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On the Extremal Wiener Polarity Index of Chemical Trees[1]

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Abstract

The Wiener polarity index $W_P(G)$ of a graph $G = (V, E)$ is the number of unordered pairs of vertices $\{u, v\}$ of G such that the distance $d_G(u, v)$ between u and v is 3. In this paper, the extremal Wiener polarity indices of all chemical trees on n vertices are given.

1 Introduction

Let $G = (V, E)$ be a connected (molecular) graph. The distance between two vertices u and v in G, denoted by $d_G(u, v)$, is the length of a shortest path between u and v in G. The Wiener polarity index of G, denoted by $W_P(G)$, is defined by

$$W_P(G) = |\{\{u, v\}|d_G(u, v) = 3, u, v \in V\}|$$

which is the number of unordered pairs of vertices $\{u, v\}$ of G such that $d_G(u, v) = 3$. The Wiener polarity index for the quantity defined in the equation above is introduced by Harold Wiener [1] for acyclic molecules in a slightly different manner. After this, it seems that less attention has been paid for the Wiener polarity index $W_P(G)$. Using the Wiener polarity index, Lukovits and Linert [2] demonstrated quantitative structure-property relationships in a series of acyclic and cycle-containing hydrocarbons. Hosoya [3] found a physico-chemical interpretation of $W_P(G)$. Very recently, Du, Li and Shi [4] described a linear time algorithm APT for computing the index

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of trees, and characterized the trees maximizing the index among all trees of given order; Deng, Xiao and Tang [5] characterized the extremal trees with respect to this index among all trees of order n and diameter k.

In this paper, we will give the extremal Wiener polarity indices of all chemical trees with order n.

2 Some transformations does not decrease the Wiener polarity index

Let T be a tree with its vertex set $V(T)$ and edge set $E(T)$. We denote by $d_T(v)$ the degree of a vertex $v \in V(T)$.

We first give a formula for computing the Wiener polarity index of trees.

Lemma 1([4,5]). Let $T = (V, E)$ be a tree. Then

$$W_P(T) = \sum_{uv \in E} (d_T(u) - 1)(d_T(v) - 1).$$

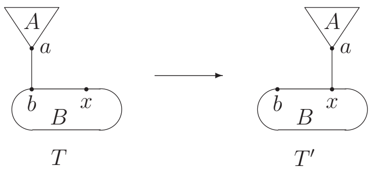

Figure 1. The (k,l)-transformation.

Then, we introduce a graph transformation which has been used to study other topological indices.

Let T be a tree and ab an edge of T. After removing ab from T we obtain two trees A and B such that $a \in V(A)$ and $b \in V(B)$. For $x \in V(B) - \{b\}$, let T' be the tree obtained by adding the edge ax to the union of A and B. We will say that T' is obtained from T by a (k,l)-transformation if $d_T(b) = k$ and $d_T(x) = l$.

This transformation is illustrated in Figure 1.

Let $\mathcal{C}_n$ be the set of chemical trees (i.e., trees for which every vertex has degree at most 4) with n vertices. We associate to $T \in \mathcal{C}_n$ the vertex sequence

$$(n_1, n_2, n_3, n_4)$$

where n_i denotes the number of vertices of T with degree i $(1 \leq i \leq 4)$. Recall the relations

$$n_1 + n_2 + n_3 + n_4 = n, \qquad n_1 + 2n_2 + 3n_3 + 4n_4 = 2n - 2$$

which implies $n_3 + 2n_4 + 2 = n_1$, and

$$n = 2 + n_2 + 2n_3 + 3n_4.$$

In the following, using transformations, we will show that for every tree $T \in \mathcal{C}_n$ there is a tree $T' \in \mathcal{C}_n$ with the vertex sequence $(n_1, 0, n_3, n_4)$ or $(n_1, 1, 0, n_4)$ such that $W_P(T') \geq W_P(T)$.

Lemma 2. Let $T \in \mathcal{C}_n$ $(n \geq 5)$ with vertex sequence (n_1, n_2, n_3, n_4) and $n_2 \geq 2$. Then there exists $T' \in \mathcal{C}_n$ obtained by a $(2,2)$-transformation on T, such that $W_P(T') \geq W_P(T)$.

Proof. We can choose $x, y \in V(T)$ such that $d_T(x) = d_T(y) = 2$. We distinguish two cases.

