

# MINIMUM WIENER INDICES OF TREES AND UNICYCLIC GRAPHS OF GIVEN MATCHING NUMBER

Zhibin Du and Bo Zhou\*

*Department of Mathematics, South China Normal University,  
Guangzhou 510631, P. R. China*

(Received January 17, 2009)

## Abstract

The Wiener index of a connected graph is defined as the sum of distances between all unordered pairs of its vertices. We determine the minimum Wiener indices of trees and unicyclic graphs with given number of vertices and matching number, respectively. The extremal graphs are characterized.

## 1. INTRODUCTION

Let  $G$  be a simple connected graph with vertex set  $V(G)$  and edge set  $E(G)$ . For  $u, v \in V(G)$ , let  $d_G(u, v)$  be the distance between the vertices  $u$  and  $v$  in  $G$  and let  $D_G(u)$  be the sum of distances between  $u$  and all other vertices of  $G$ , i.e.,  $D_G(u) = \sum_{v \in V(G)} d_G(u, v)$ . The Wiener index of  $G$  is defined as [1]

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d_G(u, v) = \frac{1}{2} \sum_{u \in V(G)} D_G(u).$$

---

\*Correspondence to B. Zhou; E-mail: zhoubo@scnu.edu.cn

The Wiener index (often also called the Wiener number) is one of the oldest topological indices [1, 2]. It has found various applications in chemical research and has been studied extensively [3–7]. For recent results on Wiener index, see, e.g., [8–13].

A matching  $M$  of the graph  $G$  is a subset of  $E(G)$  such that no two edges in  $M$  share a common vertex. A matching  $M$  of  $G$  is said to be maximum, if for any other matching  $M'$  of  $G$ ,  $|M'| \leq |M|$ . The matching number of  $G$  is the number of edges of a maximum matching in  $G$ . If  $M$  is a matching of a graph  $G$  and vertex  $v \in V(G)$  is incident with an edge of  $M$ , then  $v$  is said to be  $M$ -saturated, and if every vertex of  $G$  is  $M$ -saturated, then  $M$  is a perfect matching.

For integers  $n$  and  $m$  with  $1 \leq m \leq \lfloor n/2 \rfloor$ , let  $\mathbb{T}(n, m)$  be the set of trees with  $n$  vertices and matching number  $m$ , and let  $\mathbb{U}(n, m)$  be the set of unicyclic graphs with  $n$  vertices and matching number  $m$ . Obviously, if  $G \in \mathbb{T}(n, 1)$ , then  $G$  is the star, and if  $G \in \mathbb{U}(n, 1)$ , then  $G$  is the triangle. In the following we assume that  $2 \leq m \leq \lfloor n/2 \rfloor$ .

In this paper, we determine the minimum Wiener indices of graphs in  $\mathbb{T}(n, m)$  and  $\mathbb{U}(n, m)$ , respectively. The extremal graphs are characterized. Recall that Dankemann [14] determined the maximum Wiener index of connected graphs with  $n \geq 5$  vertices and matching number  $m \geq 2$ , and characterized the unique extremal graph, which turned out to be a tree. Thus, the maximum Wiener index of trees in  $\mathbb{T}(n, m)$  and the unique extremal graph have been known. Zhou and Trinajstić [15] determined the minimum Wiener index of connected graphs with  $n \geq 5$  vertices and matching number  $m \geq 2$ , and characterized the extremal graphs. Some properties of the Wiener index for trees may be found in [4, 10] and for unicyclic graphs in [13, 16].

## 2. PRELIMINARIES

For  $u \in V(G)$ , let  $d_G(u)$  be the degree of  $u$  in  $G$ , and the eccentricity of  $u$ , denoted by  $\text{ecc}(u)$ , is the maximum distance from  $u$  to all other vertices in  $G$ . A pendent vertex is a vertex of degree one. The following lemma is easy.

**Lemma 1.** *Let  $G \in \mathbb{T}(2m, m)$ , where  $m \geq 2$ . Then  $G$  has a pendent vertex whose unique neighbor is of degree two.*

**Lemma 2.** [17, 18] *Let  $G \in \mathbb{T}(n, m)$ , where  $n > 2m$ . Then there is a maximum matching  $M$  and a pendent vertex  $u$  of  $G$  such that  $u$  is not  $M$ -saturated.*

Let  $C_n$  be a cycle with  $n$  vertices. For a unicyclic graph  $G$  with cycle  $C_s$ , the forest formed from  $G$  by deleting the edges of  $C_s$  consists of  $s$  vertex-disjoint subtrees, each containing a vertex on  $C_s$ , which is called the root of this tree in  $G$ . These subtrees are called the branches of  $G$ .

