$

It rapidly gained popularity and numerous results on it were reported [17–21]. For the mathematical properties and extensions of hyper-Wiener index, one can be referred to [17–22] and the references cited therein.

In this paper, we shall report some recent results, mainly focus on the ordering results, of some typical variable Wiener indices, Wiener polarity index or hyper-Wiener index, in some given class of graphs.

2 The Variable Wiener indices of trees

We shall begin with some graph transformations, under which the variable Wiener index increases or decreases. Suppose v is a vertex of a tree R. As shown in Fig. 2.1, let $R_{k,l}$ ($l \geq k \geq 1$) be the graph obtained from R by attaching at v two new paths P: $v(= v_0)v_1v_2\cdots v_k$ and Q: $v(= u_0)u_1u_2\cdots u_l$ of length k and l, respectively, where v_1, v_2, ..., v_k and u_1, u_2, ..., u_l are distinct new vertices. Let $R_{k-1,l+1} = R_{k,l} - v_{k-1}v_k + u_lv_k$.

Fig. 2.1. The trees $R_{k,l}$ and $R_{k-1,l+1}$.

Proposition 2.1 [9] *Let R be a tree with at least two vertices or an isolated vertex. If $l \geq k \geq 1$, then ${}^{m}W_{\lambda}(R_{k,l}) \leq {}^{m}W_{\lambda}(R_{k-1,l+1})$ for $\lambda > 0$, and ${}^{m}W_{\lambda}(R_{k,l}) \geq {}^{m}W_{\lambda}(R_{k-1,l+1})$ for $\lambda < 0$, where both equalities hold if and only if R is an isolated vertex.*

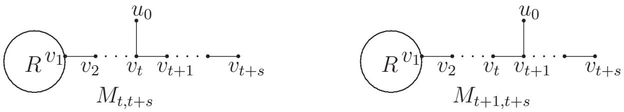

Fig. 2.2. The trees $M_{t,t+s}$ and $M_{t+1,t+s}$.

Suppose v is a vertex of a tree R, and v_2, ..., v_{t+s}, u_0 are distinct new vertices (not in R). Let R' be the graph obtained from R by attaching a new path P: $v_1 v_2 \cdots v_{t+s}$. Let $M_{t,t+s} = R' + v_t u_0$ and $M_{t+i,t+s} = R' + v_{t+i} u_0$, where $1 \leq i \leq s$. For instance, $M_{t,t+s}$ and $M_{t+1,t+s}$ are depicted in Fig. 2.2.

Proposition 2.2 *Let R be a tree with at least two vertices or an isolated vertex. If $t \geq s \geq 1$, then ${}^{m}W_{\lambda}(M_{t,t+s}) \leq {}^{m}W_{\lambda}(M_{t+i,t+s})$ for $\lambda > 0$, and ${}^{m}W_{\lambda}(M_{t,t+s}) \geq {}^{m}W_{\lambda}(M_{t+i,t+s})$ for $\lambda < 0$, where $1 \leq i \leq s$.*

Remark 2.1 In [25], Proposition 2.2 was proved to be true in the case of $\lambda = 1$, i.e., the Wiener index, since ${}^{m}W_1(T) = W(T)$. Actually, with the similar method applied in [25], we can also deduce Proposition 2.2.

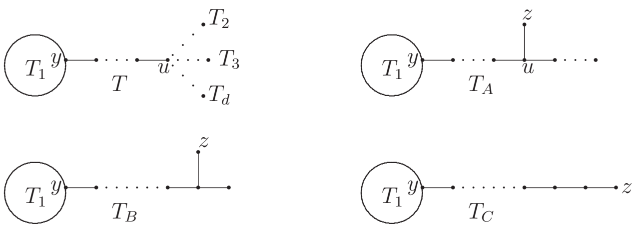

Fig. 2.3. The tree's transfer operation: $T \to T_A \to T_B \to T_C$.

A vertex u of a tree T is called a *branching vertex* of T if $d(u) \geq 3$. Furthermore, u is said to be an *out-branching vertex* if at most one of the components of $T - u$ is not a path.

Now we introduce a transfer operation, which was applied in [24–26]: $T \to T_A \to T_B \to T_C$, as shown in Fig. 2.3, where T is a tree of order n, u is an out-branching point of T, $d(u) = m \geq 3$, and all the components T_1, T_2, ..., T_m of $T - u$ except T_1 are paths.

Proposition 2.3 [26] *Let u be an out-branching vertex of a tree T of order n, $d(u) = m$ ($m \geq 3$), and let all components T_1, T_2, ..., T_m of $T - u$ except T_1 be paths.*

(1) *If $\lambda > 0$, then ${}^mW_\lambda(T) \leq {}^mW_\lambda(T_A) \leq {}^mW_\lambda(T_B) < {}^mW_\lambda(T_C)$, where ${}^mW_\lambda(T) = {}^mW_\lambda(T_A)$ if and only if $T \cong T_A$, and ${}^mW_\lambda(T_A) = {}^mW_\lambda(T_B)$ if and only if $T_A \cong T_B$.*

(2) *If $\lambda < 0$, then ${}^mW_\lambda(T) \geq {}^mW_\lambda(T_A) \geq {}^mW_\lambda(T_B) > {}^mW_\lambda(T_C)$, where ${}^mW_\lambda(T) = {}^mW_\lambda(T_A)$ if and only if $T \cong T_A$, and ${}^mW_\lambda(T_A) = {}^mW_\lambda(T_B)$ if and only if $T_A \cong T_B$.*

Fig. 2.4. The trees P_n^* and S_n^*.

As usual, let C_n, P_n, S_n and K_n be a cycle, a path, a star and a complete graph on n vertices, respectively. Let P_n^* and S_n^* be the trees as shown in Fig. 2.4. By Proposition 2.1, Gutman et al. demonstrated the following:

Theorem 2.1 [9] *Let T be an arbitrary tree on n vertices, and $T \notin \{P_n, P_n^*, S_n, S_n^*\}$.*

(1) *If $\lambda > 0$ and $n \geq 5$, then ${}^mW_\lambda(P_n) > {}^mW_\lambda(P_n^*) > {}^mW_\lambda(T) > {}^mW_\lambda(S_n^*) > {}^mW_\lambda(S_n)$.*

(2) *If $\lambda < 0$ and $n \geq 5$, then ${}^mW_\lambda(P_n) < {}^mW_\lambda(P_n^*) < {}^mW_\lambda(T) < {}^mW_\lambda(S_n^*) < {}^mW_\lambda(S_n)$.*

Remark 2.2 By the results of Theorem 2.1, it turns out that the variable Wiener indices ${}^mW_\lambda$ may be viewed as a *branching index,* namely a topological index capable of measuring the extent of branching of the carbon-atom skeleton of molecules and capable of ordering isomers according to the extent of branching [9], for all λ.

A *caterpillar* is a tree in which a removal of all pendant vertices makes a path. Let $T(n, d; n_1, n_2, ..., n_{d-1})$ be a caterpillar obtained from a path $v_0, v_1, ..., v_d$ by attaching n_i ($n_i \geq 0$) pendant vertices to v_i ($i = 1, 2, ..., d-1$). Clearly, $n = d + 1 + \sum_{i=1}^{d-1} n_i$. Let $C(v_0 \cdots v_t;\ p)$ denote a *comet*, which is a tree obtained from a path $v_0 v_1 \cdots v_t$ by attaching p pendant vertices to the vertex v_t, where $t,\ p \geq 1$. For brevity, sometimes we write $C(v_0 \cdots v_{n-\Delta}; \Delta - 1)$ as $C(n, \Delta)$. Let $\mathcal{T}_n$ be the set of trees on n vertices, and $\mathcal{T}_n^\Delta$ be the set of trees on n vertices with maximum degree Δ. In the following, let $F(n, \Delta) = T(n, n-\Delta; \Delta - 2, 0, ..., 0, 1)$, $H(n, \Delta) = T(n, n - \Delta + 1; 0, \Delta - 2, 0, ..., 0)$. Using Propositions 2.1 and 2.3 proper number of times, the next result can be achieved.

Theorem 2.2 *Let T be a tree in $\mathcal{T}_n^{\Delta} \setminus \{C(n,\Delta), F(n,\Delta), H(n,\Delta)\}$. Then,*

(1) ${}^{m}W_{\lambda}(T) < \max\{{}^{m}W_{\lambda}(F(n,\Delta)), {}^{m}W_{\lambda}(H(n,\Delta))\} < {}^{m}W_{\lambda}(C(n,\Delta))$ *for* $\lambda > 0$;

(2) ${}^{m}W_{\lambda}(T) > \min\{{}^{m}W_{\lambda}(F(n,\Delta)), {}^{m}W_{\lambda}(H(n,\Delta))\} > {}^{m}W_{\lambda}(C(n,\Delta))$ *for* $\lambda < 0$.

Remark 2.3 In [26], Theorem 2.2 was present in the restriction of $\Delta \geq \frac{n}{2}$. Actually, by employing the similar method used in [26], the condition $\Delta \geq \frac{n}{2}$ can be deleted. For detail, one can be referred to the proof of Theorems 2.1 and 2.2 of [26].

Let $\mathcal{T}_n^{1,\Delta}$ be the set of trees on n vertices, whose vertices are of degree 1 or Δ. Let $M_1(n,\Delta)$ be the caterpillar tree of order n, whose vertices are of degree 1 or Δ.

Theorem 2.3 [75] *Let T be a tree in $\mathcal{T}_n^{1,\Delta} \setminus \{M_1(n,\Delta)\}$. Then,*

(1) ${}^{m}W_{\lambda}(T) < {}^{m}W_{\lambda}(M_1(n,\Delta))$ *for* $\lambda > 0$;

(2) ${}^{m}W_{\lambda}(T) > {}^{m}W_{\lambda}(M_1(n,\Delta))$ *for* $\lambda < 0$.

