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Third Smallest Wiener Polarity Index of Unicyclic Graphs

Wei Fang[1,2], *Muhan Ma*[3], *FuYuan Chen*[4,5]* *and Hufeng Dong*[5]

[1]Anhui Province Key Laboratory of Animal Nutritional Regulation and Health, Anhui Science and Technology University, Fengyang, China, [2]School of Mathematical Sciences, Anhui University, Hefei, China, [3]Mathematics and Applied Mathematics, Reading Academy Nanjing University of Information Science and Technology, Nanjing, China, [4]Department of Applied Mathematics, Northwestern Polytechnical University, Xi'an, China, [5]Institute of Statistics and Applied Mathematics, Anhui University of Finance and Economics, Bengbu, China

The Wiener polarity index $W_P(G)$ of a graph G is the number of unordered pairs of vertices $\{u, v\}$ where the distance between u and v is 3. In this paper, we determine the third smallest Wiener polarity index of unicyclic graphs. Moreover, the corresponding extremal graphs are characterized.

Keywords: wiener polarity index, minimum, unicyclic graph, extremal graph, electrical networks

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***Correspondence:**
Fuyuan Chen
chen_fuyuan@sina.com

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1. INTRODUCTION

Graph theory is one of the most special and unique branches of mathematics. Recently, it has attained much attention among researchers because of its wide range of applications in computer science, electrical networks, interconnected networks, biological networks, chemistry, etc.

The chemical graph theory (CGT) is a fast-growing area among researchers. It helps in understanding the structural properties of a molecular graph. There are many chemical compounds that possess a variety of applications in the fields of commercial, industrial, and pharmaceutical chemistry and daily life and in the laboratory.

In a chemical graph, the vertices represent atoms and edges refer to the chemical bonds in the underlying chemical structure. A topological index is a numerical value that is computed mathematically from the molecular graph. It is associated with the chemical constitution indicating the correlation of the chemical structure with many physical and chemical properties and biological activities [1–3].

Let G be a simple and connected graph with $|V(G)| = n$ and $|E(G)| = m$. Sometimes we refer to G as a (n, m) graph. For any $u, v \in V(G)$, the *distance* $d_G(u, v)$ 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. $N_G^i(u) = \{v \in V(G) | d_G(u, v) = i\}$ is called the ith neighbor vertex set of u. Especially, if $i = 1$, then $N_G^1(u)$(or $N_G(u)$ for short) be the *neighbor vertex set* of u, and $d_G(u) = |N_G(u)|$ is called the *degree* of G. If $d_G(u) = 1$, then we call u a *pendant vertex* of G.

A unicyclic graph of order n is a connected graph with n vertices and m edges. It is well-known that every unicyclic graph has exactly one cycle. Let $\mathcal{U}_n$ denote the class of unicyclic graphs on n vertices. As usual, let $K_{1,n-1}$, C_n, and P_n be the star, cycle, and path of order n, respectively.

Let $\gamma(G, k)$ denote the number of unordered vertices pairs of G, each of whose distance is equal to k. The Wiener polarity index, denoted by $W_P(G)$, is defined to be the number of unordered vertices pairs of distance 3, i.e., $W_P(G) = \gamma(G, 3)$.

There is another important graph-based structure descriptor, called Wiener index, based on distances in a graph. The *Wiener index* $W(G)$ is denoted by [4]