(i) If $xy \in E(T)$, see Figure 2(i), then $d_T(a) + d_T(b) \geq 3$ because $n \geq 5$, and by Lemma 1,

$$W_P(T') - W_P(T) = (d_T(a) - 1) + (d_T(b) - 1) - 1 = d_T(a) + d_T(b) - 3 \geq 0.$$

(ii) Otherwise, we may choose x, y as in Figure 2(ii). Notice that $x_1 = y_1$ is possible. Without loss of generality, we assume that $d_T(y_1) \geq d_T(x_1)$. By Lemma 1,

$$\begin{aligned}
& W_P(T') - W_P(T) \\
= \; & [2(d_T(a) - 1) + 2(d_T(b) - 1) + 2(d_T(y_1) - 1)] \\
- \; & [(d_T(a) - 1) + (d_T(b) - 1) + (d_T(x_1) - 1) + (d_T(y_1) - 1)] \\
= \; & (d_T(a) - 1) + (d_T(b) - 1) + (d_T(y_1) - 1) - (d_T(x_1) - 1) \\
= \; & (d_T(a) + d_T(b) - 2) + (d_T(y_1) - d_T(x_1)) \geq 0. \qquad \square
\end{aligned}$$

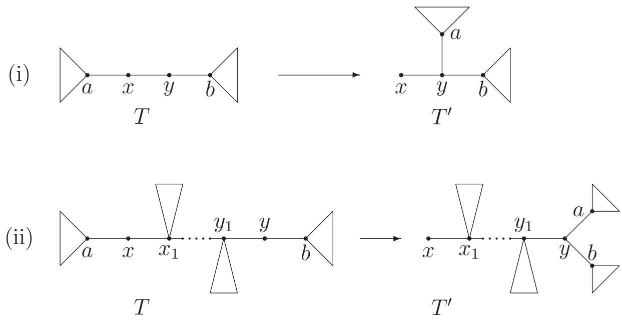

Figure 2. The transformations in Lemma 2.

Lemma 3. Let $T \in \mathcal{C}_n$ $(n \geq 6)$ with vertex sequence $(n_1, 1, n_3, n_4)$. If $n_3 \geq 1$, then there exists $T' \in \mathcal{C}_n$, obtained by a $(2,3)$-transformation on T, such that $W_P(T') \geq W_P(T)$.

Proof. We can choose $x, y \in V(T)$ such that $d_T(x) = 2$, $d_T(y) = 3$ and the distance $d_T(x, y)$ is as small as possible.

(i) If $xy \in E(T)$, see Figure 3(i). Without loss of generality, we assume that $d_T(b) \leq d_T(c)$. By Lemma 1,

$$
\begin{aligned}
& W_P(T') - W_P(T) \\
= \; & [3(d_T(a)-1) + 3(d_T(b)-1) + 3(d_T(c)-1)] \\
- \; & [(d_T(a)-1) + 2 + 2(d_T(b)-1) + 2(d_T(c)-1)] \\
= \; & 2(d_T(a)-1) - 2 + (d_T(b)-1) + (d_T(c)-1).
\end{aligned}
$$

If $d_T(a) > 1$, then $W_P(T') \geq W_P(T)$; If $d_T(a) = 1$ and $d_T(b) > 1$, then $d_T(c) > 1$ since $d_T(b) \leq d_T(c)$, so $W_P(T') \geq W_P(T)$; If $d_T(a) = 1$ and $d_T(b) = 1$, then $d_T(c) \geq 3$ since $n \geq 6$ and $n_2 = 1$, so, $W_P(T') \geq W_P(T)$.

(ii) Otherwise, we may choose x, y as in Figure 3(ii). Notice that $x_1 = y_1$ is possible. By Lemma 1,

$$
\begin{aligned}
& W_P(T') - W_P(T) \\
= \;& [3(d_T(a)-1)+3(d_T(b)-1)+3(d_T(c)-1)+3(d_T(y_1)-1)] \\
- \;& [(d_T(a)-1)+2(d_T(b)-1)+2(d_T(c)-1)+(d_T(x_1)-1)+2(d_T(y_1)-1)] \\
= \;& 2(d_T(a)-1)+(d_T(b)-1)+(d_T(c)-1)+(d_T(y_1)-1)-(d_T(x_1)-1) \\
= \;& (2d_T(a)+d_T(b)+d_T(c)-4)+(d_T(y_1)-d_T(x_1)) \\
= \;& 2d_T(a)+d_T(b)+d_T(c)-4 \geq 0.
\end{aligned}
$$