**Lemma 3.** [19] *Let  $G \in \mathbb{U}(2m, m)$ , where  $m \geq 3$ , and let  $T$  be a branch of  $G$  with root  $r$ . If  $u \in V(T)$  is a pendent vertex furthest from the root  $r$  with  $d_G(u, r) \geq 2$ , then  $u$  is adjacent to a vertex of degree two.*

**Lemma 4.** [20] *Let  $G \in \mathbb{U}(n, m)$  where  $n > 2m$ , and  $G \not\cong C_n$ . Then there is a maximum matching  $M$  and a pendent vertex  $u$  of  $G$  such that  $u$  is not  $M$ -saturated.*

**Lemma 5.** *Let  $G$  be an  $n$ -vertex connected graph with a pendent vertex  $u$  being adjacent to vertex  $v$ , and let  $w$  be a neighbor of  $v$  different from  $u$ , where  $n \geq 4$ . Then*

$$W(G) - W(G - u) \geq -d_G(v) + 3n - 4$$

with equality if and only if  $\text{ecc}(v) = 2$ . Moreover, if  $d_G(v) = 2$ , then

$$W(G) - W(G - u - v) \geq -2d_G(w) + 7n - 15$$

with equality if and only if  $\text{ecc}(w) = 2$ .

**Proof.** Note that  $D_G(u) - D_G(v) = n - 2$ . We have

$$\begin{aligned} W(G) - W(G - u) &= D_G(u) = D_G(v) + n - 2 \\ &\geq d_G(v) + 2(n - 1 - d_G(v)) + n - 2 \\ &= -d_G(v) + 3n - 4 \end{aligned}$$

with equality if and only if  $\text{ecc}(v) = 2$ .

If  $d_G(v) = 2$ , then  $D_G(v) - D_G(w) = n - 4$ , and thus

$$\begin{aligned} W(G) - W(G - u - v) &= D_G(u) + D_G(v) - 1 = 2D_G(w) + 3n - 11 \\ &\geq 2[d_G(w) + 2(n - 1 - d_G(w))] + 3n - 11 \\ &= -2d_G(w) + 7n - 15 \end{aligned}$$

with equality if and only if  $\text{ecc}(w) = 2$ . ■

For  $2 \leq m \leq \lfloor n/2 \rfloor$ , let  $T_{n,m}$  be the tree obtained by attaching a pendent vertex to  $m - 1$  noncentral vertices of the star  $S_{n-m+1}$ , and let  $U_{n,m}$  be the unicyclic graph

obtained by attaching a pendent vertex to  $m - 2$  noncentral vertices and adding an edge between two other noncentral vertices of the star  $S_{n-m+2}$ ; see also Fig. 1. Obviously,  $T_{n,m} \in \mathbb{T}(n, m)$  and  $U_{n,m} \in \mathbb{U}(n, m)$ . It is easily checked that  $W(T_{n,m}) = n^2 + (m - 3)n - 3m + 4$  and  $W(U_{n,m}) = n^2 + (m - 4)n - 3m + 6$ .

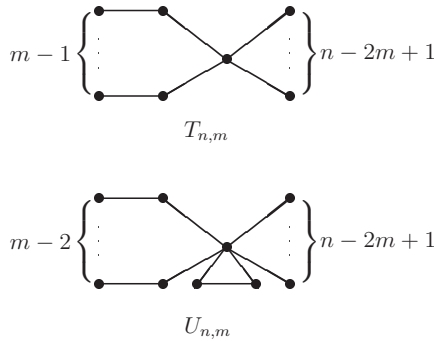


Fig. 1. The graphs  $T_{n,m}$  and  $U_{n,m}$ .

### 3. WIENER INDICES OF TREES

We first consider trees with a perfect matching.

**Theorem 1.** *Let  $G \in \mathbb{T}(2m, m)$ , where  $m \geq 2$ . Then*

$$W(G) \geq 6m^2 - 9m + 4$$

*with equality if and only if  $G = T_{2m,m}$ .*

**Proof.** Let  $f(m) = 6m^2 - 9m + 4$ . We prove the result by induction on  $m$ . It is easily checked that  $G = T_{4,2}$  if  $m = 2$ .

