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On the hyper-Wiener index of unicyclic graphs with given matching number

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Abstract. We determine the minimum hyper-Wiener index of unicyclic graphs with given number of vertices and matching number, and characterize the extremal graphs.

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1. Introduction

Let G be a simple connected graph with vertex set $V(G)$. For $u, v \in V(G)$, the distance $d_G(u,v)$ or d_{uv} between u and v in G is the length of a shortest path connecting them. The Wiener index of G is defined as [7, 13]

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

The Wiener index has found various applications in chemical research [11] and has been studied extensively in mathematics [3, 4].

As a variant of the Wiener index, the hyper-Wiener index of the graph G is defined as [8]

$$WW(G) = \sum_{\{u,v\} \subseteq V(G)} \binom{d_{uv}+1}{2} = \frac{1}{2} \sum_{\{u,v\} \subseteq V(G)} \left(d_{uv}^2 + d_{uv}\right).$$

This graph invariant was proposed by Randić [12] for a tree and extended by Klein et al. [8] to a connected graph. It is used to predict physicochemical properties of organic compounds [1], and has also been extensively studied, see, e.g., [2, 5, 9, 10, 14].

Du and Zhou [4] determined the minimum Wiener indices of trees and unicyclic graphs with given number of vertices and matching number, respectively, and characterize the extremal graphs. Recently, Yu et al. [15] gave the minimum hyper-Wiener index of trees with given number of vertices and matching number, and characterized the unique extremal graph. We now determine the minimum hyper-Wiener index of unicyclic graphs with given number of vertices and matching number, and characterize the extremal graphs.

2. Preliminaries

For a connected graph G with $u \in V(G)$, let $W_G(u) = \sum_{v \in V(G)} d_{uv}$, and

$$WW_G(u) = \sum_{v \in V(G)} \binom{d_{uv}+1}{2}.$$

For $u \in V(G)$, let $d_G(u)$ be the degree of u in G, and the eccentricity of u, denoted by $ecc(u)$, is the maximum distance from u to all other vertices in G. Let S_n be the n-vertex star.

Lemma 2.1. *Let G be an n-vertex connected graph with a pendent vertex x being adjacent to vertex y, and let z be a neighbor of y different from x, where $n \geq 4$. Then*

$$WW(G) - WW(G-x) \geq 6n - 8 - 3d_G(y)$$

with equality if and only if $ecc(y) = 2$. Moreover, if $d_G(y) = 2$, then

$$WW(G) - WW(G-x-y) \geq 16n - 36 - 7d_G(z)$$

with equality if and only if $ecc(z) = 2$.

Proof. Note that

$$\begin{aligned} WW_G(x) &= \sum_{u \in V(G)\setminus\{x\}} \binom{1+d_{uy}+1}{2} \\ &= \sum_{u \in V(G)\setminus\{x\}} \binom{d_{uy}+1}{2} + \sum_{u \in V(G)\setminus\{x\}} (d_{uy}+1) \\ &= WW_G(y) - 1 + W_G(y) - 1 + n - 1 \\ &= WW_G(y) + W_G(y) + n - 3. \end{aligned}$$

Then

$$\begin{aligned} WW(G) - WW(G-x) &= WW_G(x) = WW_G(y) + W_G(y) + n - 3 \\ &\geq \binom{1+1}{2} d_G(y) + \binom{2+1}{2}(n-1-d_G(y)) \\ &\quad + d_G(y) + 2(n-1-d_G(y)) + n - 3 \\ &= 6n - 8 - 3d_G(y) \end{aligned}$$

with equality if and only if $ecc(y) = 2$.

If $d_G(y) = 2$, then $W_G(y) = W_G(z) + n - 4$,

$$\begin{aligned} WW_G(y) &= 1 + \sum_{u \in V(G)\setminus\{x,y\}} \binom{1 + d_{uz} + 1}{2} \\ &= 1 + \sum_{u \in V(G)\setminus\{x,y\}} \binom{d_{uz} + 1}{2} + \sum_{u \in V(G)\setminus\{x,y\}} (d_{uz} + 1) \\ &= 1 + WW_G(z) - 1 - 3 + W_G(z) - 1 - 2 + n - 2 \\ &= WW_G(z) + W_G(z) + n - 8, \end{aligned}$$

and thus

$$\begin{aligned} & WW(G) - WW(G - x - y) \\ = \; & WW_G(x) + WW_G(y) - 1 = 2WW_G(y) + W_G(y) + n - 4 \\ = \; & 2(WW_G(z) + W_G(z) + n - 8) + (W_G(z) + n - 4) + n - 4 \\ = \; & 2WW_G(z) + 3W_G(z) + 4n - 24 \\ \geq \; & 2\left(\binom{1+1}{2} d_G(z) + \binom{2+1}{2}(n - 1 - d_G(z))\right) \\ & +3\left[d_G(z) + 2(n - 1 - d_G(z))\right] + 4n - 24 \\ = \; & 16n - 36 - 7d_G(z) \end{aligned}$$

with equality if and only if $ecc(z) = 2$. □

Let C_n be a cycle with n vertices.