Let $\mathcal{T}_{n,\ k}$ $(n \geq 3)$ be the set of trees with n vertices and k pendant vertices. It is easy to see that $\mathcal{T}_{n,\ 2} = \{P_n\}$ and $\mathcal{T}_{n,\ n-1} = \{S_n\}$. Paths P_{l_1}, ..., P_{l_k} are said to *have almost equal lengths* if l_1, ..., l_k satisfy $|l_i - l_j| \leq 1$ for $1 \leq i \leq j \leq k$. The notation $B_{n,k}$ denotes the tree on n vertices formed by attaching k paths of almost equal lengths to one common vertex v. Obviously, $B_{n,k} \in \mathcal{T}_{n,\ k}$. Let $S(p; n_1, n_2)$ be a tree on n vertices obtained from a path $v_1 v_2 \cdots v_p$ by attaching n_1 and n_2 pendant vertices to the vertices v_1 and v_p, respectively, where $n_1 + n_2 + p = n$. For $3 \leq k \leq n-2$, the maximum and minimum variable Wiener indices in $\mathcal{T}_{n,\ k}$ were determined.

Theorem 2.4 [23] *Suppose $T \in \mathcal{T}_{n,\ k} \setminus \{B_{n,k}, S(n-k; \lfloor \frac{k}{2} \rfloor, \lceil \frac{k}{2} \rceil)\}$, where $3 \leq k \leq n-2$. Then,*

(1) ${}^{m}W_{\lambda}(B_{n,k}) < {}^{m}W_{\lambda}(T) < {}^{m}W_{\lambda}(S(n-k; \lfloor \frac{k}{2} \rfloor, \lceil \frac{k}{2} \rceil))$ *if* $\lambda > 0$;

(2) ${}^{m}W_{\lambda}(S(n-k; \lfloor \frac{k}{2} \rfloor, \lceil \frac{k}{2} \rceil)) < {}^{m}W_{\lambda}(T) < {}^{m}W_{\lambda}(B_{n,k})$ *if* $\lambda < 0$.

Let $\mathcal{T}(n,d)$ be the set of trees with n vertices and diameter d. It is easy to see that $\mathcal{T}(n,2) = \{S_n\}$, and $\mathcal{T}(n,n-1) = \{P_n\}$. Let $C_{n,d}$ be the caterpillar obtained from a path P_d with vertices $\{v_0, v_1, ..., v_d\}$ by attaching $n-d-1$ pendent edges to vertex $v_{\lfloor \frac{d}{2} \rfloor}$. Zhang and Zhou [87] determined the extremal variable Wiener index in $\mathcal{T}(n,d)$ via the next result.

Theorem 2.5 [87] *Suppose $T \in \mathcal{T}(n,d) \setminus \{C_{n,d}\}$, where $3 \leq d \leq n-1$. Then,* ${}^{m}W_{\lambda}(C_{n,d}) < {}^{m}W_{\lambda}(T)$ *if* $\lambda > 0$, *and* ${}^{m}W_{\lambda}(C_{n,d}) > {}^{m}W_{\lambda}(T)$ *if* $\lambda < 0$.

3 The Modified Wiener indices of trees

For modified Wiener index, Theorem 2.2 can be improved to

Theorem 3.1 [26] *Let T be a tree in $\mathcal{T}_n^{\Delta}\backslash\{C(n,\Delta)\}$. Then, ${}^mW(T) \geq {}^mW(H(n,\Delta)) > {}^mW(C(n,\Delta))$, and the first equality holds if and only if $T \cong H(n,\Delta)$.*

The tree $S(i, n-i)$ on n vertex is called a *double star* graph, which is obtained by joining the center of S_i to that of S_{n-i} by an edge. In particularly, $S(n-1,1)$ is the star S_n and $S(\Delta, n-\Delta) \cong T(n,3;\Delta-2, n-\Delta-2)$. The next result determines the first two largest values of ${}^mW(T)$ in $\mathcal{T}_n^{\Delta}$, where $\Delta \geq \frac{n}{2}$ and $n \geq 10$.

Theorem 3.2 [26] *Suppose $T \in \mathcal{T}_n^{\Delta}$, where $\Delta \geq \frac{n}{2}$ and $n \geq 10$. If $T \neq S(\Delta, n-\Delta)$, then*

$$ {}^mW(T) \leq {}^mW(T(n,4;n-\Delta-3,\Delta-2,0)) < {}^mW(S(\Delta,n-\Delta)), $$

where the first equality holds if and only if $T \cong T(n,4;n-\Delta-3,\Delta-2,0)$.

A *starlike tree* is a tree with only one branching point. Let $T(n;n_1,n_2,...,n_d)$ denote the starlike tree of order n obtained by inserting n_1-1, ..., n_d-1 vertices into the d edges of the star S_{d+1} of order $d+1$ respectively, where $n_1+\cdots+n_d = n-1$. For example, $P_n^* \cong T(n;n-3,1,1)$. The first k-th greatest and smallest modified Wiener indices in the class of trees on n vertices for all k up to $\lfloor \frac{n}{2} \rfloor + 1$, respectively, are characterized by the following two results.

Theorem 3.3 [24] *Suppose $T \in \mathcal{T}_n\backslash\{S_n, S_n^*, S(n-3,3), S(n-4,4), ..., S(\lceil \frac{n}{2} \rceil, \lfloor \frac{n}{2} \rfloor), T(n,4;0,n-5,0)\}$. If $n \geq 6$, then ${}^mW(S_n) > {}^mW(S_n^*) > {}^mW(S(n-3,3)) > {}^mW(S(n-4,4)) > \cdots > {}^mW(S(\lceil \frac{n}{2} \rceil, \lfloor \frac{n}{2} \rfloor)) > {}^mW(T(n,4;0,n-5,0)) > {}^mW(T)$.*

Theorem 3.4 [24] *If T is a tree with $n \geq 45$ vertices, then ${}^mW(P_n) < {}^mW(P_n^*) < {}^mW(T(n;n-4,2,1)) < \cdots < {}^mW(T(n;n-13,11,1)) < {}^mW(T(n;n-5,2,2)) < {}^mW(T(n;n-14,12,1)) < \cdots < {}^mW(T(n;\lceil \frac{n}{2} \rceil, \lfloor \frac{n}{2} \rfloor - 2, 1)) < {}^mW(T(n;\lceil \frac{n}{2} \rceil - 1, \lfloor \frac{n}{2} \rfloor - 1, 1))$, and for any other tree T, ${}^mW(T(n;\lceil \frac{n}{2} \rceil - 1, \lfloor \frac{n}{2} \rfloor - 1, 1)) < {}^mW(T)$.*

By Theorem 2.4, it immediately follows that

Theorem 3.5 *Suppose $T \in \mathcal{T}_{n,\ k}\backslash\{B_{n,k}, S(n-k; \lfloor \frac{k}{2} \rfloor, \lceil \frac{k}{2} \rceil)\}$, where $3 \leq k \leq n-2$. Then, ${}^mW(S(n-k; \lfloor \frac{k}{2} \rfloor, \lceil \frac{k}{2} \rceil)) < {}^mW(T) < {}^mW(B_{n,k})$.*

By Theorem 2.5, we have

Theorem 3.6 *Suppose $T \in \mathcal{T}(n,d) \setminus \{C_{n,d}\}$, where $3 \le d \le n-1$. Then, ${}^{m}W(C_{n,d}) > {}^{m}W(T)$.*

4 The Wiener index and hyper-Wiener index of graphs

In this section, we shall consider the ordering results of Wiener index and hyper-Wiener index in some given class of graphs. The reason for us to combine them together here is that they have many similar ordering results, for instance, see Remarks 4.1, 4.2, 4.3 and 4.4.

Let $\mathcal{G}(n)$ be the set of all the connected graphs on n vertices. Suppose k is a nonnegative integer, the notation $\mathcal{S}(K_n - ke)$ denotes the set of all connected graphs obtained from K_n by deleting k edges. By the definition, $\mathcal{S}(K_n - 0e) = \{K_n\}$. The *diameter* of G, denoted by $d(G)$, is $d(G) = max\{d(u,v) : u, v \in V(G)\}$. By some observations to Eqs. (1.1) and (1.5), it is straightforward to see that the smaller diameter, the smaller Wiener index and the smaller hyper-Wiener index. The next result will confirm this observation.

Theorem 4.1 [27] *Let n and k be two nonnegative integers with $n > 2k$. The first to $(k+1)$-th smallest Wiener indices of $\mathcal{G}(n)$ is $\binom{n}{2}$, $\binom{n}{2}+1$, ..., $\binom{n}{2}+k$, and the first to $(k+1)$-th smallest hyper-Wiener indices of $\mathcal{G}(n)$ is $\binom{n}{2}$, $\binom{n}{2}+2$, ..., $\binom{n}{2}+2k$. Moreover, $W(G) = \binom{n}{2}+i$ or $WW(G) = \binom{n}{2}+2i$ if and only if $G \in \mathcal{S}(K_n - ie)$, where $0 \le i \le k$.*

Remark 4.1 Suppose n and k are two nonnegative integers with $n > 2k$. Theorem 4.1 implies that the graphs which reach the i-th smallest Wiener indices even share the i-th smallest hyper-Wiener indices in the class of connected graphs on n vertices for every $i \in \{1, 2, ..., k+1\}$.

As early as in 1997, it has been demonstrated [28] that the S_n and P_n have the maximum and minimum Wiener indices in $\mathcal{T}_n$, respectively. After then, the first up to twelfth smallest (resp. fifteenth greatest) Wiener indices in $\mathcal{T}_n$ were identified in [29] (resp. [25]). Also, Gutman considered the similar order of hyper-Wiener index in $\mathcal{T}_n$, and he found that S_n and P_n also have the minimum and maximum hyper-Wiener indices in $\mathcal{T}_n$ [30]. In the sequel, Liu et al. identified the second up to ninth smallest hyper-Wiener indices of trees on $n \geq 17$ vertices and the second up to fifteenth greatest hyper-Wiener indices of trees on $n \geq 20$ vertices in [31, 32]. Next we shall introduce these results. We first would like to report some operations that increase or decrease the hyper-Wiener indices of trees.