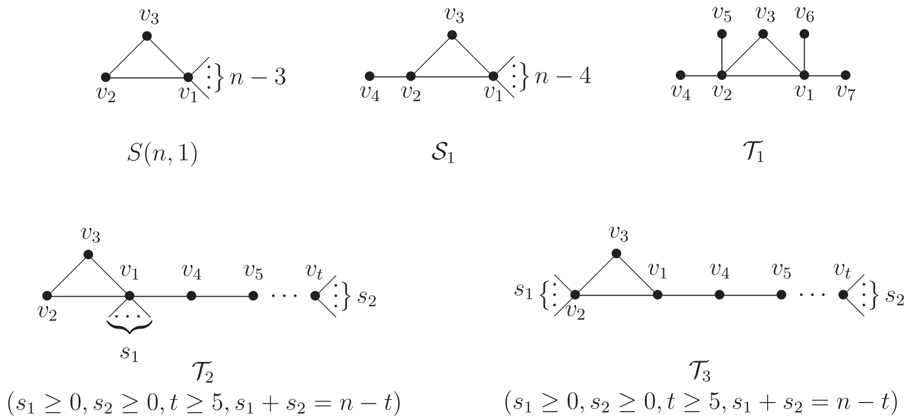

FIGURE 1 | Graphs $S(n,1)$,$\mathcal{S}_1$,$\mathcal{T}_1$, $\mathcal{T}_2$, and $\mathcal{T}_3$.

$$W(G) = \frac{1}{2}\sum_{u,v \in V(G)} d(u,v) = \sum_{k \geq 1} \gamma(G,k).$$

The name Wiener polarity index is introduced by Harold Wiener [4] in 1947. In Ref. [4], Wiener used a linear formula of $W(G)$ and $W_P(G)$ to calculate the boiling points t_B of the paraffins, i.e.,

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

where a, b, and c are constants for a given isomeric group.

If $G_1, \cdots, G_t$ are the connected components of a graph G, then $W_P(G) = \sum_{i=1}^{t} W_P(G_i)$. Therefore, it will suffice to consider the Wiener polarity index of connected graphs.

In 1998, Lukovits and Linert [5] demonstrated quantitative structure-property relationships in a series of acyclic and cycle-containing hydrocarbons by using the Wiener polarity index. In 2002, Hosoya [6] found a physicochemical interpretation of $W_P(G)$. Du et al. [7] obtained the smallest and largest Wiener polarity indices together with the corresponding graphs among all trees on n vertices, respectively. Deng [8] characterized the extremal Wiener polarity indices among all chemical trees of order n. Hou [9] determined the maximum Wiener polarity index of unicyclic graphs and characterized the corresponding extremal graphs. Lei [8] determined the extremal trees with the given degree sequence with respect to the Wiener polarity index. In a previous study [10], the authors obtained the first and second smallest Wiener polarity indexes of unicyclic graphs. In this paper, we determine the third smallest Wiener polarity index of unicyclic graphs. Moreover, all the corresponding extremal graphs are characterized.

2. THE THIRD SMALLEST WIENER POLARITY INDEX OF UNICYCLIC GRAPHS

The girth $g(G)$ of a connected graph G is the length of a shortest cycle in G. Let $S(n,1)$ be the unicyclic graph obtained from $K_{1,n-1}$ by adding one edge to two pendant vertices of $K_{1,n-1}$.

A *non − pendant vertex* of G is a vertex of G which is not a pendant vertex. Suppose U is a unicyclic graph with unique cycle C_t, in the sequel, we agree that $V(C_t) = \{v_1, v_2, \ldots, v_t\}$ and $E(C_t) = \{v_1v_2, v_2v_3, \ldots, v_{t-1}v_t, v_1v_t\}$. For $1 \leq i \leq t$, let $l_i = \max\{d(v_i, x)$, where w is a non-pendant vertex and there is exactly one path connecting v_i with $x\}$.

Lemma 2.1. [10] Let $U \in \mathcal{U}_n$, then $W_P(G) \geq 0$, where equality holds if and only if $U \in S(n,1)$ *or* $U \cong C_4$ *or* $U \cong C_5$ ($S(n,1)$ is shown in **Figure 1**).

Lemma 2.2. Let $G \in \mathcal{U}_n$ and $|N_G^2(u)| \geq k$ for any $u \in V(G)$. $G + w$ be the new graph obtained from G by adding one vertex w and one edge adjacent to u in G. Then, $W_P(G+w) \geq W_P(G) + k$.