Lemma 2.2. [6, 8] *Let u be a vertex on the cycle C_r with $r \geq 3$. Then*

$$W_{C_r}(u) = \begin{cases} \frac{r^2-1}{4} & \text{if } r \text{ is odd,} \\ \frac{r^2}{4} & \text{if } r \text{ is even,} \end{cases}$$

$$WW_{C_r}(u) = \begin{cases} \frac{(r-1)(r+1)(r+3)}{24} & \text{if } r \text{ is odd,} \\ \frac{r(r+1)(r+2)}{24} & \text{if } r \text{ is even.} \end{cases}$$

For integers n and r with $3 \leq r \leq n$, let $S_{n,r}$ be the graph formed by attaching $n - r$ pendent vertices to a vertex of the cycle C_r.

Lemma 2.3. [14] *Let G be an n-vertex unicyclic graph with cycle length r, where $3 \leq r \leq n$. Then*

$$WW(G) \geq \begin{cases} \frac{72n^2+(2r^3+18r^2-98r-90)n-r^4-15r^3+25r^2+87r}{48} & \text{if } r \text{ is odd} \\ \frac{72n^2+(2r^3+18r^2-92r-72)n-r^4-15r^3+22r^2+72r}{48} & \text{if } r \text{ is even} \end{cases}$$

with equality if and only if $G = S_{n,r}$.

3. Results

For integers n and m with $2 \le m \le \lfloor \frac{n}{2} \rfloor$, let $\mathbb{U}(n,m)$ be the set of unicyclic graphs with n vertices and matching number m, 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}. Obviously, $U_{n,m} \in \mathbb{U}(n,m)$. By direct calculation, $WW(U_{n,m}) = \frac{1}{2}(3n^2 + m^2 + 6nm - 19n - 23m + 42)$.

For integer $m \ge 3$, let $\mathbb{U}_1(m)$ be the set of graphs in $\mathbb{U}(2m,m)$ containing a pendent vertex whose neighbor is of degree two. Let $\mathbb{U}_2(m) = \mathbb{U}(2m,m) \setminus \mathbb{U}_1(m)$. Let $H_{8,5}$ be the graph obtained by attaching three pendent vertices to three consecutive vertices of C_5. Let $H_{8,6}$ be the graph obtained by attaching two pendent vertices to two adjacent vertices of C_6. Let $H'_{8,6}$ be the graph obtained by attaching two pendent vertices to two vertices of distance two of C_6. Let $H''_{8,6}$ be the graph obtained by attaching two pendent vertices to two vertices of distance three of C_6.

Lemma 3.1. *Let $G \in \mathbb{U}_2(m)$ with $m \ge 4$. Then $WW(G) \ge \frac{1}{2}(25m^2 - 61m + 42)$ with equality if and only if $G = H_{8,5}$.*

Proof. Since $G \in \mathbb{U}_2(m)$, it is easily seen 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 by Lemma 2.2,

$$WW(C_{2m}) = \frac{(2m)^2(2m+1)(2m+2)}{48} = \frac{1}{6}(2m^4 + 3m^3 + m^2) > \frac{1}{2}(25m^2 - 61m + 42).$$

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_r, where $m \le r \le 2m-1$.