Proposition 4.1 [32] *Let R be a tree with at least two vertices, or an isolated vertex. If $l \geq k \geq 1$, then $WW(R_{k,l}) \leq WW(R_{k-1,l+1})$, where the equality holds if and only if R is an isolated vertex.*

Proposition 4.2 [32] *Let R be a tree with at least two vertices, or an isolated vertex. If $t \geq s \geq 1$, then $WW(M_{t,t+s}) \leq WW(M_{t+i,t+s})$, where $1 \leq i \leq s$.*

Proposition 4.3 [32] *Let u be an out-branching point of a tree T of order n, $d(u) = m$ ($m \geq 3$), and let all components T_1, T_2, ..., T_m of $T - u$ except T_1 be paths. Then, $WW(T) \leq WW(T_A) \leq WW(T_B) < WW(T_C)$, where $WW(T) = WW(T_A)$ if and only if $T \cong T_A$, and $WW(T_A) = WW(T_B)$ if and only if $T_A \cong T_B$.*

If T is a tree of order n with exactly two branching points u_1 and u_2, with $d(u_1) = r$ and $d(u_2) = t$. The orders of those $r-1$ components of $T-u_1$, which are paths, are p_1, ..., p_{r-1}, the order of the component which is not a path of $T-u_1$ is $p_r = n-p_1-\cdots-p_{r-1}-1$. The orders of $t-1$ components, which are paths, of $T-u_2$ are q_1, ..., q_{t-1}, the order of the component which is not a path of $T-u_2$ is $q_t = n-q_1-\cdots-q_{t-1}-1$. We denote this tree by $T(n; p_1, ..., p_{r-1}; q_1, ..., q_{t-1})$, where $r \leq t$, $p_1 \geq \cdots \geq p_{r-1}$ and $q_1 \geq \cdots \geq q_{t-1}$. For example, $T(n; 1, 1; 1, 1) = T(n, n-3; 1, 0, ..., 0, 1)$. The next result, which can be proved by invoking Propositions 2.1–2.3 and Propositions 4.1–4.3, gives some largest Wiener indices and hyper-Wiener indices in $\mathcal{T}_n$, respectively.

Theorem 4.2 *Let $T \in \mathcal{T}_n$.* (1) [25, 28] *If $n \geq 28$, then* $W(P_n) > W(T(n; n-3, 1, 1)) > W(T(n; n-4, 2, 1)) > W(T(n; 1, 1; 1, 1)) > W(T(n; n-5, 3, 1)) > W(T(n; n-4, 1, 1, 1)) = W(T(n; 1, 1; 2, 1)) > W(T(n; n-6, 4, 1)) > W(T(n; n-5, 2, 2)) > W(T(n; 1, 1; n-5, 1)) = W(T(n; 1, 1; 3, 1)) > W(T(n; 2, 1; 2, 1)) > W(T(n; 1, 1; 1, 1, 1)) > W(T(n; n-7, 5, 1)) > W(T(n; 1, 1; n-6, 1)) = W(T(n; 1, 1; 4, 1)) > W(T(n; n-5, 2, 1, 1)) = W(T(n; 1, 1; 2, 2)) = W(T(n; 2, 1; 3, 1)) > W(T(n, n-4; 1, 1, 0, ..., 0, 1)) > W(T)$.
(2) [30, 32] *If $n \geq 20$, then* $WW(P_n) > WW(T(n; n-3, 1, 1)) > WW(T(n; n-4, 2, 1)) > WW(T(n; 1, 1; 1, 1)) > WW(T(n; n-5, 3, 1)) > WW(T(n; n-4, 1, 1, 1)) > WW(T(n; 1, 1; 2, 1)) > WW(T(n; n-6, 4, 1)) > WW(T(n; n-5, 2, 2))$

$> WW(T(n;1,1;n-5,1)) > WW(T(n;1,1;3,1)) > WW(T(n;2,1;2,1))$
$> WW(T(n;1,1;1,1,1)) > WW(T(n;n-7,5,1)) > WW(T(n;1,1;n-6,1)) > WW(T).$

Remark 4.2 Theorem 4.2 implies that the trees which reach the first to fifteenth greatest hyper-Wiener indices even share the first to thirteenth greatest Wiener indices in $\mathcal{T}_n$ when $n \geq 28$.

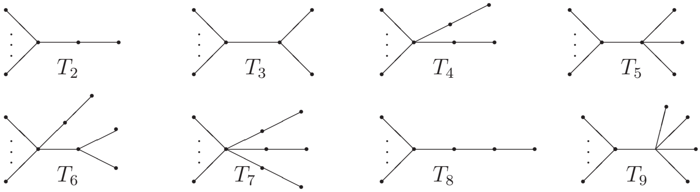

Fig. 4.1. The trees $T_2, ..., T_9$.

Theorem 4.3 *Let $T \in \mathcal{T}_n \backslash \{T_1, T_2, T_3, T_4, T_5, T_6, T_7, T_8, T_9\}$, where $T_1 = S_n$, T_2, ..., T_9 are the trees as shown in Fig.* 4.1. (1) [30–32] *If $n \geq 18$, then $WW(T) > WW(T_9) > WW(T_8) > WW(T_7) > WW(T_6) > WW(T_5) > WW(T_4) > WW(T_3) > WW(T_2) > WW(T_1)$.* (2) [28, 29] *If $n \geq 24$, then $W(T) > W(T_9) > W(T_8) > W(T_7) = W(T_6) > W(T_5) > W(T_4) > W(T_3) > W(T_2) > W(T_1)$.*

Remark 4.3 Theorem 4.3 implies that the trees which reach the first to ninth smallest hyper-Wiener indices even share the first to eighth smallest Wiener indices in $\mathcal{T}_n$ when $n \geq 24$. Actually, Dong and Guo [29] had determined the first twelfth smallest Wiener indices in $\mathcal{T}_n$ when $n \geq 24$.

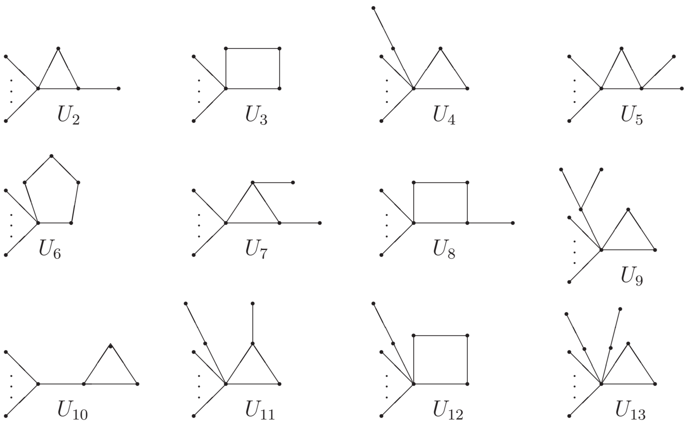

Fig. 4.2. The unicyclic graphs U_2, ..., U_{13}.

Let $\mathbb{U}(n)$ and $\mathbb{B}(n)$ be the set of unicyclic graphs and bicyclic graphs on n vertices, respectively. Next we shall introduce some ordering results of the Wiener indices and hyper-Wiener indices in $\mathbb{U}(n)$ and $\mathbb{B}(n)$, respectively. Let U_1 be the unicyclic graph obtained from S_n by adding one edge to two pendent vertices of S_n, and let U_2, ..., U_{13} be the unicyclic graphs on n vertices as depicted in Fig. 4.2.

Theorem 4.4 *Suppose* $n \geq 13$ *and* $U \in \mathbb{U}(n) \backslash \{U_1, U_2, ..., U_{13}\}$. *Then,* (1) [31] $WW(U) > WW(U_{13}) > WW(U_{12}) = WW(U_{11}) > WW(U_{10}) = WW(U_9) > WW(U_8) = WW(U_7) > WW(U_6) = WW(U_5) > WW(U_4) > WW(U_3) = WW(U_2) > WW(U_1)$; (2) [31, 84] $W(U) > W(U_{13}) > W(U_{12}) = W(U_{11}) > W(U_{10}) = W(U_9) > W(U_8) = W(U_7) > W(U_6) = W(U_5) > W(U_4) > W(U_3) = W(U_2) > W(U_1)$.

Remark 4.4 Theorem 4.4 implies that the unicyclic graphs which reach the first to eighth smallest hyper-Wiener indices even share the first to eighth smallest Wiener indices in $\mathbb{U}(n)$ when $n \geq 13$.

Let $C_g(P_{n-g})$ be the unicyclic graph on n vertices formed by attaching a path P_{n-g} to one vertex of C_g. Let $C^1_{n,g}$ be the unicyclic graph obtained from a cycle C_g by attaching a path P_{n-g-1} to a vertex u_0 of C_g, and one pendent vertex to another vertex v_0 of C_g.

Theorem 4.5 *Let* $U \in \mathbb{U}(n) \setminus \{C_3(P_{n-3})\}$. *If* $n \geq 6$, *then* (1) [72, 73, 84] $W(U) \leq W(C_4(P_{n-4})) = W(C^1_{n,3}) < W(C_3(P_{n-3}))$, *where the first equality holds if and only if* $U \cong C_4(P_{n-4})$ *or* $U \cong C^1_{n,3}$; (2) [43] $WW(U) < WW(C_3(P_{n-3}))$.

B_1 B_2

Fig. 4.3. The bicyclic graphs B_1 and B_2.

Let D_n be the bicyclic graph on n vertices formed by attaching a path of order $n-4$ to one vertex of degree two of $K_4 - e$. Let B_1 and B_2 be the bicyclic graphs as shown in Fig. 4.3.

Theorem 4.6 *Let* $B \in \mathbb{B}(n)$. *If* $n \geq 6$, *then* (1) [44, 45] $W(B_2) = W(B_1) \leq W(B) \leq W(D_n)$; (2) [45] $WW(B_2) = WW(B_1) \leq WW(B) \leq WW(D_n)$, *where the left equality holds if and only if* $B \cong B_1$ *or* $B \cong B_2$, *and the right if and only if* $B \cong D_n$.