$\square$

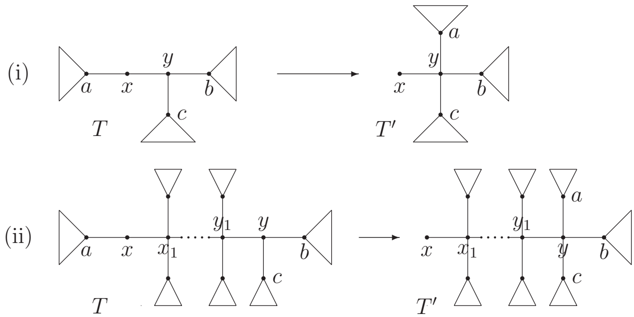

Figure 3. The transformations in Lemma 3.

By Lemma 2 and an inductive argument, we can show that if $T \in \mathcal{C}_n$ with vertex sequence (n_1, n_2, n_3, n_4) and $n_2 = 2l$ or $n_2 = 2l+1$, where l is a positive integer, we can construct a tree $T' \in \mathcal{C}_n$ such that $W_P(T') \geq W_P(T)$ and the vertex sequence of T' is

$$(n_1 + l, 0, n_3 + l, n_4) \qquad \text{if } n_2 = 2l$$

$$(n_1 + l, 1, n_3 + l, n_4) \quad \text{if } n_2 = 2l+1$$

Now, by Lemma 3, if T' has vertex sequence $(n_1 + l, 1, n_3 + l, n_4)$ with $n_3 + l \geq 1$, then, using a $(2,3)$-transformation on T', we can construct a tree $T'' \in \mathcal{C}_n$ such that $W_P(T'') \geq W_P(T')$ and T'' has the vertex sequence $(n_1 + l + 1, 0, n_3 + l - 1, n_4 + 1)$. In this way, we have shown the following result.

Theorem 1. Let $T \in \mathcal{C}_n$ $(n \geq 6)$ with vertex sequence (n_1, n_2, n_3, n_4). Then there exists $T' \in \mathcal{C}_n$ such that $W_P(T') \geq W_P(T)$ and T' has the vertex sequence

$$\begin{cases} \left(n_1 + \frac{n_2}{2}, 0, n_3 + \frac{n_2}{2}, n_4\right), & \text{if } n_2 \text{ is even;} \\ \left(n_1 + \frac{n_2+1}{2}, 0, n_3 + \frac{n_2-3}{2}, n_4 + 1\right) \text{ or } (n_1, 1, 0, n_4), & \text{if } n_2 \text{ is odd.} \end{cases}$$

Therefore, we have reduced the problem to the chemical trees with no vertices of degree 2, or with one vertex of degree 2 and no vertices of degree 3.

Lemma 4. Let $T \in \mathcal{C}_n$ $(n \geq 7)$ with vertex sequence $(n_1, 0, n_3, n_4)$. If $n_3 \geq 2$, then there exists $T' \in \mathcal{C}_n$, obtained by a $(3,3)$-transformation on T, such that $W_P(T') \geq W_P(T)$.

Proof. We can choose $x, y \in V(T)$ such that $d_T(x) = d_T(y) = 3$ and the distance $d_T(x, y)$ is as small as possible.

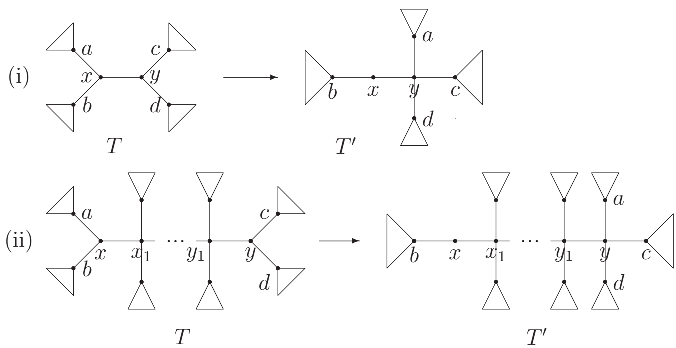

Figure 4. The transformations in Lemma 4.