Suppose that  $m \geq 3$  and the result holds for trees in  $\mathbb{T}(2m - 2, m - 1)$ . Let  $G \in \mathbb{T}(2m, m)$  with a perfect matching  $M$ . By Lemma 1, there exists a pendent vertex  $u$  in  $G$  adjacent to a vertex  $v$  of degree two. Then  $uv \in M$  and  $G - u - v \in \mathbb{T}(2m - 2, m - 1)$ . Let  $w$  be the neighbor of  $v$  different from  $u$ . Since  $|M| = m$  and every pendent vertex is  $M$ -saturated, we have  $d_G(w) \leq m$ . By Lemma 5 and the induction hypothesis,

$$W(G) \geq W(G - u - v) - 2d_G(w) + 14m - 15$$

$$\geq f(m-1) - 2m + 14m - 15 = f(m)$$

with equalities if and only if  $G - u - v = T_{2(m-1), m-1}$ ,  $d_G(w) = m$  and  $\text{ecc}(w) = 2$ , i.e.,  $G = T_{2m, m}$ . ■

For trees with given matching number, we have

**Theorem 2.** *Let  $G \in \mathbb{T}(n, m)$ , where  $2 \leq m \leq \lfloor n/2 \rfloor$ . Then*

$$W(G) \geq n^2 + (m-3)n - 3m + 4$$

*with equality if and only if  $G = T_{n, m}$ .*

**Proof.** Let  $f(n, m) = n^2 + (m-3)n - 3m + 4$ . We prove the result by induction on  $n$ . If  $n = 2m$ , then the result follows from Theorem 1.

Suppose that  $n > 2m$  and the result holds for trees in  $\mathbb{T}(n-1, m)$ . Let  $G \in \mathbb{T}(n, m)$ . By Lemma 2, there is a maximum matching  $M$  and a pendent vertex  $u$  of  $G$  such that  $u$  is not  $M$ -saturated. Then  $G - u \in \mathbb{T}(n-1, m)$ . Let  $v$  be the unique neighbor of  $u$ . Since  $M$  is a maximum matching,  $M$  contains one edge incident with  $v$ . Note that there are  $n-1-m$  edges of  $G$  outside  $M$ . Then  $d_G(v) - 1 \leq n-1-m$ , i.e.,  $d_G(v) \leq n-m$ . By Lemma 5 and the induction hypothesis,

$$\begin{aligned} W(G) &\geq W(G-u) - d_G(v) + 3n - 4 \\ &\geq f(n-1, m) - (n-m) + 3n - 4 = f(n, m) \end{aligned}$$

with equalities if and only if  $G - u = T_{n-1, m}$ ,  $d_G(v) = n-m$  and  $\text{ecc}(v) = 2$ , i.e.,  $G = T_{n, m}$ . ■

Let  $G$  be a connected graph of order  $n$  and matching number  $m$ , where  $2 \leq m \leq \lfloor n/2 \rfloor$ . Dankelmann [14] showed that  $W(G) \leq W(T^{n, m})$  with equality if and only if  $G = T^{n, m}$ , where  $T^{n, m}$  is the tree formed by attaching respectively  $\lceil \frac{n+1}{2} \rceil - m$  and  $\lfloor \frac{n+1}{2} \rfloor - m$  pendent vertices to the two end vertices of the path  $P_{2m-1}$ . Thus  $T^{n, m}$  is the unique tree with maximum Wiener index in  $\mathbb{T}(n, m)$ .

#### 4. WIENER INDICES OF UNICYCLIC GRAPHS

In this section, we determine the unicyclic graph(s) of a given matching number with minimum Wiener index.

**Lemma 6.** [21] *Let  $G_0$  be a connected graph with at least three vertices and let  $u$  and  $v$  be two distinct vertices of  $G_0$ . Let  $G_{s,t}$  be the graph obtained from  $G_0$  by attaching  $s$  and  $t$  pendent vertices to  $u$  and  $v$ , respectively. If  $s, t \geq 1$ , then  $W(G_{s,t}) > \min\{W(G_{s+t,0}), W(G_{0,s+t})\}$ .*