Let $PK_{n,m}$ be the path-complete graph obtained from the disjoint union of a path and a complete graph by the addition of edges between one end-vertex of the path and some, but not all, vertices of a complete graph.

Theorem 4.7 [64] *Suppose G has n vertices and m edges, where $n-1 \leq m \leq \binom{n}{2}$, then the path-complete graph $PK_{n,m}$ has maximum Wiener index.*

A connected graph G is called a *cactus* if each block of G is either an edge or a cycle. Denote by $Cat(n,t)$ the set of connected cacti possessing n vertices and t cycles. Let $C^0(n,t)$ be the cactus graph obtained from a star S_n by adding t independent edges between the pendent vertices of S_n.

Theorem 4.8 *Among all graphs in $Cat(n,t)$ with $n \geq 8$, (2) [69] $C^0(n,t)$ is the unique graph having the minimum Wiener index for $t \geq 0$; (2) [70] $C^0(n,t)$ is the unique graph having the minimum hyper-Wiener index for $t \geq 1$.*

By Theorem 2.4, the next known result follows at once.

Theorem 4.9 [46–48] *Suppose $T \in \mathcal{T}_{n,\,k} \backslash \{B_{n,k}, S(n-k; \lfloor \frac{k}{2} \rfloor, \lceil \frac{k}{2} \rceil)\}$, where $3 \leq k \leq n-2$. Then, $W(B_{n,k}) < W(T) < W(S(n-k; \lfloor \frac{k}{2} \rfloor, \lceil \frac{k}{2} \rceil))$.*

Recently, Yu et al. also considered the extremal value of hyper-Wiener index in the class of trees with n vertices and k pendent vertices, and they showed that

Theorem 4.10 [49] (1) *Suppose $T \in \mathcal{T}_{n,\,k} \setminus \{B_{n,k}\}$, where $3 \leq k \leq n-2$. Then, $WW(B_{n,k}) < WW(T)$.* (2) *Let T be a starlike tree on n vertices and k pendent vertices. If $T \neq B_{n,k}$ and $T \neq C(n,k)$, then $WW(B_{n,k}) < WW(T) < WW(C(n,k))$.*

In [61], Ilić et al. obtained a generalization to Theorem 4.9, and they also showed the following interesting result.

Theorem 4.11 [61] *Among trees on n vertices and $0 \leq p \leq n-2$ vertices of degree two, $B_{n,n-1-p}$ is the unique tree having minimum Wiener index.*

Let n, g and k be integers with $g \geq 3$, $k \geq 2$ and $g+k \leq n$. For integer a with $0 \leq a \leq n-g-k$, let $p(a) = \lfloor \frac{n-g-a}{k} \rfloor$ and $s = n-g-a-k \cdot p(a)$, and let $U_{n,g,k}(a)$ be the unicyclic graph obtained from the cycle $C_g = v_0 v_1 ... v_{g-1} v_0$ by attaching the path P_a at an end vertex to v_0, and then attaching to the other end vertex of the path the end vertices of $k-s$ paths with $p(a)$ vertices, and s paths with $p(a)+1$ vertices (if $a=0$, then these k paths are attached to v_0).

For integers n, g and k with $g \geq 3$, $k \geq 0$ and $g+k \leq n$, let $\mathbb{U}(n,g,k)$ be the set of unicyclic graphs with n vertices, cycle length g and k pendent vertices. Du et al. [55], later Hong et al. [83] independently determined the minimum Wiener index in the class of $\mathbb{U}(n,g,k)$.

Theorem 4.12 [55, 83] *Let n, g and k be integers with $n \geq 6$, $g \geq 3$, $k \geq 2$ and $g+k \leq n$. Let $\gamma = \gamma(n,g,k) = \max\{\lfloor \frac{n-2}{k+1} \rfloor + 2 - g, 0\}$. Then, $U_{n,g,k}(\gamma)$ and $U_{n,g,k}(\gamma-1)$ if $\gamma \geq 1$ and $\frac{n-1}{k+1}$ is not an integer, and $U_{n,g,k}(\gamma)$ otherwise are the unique graphs in $\mathbb{U}(n,g,k)$ with minimum Wiener index.*

Denote by K_n^k the graph obtained by attaching k pendent vertices to one vertex of complete graph K_{n-k}. Let $\mathcal{G}_{n,k}$ be the set of connected graphs with n vertices and k cut edges. The following result implies that K_n^k is the unique graph sharing the minimum hyper-Wiener index and the minimum Wiener index in $\mathcal{G}_{n,k}$, respectively.

Theorem 4.13 *If $G \in \mathcal{G}_{n,k} \setminus \{K_n^k\}$, then* (1) [66] $W(G) > W(K_n^k)$; (2) [67] $WW(G) > WW(K_n^k)$.

The *join graph* $G_1 \vee G_2$ of two vertex disjoint graphs G_1 and G_2 is the graph having vertex set $V(G_1 \vee G_2) = V(G_1 \cup G_2)$ and edge set $E(G_1 \vee G_2) = E(G_1) \cup E(G_2) \cup \{(u,v) : u \in V(G_1), v \in V(G_2)\}$. Let $\overline{G}$ be the complement graph of G. For $\overline{K_2} = \{u,v\}$, the graph G_{l_1,l_2} is obtained from $K_{n-d} \vee \overline{K_2}$ by identifying one end vertex of each path of length l_1 and l_2 with u and v, respectively, $l_1 \geq l_2$, $l_1 + l_2 = d-2$. It is easy to see that G_{l_1,l_2} has diameter d. If $l_1 - l_2 \leq 1$, we denote the graph by G_d^*. Let $\mathcal{G}(n,d)$ be the set of connected graphs with n vertices and diameter d. Plesnik [50] firstly obtained the graphs (may not be unique) with minimum Wiener index in $\mathcal{G}(n,d)$. Very recently, Feng et al. considered the similar problem for hyper-Wiener index. They showed that

Theorem 4.14 *Let $G \in \mathcal{G}(n,d) \setminus \{G_d^*\}$, where $n \geq 2$ and $d \geq 2$. Then,* (1) [50] $W(G) > W(G_d^*)$; (2) [54] $WW(G) > WW(G_d^*)$.

Denote by G^{**} a graph of diameter d ($3 \leq d \leq 4$ and $|V(G^{**})| \geq d+2$), having the following property: Assume P_{d+1} is a path contained in G^{**}, then for any $v_i \in V(G^{**}) \setminus V(P_{d+1})$ and $v_j \in V(G^{**})$, $j \neq i$, it should be either $d(v_i,v_j) = 1$ or $d(v_i,v_j) = 2$.

Theorem 4.15 [54] *Suppose* $G \in \mathcal{G}(n,d)$ *with* m *edges. If* $n \geq 2$*, and* $d \geq 2$*, then* (1) $WW(G) \geq \frac{1}{2}\left(3n(n-1) - 4m + \frac{1}{12}d(d-1)(d-2)(d+9)\right)$*, where the equality holds if and only if* G *is a graph of diameter at most* 2 *or* $G \cong P_n$ *or* G *is one graph of* G^{**}; (2) $WW(G) \leq \frac{1}{2}\left(\frac{1}{2}d(d+1)n(n-1) + (2-d-d^2)m - \frac{1}{12}d(d-1)(d-2)(5d+9)\right)$, *where the equality holds if and only if* G *is a graph of diameter at most* 2 *or* $G \cong P_n$.

Wang and Guo [51] determined the minimum Wiener index in $\mathcal{T}(n,d)$. This bound was also independently obtained by Liu and Pan [52]. In the sequel, Ilić et al. [53] gave a generalization to the former results of [51,52]. Recently, Yu et al. [49] also determined the minimum hyper-Wiener index in $\mathcal{T}(n,d)$.

Theorem 4.16 *Suppose* $T \in \mathcal{T}(n,d) \setminus \{C_{n,d}\}$*, where* $3 \leq d \leq n-1$*. Then,* (1) [51–53] $W(C_{n,d}) < W(T)$; (2) [49] $WW(C_{n,d}) < WW(T)$.

It is easy to see that (1) of Theorem 4.16 is also a corollary of Theorem 2.5. Actually, Liu and Pan [52] also determined the second minimum Wiener indices in $\mathcal{T}(n,d)$. Wang and Guo [51] also considered the maximum Wiener index in $\mathcal{T}(n,d)$, they obtained the extremal trees when $d \leq 4$. Furthermore, they claimed that it is impossible to give a universal characterization for the trees with maximum Wiener indices in $\mathcal{T}(n,d)$ for $5 \leq d \leq n-4$. For the case of caterpillar trees, Wang and Guo showed that

Theorem 4.17 [51] *Let* T *be an arbitrary caterpillar trees of order* n *and diameter* d*. Then,* $W(C_{n,d}) \leq W(T) \leq W(S(d-1; \lfloor\frac{n-d+1}{2}\rfloor, \lceil\frac{n-d+1}{2}\rceil))$*, where the lower bound is realized if and only if* $T \cong C_{n,d}$*, and the upper bound if and only if* $T \cong S(d-1; \lfloor\frac{n-d+1}{2}\rfloor, \lceil\frac{n-d+1}{2}\rceil)$.

Theorem 4.18 *Let* T *be a caterpillar tree on* n *vertices with radius* r*. If* $T \neq C_{n,2r-1}$*, then* (1) [53] $W(C_{n,2r-1}) < W(T)$; (2) [49] $WW(C_{n,2r-1}) < WW(T)$.

For the Wiener indices of connected graphs with fixed radius, Ilić et al. [53] verified that

Theorem 4.19 [53] *Among connected graphs on* n *vertices and radius* r*, the caterpillar* $C_{n,2r-1}$ *is the unique graph with minimum Wiener index.*

For integers n and d with $4 \leq d \leq n-3$, let $N_{n,d}$ be the tree obtained from the path P_{d+1} labeled as v_0, v_1, ..., v_d by attaching the path P_2 and $n-d-3$ pendant vertices to the vertex $v_{\lfloor \frac{d}{2} \rfloor}$. The unique tree with minimum Wiener index in the class of all n-vertex non-caterpillars with given diameter d is determined for $4 \le d \le n-3$ by the following result.