Case 1. $r = m$. Then every vertex on the cycle has degree three, and for any pendent vertex x and its neighbor y, by Lemmas 2.1 and 2.2, we have

$$\begin{aligned}
WW(G) &= \frac{1}{2}m(WW_G(x) + WW_G(y)) \\
&= \frac{1}{2}m(2WW_G(y) + W_G(y) + 2m - 3) \\
&= \frac{1}{2}m\left(2\sum_{u\in V(C_m)}\binom{d_{uy}+1}{2} + 2\sum_{u\in V(G)\setminus V(C_m)}\binom{d_{uy}+1}{2}\right. \\
&\quad \left. + \sum_{u\in V(C_m)} d_{uy} + \sum_{u\in V(G)\setminus V(C_m)} d_{uy} + 2m - 3\right) \\
&= \frac{1}{2}m\left(2WW_{C_m}(y) + 2\sum_{u\in V(C_m)}\binom{1 + d_{uy} + 1}{2}\right. \\
&\quad \left. + W_{C_m}(y) + \sum_{u\in V(C_m)}(d_{uy}+1) + 2m - 3\right)
\end{aligned}$$

$$= \frac{1}{2}m\left(2WW_{C_m}(y) + 2\sum_{u\in V(C_m)}\binom{d_{uy}+1}{2} + 2\sum_{u\in V(C_m)}(d_{uy}+1)\right.$$
$$\left. + W_{C_m}(y) + \sum_{u\in V(C_m)}(d_{uy}+1) + 2m - 3\right)$$
$$= \frac{1}{2}m\left(4WW_{C_m}(y) + 4W_{C_m}(y) + 5m - 3\right)$$
$$= \begin{cases} \frac{1}{12}(m^4+9m^3+29m^2-27m) & \text{if } m \text{ is odd} \\ \frac{1}{12}(m^4+9m^3+32m^2-18m) & \text{if } m \text{ is even} \end{cases}$$
$$> \frac{1}{2}(25m^2-61m+42).$$

Case 2. $r = m+1$. Then there are precisely two adjacent vertices on the cycle of degree two in G. Let G' be the graph obtained from G by attaching two pendent vertices to the two adjacent vertices of degree two in G. For any pendent vertex x and its neighbor y in G', by the above conclusion and Lemma 2.2, we have

$$\begin{aligned} WW(G) &= WW(G') - 2WW_{G'}(x) + \binom{3+1}{2} \\ &= \frac{1}{2}(m+1)\big(4WW_{C_{m+1}}(y) + 4W_{C_{m+1}}(y) + 5(m+1) - 3\big) \\ &\quad -2(2WW_{C_{m+1}}(y) + 3W_{C_{m+1}}(y) + 4m + 1) + 6 \\ &= \frac{1}{2}\big((4m-4)WW_{C_{m+1}}(y) + (4m-8)W_{C_{m+1}}(y) + 5m^2 - 9m + 10\big) \\ &= \begin{cases} \frac{1}{12}(m^4+11m^3+35m^2-77m+42) & \text{if } m \text{ is odd} \\ \frac{1}{12}(m^4+11m^3+32m^2-86m+60) & \text{if } m \text{ is even} \end{cases} \\ &\geq \frac{1}{2}(25m^2-61m+42) \end{aligned}$$

with equality if and only if $m = 4$, i.e., $G = H_{8,5}$.

Case 3. $m+2 \leq r \leq 2m-1$. First we consider the subcase $m \geq 5$. By Lemma 2.3,

$$\begin{aligned} WW(G) &\geq WW(S_{2m,r}) \\ &= \begin{cases} \frac{1}{48}\big(-r^4 + (4m-15)r^3 + (36m+25)r^2 \\ +(87-196m)r + 288m^2 - 180m\big) & \text{if } r \text{ is odd,} \\ \frac{1}{48}\big(-r^4 + (4m-15)r^3 + (36m+22)r^2 \\ +(72-184m)r + 288m^2 - 144m\big) & \text{if } r \text{ is even.} \end{cases} \end{aligned}$$

Let $f(r) = 48WW(S_{2m,r})$. For odd r, we have

$$f'(r) = -4r^3 + (12m-45)r^2 + (72m+50)r + 87 - 196m,$$

from which it is easy to check that $f'(r) > 0$, and thus $f(r)$ is increasing with respect to r, implying that

$$\begin{aligned} WW(G) &\geq \frac{1}{48}f(r) \geq \frac{1}{48}f(m+2) \\ &= \frac{1}{48}(3m^4 + 37m^3 + 195m^2 - 421m + 138) \\ &> \frac{1}{2}(25m^2 - 61m + 42). \end{aligned}$$

For even r, by similar arguments as above,

$$\begin{aligned} WW(G) &\geq \frac{1}{48}f(r) \geq \frac{1}{48}f(m+2) \\ &= \frac{1}{48}(3m^4 + 37m^3 + 204m^2 - 388m + 96) \\ &> \frac{1}{2}(25m^2 - 61m + 42). \end{aligned}$$

Now we consider the subcase $m = 4$. Then $r = 6, 7$, $G = H_{8,6}, H'_{8,6}, H''_{8,6}$ or $H_{8,7}$, and the hyper-Wiener indices of these four graph are respectively equal to 106, 110, 115, and 109, all larger than $99 = \frac{1}{2}(25 \times 4^2 - 61 \times 4 + 42)$.