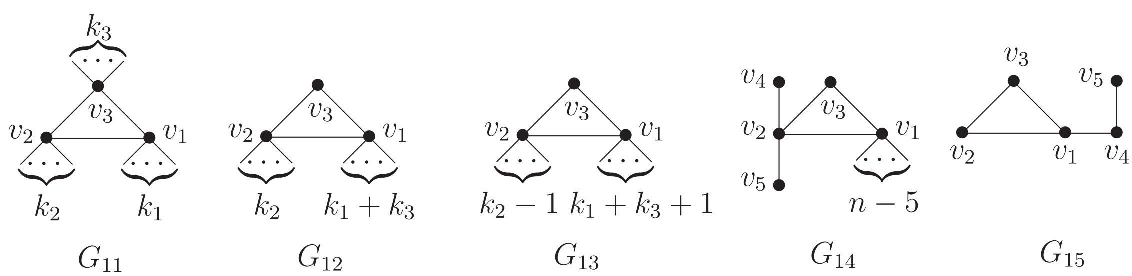

FIGURE 2 | Graphs G_{1i} $(1 \leq i \leq 4)$.

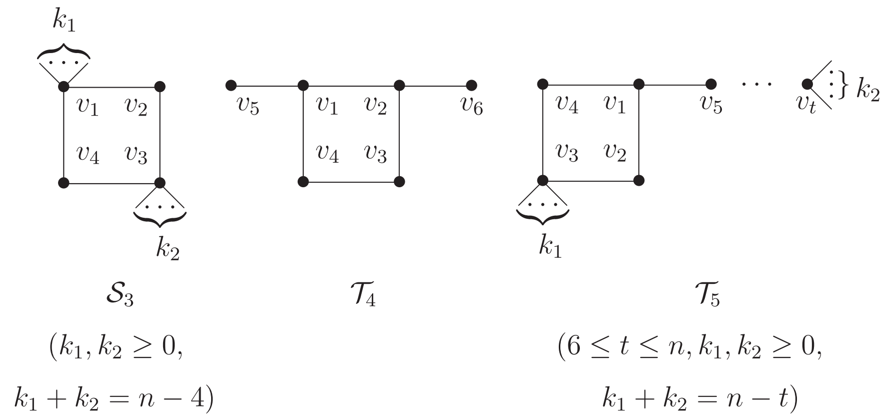

FIGURE 3 | Graphs $\mathcal{S}_2$, $\mathcal{T}_4$, and $\mathcal{T}_5$.

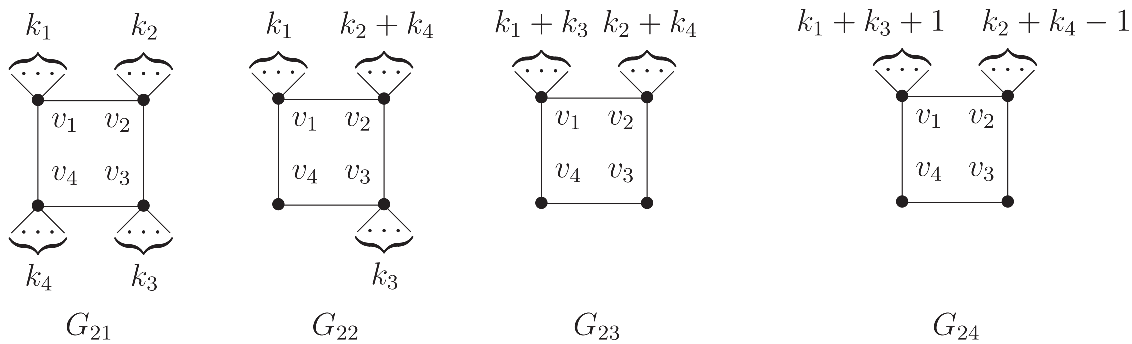

FIGURE 4 | Graphs $G_{2i}\,(1 \leq i \leq 4)$.

Proof. Since $N_{G+w}(w) = \{u\}$ and $\left|N_G^2(u)\right| \geq k$, then $W_P(G+w) = W_P(G) + \left|N_G^3(w)\right| = W_P(G) + \left|N_G^2(u)\right| \geq W_P(G) + k$.