Let  $U_n(k)$  be the unicyclic graph obtained from  $C_k = v_0v_1 \dots v_{k-1}v_0$  by attaching a pendent vertex and  $n - k - 1$  pendent vertices to  $v_0$  and  $v_1$ , respectively, where  $3 \leq k \leq n - 2$ . Note that  $W(C_k) = \frac{k}{2} \lfloor \frac{k^2}{4} \rfloor$ . It is easily checked that

$$\begin{aligned} W(U_n(k)) &= W(C_k) + (n - k) \left( k + \left\lfloor \frac{k^2}{4} \right\rfloor \right) + 2 \binom{n - k}{2} + n - k - 1 \\ &= \frac{k}{2} \left\lfloor \frac{k^2}{4} \right\rfloor + (n - k) \left( n + \left\lfloor \frac{k^2}{4} \right\rfloor \right) - 1. \end{aligned}$$

**Lemma 7.** *Suppose that  $m + 1 \leq k \leq 2m - 2$ . If  $m \geq 5$  or  $(m, k) = (4, 6)$ , then  $W(U_{2m}(k)) > 6m^2 - 11m + 6$ .*

**Proof.** Let  $f(k) = W(U_{2m}(k)) = \frac{k}{2} \lfloor \frac{k^2}{4} \rfloor + (2m - k) \left( 2m + \lfloor \frac{k^2}{4} \rfloor \right) - 1$  with  $m + 1 \leq k \leq 2m - 2$ .

Suppose that  $k$  is even. If  $m = 4$ , then  $k = 6$ , and thus  $f(k) - (6m^2 - 11m + 6) = 2 > 0$ . Suppose that  $m \geq 5$ . Then  $f(k) = -\frac{1}{8}k^3 + \frac{1}{2}mk^2 - 2mk + 4m^2 - 1$ , and thus  $f'(k) = -\frac{3}{8}k^2 + mk - 2m$ . Since  $f'(m + 1) = \frac{5}{8}m^2 - \frac{7}{4}m - \frac{3}{8} > 0$  and  $f'(2m - 2) = \frac{1}{2}m^2 - m - \frac{3}{2} > 0$ , for  $m + 1 \leq k \leq 2m - 2$ , we have  $f'(k) > 0$ , i.e.,  $f(k)$  is increasing on  $k$ . Thus,  $f(k) \geq f(m + 1) = \frac{3}{8}(m^3 + 7m^2 - 5m - 3) > 6m^2 - 11m + 6$ .

Suppose that  $k$  is odd. If  $m = 5$ , then  $k = 7$ , and thus  $f(k) - (6m^2 - 11m + 6) = 6 > 0$ . If  $m \geq 6$ , then by similar arguments as above, we have  $f(k) \geq f(m + 1) > 6m^2 - 11m + 6$ . ■

For integer  $m \geq 3$ , let  $U_1(m)$  be the set of graphs in  $\mathbb{U}(2m, m)$  containing a pendent vertex whose neighbor is of degree two. Let  $U_2(m) = \mathbb{U}(2m, m) \setminus U_1(m)$ .

Let  $H_8$  be the graph obtained by attaching three pendent vertices to three consecutive vertices of  $C_5$ .

**Lemma 8.** *Let  $G \in U_2(m)$ , where  $m \geq 4$ . If  $G = H_8$ , then  $W(G) = 6m^2 - 11m + 6$ , and if  $G \neq H_8$ , then  $W(G) > 6m^2 - 11m + 6$ .*

**Proof.** If  $G = H_8$ , then the result follows easily. Suppose that  $G \neq H_8$ . By Lemma 3,  $G \in U_2(m)$  implies that  $G = C_{2m}$  or  $G$  is a graph of maximum degree

three obtained by attaching some pendent vertices to a cycle. If  $G = C_{2m}$ , then  $W(G) = m^3 > 6m^2 - 11m + 6$ . Suppose that  $G \neq C_{2m}$ . Then  $G$  is a graph of maximum degree three obtained by attaching some pendent vertices to a cycle  $C_k$ , where  $m \leq k \leq 2m - 1$ .

If  $k = m$ , then every vertex on the cycle has degree three, and for any pendent vertex  $x$  and its neighbor  $y$ ,

$$\begin{aligned} W(G) &= \frac{1}{2}m[D_G(x) + D_G(y)] \\ &= \frac{1}{2}m \left[ \left( 2 \left\lfloor \frac{m^2}{4} \right\rfloor + 3m - 2 \right) + \left( 2 \left\lfloor \frac{m^2}{4} \right\rfloor + m \right) \right] \\ &= m \left( 2 \left\lfloor \frac{m^2}{4} \right\rfloor + 2m - 1 \right) > 6m^2 - 11m + 6. \end{aligned}$$