Theorem 4.20 [60] *Let T be a non-caterpillar tree on n vertices with diameter d, where $4 \le d \le n-3$. Then,*

$$W(T) \ge \frac{d(d+1)(d+2)}{6} + (n-d-1)\left(n + \frac{1}{2}\left\lfloor \frac{(d+1)^2}{2} \right\rfloor\right) + d - 2,$$

where equality holds if and only if $T = N_{n,d}$.

Du and Zhou [56] also considered the extremal problem in the case of unicyclic graphs, and they determined the minimum Wiener index in the class of unicyclic graphs with n vertices, cycle length t and diameter d. For detail, one can be referred to [56]. Moreover, for any connected graph G, some lower and upper bounds, respectively, of $W(G)$ in terms of the order, the size and the diameter of G were given in [33].

Let $\beta(G)$, β for short if there is no confusion, be the matching number of G, i.e., the maximum size of an independent (pair-wise nonadjacent) set of edges of G. Let $\mathbb{G}_{n,\beta}$ be the set of connected graphs with n vertices and matching number β. Similarly, let $\mathbb{U}_{n,\beta}$ and $\mathbb{T}_{n,\beta}$ be the class of unicyclic graphs and trees with n vertices and matching number β, respectively. As early as in 1994, the maximum Wiener index in $\mathbb{G}_{n,\beta}$ was determined by Dankelmann, that is

Theorem 4.21 [63] *Suppose $G \in \mathbb{G}_{n,\beta}$, where $2 \le \beta \le \lfloor \frac{n}{2} \rfloor$. If $G \ne S(2\beta - 1; \lceil \frac{n+1}{2} \rceil - \beta, \lfloor \frac{n+1}{2} \rfloor - \beta)$, then $W(G) < W(S(2\beta - 1; \lceil \frac{n+1}{2} \rceil - \beta, \lfloor \frac{n+1}{2} \rfloor - \beta))$.*

As the next result shown, the extremal graphs with the minimum Wiener index in $\mathbb{G}_{n,\beta}$ is somewhat difficultly described, by comparing to the maximum case.

Theorem 4.22 [65] *Suppose $G \in \mathbb{G}_{n,\beta}$, where $n \ge 4$ and $2 \le \beta \le \lfloor \frac{n}{2} \rfloor$. (1) If $2 \le \beta \le [\frac{2n}{5}]$ and $\beta \ne \frac{2n}{5}$, then $W(G) \ge n(n-1) - \frac{1}{2}\beta(2n - \beta - 1)$, with equality if and only if $G \cong K_\beta \vee \overline{K_{n-\beta}}$; (2) If $[\frac{2n}{5}] \le \beta \le [\frac{n}{2}] - 1$ and $\beta \ne \frac{2n}{5}$, then $W(G) \ge n^2 - 2n - 2\beta^2 + 3\beta$, with equality if and only if $G \cong K_1 \vee \left(\overline{K_{n-2\beta}} \cup K_{2\beta-1}\right)$; (3) If $\beta = \frac{2n}{5}$, then $W(G) \ge \frac{1}{25}(17n^2 - 20n)$, with equality if and only if $G \cong K_1 \vee \left(\overline{K_{n-2\beta}} \cup K_{2\beta-1}\right)$ or $G \cong K_\beta \vee \overline{K_{n-\beta}}$.*

Recently, Feng et al. characterized the minimum hyper-Wiener index together with its corresponding graphs in $\mathbb{G}_{n,\beta}$ via the next Theorem.

Theorem 4.23 [68] *Suppose $G \in \mathbb{G}_{n,\beta}$, where $n \geq 4$ and $2 \leq \beta \leq \lfloor \frac{n}{2} \rfloor$. (1) If $\beta = \lfloor \frac{n}{2} \rfloor$, then $WW(G) \geq \frac{1}{2}n(n-1)$, with equality if and only if $G \cong K_n$; (2) If $\frac{2n}{5} < \beta \leq \lfloor \frac{n}{2} \rfloor - 1$, then $WW(G) \geq \frac{1}{2}n(3n-7) - 4\beta^2 + 6\beta$, with equality if and only if $G \cong K_1 \vee \left(\overline{K_{n-2\beta}} \cup K_{2\beta-1}\right)$; (3) If $2 \leq \beta < \frac{2n}{5}$, then $WW(G) \geq \frac{3}{2}n(n-1) + \beta^2 + \beta - 2n\beta$, with equality if and only if $G \cong K_\beta \vee \overline{K_{n-\beta}}$; (4) If $\beta = \frac{2n}{5}$, then $W(G) \geq \frac{1}{50}n(43n-55)$, with equality if and only if $G \cong K_1 \vee \left(\overline{K_{n-2\beta}} \cup K_{2\beta-1}\right)$ or $G \cong K_\beta \vee \overline{K_{n-\beta}}$.*

For $2 \leq b \leq \lfloor \frac{n}{2} \rfloor$, let $H_{n,b}$ be the tree obtained by attaching a pendent vertex to each of $b-1$ noncentral vertices of the star S_{n-b+1}, and let $F_{n,b}$ be the unicyclic graph obtained by attaching a pendent vertex to each of $b-2$ noncentral vertices and adding an edge between two other noncentral vertices of the star S_{n-b+2}. By Theorem 4.21, we can conclude that $S(2\beta-1; \lceil \frac{n+1}{2} \rceil - \beta, \lfloor \frac{n+1}{2} \rfloor - \beta)$ is also the unique tree with the maximum Winer index in $\mathbb{T}_{n,\beta}$. The next result determines the extremal trees for the minimum cases of Wiener index and hyper-Wiener index, respectively, of $\mathbb{T}_{n,\beta}$.

Theorem 4.24 *Suppose $T \in \mathbb{T}_{n,\beta}$, where $2 \leq \beta \leq \lfloor \frac{n}{2} \rfloor$. Then,* (1) [62] *$W(T) \geq n^2 + (\beta-3)n - 3\beta + 4$, with equality if and only if $T \cong H_{n,\beta}$;* (2) [49] *$WW(T) \geq \frac{1}{2}(3n^2 + 6n\beta - 13n + \beta^2 - 21\beta$
$+24)$, with equality if and only if $T \cong H_{n,\beta}$.*

As the following Theorem shown, the minimum Wiener index and hyper-Wiener index, respectively, in $\mathbb{U}_{n,\beta}$ were also determined.

Theorem 4.25 *Suppose $U \in \mathbb{U}_{n,\beta}$, where $2 \leq \beta \leq \lfloor \frac{n}{2} \rfloor$. If $n \geq 9$ and $U \neq F_{n,\beta}$, then* (1) [62] *$W(U) > W(F_{n,\beta})$;* (2) [74] *$WW(U) > WW(F_{n,\beta})$.*

Moreover, Du and Zhou [62] had characterized the maximum Wiener index together with its corresponding unicyclic graphs in $\mathbb{U}_{n,\beta}$ for $\beta = 2$ and $\beta = \lfloor \frac{n}{2} \rfloor$. Simultaneously, for the case of $3 \leq \beta \leq \lfloor \frac{n}{2} \rfloor - 1$, they claimed that it seems to be difficult and remains a task for the future.

Assume that $n \geq 2\beta \geq 3g \geq 9$, and $C_g = u_1u_2...u_gu_1$. If g is odd, let $F_{n,g,\beta}$ be the unicyclic graph formed by attaching $n-2\beta+1$ pendent vertices and $\beta - \frac{g+1}{2}$ independent edges to the vertices u_1 of C_g. If g is even, let $F_{n,g,\beta}$ be the unicyclic graph formed by attaching $n-2\beta+1$ pendent vertices and $\beta - \frac{g}{2} - 1$ independent edges to the vertices u_1 of C_g, and attaching a pendent vertex to u_2 of C_g. It is easy to see that $F_{n,g,\beta}$ is a unicyclic graph on n vertices with girth g and matching number β. Very recently, Chen and Zhang showed that

Theorem 4.26 [76] *Let U be a unicyclic graph of order n with girth g and the matching number β. If $\beta \geq \frac{3g}{2}$ and $U \neq F_{n,g,\beta}$, then $W(U) > W(F_{n,g,\beta})$.*

A subset S of V is called a *dominating set* of G if for every vertex $v \in V - S$, there exists a vertex $u \in S$ such that v is adjacent to u. The *domination number* of G is the minimum cardinality of a dominating set of G.

Theorem 4.27 [49] *Let T be a tree on n vertices with domination number γ. Then, $WW(T) \geq \frac{1}{2}\left(3n^2 + 6n\gamma - 13n + \gamma^2 - 21\gamma + 24\right)$, with equality if and only if $T \cong H_{n,\gamma}$.*

As usually, let $\alpha(G)$ be the *independence number*, namely, the size of a maximum independent (pair-wise nonadjacent) set of vertices of G. Recall that the *clique number* of G, $\omega(G)$, is the largest number of pairwise adjacent vertices of G. Let $L_{n,k}$ be the *Kite graph*, obtained by attaching one end vertex of P_{n-k} to a vertex of K_k. Let $R(n,t)$ be the Turán graph, i.e., a complete t-partite graph of order n with partition sets differ in size by at most one. Recently, Došlić et al. [85] and Feng et al. [71] showed that

Theorem 4.28 [85] *Let G be a nontrivial graph with clique number ω and independence number α. Then, $W(G) \geq \frac{1}{2}(\omega - 1)\omega + \alpha(\alpha - 1) + (\omega - 1)(\alpha - 1)$, with equality if and only if $G \cong K_{\omega-1} \vee \overline{K_\alpha}$.*

Theorem 4.29 [71] *Let G be a connected graph with $n \geq 2$ vertices and clique number $\omega \geq 2$. If $G \neq L_{n,\omega}$, then $W(G) < W(L_{n,\omega})$ and $WW(G) < WW(L_{n,\omega})$. Moreover, if $G \neq R(n,\omega)$, then $W(G) > W(R(n,\omega))$ and $WW(G) > WW(R(n,\omega))$.*

For the relation between (resp. hyper-Wiener) Wiener index and the independence number of an arbitrary graph (resp. tree), we have

Theorem 4.30 [85] *Let G be a nontrivial graph with n vertices and independence number α. Then, $W(G) \geq \frac{1}{2}(n-\alpha)(n-\alpha-1)+\alpha(n-1)$, with equality if and only if $G \cong K_{n-\alpha} \vee \overline{K_\alpha}$.*

Theorem 4.31 [49] *Let T be a tree on n vertices with independence number α. Then, $WW(T) \geq \frac{1}{2}\left(10n^2 + \alpha^2 - 8n\alpha + 21\alpha - 34n + 24\right)$, with equality if and only if $T \cong H_{n,n-\alpha}$.*

The *chromatic number*, $\chi(G)$, of G is the minimum number of colors to be assigned to the vertices of G such that no two adjacent vertices receive the same color.