Lemma 2.3 [10]. Suppose $U \in \mathcal{U}_n \backslash \{S(n,1)\}$. If $g(U) = 3$ and $n \geq 5$, then $W_P(U) \geq n-4$, where equality holds if and only if $U \cong \mathcal{S}_1$ ($\mathcal{S}_1$ is shown in **Figure 1**).

Lemma 2.4. Let $U \in \mathcal{U}_n$. If $g(U) = 3$, then the third smallest Wiener polarity index $W_P(U) = n-3$, the equality holds if and only if $U \cong \mathcal{T}_i, 1 \leq i \leq 3$ ($\mathcal{T}_1, \mathcal{T}_2$, and $\mathcal{T}_3$ are shown in **Figure 1**).

Proof. Let $C_3 = \{v_1, v_2, v_3\}$; we consider the next cases.

Case 1. $\max\{l_1, l_2, l_3\} = 0$.

This implies that U is a unicyclic graph obtained by attaching $k_i \geq 0$ pendant vertices to v_i, where $1 \leq i \leq 3$. Without loss of generality, let $k_1 + k_3 \geq k_2$. The graph $G_{1i}\,(1 \leq i \leq 4)$ is shown in **Figure 2**; by the definition of Wiener polarity index, we have

$$\begin{aligned}
W_P(G_{11}) &= k_1k_2 + k_2k_3 + k_1k_3;\\
W_P(G_{12}) &= k_1k_2 + k_2k_3;\\
W_P(G_{13}) &= (k_1 + k_3 + 1)(k_2 - 1)\\
&= k_1k_2 + k_2k_3 - (k_1 + k_3 + 1 - k_2);\\
W_P(G_{14}) &= 2(n-5) \geq n-4\,(n \geq 6);\\
W_P(\mathcal{S}_1) &= n-4\,(n \geq 5).
\end{aligned}$$

Obviously, $W_P(G_{11}) \geq W_P(G_{12}) > W_P(G_{13})$; the equality holds if and only if $G_{11} \cong G_{12}$. Then the third smallest Wiener polarity index is $W_P(\mathcal{T}_1) = 4 = n-3$.

Case 2. $\max\{l_1, l_2, l_3\} \geq 1$.

G_{15} is the subgraph of U and $W_P(G_{15}) = 2, \left|N_{G_{15}}^2(u)\right| \geq 1$, the equality holds if and only if $u \neq v_4$ by Lemma 2.2; we have

$$W_P(U) \geq W_P(G_{15}) + n - 5 = n - 3,$$

the equality holds if and only if $\mathcal{T}_2$ or $\mathcal{T}_3$.

By combining the above arguments, the result follows.

Lemma 2.5 *Let $U \in \mathcal{U}_n$. If $g(U) = 4$, then the third smallest Wiener polarity index $W_P(U) = n-3$, the equality holds if and only if $U \cong \mathcal{T}_4$ or $\mathcal{T}_5$ ($\mathcal{T}_4$ and $\mathcal{T}_5$ are shown in* **Figure 3**).

Proof. Let $C_4 = \{v_1, v_2, v_3, v_4\}$, we consider the next cases.

Case 1. $\max\{l_1, l_2, l_3, l_4\} = 0$.

This implies that U is a unicyclic graph obtained by attaching $k_i \geq 0$ pendant vertices to v_i, where $1 \leq i \leq 4$. Without loss of generality, let $k_1 + k_3 \geq k_2 + k_4$. The graph $G_{2i}\,(1 \leq i \leq 4)$ is shown in **Figure 4**; by the definition of Wiener polarity index, we have