The result follows by combining Cases 1-3. □

Let $H_{6,3}$ be the graph obtained by attaching a vertex to every vertex of a triangle. Let $H_{6,4}$ be the graph obtained by attaching two pendent vertices to two adjacent vertices of a quadrangle. Let $H_{6,5}$ be the graph obtained by attaching a pendent vertex to C_5. Then the following Lemma may be checked easily.

Lemma 3.2. *Among the graphs in* $\mathbb{U}(6,3)$, $H_{6,5}$ *is the unique graph with minimum hyper-Wiener index* 39, *and* $U_{6,3}$, $H_{6,3}$, $H_{6,4}$ *and* C_6 *are the unique graphs with the second minimum hyper-Wiener index* 42.

For $G \in \mathbb{U}_1(m)$, a vertex triple of G, denoted by (x, y, z), consist of three vertices x, y and z, where x is a pendent vertex of G whose neighbor y is of degree two, and z is the neighbor of y different from x. For the vertex triple (x, y, z) and a perfect matching M with $|M| = m$, we have $xy \in M$ and $d_G(z) \leq m + 1$.

Lemma 3.3. *Let* $G \in \mathbb{U}(8,4)$. *Then* $WW(G) \geq 99$ *with equality if and only if* $G = U_{8,4}$ *or* $H_{8,5}$.

Proof. If $G \in \mathbb{U}_2(4)$, then by Lemma 3.1, $WW(G) \geq \frac{1}{2}(25 \times 4^2 - 61 \times 4 + 42) = 99$ with equality if and only if $G = H_{8,5}$. Suppose that $G \in \mathbb{U}_1(4)$. Let (x, y, z) be a vertex triple of G. Then $G - x - y \in \mathbb{U}(6,3)$. If $G - x - y \neq H_{6,5}$, then by Lemma 2.1,

$$WW(G) \geq WW(G - x - y) + 16 \times 8 - 36 - 7d_G(z) \geq 42 + 92 - 7 \times 5 = 99$$

with equalities if and only if $G - x - y = U_{6,3}$, $H_{6,3}$, $H_{6,4}$ or C_6, $d_G(z) = 5$ and $ecc(z) = 2$, i.e., $G = U_{8,4}$. If $G - x - y = H_{6,5}$, then $d_G(z) \leq 4$, and by Lemma 2.1,

$$WW(G) \geq WW(H_{6,5}) + 16 \times 8 - 36 - 7d_G(z) \geq 39 + 92 - 7 \times 4 = 103 > 99.$$

The result follows. □

Lemma 3.4. *Let* $G \in \mathbb{U}(10,5)$. *Then* $WW(G) \geq 181$ *with equality if and only if* $G = U_{10,5}$.

Proof. If $G \in \mathbb{U}_2(5)$, then by Lemma 3.1, $WW(G) > \frac{1}{2}(25 \times 5^2 - 61 \times 5 + 42) = 181$. Suppose that $G \in \mathbb{U}_1(5)$. Let (x, y, z) be a vertex triple of G. Then $G-x-y \in \mathbb{U}(8,4)$, and by Lemmas 2.1 and 3.3,

$$WW(G) \geq WW(G-x-y) + 16 \times 10 - 36 - 7d_G(z) \geq 99 + 124 - 7 \times 6 = 181$$

with equalities if and only if $G - x - y = U_{8,4}$ or $H_{8,5}$, $d_G(z) = 6$ and $ecc(z) = 2$, i.e., $G = U_{10,5}$. □

Proposition 3.5. *Let* $G \in \mathbb{U}(2m, m)$, *where* $m \geq 2$.
(i) If $m = 3$, *then* $WW(G) \geq 39$ *with equality if and only if* $G = H_{6,5}$;
(ii) If $m \neq 3$, *then*

$$WW(G) \geq \frac{1}{2}(25m^2 - 61m + 42)$$

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

Proof. The case $m = 2$ is obvious since $\mathbb{U}(4,2) = \{U_{4,2}, C_4\}$ and $WW(U_{4,2}) = WW(C_4) = 10$. The cases $m = 3$ and $m = 4$ follow from Lemmas 3.2 and 3.3, respectively.