Theorem 4.32 [71] *Let G be a connected graph with $n \geq 2$ vertices and chromatic number $\chi \geq 2$. If $G \neq L_{n,\chi}$, then $W(G) < W(L_{n,\chi})$ and $WW(G) < WW(L_{n,\chi})$. Moreover, if $G \neq R(n,\chi)$, then $W(G) > W(R(n,\chi))$ and $WW(G) > WW(R(n,\chi))$.*

Došlić et al. [85] also demonstrated a lower bound of $W(G)$ in terms of the order and the cardinality of every color class of a coloring of G. We denote by $C_{n,g}$ the unicyclic graph obtained from C_g by adding $n-g$ pendent vertices to a vertex of C_g. Let $C^2_{n,g}$ be the unicyclic graph obtained from a cycle C_g by attaching $n-g-1$ pendent vertices to a vertex u_0 of C_g, and one pendent vertex to another vertex v_0 of C_g. Let $C^3_{n,g}$ be the unicyclic graph obtained from a cycle C_g by attaching a path P_{n-g-1} to a vertex u_0 of C_g, and one pendent vertex to the vertex of degree two in P_{n-g-1}, which has the maximum distance from u_0. Let $\mathbb{U}(n,g)$ be the set of unicyclic graph with n vertices and girth g. The first two largest and first two smallest Wiener indices of $\mathbb{U}(n,g)$, respectively, are determined by the following two results.

Theorem 4.33 [72,73] *Suppose $U \in \mathbb{U}(n,g) \setminus \{C_{n,g}, C^2_{n,g}\}$, where $3 \leq g \leq n-2$. Then, $W(U) > W(C^2_{n,g}) > W(C_{n,g})$.*

Theorem 4.34 [72,73] *Suppose $U \in \mathbb{U}(n,g) \setminus \{C_g(P_{n-g})\}$, where $3 \leq g \leq n-2$ and $n \geq 13$. (1) If $g=3$ or $g=4$ or $g=n-3$ or $g=n-2$, then $W(U) \leq W(C^1_{n,g}) < W(C_g(P_{n-g}))$. Moreover, the equality holds if and only if $U \cong C^1_{n,g}$, where $d(u_0,v_0) = \lfloor \frac{g}{2} \rfloor$. (2) If $5 \leq g \leq n-4$, then $W(U) \leq W(C^3_{n,g}) < W(C_g(P_{n-g}))$, where the equality holds if and only if $U \cong C^3_{n,g}$.*

Moreover, Feng et al. determined the maximum and minimum hyper-Wiener indices in $\mathbb{U}(n,g)$, respectively, via the next Theorem.

Theorem 4.35 [43] *Suppose $U \in \mathbb{U}(n,g)$, where $3 \leq g \leq n-2$. Then, $WW(C_{n,g}) \leq WW(U) \leq WW(C_g(P_{n-g}))$. The left equality holds if and only if $U \cong C_{n,g}$, and the right equality holds if and only if $U \cong C_g(P_{n-g})$.*

For any connected graph G with n vertices and girth g, Bekkai and Kouider [34] demonstrated an upper bound for $W(G)$ in terms of n and g according to the parity of g.

A *dendrimer* of degree Δ on n vertices, $D_{n,\Delta}$ is a tree with maximum degree Δ defined inductively as follows: The tree $D_{1,\Delta}$ consists of a single vertex labeled 1. The tree $D_{n,\Delta}$ has vertex set {1, 2,..., n} and is obtained by attaching a pendant vertex to the vertex with smallest degree of $D_{n-1,\Delta}$, which has degree $< \Delta$. The trees attaining the minimum Wiener index among trees with maximum degree at most Δ had been determined by Fischermann et al. in [35] and, independently, by Jelen et al. in [59]. Moreover, Liu et al. [58] determined the unique trees which minimizes the Wiener index in the class of $\mathcal{T}_n^{\Delta}$.

Theorem 4.36 [58] *If* $T \in \mathcal{T}_n^{\Delta} \setminus \{D_{n,\Delta}\}$, *then* $W(T) > W(D_{n,\Delta})$.

Note that $D_{n,\Delta} = S(\Delta, n-\Delta)$ if $\Delta \geq \frac{n}{2}$. When $\Delta \geq \frac{n}{2}$, Theorem 4.36 can be extended to

Theorem 4.37 [26] *Suppose* $T \in \mathcal{T}_n^{\Delta} \setminus \{S(\Delta, n-\Delta), T(n, 4; n-\Delta-3, \Delta-2, 0)\}$, *where* $\Delta \geq \frac{n}{2}$. *If* $n \geq 6$, *then* $W(T) > W(T(n, 4; n-\Delta-3, \Delta-2, 0)) > W(S(\Delta, n-\Delta))$.

Theorem 4.38 [26] *Suppose* $T \in \mathcal{T}_n^{\Delta} \setminus \{S(\Delta, n-\Delta), T(n, 4; n-\Delta-3, \Delta-2, 0)\}$, *where* $\Delta \geq \frac{n}{2}$. (1) *If* $\Delta > \frac{3n-9}{4}$, *then* $W(T) \geq W(T(n, 4; n-\Delta-4, \Delta-2, 1))$, *where the equality holds if and only if* $T \cong T(n, 4; n-\Delta-4, \Delta-2, 1)$; (2) *If* $\frac{n}{2} \leq \Delta \leq \frac{3n-9}{4}$, *then* $W(T) \geq W(T(n, 4; \Delta-2, n-\Delta-3, 0))$. *Moreover, if* $\Delta \neq \frac{3n-9}{4}$, *then equality holds if and only if* $T \cong T(n, 4; \Delta-2, n-\Delta-3, 0)$.

Wang et al. [51] (resp. Yu et al.) characterized the tree with the maximum Wiener (resp. hyper-Wiener) index in $\mathcal{T}_n^{\Delta}$. In the sequel, Liu et al. [26] determined the second maximum Wiener index in $\mathcal{T}_n^{\Delta}$ when $\Delta \geq \frac{n}{2}$.

Theorem 4.39 *Let* T *be a tree in* $\mathcal{T}_n^{\Delta} \setminus \{C(n, \Delta)\}$. *If* $T \neq C(n, \Delta)$, *then* (1) [51] $W(T) < W(C(n, \Delta))$; (2) [49] $WW(T) < WW(C(n, \Delta))$.

Theorem 4.40 [26] *Let* T *be a tree in* $\mathcal{T}_n^{\Delta} \setminus \{C(n, \Delta)\}$, $n \geq 10$. *If* $\Delta = n-3$, *then* $W(T) \leq W(H(n, \Delta)) < W(C(n, \Delta))$, *with the equality if and only if* $T \cong H(n, \Delta)$; *If* $\frac{n}{2} \leq \Delta \leq n-4$, *then* $W(T) \leq W(F(n, \Delta)) < W(C(n, \Delta))$, *with the equality if and only if* $T \cong F(n, \Delta)$.

Stevanović [57] generalized (1) of Theorem 4.39 to

Theorem 4.41 [57] *Let* G *be a connected graph with* n *vertices and maximum degree* Δ. *If* $G \neq C(n, \Delta)$, *then* $W(G) < W(C(n, \Delta))$.

Let $b = \frac{n-2}{\Delta-1} \geq 4$. Let $M_2(n,\Delta)$ be the tree of $\mathcal{T}_n^{1,\Delta}$ obtained by attaching $\Delta-1$ pendant vertices to one pendant vertex being adjacent to v_2 of $T(n+1-\Delta, b; \Delta-2, ..., \Delta-2)$, and $M_3(n,\Delta)$ be the tree of $\mathcal{T}_n^{1,\Delta}$ obtained by attaching $\Delta-1$ pendant vertices to one pendant vertex being adjacent to v_3 of $T(n+1-\Delta, b; \Delta-2, ..., \Delta-2)$. Fischermann et al. [35] also considered the extremal Wiener index in $\mathcal{T}_n^{1,\Delta}$, and they showed that

Theorem 4.42 [35] *If* $T \in \mathcal{T}_n^{1,\Delta} \backslash \{M_1(n,\Delta)\}$, *then* $W(T) < W(M_1(n,\Delta))$.

Clearly, Theorem 4.42 can be immediately deduced by Theorem 2.3. Wang et al. [51] extended the order of Theorem 4.42 to the third largest value, but in the class of trees with more restrictions.

Theorem 4.43 [51] *Suppose* $T \in \mathcal{T}_n^{1,\Delta}$ *with* $\Delta \geq 3$. *(1) If* $T \notin \{M_1(n,\Delta), M_2(n,\Delta)\}$ *and* $n \geq 4\Delta - 2$, *then* $W(T) < W(M_2(n,\Delta)) < W(M_1(n,\Delta))$;
(2) If $T \notin \{M_1(n,\Delta), M_2(n,\Delta), M_3(n,\Delta)\}$ *and* $n \geq 6\Delta - 4$, *then* $W(T) < W(M_3(n,\Delta)) < W(M_2(n,\Delta)) < W(M_1(n,\Delta))$.