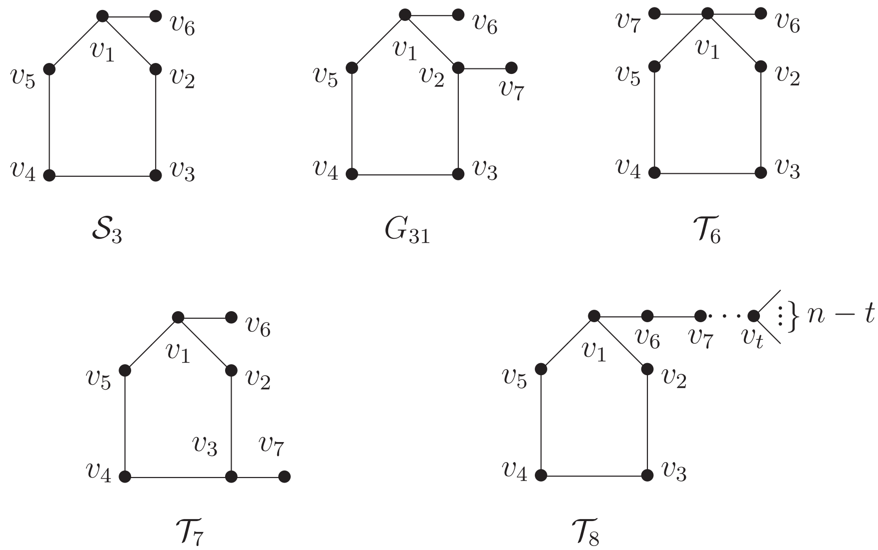

FIGURE 5 | Graphs $\mathcal{S}_3$,G_{31},$\mathcal{T}_6$,$\mathcal{T}_7$, and $\mathcal{T}_8$.

$$W_P(G_{21}) = k_1k_2 + k_2k_3 + k_3k_4 + k_1k_4 + \sum_{i=1}^{4} k_i,$$

$$W_P(G_{22}) = k_1k_2 + k_2k_3 + k_3k_4 + k_1k_4 + \sum_{i=1}^{4} k_i,$$

$$W_P(G_{23}) = k_1k_2 + k_2k_3 + k_3k_4 + k_1k_4 + \sum_{i=1}^{4} k_i,$$

$$W_P(G_{24}) = (k_1 + k_3 + 1)(k_2 + k_4 - 1) + \sum_{i=1}^{4} k_i.$$

Obviously, $W_P(G_{21}) = W_P(G_{22}) = W_P(G_{23}) > W_P(G_{24}) \geq n-3$; the equality holds if and only if $G_{24} \cong \mathcal{T}_4$. Then the third smallest Wiener polarity index is $W_P(\mathcal{T}_4) = 3 = n-3$.

Case 2. $\max\{l_1, l_2, l_3, v_4\} \geq 1$.

$\mathcal{S}_2(k_1 = 1 \text{ and } k_2 = 0)$ is the subgraph of U and $W_P(\mathcal{S}_2) = 1\,(k_1 = 1 \text{ and } k_2 = 0)$, by Lemma 2.2, we have

$$W_P(U) \geq 1 + n - 5 = n - 4,$$

the equality holds if and only if $U \cong \mathcal{S}_2(k_1 = 1, k_2 = 1)$. If $\mathcal{S}_2(k_1 = 1, k_2 = 1)$ is the induced subgraph of U, by Lemma 2.2, we have

$$W_P(U) \geq 2 + n - 5 = n - 3,$$

the equality holds if and only if $U \cong \mathcal{T}_5$.

By combining the above arguments, the result follows.

Lemma 2.6 *Let $U \in \mathcal{U}_n$. If $g(U) = 5$, then the third smallest Wiener polarity index $W_P(U) = n-3$, the equality holds if and only if $U \cong \mathcal{T}_i$, $(i = 6, 7, 8)$ ($\mathcal{T}_6$, $\mathcal{T}_7$, and $\mathcal{T}_8$ are shown in* **Figure 5***).*

Proof. Let $C_5 = \{v_1, v_2, v_3, v_4, v_5\}$, we consider the next cases.

Case 1. $\max\{l_1, l_2, l_3, l_4, l_5\} = 0$.

This implies that U is a unicyclic graph obtained by attaching $k_i \geq 0$ pendant vertices to v_i, where $1 \leq i \leq 5$.

If $n = 5$, then there exists only one graph C_5 and $W_P(C_5) = 0$.