Suppose that $m \geq 5$. Let $g(m) = \frac{1}{2}(25m^2 - 61m + 42)$. We prove the result by induction on m. If $m = 5$, then the result follows from Lemma 3.4. 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 $G \in \mathbb{U}_2(m)$, then by Lemma 3.1, $WW(G) > g(m)$. If $G \in \mathbb{U}_1(m)$, then for a vertex triple (x, y, z) of G, $G - x - y \in \mathbb{U}(2m-2, m-1)$, and thus by Lemma 2.1 and the induction hypothesis,

$$\begin{aligned} WW(G) &\geq WW(G-x-y) + 32m - 36 - 7d_G(z) \\ &\geq g(m-1) + 32m - 36 - 7(m+1) \\ &= \frac{1}{2}(25m^2 - 61m + 42) = g(m) \end{aligned}$$

with equality if and only if $G - x - y = U_{2m-2,m-1}$, $d_G(z) = m + 1$ and $ecc(z) = 2$, i.e., $G = U_{2m,m}$. □

Let $H_{7,5}$ be the graph obtained by attaching two pendent vertices to a vertex of C_5.

Theorem 3.6. *Let* $G \in \mathbb{U}(n, m)$, *where* $2 \leq m \leq \lfloor \frac{n}{2} \rfloor$.
(i) If $(n, m) = (6, 3)$, *then* $WW(G) \geq 39$ *with equality if and only if* $G = H_{6,5}$;
(ii) If $(n, m) \neq (6, 3)$, *then*

$$WW(G) \geq \frac{1}{2}(3n^2 + m^2 + 6nm - 19n - 23m + 42)$$

with equality if and only if $G = U_{4,2}$, C_4 *for* $(n, m) = (4, 2)$, $G = U_{5,2}$, C_5 *for* $(n, m) = (5, 2)$, $G = U_{7,3}$, $H_{7,5}$ *for* $(n, m) = (7, 3)$, $G = U_{8,4}$, $H_{8,5}$ *for* $(n, m) = (8, 4)$ *and* $G = U_{n,m}$ *otherwise.*

Proof. The case $(n,m)=(6,3)$ follows from Lemma 3.2. Suppose that $(n,m)\neq(6,3)$. Let $g(n,m)=\frac{1}{2}(3n^2+m^2+6nm-19n-23m+42)$.

If $G=C_n$ with $n\geq 7$, then by Lemma 2.2, $WW(G)>g(n,m)$.

If $G\neq C_n$ with $n>2m$, then there exist a pendent vertex x and a maximum matching M such that x is not M-saturated in G [16], 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 $n=4$ follows from Proposition 3.5. If $n=5$, then by Lemma 2.3, the minimum hyper-Wiener index is achieved only by $S_{5,3}$, $S_{5,4}$, or C_5, and thus the result follows by noting that $WW(S_{5,3})=WW(C_5)=20<23=WW(S_{5,4})$ and $S_{5,3}=U_{5,2}$. If $n\geq 6$, then by Lemma 2.3, the minimum hyper-Wiener index is achieved only by $S_{n,3}$ or $S_{n,4}$, and thus the result follows by noting that $WW(S_{n,3})=\frac{1}{2}(3n^2-7n)<\frac{1}{2}(3n^2-n-24)=WW(S_{n,4})$ and $S_{n,3}=U_{n,2}$.

Case 2. $m=3$. Suppose first that $n=7$. Then $G-x\in\mathbb{U}(6,3)$. If $G-x=H_{6,5}$, then $d_G(y)\leq 4$, and by Lemma 2.1,

$$WW(G)\geq WW(G-x)+6\times 7-8-3d_G(y)\geq 39+34-12=61$$

with equalities if and only if $d_G(y)=4$ and $ecc(y)=2$, i.e., $G=H_{7,5}$, while if $G-x\neq H_{6,5}$, then by Lemmas 2.1 and 3.2,

$$WW(G)\geq WW(G-x)+6\times 7-8-3d_G(y)\geq 42+34-15=61$$

with equalities if and only if $G-x=U_{6,3}$, $H_{6,3}$, $H_{6,4}$ or C_6, $d_G(y)=5$ and $ecc(y)=2$, i.e., $G=U_{7,3}$. It follows that $WW(G)\geq 61$ with equality if and only if $G=H_{7,5}$ 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 2.1,

$$WW(G)\geq WW(G-x)+6\times 8-8-3d_G(y)\geq 61+40-3\times 6=83$$

with equalities if and only if $G=H_{7,5}$ or $U_{7,3}$, $d_G(y)=6$ and $ecc(y)=2$, i.e., $G=U_{8,4}$. Suppose that $n\geq 9$ and the result holds for graphs in $\mathbb{U}(n-1,3)$. By Lemma 2.1 and the induction hypothesis,

$$\begin{aligned} WW(G) &\geq WW(G-x)+6n-8-3d_G(y)\\ &\geq g(n-1,3)+6n-8-3(n-2)\\ &= \frac{1}{2}(3n^2-n-18)=g(n,3)\end{aligned}$$