If  $m + 1 \leq k \leq 2m - 2$ , then  $m \geq 5$  or  $(m, k) = (4, 6)$  since  $G \neq H_8$ , and by Lemmas 6 and 7, for some  $U_{2m}(k)$ , we have  $W(G) \geq W(U_{2m}(k)) > 6m^2 - 11m + 6$ . If  $k = 2m - 1$ , then it is easily checked that  $W(G) = m^3 - \frac{1}{2}m^2 + \frac{3}{2}m - 1 > 6m^2 - 11m + 6$ . ■

In the following, if  $G$  is a graph in  $U_1(m)$  with a perfect matching  $M$ , then  $u$  is a pendent vertex whose neighbor  $v$  is of degree two in  $G$ , and  $w$  is the neighbor of  $v$  different from  $u$ . Obviously,  $uv \in M$ . Since  $|M| = m$ , we have  $d_G(w) \leq m + 1$ .

Let  $H_6$  be the graph obtained by attaching a pendent vertex to  $C_5$ . Let  $H'_6$  be the graph obtained by attaching a pendent vertex to every vertex of a triangle. Let  $H''_6$  be the graph obtained by attaching two pendent vertices to two adjacent vertices of a quadrangle. It may be easily verified that the following lemma holds.

**Lemma 9.** *Among the graphs in  $\mathbb{U}(6, 3)$ ,  $H_6$  is the unique graph with minimum Wiener index 26, and  $H'_6, H''_6, C_6$  and  $U_{6,3}$  are the unique graphs with the second minimum Wiener index 27.*

**Lemma 10.** *Let  $G \in \mathbb{U}(8, 4)$ . Then  $W(G) \geq 58$  with equality if and only if  $G = H_8$  or  $U_{8,4}$ .*

**Proof.** If  $G \in U_2(4)$ , then by Lemma 8,  $W(G) \geq 58$  with equality if and only if  $G = H_8$ . Suppose that  $G \in U_1(4)$ . Then  $G - u - v \in \mathbb{U}(6, 3)$ . If  $G - u - v \neq H_6$ , then by Lemma 5,

$$W(G) \geq W(G - u - v) - 2d_G(w) + 41 \geq 27 - 2 \times 5 + 41 = 58$$

with equalities if and only if  $G - u - v = H'_6, H''_6, C_6$  or  $U_{6,3}$ ,  $d_G(w) = 5$  and  $\text{ecc}(w) = 2$ , i.e.,  $G = U_{8,4}$ . If  $G - u - v = H_6$ , then  $d_G(w) \leq 4$ , and by Lemma 5,

$$W(G) \geq W(H_6) - 2d_G(w) + 41 \geq 26 - 2 \times 4 + 41 = 59 > 58.$$

The result follows. ■

**Lemma 11.** *Let  $G \in \mathbb{U}(10, 5)$ . Then  $W(G) \geq 101$  with equality if and only if  $G = U_{10,5}$ .*

**Proof.** If  $G \in U_2(5)$ , then by Lemma 8,  $W(G) > 101$ . If  $G \in U_1(5)$ , then by Lemmas 5 and 10,

$$W(G) \geq W(G - u - v) - 2d_G(w) + 55 \geq 58 - 2 \times 6 + 55 = 101$$

with equalities if and only if  $G - u - v = H_8$  or  $U_{8,4}$ ,  $d_G(w) = 6$  and  $\text{ecc}(w) = 2$ , i.e.,  $G = U_{10,5}$ . ■

**Theorem 3.** *Let  $G \in \mathbb{U}(2m, m)$ , where  $m \geq 2$ .*

(i) *If  $m = 3$ , then  $W(G) \geq 26$  with equality if and only if  $G = H_6$ .*

(ii) *If  $m \neq 3$ , then*

$$W(G) \geq 6m^2 - 11m + 6$$

*with equality if and only if  $G = C_4, U_{4,2}$  for  $m = 2$ ,  $G = H_8, U_{8,4}$  for  $m = 4$ , and  $G = U_{2m,m}$  for  $m \geq 5$ .*

**Proof.** The case  $m = 2$  is obvious since  $\mathbb{U}(4, 2) = \{C_4, U_{4,2}\}$ . The cases  $m = 3$  and  $m = 4$  follow from Lemmas 9 and 10, respectively.

Suppose that  $m \geq 5$ . Let  $g(m) = 6m^2 - 11m + 6$ . We prove the result by induction on  $m$ . If  $m = 5$ , then the result follows from Lemma 11.