If $n = 6$, then there exists only one graph $\mathcal{S}_3$ and $W_P(\mathcal{S}_3) = 2 = n-4$.

If $n = 7$, then there exists three graphs G_{31}, $\mathcal{T}_6$, and $\mathcal{T}_7$, $W_P(G_{31}) = 5 = n-2$, $W_P(\mathcal{T}_6) = W_P(\mathcal{T}_7) = 4 = n-3$.

If $n > 7$, then G_{31} or $\mathcal{T}_6$ or $\mathcal{T}_7$ is the subgraph of U and $\min\{|N^2_{G_{31}}(u)|, |N^2_{\mathcal{T}_6}(u)|, |N^2_{\mathcal{T}_7}(u)|\} \geq 2$. By Lemma 2.2, we have $W_P(U) \geq 4 + 2 + n - 8 = n - 2$.

Case 2. $\max\{l_1, l_2, l_3, l_4, l_5\} \geq 1$.$\mathcal{T}_8\,(n = t = 7)$ is the subgraph of U and $W_P(\mathcal{T}_8) = 4\,(n = t = 7)$; meanwhile, $|N^2_{\mathcal{T}_8}(u)| \geq 1$, the equality holds if and only if $u = v_7$. By Lemma 2.2, we have $W_P(U) \geq 4 + n - 7 = n - 3$, the equality holds if and only if $U = \mathcal{T}_8$.

By combining the above arguments, the result follows.

Lemma 2.7 *Let $U \in \mathcal{U}_n$ and $g(U) = 6$. If $n = 6$, then $W_P(C_6) = n-3$; if $n > 7$, then $W_P(U) \geq n-2$.*

Proof. When $g(U) = 6$ and $n = 6$, then there exists only one graph C_6 and $W_P(C_6) = 3 = n-3$.

When $n \geq 7$, C_6 is the subgraph of U and $|N^2_{C_6}(u)| \geq 2$, by Lemma 2.2, we have $W_P(U) \geq 3 + 2 + n - 7 = n - 2$.

Lemma 2.8 Let $U \in \mathcal{U}_n$, if $g(U) = s \geq 7$, then $W_P(U) \geq n$, the equality holds if and only if $U \cong C_s$.

Proof. If $U \cong C_s$, then by the definition of Wiener polarity index, we have $W_P(U) = n$.

If $U \ncong C_s$, then $C_s\,(s \geq 7)$ is the subgraph of U and $|N^2_{C_s}(u)| \geq 2$. By Lemma 2.2, we have $W_P(U) \geq W_P(C_s) + 2 + (n - s - 1) = n + 1$.

By combining the above arguments, the result follows.

Theorem 2.9. Let $U \in \mathcal{U}_n$; then the third smallest Wiener polarity index $W_P(U) = n-3$, the equality holds if and only if $U \cong C_6$ or $\mathcal{T}_i, 1 \leq i \leq 8$ ($\mathcal{T}_1$,$\mathcal{T}_2$, and $\mathcal{T}_3$ are shown in **Figure 1**; $\mathcal{T}_4$ and $\mathcal{T}_5$ are shown in **Figure 3**; $\mathcal{T}_6$,$\mathcal{T}_7$, and $\mathcal{T}_8$ are shown in **Figure 5**).

Proof. By Lemma 2.4–2.8, the result follows.

3. CONCLUSIONS

Chemical graph theory is an important area of research in mathematical chemistry which deals with topology of molecular structure such as the mathematical study of isomerism and the development of topological descriptors or indices. In this paper, we first introduce some useful graph transformations and determine the third smallest Wiener polarity index of unicyclic graphs. In addition, all the corresponding extremal graphs are characterized.

DATA AVAILABILITY STATEMENT

All datasets presented in this study are included in the article.

AUTHOR CONTRIBUTIONS

WF performed conceptualization. FC and HD were responsible for methodology. WF and MM wrote the original manuscript. WF and FC reviewed and edited the article.

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Conflict of Interest: The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.