(i) If $xy \in E(T)$, see Figure 4(i). Without loss of generality, we assume that $d_T(a) \geq d_T(b)$ and $d_T(a) + d_T(b) \leq d_T(c) + d_T(d)$. By Lemma 1,

$$\begin{aligned} & W_P(T') - W_P(T) \\ = \; & [3(d_T(a) - 1) + (d_T(b) - 1) + 3 + 3(d_T(c) - 1) + 3(d_T(d) - 1)] \\ - \; & [2(d_T(a) - 1) + 2(d_T(b) - 1) + 4 + 2(d_T(c) - 1) + 2(d_T(d) - 1)] \end{aligned}$$

$$= (d_T(a)-1)-(d_T(b)-1)-1+(d_T(c)-1)+(d_T(d)-1)$$

$$= (d_T(a)-d_T(b))+(d_T(c)+d_T(d)-3).$$

If $d_T(a) > 1$, then $d_T(c)+d_T(d) \geq d_T(a)+d_T(b) \geq 3$, so $W_P(T') \geq W_P(T)$; If $d_T(a)=1$, then $d_T(b)=1$ since $d_T(a) \geq d_T(b)$, and $d_T(c)+d_T(d) \geq 3$ since $n \geq 7$. So, $W_P(T') \geq W_P(T)$.

(ii) Otherwise, we may choose x, y as in Figure 4(ii). Notice that $x_1 = y_1$ is possible. Without loss of generality, we assume that $d_T(a) \geq d_T(b)$. By Lemma 1,

$$\begin{aligned}
& W_P(T')-W_P(T) \\
= \; & [3(d_T(a)-1)+(d_T(b)-1)+3+9+3(d_T(c)-1)+3(d_T(d)-1)] \\
- \; & [2(d_T(a)-1)+2(d_T(b)-1)+6+6+2(d_T(c)-1)+2(d_T(d)-1)] \\
= \; & (d_T(a)-1)-(d_T(b)-1)+(d_T(c)-1)+(d_T(d)-1) \\
= \; & (d_T(a)-d_T(b))+(d_T(c)+d_T(d)-2) \geq 0.
\end{aligned}$$

□

Let $T \in \mathcal{C}_n$ with vertex sequence $(n_1, 0, n_3, n_4)$ and $n_3 \geq 2$. By Lemma 4, there is a tree $T' \in \mathcal{C}_n$ with vertex sequence $(n_1, 1, n_3-2, n_4+1)$ and $W_P(T') \geq W_P(T)$. If $n_3-2>0$, then we can apply Lemma 3 to obtain a tree $T'' \in \mathcal{C}_n$ with vertex sequence $(n_1+1, 0, n_3-3, n_4+2)$ and $W_P(T'') \geq W_P(T')$. If $n_3-3 \geq 2$, then we again apply Lemma 4 to T''. Continuing this (finite) process, we can obtain the next result.

Theorem 2. Let $T \in \mathcal{C}_n$ $(n \geq 7)$ with vertex sequence $(n_1, 0, n_3, n_4)$. Then there exists $T' \in \mathcal{C}_n$ such that $W_P(T') \geq W_P(T)$ and T' has the vertex sequence

$$\begin{cases}
\left(n_1+\dfrac{n_3}{3}, 0, 0, n_4+\dfrac{2n_3}{3}\right), & \text{if } n_3 \equiv 0(mod3); \\[2ex]
\left(n_1+\dfrac{n_3-1}{3}, 0, 1, n_4+\dfrac{2n_3-2}{3}\right), & \text{if } n_3 \equiv 1(mod3); \\[2ex]
\left(n_1+\dfrac{n_3-2}{3}, 1, 0, n_4+\dfrac{2n_3-1}{3}\right), & \text{if } n_3 \equiv 2(mod3).
\end{cases}$$

From Theorems 1, 2 and the relation $n = 2 + n_2 + 2n_3 + 3n_4$, we have

Theorem 3. Let $T \in \mathcal{C}_n$ $(n \geq 7)$. Then there exists $T' \in \mathcal{C}_n$ such that $W_P(T') \geq W_P(T)$ and T' has the vertex sequence

$$\begin{cases} (n_1, 1, 0, n_4), & \text{if } n \equiv 0(mod3); \\ (n_1, 0, 1, n_4), & \text{if } n \equiv 1(mod3); \\ (n_1, 0, 0, n_4), & \text{if } n \equiv 2(mod3). \end{cases}$$

3 The extremal Wiener polarity index of chemical trees

In [5], we showed that $W_P(T) \geq n - 3$ for any tree T of order n and diameter $k \geq 3$, and $W_P(P_n) = n - 3$ for $n \geq 3$. So, the minimum Wiener polarity index of chemical trees with order $n \geq 6$ is $n - 3$.