Suppose that  $m \geq 6$  and the result holds for graphs in  $\mathbb{U}(2m - 2, m - 1)$ . Let  $G \in \mathbb{U}(2m, m)$ . If  $G \in U_2(m)$ , then by Lemma 8,  $W(G) > g(m)$ . If  $G \in U_1(m)$ , then  $G - u - v \in \mathbb{U}(2m - 2, m - 1)$ , and thus by Lemma 5 and the induction hypothesis, it is easily seen that

$$\begin{aligned} W(G) &\geq W(G - u - v) - 2d_G(w) + 14m - 15 \\ &\geq g(m - 1) - 2(m + 1) + 14m - 15 = g(m) \end{aligned}$$



with equalities if and only if  $G - u - v = U_{2(m-1), m-1}$ ,  $d_G(w) = m + 1$  and  $\text{ecc}(w) = 2$ , i.e.,  $G = U_{2m, m}$ . ■

Let  $H_7$  be the graph obtained by attaching two pendent vertices to a vertex of  $C_5$ .

**Theorem 4.** *Let  $G \in \mathbb{U}(n, m)$ , where  $2 \leq m \leq \lfloor n/2 \rfloor$ .*

(i) *If  $(n, m) = (6, 3)$ , then  $W(G) \geq 26$  with equality if and only if  $G = H_6$ .*

(ii) *If  $(n, m) \neq (6, 3)$ , then*

$$W(G) \geq n^2 + (m - 4)n - 3m + 6$$

*with equality if and only if  $G = C_n, U_{n, 2}$  for  $(n, m) = (4, 2), (5, 2)$ ,  $G = H_7, U_{7, 3}$  for  $(n, m) = (7, 3)$ ,  $G = H_8, U_{8, 4}$  for  $(n, m) = (8, 4)$  and  $G = U_{n, m}$  otherwise.*

**Proof.** The case  $(n, m) = (6, 3)$  follows from Lemma 9. Suppose that  $(n, m) \neq (6, 3)$ . Let  $g(n, m) = n^2 + (m - 4)n - 3m + 6$ .

For  $C_7$ , we have  $W(C_7) > g(7, 3)$ . For  $C_n$  with  $n \geq 8$ , we have either  $n = 2m$ ,  $W(C_n) = m^3 > g(n, m)$ , or  $n = 2m + 1$ ,  $W(C_n) = m^3 + \frac{3m^2}{2} + \frac{m}{2} > g(n, m)$ .

If  $G \neq C_n$  with  $n > 2m$ , then by Lemma 4, there exists a pendent vertex  $x$  and a maximum matching  $M$  such that  $x$  is not  $M$ -saturated in  $G$ , and thus  $G - x \in \mathbb{U}(n - 1, m)$ . Let  $y$  be the unique neighbor of  $x$ . Since  $M$  contains one edge incident with  $y$ , and there are  $n - m$  edges of  $G$  outside  $M$ , we have  $d_G(y) \leq n - m + 1$ .

**Case 1.**  $m = 2$ . The result for  $n = 4$  is obvious as in previous theorem. The result for  $n = 5$  may be checked directly as there are only five possibilities for  $G$ . For  $n \geq 6$ , it is easily checked that  $U_{n, 2}$  is the unique unicyclic graph on  $n$  vertices with minimum Wiener index, and thus the unique graph in  $\mathbb{U}(n, 2)$  with minimum Wiener index.

**Case 2.**  $m = 3$ . If  $n = 7$ , then  $G - x \in \mathbb{U}(6, 3)$ : if  $G - x = H_6$ , then  $d_G(y) \leq 4$ , and by Lemma 5,

$$W(G) \geq W(H_6) - d_G(y) + 17 \geq 26 - 4 + 17 = 39$$

with equalities if and only if  $d_G(y) = 4$  and  $\text{ecc}(y) = 2$ , i.e.,  $G = H_7$ , while if  $G - x \neq H_6$ , then by Lemmas 5 and 9,

$$W(G) \geq W(G - x) - d_G(y) + 17 \geq 27 - 5 + 17 = 39$$

with equalities if and only if  $G - x = H'_6, H''_6, C_6$  or  $U_{6,3}$ ,  $d_G(y) = 5$  and  $\text{ecc}(y) = 2$ , i.e.,  $G = U_{7,3}$ . Thus, for  $n = 7$ , we have  $W(G) \geq 39$  with equality if and only if  $G = H_7$  or  $U_{7,3}$ .

