Third Smallest Wiener Polarity Index of Unicyclic Graphs

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The Wiener polarity index WP(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

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 \( v \). \( N_G(u) = \{v \in V(G) | d_G(u, v) = 1\} \) is called the first neighbor vertex set of \( u \). Especially, if \( i = 1 \), then \( N_G(u) \) (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 \( U_n \) 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 \( r(G, k) \) denote the number of unordered vertices pairs of \( G \), each of whose distance is equal to \( k \). The Wiener polarity index, denoted by \( WP(G) \), is defined to be the number of unordered vertices pairs of distance 3, i.e., \( WP(G) = r(G, 3) \).

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]
The Wiener polarity index is introduced by Harold Wiener [4] in 1947. In Ref. [4], Wiener used a linear formula of paraf:

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

where \(a, b, c\) are constants for a given isomeric group.

If \(G_1, \ldots, G_t\) 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 the Wiener polarity index of connected graphs. Moreover, all the corresponding extremal graphs are characterized.

In the 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.

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 \(K_{i,n-1}\) by adding one edge to two pendant vertices of \(K_{i,n-1}\).

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 \(E(C_t) = \{v_1v_2, v_2v_3, \ldots, v_{t-1}v_t, v_tv_1\}\). 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 \(U \in U_n\), then \(W_p(G) \geq 0\), where equality holds if and only if \(U \in S(n,1)\) or \(U \equiv C_t\) or \(U \equiv C_5\) \((S(n,1)\) is shown in Figure 1).

**Lemma 2.2.** Let \(G \in U_n\) and \(|N^2_v(u)| \geq k\) 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, \(W_p(G + w) \geq W_p(G) + k\).
Without loss of generality, let $G = (V(G), E(G))$, where $|V(G)| = n$.

**Proof.** Since $N_{G,w}(v) = \{u\}$ and $N_{G}^{2}(u) \geq k$, then $W_{p}(G + w) = W_{p}(G) + |N_{G}^{2}(u)| = W_{p}(G) + N_{G}^{2}(u) \geq W_{p}(G) + k$.

**Lemma 2.3** [10]. Suppose $U \in \mathcal{U}_{n} \setminus \{S(n, 1)\}$. If $g(U) = 3$ and $n \geq 5$, then $W_{p}(U) \geq n - 4$, where equality holds if and only if $U \equiv S_{1}(1)$ is 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 $1 \leq i \leq 5$. 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

\[
W_{p}(G_{1i}) = k_{1}k_{2} + k_{2}k_{3} + k_{1}k_{3};
\]

\[
W_{p}(G_{12}) = k_{1}k_{2} + k_{2}k_{3};
\]

\[
W_{p}(G_{13}) = (k_{1} + k_{3} + 1)(k_{2} - 1) = k_{1}k_{2} + k_{2}k_{3} - (k_{1} + k_{3} + 1 - k_{2});
\]

\[
W_{p}(G_{14}) = 2(n - 5) \geq n - 4(n \geq 6);
\]

\[
W_{p}(S_{1}) = n - 4(n \geq 5).
\]

Obviously, $W_{p}(G_{11}) \geq W_{p}(G_{12}) > W_{p}(G_{13});$ the equality holds if and only if $G_{11} \equiv G_{12}$. Then the third smallest Wiener polarity index is $W_{p}(T_{1}) = 4 = n - 3$.

Case 2. $\max\{|l_{1}, l_{2}, l_{3}\} \geq 1$.

$G_{15}$ is the subgraph of $U$ and $W_{p}(G_{15}) = 2N_{G_{15}}^{2}(u) \geq 1$, 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 $T_{2}$ or $T_{3}$.

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 $U \equiv T_{4}$ or $T_{5}$ ($T_{4}$ and $T_{5}$ 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
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 $G_{24} \cong T_4$. Then the third smallest Wiener polarity index is $W_P(T_4) = 3 = n - 3$.

Case 2. $\max\{l_1,l_2,l_3,l_4\} \geq 1$.

$S_2(k_1 = 1 \text{ and } k_2 = 0)$ is the subgraph of $U$ and $W_P(S_2) = 1(k_1 = 1 \text{ and } k_2 = 0)$, by Lemma 2.2, we have

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

the equality holds if and only if $U \cong S_2(k_1 = 1, k_2 = 1)$. If $S_2(k_1 = 1, k_2 = 1)$ 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 $U \cong T_5$.

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 $U \cong T_n$, ($n = 6,7,8$) ($T_6$, $T_7$, and $T_8$ 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. $\max\{l_1,l_2,l_3,l_4\} = 0$.

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 $S_3$ and $W_P(S_3) = 2 = n - 4$.

If $n = 7$, then there exists three graphs $G_{31}$, $T_6$, and $T_7$, $W_P(G_{31}) = 5 = n - 2$, $W_P(T_6) = W_P(T_7) = 4 = n - 3$.

If $n > 7$, then $G_{31}$ or $T_6$ or $T_7$ is the subgraph of $U$ and $\min\{|N_{G_{31}}^2(u)|,|N_{T_6}^2(u)|,|N_{T_7}^2(u)|\} \geq 2$. By Lemma 2.2, we have $W_P(U) \geq 4 + 2 + n - 8 = n - 2$.

Case 2. $\max\{l_1,l_2,l_3,l_4\} \geq 1$.

$T_n (n = 7)$ is the subgraph of $U$ and $W_P(T_n) = 4 (n = 7)$; meanwhile, $|N_{T_n}^2(u)| \geq 1$, 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 $U \cong T_7$.

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 $|N_{C_6}^2(u)| \geq 2$, 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 $g(U) = 7$, then $W_P(U) \geq n$, the equality holds if and only if $U \cong C_7$.

**Proof.** If $U \cong C_7$, then by the definition of Wiener polarity index, we have $W_P(U) = n$.

If $U \neq C_7$, then $C_i (i \geq 7)$ is the subgraph of $U$ and $|N_{C_i}^2(u)| \geq 2$. By Lemma 2.2, we have $W_P(U) \geq W_P(C_i) + 2 + (n - s - 1) = n + 1$.

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 $T_i$, $1 \leq i \leq 8$ ($T_1, T_2$, and $T_3$ are shown in Figure 1; $T_4$ and $T_5$ are shown in Figure 3; $T_6$, $T_7$, and $T_8$ 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.

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