Recently, by using different approaches, Wang [77] and Zhang et al. [78] independently characterized the tree that minimizes the Wiener index among trees of given degree sequences. Moreover, the maximum Wiener index among trees of given degree sequences was also investigated in [77] and [79], respectively.

5 The Wiener Polarity index of trees and unicyclic graphs

As mentioned before, the Wiener index is popular in chemical and mathematical literatures. However, it seems that less attention has been paid for the Wiener polarity index $W_P(G)$ up to now. Actually, $W_P(G)$ was received earlier attention in the chemical literatures than mathematical literatures. For instance, by employing the Wiener polarity index, the authors in [80] demonstrated quantitative structure-property relationships in a series of acyclic and cycle-containing hydrocarbons, and Hosoya gave a physical-chemical interpretation of $W_P(G)$ in [81]. In this section, some results invoking the extremal Wiener polarity indices in the class of trees or unicyclic graphs on n vertices are present.

Denote by $V^{(\Delta)}(T) = \{v \in V(T) \mid d_T(v) = \Delta\}$, and $N^{(\Delta)}(T) = \bigcup_{u \in V^{(\Delta)}(T)} N_T(u)$. Let $h = n - (\Delta+1)$ and $T_0 = S_{\Delta+1}$. Let T_i be a tree obtained from T_{i-1} by attaching a pendant vertex to one vertex of $N^{(\Delta)}(T_{i-1}) \setminus V^{(\Delta)}(T_{i-1})$, where $i = 1,\ 2,\ ...,\ h$. Then we can construct a tree T_h after h steps, and the set of all T_h is denoted by $\mathcal{T}_{max}^{(n,\ \Delta)}$. From the forgoing construction, it is easy to see that

$$W_P(T) = h \cdot (\Delta - 1) = (n - \Delta - 1)(\Delta - 1)\ for\ T \in \mathcal{T}_{max}^{(n,\ \Delta)}.$$

Du et al. firstly characterized the trees maximizing the Wiener polarity index in $\mathcal{T}_n$.

Theorem 5.1 [37] *Let T be a tree of order n (≥ 4). Then, $W_P(T) \leq \lceil \frac{n-2}{2} \rceil \cdot \lfloor \frac{n-2}{2} \rfloor$, and the equality holds if and only if $T \in \mathcal{T}_{max}^{(n,\ \lceil \frac{n}{2} \rceil)}$ or $T \in \mathcal{T}_{max}^{(n,\ \lfloor \frac{n}{2} \rfloor)}$.*

In the sequel, Liu et al. considered the minimum case, and they verified that

Theorem 5.2 [36] *Suppose $T \in \mathcal{T}_n \setminus \{S_n\}$, then $W_P(T) \geq n-3$. Moreover, the equality holds if and only if $T \cong S(k; n-k-b, b)$, where $k \geq 3$, $n-k \geq b \geq 0$.*

A chemical graph is a graph with the maximum degree not larger than 4. Deng obtained the maximum Wiener polarity index in the class of chemical trees on n vertices.

Theorem 5.3 [39] *Let T be a chemical tree of order n (≥ 7). Then, $W_P(T) \leq 3(n-5)$, and the equality holds if and only if $T \in \mathcal{T}_{max}^{(n,\ 4)}$.*

Deng merely determined the upper bound of Theorem 5.3 without characterizing the extremal tree, and the extremal tree is given by the following results, which determine the maximum and minimum Wiener polarity indices in $\mathcal{T}_n^{\Delta}$, respectively.

Theorem 5.4 [38] *Let $T \in \mathcal{T}_n^{\Delta}$, where $3 \leq \Delta \leq n-3$. Then $W_P(T) \leq (n-\Delta-1)(\Delta-1)$, and the equality holds if and only if $T \in \mathcal{T}_{max}^{(n,\ \Delta)}$.*

Theorem 5.5 [38] *Let $T \in \mathcal{T}_n^{\Delta}$, where $3 \leq \Delta \leq n-3$. Then, $W_P(T) \geq n-3$, and the equality holds if and only if $T \cong S(n-\Delta+1-l; \Delta-1,\ l)$, where $0 \leq l \leq min\{\Delta-1,\ n-\Delta-2\}$.*

For $T \in \mathcal{T}_n^{\Delta}$, by Theorem 5.4 it follows that

$$W_P(T) \leq (n-\Delta-1)(\Delta-1) \leq \left\lceil \frac{n-2}{2} \right\rceil \cdot \left\lfloor \frac{n-2}{2} \right\rfloor,$$

the first equality holds if and only if $T \in \mathcal{T}_{max}^{(n,\ \Delta)}$, the second equality holds if and only if $\Delta = \lceil \frac{n}{2} \rceil$ or $\lfloor \frac{n}{2} \rfloor$. Thus, Theorem 5.1 is a corollary of Theorem 5.4. With the similar reason, Theorem 5.3 is also a corollary of Theorem 5.4.

By the definition of $W_P(G)$, if $d(G) \leq 2$, then $W_P(G) = 0$. For $3 \leq d(G) \leq n-1$, we have

Theorem 5.6 [42] *Let* $T \in \mathcal{T}(n,\ d)$*, where* $3 \le d \le n-1$*. Then,* $W_P(T) \ge n-3$*, where equality holds if and only if* $T \cong S(d-2; n+2-d-t, t)$*, where* $n+2-d-t \ge t \ge 1$*, if* $d > 3$*; and* $T \cong T_2$ *if* $d = 3$*.*

When $3 \le d \le 4$, Theorem 5.1 implies that $W_P(T) \le \lceil \frac{n-2}{2} \rceil \cdot \lfloor \frac{n-2}{2} \rfloor$ if $T \in \mathcal{T}(n,\ d)$. For detail discussion, one can be referred to [37,42]. For the case of $d \ge 5$, the maximum value of $W_P(T)$ in $\mathcal{T}(n,\ d)$ is determined by the next result.

Theorem 5.7 [42] *Let* $T \in \mathcal{T}(n, d)$*, where* $5 \le d \le n-1$*. Then,*

$$W_P(T) \le \left\lfloor \frac{n-d-1}{2} \right\rfloor \left\lceil \frac{n-d-1}{2} \right\rceil + 2n - d - 4\ .$$

Moreover, the equality holds if and only if $T \cong T(n, d; 0, ..., 0, x_i, x_{i+1}, x_{i+2}, 0, ..., 0)$*, where* $2 \le i \le d-4$*,* $x_i \ge 0$*,* $x_{i+2} \ge 0$*, and* $x_{i+1} = \lfloor \frac{n-d-1}{2} \rfloor$ *or* $x_{i+1} = \lceil \frac{n-d-1}{2} \rceil$*.*

Actually, Tong and Deng [82] had characterized the trees with the first three smallest Wiener polarity indices in $\mathcal{T}(n, d)$. Next we shall gave the extremal values for trees in $\mathcal{T}_{n,k}$. It is easy to see that $\mathcal{T}_{n,\ 2} = \{P_n\}$ with $W_P(P_n) = n-3$; and $\mathcal{T}_{n,\ n-1} = \{S_n\}$ with $W_P(S_n) = 0$. For $3 \le k \le n-2$, we have

Theorem 5.8 [38,41] $\mathcal{T}_{n,\ n-2} = \{S(n_1,\ n_2)$*, where* $n_1 + n_2 = n$ *and* $n_1 \ge n_2 \ge 2\}$*. Moreover, if* $T \in \mathcal{T}_{n,\ n-2}$*, then* $n-3 \le W_P(T) \le \lfloor \frac{n-2}{2} \rfloor \lceil \frac{n-2}{2} \rceil$*, where the left equality holds if and only if* $T \cong S(n-2,\ 2)$*, and the right equality holds if and only if* $T \cong S(\lceil \frac{n-2}{2} \rceil + 1, \lfloor \frac{n-2}{2} \rfloor + 1)$*.*

Theorem 5.9 [38] *Let* $T \in \mathcal{T}_{n,\ k}$*, where* $3 \le k \le n-3$*. Then,* $W_P(T) \ge n-3$*, with the equality if and only if* $T \cong S(n-k; n_1, k-n_1)$*, where* $0 < n_1 \le k - n_1$*.*

Suppose the neighbor vertices of v_2 of $T(n-l_1-\cdots-l_s, 4; k_1, s+k_2, k_3)$ are u_1, ..., u_s, w_1, ..., w_{k_2}. Let $T(k_1, k_2, k_3, l_1, ..., l_s)$ be a tree obtained from $T(n-l_1-\cdots-l_s, 4; k_1, s+k_2, k_3)$ by attaching l_i pendent vertices to u_i for $1 \le i \le s$. Clearly, $T(k_1, k_2, k_3, l_1, ..., l_s)$ is a tree on n vertices with $n-s-3$ pendent vertices.

Theorem 5.10 [41] *Let* $T \in \mathcal{T}_{n,\ k}$*, where* $k+2 \le n \le 2k$ *and* $n \ge 4$*. Then,* $W_P(T) \le \lfloor \frac{n-2}{2} \rfloor \lceil \frac{n-2}{2} \rceil$*, where the equality holds if and only if (i)* $T \cong T(k_1, k_2, k_3, l_1, ..., l_s)$ *with* $k_2 = k+1-\lceil \frac{n}{2} \rceil$ *or* $k_2 = k+1-\lfloor \frac{n}{2} \rfloor$*, or (ii)* $T \cong S(\lceil \frac{n}{2} \rceil, \lfloor \frac{n}{2} \rfloor)$*.*

Theorem 5.11 [41] *Let $T \in \mathcal{T}_{n,\ k}$. If $n \geq 2k+1$, then $W_P(T) \leq k^2 - 3k + n - 1$, with equality if and only if T is a starlike tree of order n in which the lengths of all pendant chains are at least 2.*

Let l be a nonnegative integer, and $l_1,\ l_2$ be two positive integers. Let $C_g = u_1u_2 \cdots u_gu_1$ be a cycle of order g. Let $C^{(j)}_{g,\ l_1,\ l_2}$ be a unicyclic graph obtained from C_g by attaching l_1 and l_2 pendant vertices to u_i and u_{i+j} respectively, where $i,\ j \in \{1,\ ...,\ g\ (mod\ g)\}$.