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

Case 3. $m=4$. The case $n=8$ follows from Lemma 3.3. 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 2.1 and 3.3,

$$WW(G)\geq WW(G-x)+6\times 9-8-3d_G(y)\geq 99+46-3\times 6=127$$

with equalities if and only if $G=U_{8,4}$ or $H_{8,5}$, $d_G(y)=6$ and $ecc(y)=2$, 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 2.1 and the induction hypothesis,

$$\begin{aligned} WW(G) &\geq WW(G-x)+6n-8-3d_G(y) \\ &\geq g(n-1,4)+6n-8-3(n-3) \\ &= \frac{1}{2}(3n^2+5n-34)=g(n,4) \end{aligned}$$

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

Case 4. $m\geq 5$. We prove the result by induction on n (for fixed m). If $n=2m$, then the result follows from Proposition 3.5. 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 2.1 and the induction hypothesis,

$$\begin{aligned} WW(G) &\geq WW(G-x)+6n-8-3d_G(y) \\ &\geq g(n-1,m)+6n-8-3(n-m+1) \\ &= \frac{1}{2}(3n^2+m^2+6nm-19n-23m+42)=g(n,m) \end{aligned}$$

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

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References

[1] Devillers, J., Balaban, A. T., *Topological Indices and Related Descriptors in QSAR and QSPR*, Gordon and Breach, Amsterdam, 1999.

[2] Diudea, M.V., Parv, B., *Molecular topology. 25. Hyper-Wiener index of dendrimers*, J. Chem. Inf. Comput. Sci., **35**(1995), 1015-1018.

[3] Dobrynin, A.A., Entringer, R., Gutman, I., *Wiener index of Trees: Theory and applications*, Acta Appl. Math., **66**(2001), 211-249.

[4] Du, Z., Zhou, B., *Minimum Wiener indices of trees and unicyclic graphs of given matching number*, MATCH Commun. Math. Comput. Chem., **63**(2010), 101-112.

[5] Gutman, I., Linert, W., Lukovits, I., Dobrynin, A.A., *Trees with extremal hyper-Wiener index: Mathematical basis and chemical applications*, J. Chem. Inf. Comput. Sci., **37**(1997), 349-354.

[6] Gutman, I., Polansky, O.E., *Mathematical Concepts in Organic Chemistry*, Berlin, Springer, 1986.

[7] Hosoya, H., *Topological index. A newly proposed quantity characterizing the topological nature of structural isomers of saturated hydrocarbons*, Bull. Chem. Soc. Japan, **44**(1971), 2332-2339.

[8] Klein, D.J., Lukovits, I., Gutman, I., *On the definition of the hyper-Wiener index for cycle-containing structures*, J. Chem. Inf. Comput. Sci., **35**(1995), 50-52.

[9] Klavžar, S., Žigert, P., Gutman, I., *An algorithm for the calculation of the hyper-Wiener index of benzenoid hydrocarbons*, Match Commun. Math. Comput. Chem., **24**(2000), 229-233.

[10] Lukovits, I., *Formulas for the hyper-Wiener index of trees*, J. Chem. Inf. Comput. Sci., **34**(1994), 1079-1081.

[11] Nikolić, S., Trinajstić, N., Mihalić, Z., *The Wiener index: Developments and applications*, Croat. Chem. Acta, **68**(1995), 105-129.

[12] Randić, M., *Novel molecular description for structure-property studies*, Chem. Phys. Lett., **211**(1993), 478-483.

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

[14] Xing, R., Zhou, B., Qi, X., *Hyper-Wiener index of unicyclic graphs*, Match Commun. Math. Comput. Chem., **66**(2011), 315-328.

[15] Yu, G., Feng, L., Ilić, A., *The hyper-Wiener index of trees with given parameters*, Ars Combin., **96**(2010), 395-404.

[16] Yu, A., Tian, F., *On the spectral radius of unicyclic graphs*, Match Commum. Math. Comput. Chem., **51**(2004), 97-109.

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