For  $n \geq 8$ , we prove the result by induction on  $n$ . If  $n = 8$ , then  $G - x \in \mathbb{U}(7, 3)$ , and by Lemma 5,

$$W(G) \geq W(G - x) - d_G(y) + 20 \geq 39 - 6 + 20 = 53$$

with equalities if and only if  $G - x = H_7$  or  $U_{7,3}$ ,  $d_G(y) = 6$  and  $\text{ecc}(y) = 2$ , i.e.,  $G = U_{8,3}$ . Suppose that  $n \geq 9$  and the result holds for graphs in  $\mathbb{U}(n - 1, 3)$ . By Lemma 5 and the induction hypothesis,

$$\begin{aligned} W(G) &\geq W(G - x) - d_G(y) + 3n - 4 \\ &\geq n^2 - 3n - 1 - (n - 2) + 3n - 4 = n^2 - n - 3 \end{aligned}$$

with equalities if and only if  $G - x = U_{n-1,3}$ ,  $d_G(y) = n - 2$  and  $\text{ecc}(y) = 2$ , i.e.,  $G = U_{n,3}$ .

**Case 3.**  $m = 4$ . The case  $n = 8$  follows from Lemma 10. For  $n \geq 9$ , we prove the result by induction on  $n$ . If  $n = 9$ , then  $G - x \in \mathbb{U}(8, 4)$ , and by Lemmas 5 and 10,

$$W(G) \geq W(G - x) - d_G(y) + 23 \geq 58 - 6 + 23 = 75$$

with equalities if and only if  $G - x = H_8$  or  $U_{8,4}$ ,  $d_G(y) = 6$  and  $\text{ecc}(y) = 2$ , i.e.,  $G = U_{9,4}$ . Suppose that  $n \geq 10$  and the result holds for graphs in  $\mathbb{U}(n - 1, 4)$ . By Lemma 5 and the induction hypothesis,

$$\begin{aligned} W(G) &\geq W(G - x) - d_G(y) + 3n - 4 \\ &\geq n^2 - 2n - 5 - (n - 3) + 3n - 4 = n^2 - 6 \end{aligned}$$

with equalities if and only if  $G - x = U_{n-1,4}$ ,  $d_G(y) = n - 3$  and  $\text{ecc}(y) = 2$ , i.e.,  $G = U_{n,4}$ .

**Case 4.**  $m \geq 5$ . We prove the result by induction on  $n$ . If  $n = 2m$ , then the result follows from Theorem 3. Suppose that  $n > 2m$  and the result holds for graphs in  $\mathbb{U}(n - 1, m)$ . Let  $G \in \mathbb{U}(n, m)$ . By Lemma 5 and the induction hypothesis,

$$\begin{aligned} W(G) &\geq W(G - x) - d_G(y) + 3n - 4 \\ &\geq g(n - 1, m) - (n - m + 1) + 3n - 4 = g(n, m) \end{aligned}$$

with equalities if and only if  $G - x = U_{n-1,m}$ ,  $d_G(y) = n - m + 1$  and  $\text{ecc}(y) = 2$ , i.e.,  $G = U_{n,m}$ . ■

Šoltés [22] showed that, of all connected graphs with  $n$  vertices and  $e$  edges, where  $n - 1 \leq e \leq \frac{n(n-1)}{2}$ , the graph  $PK_{n,e}$  has the maximum Wiener index, where  $PK_{n,e}$  is the path-complete graph consisting of a path, an end vertex of which is adjacent to one or more, but not all, vertices of a complete graph, and it can be easily shown that there is a unique such path-complete graph for given  $n$  and  $e$ . Šoltés's result was refined by Goddard, Swart and Swart [23], who showed that  $PK_{n,e}$  is the only extremal graph except for  $e \geq \frac{n(n-1)}{2} - (n-1)$ . Thus, for  $n \geq 5$ , the graph  $U^n$  formed from the path whose vertices are labeled consecutively by  $1, 2, \dots, n$  by adding an edge between vertices 1 and 3 is the unique graph with maximum Wiener index in the class of  $n$ -vertex unicyclic graphs. As a consequence,  $U^n$  is the unique graph in  $\mathbb{U}(n, \lfloor \frac{n}{2} \rfloor)$  with maximum Wiener index, which is equal to  $\frac{1}{6}(n^3 - 7n + 12)$ . On the other hand, it may be easily checked that the graph formed by attaching  $n-5$  pendent vertices to the neighbor of the pendent vertex of  $U^5$  is the unique graph in  $\mathbb{U}(n, 2)$  with maximum Wiener index, which is equal to  $n^2 - 8$ . However, the determination of the maximum Wiener index and the extremal graphs for the graph class  $\mathbb{U}(n, m)$ ,  $3 \leq m \leq \lfloor \frac{n}{2} \rfloor - 1$ , seems to be difficult and remains a task for the future.