Theorem 5.12 [40] *Suppose $n \geq 9$. Then,*
(1) $\mathbb{U}(n,\ n) = \{C_n\}$, and $W_P(C_n) = n$;
(2) $\mathbb{U}(n,\ n-1) = \{C_{n,n-1}\}$, and $W_P(C_{n,n-1}) = n+1$;
(3) $\mathbb{U}(n,\ n-2) = \{C_{n-2}(P_2), C_{n,n-2},\ C^{(j)}_{n-2,\ 1,\ 1}\}$, where $1 \leq j \leq \lfloor \frac{n-2}{2} \rfloor$.
And $W_P(C^{(1)}_{n-2,\ 1,\ 1}) = n+3 > n+2 = W_P(C_{n-2}(P_2)) = W_P(C_{n,n-2}) = W_P(C^{(j)}_{n-2,\ 1,\ 1})$, where $1 < j \leq \lfloor \frac{n-2}{2} \rfloor$.

Let $C_g(k_1,\ k_2,\ ...,\ k_g)$ denote a *caterpillar cycle*, which is a unicyclic graph obtained from C_g by attaching k_i pendant vertices to the vertex u_i, where $k_i \geq 0$ for $i = 1,\ 2,\ ...,\ g$. Let $C_g \odot C(v_0 \cdots v_t;\ n-t-g)$ be a unicyclic graph obtained from a cycle C_g and $C(v_0 \cdots v_t;\ n-t-g)$ by identifying a vertex of C_g and v_0.

Theorem 5.13 [40] *Let $U \in \mathbb{U}(n,\ g)$, where $5 \leq g \leq n-3$. Then, $W_P(U) \geq n+2$ (resp. $n-1$, $n-3$) if $g \geq 7$ (resp. $g = 6,\ 5$), where all the equalities hold if and only if $U \cong C_g \odot C(v_0 \cdots v_t;\ n-t-g)$ with $t \geq 2, n-t-g \geq 1$.*

Theorem 5.14 [36] *Suppose $n \geq 7$. If $U \in \mathbb{U}(n,3) \setminus \{U_1\}$, then $W_P(U) \geq n-4$, with equality if and only if $U \cong U_2$. If $U \in \mathbb{U}(n,\ 4)$, then $W_P(U) \geq n-4$, with equality if and only if $U \cong C_{n,\ 4}$ or $C^{(2)}_{4,\ l,\ n-4-l}$, where $1 \leq l \leq n-5$.*

By combining Theorems 5.12–5.14, we can conclude that

Remark 5.1 The minimum Wiener polarity index together with its corresponding unicyclic graphs of $\mathbb{U}(n,g)$ are determined for $3 \leq g \leq n$. And the first three smallest Wiener polarity indices of $\mathbb{U}(n)$ are 0, $n-4$, and $n-3$, respectively.

Theorem 5.15 [40] *Let $U \in \mathbb{U}(n,\ g)$, where $5 \leq g \leq n-3$. Then,*

$$W_P(U) \leq \left\lfloor \frac{n-g}{2} \right\rfloor \cdot \left\lceil \frac{n-g}{2} \right\rceil + \begin{cases} 2n-10, & g=5, \\ 2n-9, & g=6, \\ 2n-g, & g \geq 7, \end{cases}$$

with equality if and only if $U \cong C_g(k_1,\ k_2,\ k_3,\ 0,\ ...,\ 0)$, where $k_1,\ k_2,\ k_3 \geq 0$, $\sum_{i=1}^{3} k_i = n-g$, and $k_2 = \lfloor \frac{n-g}{2} \rfloor$ or $\lceil \frac{n-g}{2} \rceil$.

Let $C_4(k_1,\ k_2,\ k_3,\ 0) \otimes (t)$ denote the unicyclic graph obtained from t isolated vertices and $C_4(k_1,\ k_2,\ k_3,\ 0)$ by attaching each of the t isolated vertices to any pendant vertices of $N_{C_4(k_1,\ k_2,\ k_3,\ 0)}(v_2)$, where $k_1,\ k_2,\ k_3 \geq 0$ and $t \geq 1$.

Theorem 5.16 [40] *Let $U \in \mathbb{U}(n,\ 4)$. Then, $W_P(U) \leq \lfloor \frac{n-4}{2} \rfloor \cdot \lceil \frac{n-4}{2} \rceil + n-4$, with equality if and only if $U \cong C_4(k_1,\ k_2,\ k_3,\ k_4)$, where $k_1,\ k_2,\ k_3,\ k_4 \geq 0$ and $n-4-k_1-k_3 = k_2+k_4 = \lfloor \frac{n-4}{2} \rfloor$ or $\lceil \frac{n-4}{2} \rceil$, or $U \cong C_4(k_1,\ k_2,\ k_3,\ 0) \otimes (t)$, where $k_1,\ k_2,\ k_3 \geq 0,\ t \geq 1$ and $n-4-k_1-k_3-t = k_2 = \lfloor \frac{n-4}{2} \rfloor$ or $\lceil \frac{n-4}{2} \rceil$.*

Let $\Delta_3(n)$ be the caterpillar cycle $C_3(k_1,\ k_2,\ k_3)$ with $|k_i - k_j| \leq 1$, where $i,\ j \in \{1,\ 2,\ 3\}$.

Theorem 5.17 [40] *Let $U \in \mathbb{U}(n,\ 3)$, where $n \geq 11$. Then,*

$$W_P(U) \quad \leq \quad \begin{cases} \frac{1}{3}\,(n-3)^2\,, & n \equiv 0\ (mod\ 3), \\ \frac{1}{3}(n-2)(n-4), & n \not\equiv 0\ (mod\ 3), \end{cases}$$

where the equality holds if and only if $U \cong \Delta_3(n)$.

By Theorems 5.15–5.17, we can conclude that

Remark 5.2 When $n \geq 12$, the maximum Wiener polarity index of $\mathbb{U}(n)$ is $\frac{1}{3}\,(n-3)^2$ if $n \equiv 0\ (mod\ 3)$, or $\frac{1}{3}(n-2)(n-4)$ if $n \not\equiv 0\ (mod\ 3)$. Moreover, the maximum Wiener polarity index together with its corresponding unicyclic graphs of $\mathbb{U}(n, g)$ are determined for $3 \leq g \leq n$.

For the chemical unicyclic graphs on n vertices, the maximum and minimum Wiener polarity indices are determined by the next result.

Theorem 5.18 [86] *Let U be a unicyclic chemical graph with $n \geq 9$ vertices, then $n-3 \leq W_P(U) \leq 3n+12$.*

Let $\mathcal{U}_{n,\ k}$ be the set of unicyclic graphs on n vertices with k pendent vertices. Clearly, $0 \leq k \leq n-3$. The next result determines the minimum Wiener polarity index in $\mathcal{U}_{n,k}$ for arbitrary k.

Theorem 5.19 [40] *Suppose* $n \geq 9$. (1) $\mathcal{U}_{n,\ 0} = \{C_n\}$, *and* $W_P(U) = n$; (2) $\mathcal{U}_{n,1} = \{C_g(P_{n-g})\}$ $(n > g \geq 3)$, *where* $W_P(C_{n-1}(P_1)) = n+1$, *and* $W_P(C_g(P_{n-g})) = n+2$ *for* $g \leq n-2$. (3) *Let* $U \in \mathcal{U}_{n,n-3}$. *Then,* $W_P(U) \geq 0$, *where the equality holds if and only if* $U \cong U_1$. (4) *Let* $U \in \mathcal{U}_{n,n-4}$. *Then,* $W_P(U) \geq n-4$, *where the equality holds if and only if* $U \cong C_{n,4}$ *or* $C^{(2)}_{4,\ l,\ n-4-l}$, *where* $1 \leq l \leq n-5$. (5) *If* $2 \leq k \leq n-5$ *and* $U \in \mathcal{U}_{n,k}$, *then* $W_P(U) \geq n-3$.

Actually, for $2 \leq k \leq n-5$, the extremal unicyclic graphs of Theorem 5.19 were also characterized in [40]. Let $\mathcal{U}_n^{\Delta}$ be the set of unicyclic graphs on n vertices with maximum degree Δ. Clearly, $2 \leq \Delta \leq n-1$. It is easy to see that $\mathcal{U}_n^2 = \{C_n\}$ and $\mathcal{U}_n^{n-1} = \{U_1\}$. For $3 \leq \Delta \leq n-2$, we have

Theorem 5.20 [40] *Let* $U \in \mathcal{U}_n^{\Delta}$ *and* $n \geq 7$. (1) *If* $3 \leq \Delta < \lceil \frac{n}{2} \rceil$, *then* $W_P(U) \geq n-3$. (2) *If* $\lceil \frac{n}{2} \rceil \leq \Delta \leq n-2$, *then* $W_P(U) \geq n-4$, *where the equality holds if and only if* $U \cong C^{(1)}_{3,n-4,1}$ *or* $C_{n,4}$ *if* $\Delta = n-2$, *and* $U \cong C^{(2)}_{4,\Delta-2,n-2-\Delta}$ *if* $\lceil \frac{n}{2} \rceil \leq \Delta \leq n-3$.

Clearly, Theorem 5.20 determines the minimum Wiener polarity index in $\mathcal{U}_n^{\Delta}$ for arbitrary Δ, since $W_P(C_n) = n$ and $W_P(U_1) = 0$ for $n \geq 7$. Moreover, the extremal unicyclic graphs for $3 \leq \Delta < \lceil \frac{n}{2} \rceil$ of Theorem 5.20 were also characterized in [40].

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