**Acknowledgement.** This work was supported by the Guangdong Provincial Natural Science Foundation of China (no. 8151063101000026).

## References

- [1] I. Gutman, O. E. Polansky, *Mathematical Concepts in Organic Chemistry*, Springer-Verlag, Berlin 1986.
- [2] H. Wiener, Structural determination of paraffin boiling points, *J. Am. Chem. Soc.* **69** (1947) 17–20.
- [3] S. Nikolić, N. Trinajstić, Z. Mihalić, The Wiener index: Development and applications, *Croat. Chem. Acta* **68** (1995) 105–128.
- [4] A. A. Dobrynin, R. Entringer, I. Gutman, Wiener index of trees: Theory and applications, *Acta Appl. Math.* **66** (2001) 211–249.
- [5] A. A. Dobrynin, I. Gutman, S. Klavžar, P. Žigert, Wiener index of hexagonal systems, *Acta Appl. Math.* **72** (2002) 247–294.

- [6] I. Gutman, S. Klavžar, B. Mohar (Eds.), Fifty years of the Wiener index, *MATCH Commun. Math. Comput. Chem.* **35** (1997) 1–259.
- [7] I. Gutman, S. Klavžar, B. Mohar (Eds.), Fiftieth anniversary of the Wiener index, *Discr. Appl. Math.* **80** (1997) 1–113.
- [8] B. Zhou, I. Gutman, Relations between Wiener, hyper-Wiener and Zagreb indices, *Chem. Phys. Lett.* **394** (2004) 93–95.
- [9] S. Yousefi, A. R. Ashrafi, An exact expression for the Wiener index of polyhex nanotorus, *MATCH Commun. Math. Comput. Chem.* **56** (2006) 169–178.
- [10] B. Zhang, B. Zhou, On modified and reverse Wiener indices of trees, *Z. Naturforsch.* **61a** (2006) 536–540.
- [11] S. Yousefi, A. R. Ashrafi, An exact expression for the Wiener index of a  $TUC_4C_8(R)$  nanotorus, *J. Math. Chem.* **42** (2007) 1031–1039.
- [12] D. Stevanović, Maximizing Wiener index of graphs with fixed maximum degree, *MATCH Commun. Math. Comput. Chem.* **60** (2008) 71–83.
- [13] Z. Du, B. Zhou, A note on Wiener indices of unicyclic graphs, *Ars Combin.* **93** (2009), in press.
- [14] P. Dankelmann, Average distance and independence number, *Discr. Appl. Math.* **51** (1994) 75–83.
- [15] B. Zhou, N. Trinajstić, The Kirchhoff index and the matching number, *Int. J. Quantum Chem.* **109** (2009), in press.
- [16] I. Gutman, L. Popović, P. V. Khadikar, S. Karmarkar, S. Joshi, M. Mandloi, Relations between Wiener and Szeged indices of monocyclic molecules, *MATCH Commun. Math. Comput. Chem.* **35** (1997) 91–103.
- [17] R. A. Brualdi, J. L. Goldwasser, Permanent of the Laplacian matrix of trees and bipartite graphs, *Discr. Math.* **48** (1984) 1–21.
- [18] Y. Hou, J. Li, Bounds on the largest eigenvalues of trees with a given size of matching, *Lin. Algebra Appl.* **342** (2002) 203–217.
- [19] A. Chang, F. Tian, On the spectral radius of unicyclic graphs with perfect matching, *Lin. Algebra Appl.* **370** (2003) 237–250.
- [20] A. Yu, F. Tian, On the spectral radius of unicyclic graphs, *MATCH Commun. Math. Comput. Chem.* **51** (2004) 97–109.
- [21] Z. Du, B. Zhou, On the reverse Wiener indices of unicyclic graphs, *Acta Appl. Math.*, in press.
- [22] L. Šoltés, Transmission in graphs: a bound and vertex removing, *Math. Slovaca* **41** (1991) 11–16.
- [23] W. Goddard, C. S. Swart, H. C. Swart, On the graphs with maximum distance or  $k$ -diameter, *Math. Slovaca* **55** (2005) 131–139.