In the following, we will give the maximum Wiener polarity index of chemical trees.

Let m_{ij} be the number of edges in T between vertices of degrees i and j. By Lemma 1, we have

$$W_P(T) = \sum_{uv \in E(T)} (d_T(u) - 1)(d_T(v) - 1) = \sum_{1 \leq i \leq j \leq n-1} (i-1)(j-1)m_{ij}.$$

Specially, if T is a chemical tree, then

$$W_P(T) = m_{22} + 2m_{23} + 3m_{24} + 4m_{33} + 6m_{34} + 9m_{44}.$$

Now, we compute the maximal Wiener polarity indices of chemical trees with order $n \geq 7$ by Theorem 3 and the formula above.

Case I. $n \equiv 2(mod3)$ and $T \in \mathcal{C}_n$ with vertex sequence $(n_1, 0, 0, n_4)$. Then $m_{22} = m_{23} = m_{24} = m_{33} = m_{34} = 0$, and

$$W_P(T) = 9m_{44}.$$

Because $m_{14} + m_{44} = n - 1$ and $m_{14} = n_1$, $m_{44} = n - 1 - n_1$. Also, $n_1 + n_4 = n$ and $n_1 + 4n_4 = 2n - 2$, we have $n_1 = \frac{2n+2}{3}$ and $m_{44} = \frac{n-5}{3}$. So,

$$W_P(T) = 3n - 15.$$

Case II. $n \equiv 1(mod3)$ and $T \in \mathcal{C}_n$ with vertex sequence $(n_1, 0, 1, n_4)$. Then $m_{22} = m_{23} = m_{24} = m_{33} = 0$. We distinguish three cases according to $m_{13} = 2, 1, 0$.

(i) $m_{13} = 2$. Then $m_{34} = 1$, and

$$W_P(T) = 6m_{34} + 9m_{44} = 6 + 9m_{44}.$$

Because $m_{13} + m_{14} + m_{34} + m_{44} = n - 1$ and $m_{13} + m_{14} = n_1$, $m_{44} = n - 2 - n_1$. Also, $n = n_1 + n_3 + n_4 = n_1 + 1 + n_4$ and $2n - 2 = n_1 + 3n_3 + 4n_4 = n_1 + 3 + 4n_4$, we have $n_1 = \frac{2n+1}{3}$ and $m_{44} = \frac{n-7}{3}$. So,

$$W_P(T) = 3n - 15.$$

(ii) $m_{13} = 1$. Then $m_{34} = 2$, and

$$W_P(T) = 6m_{34} + 9m_{44} = 12 + 9m_{44}.$$

Because $m_{13} + m_{14} + m_{34} + m_{44} = n - 1$ and $m_{13} + m_{14} = n_1$, $m_{44} = n - 3 - n_1$. Also, $n = n_1 + n_3 + n_4 = n_1 + 1 + n_4$ and $2n - 2 = n_1 + 3n_3 + 4n_4 = n_1 + 3 + 4n_4$, we have $n_1 = \frac{2n+1}{3}$ and $m_{44} = \frac{n-10}{3}$. So,

$$W_P(T) = 3n - 18.$$

(iii) $m_{13} = 0$. Then $m_{34} = 3$, and

$$W_P(T) = 6m_{34} + 9m_{44} = 18 + 9m_{44}.$$

Because $m_{14} + m_{34} + m_{44} = n - 1$ and $m_{14} = n_1$, $m_{44} = n - 4 - n_1$. Also, $n = n_1 + n_3 + n_4 = n_1 + 1 + n_4$ and $2n - 2 = n_1 + 3n_3 + 4n_4 = n_1 + 3 + 4n_4$, we have $n_1 = \frac{2n+1}{3}$ and $m_{44} = \frac{n-13}{3}$. So,

$$W_P(T) = 3n - 21.$$

Case III. $n \equiv 0(mod3)$ and $T \in \mathcal{C}_n$ with vertex sequence $(n_1, 1, 0, n_4)$. Then $m_{13} = m_{22} = m_{23} = m_{33} = m_{34} = 0$. We distinguish two cases according to $m_{12} = 1, 0$.

(i) $m_{12} = 1$. Then $m_{24} = 1$, and

$$W_P(T) = 3m_{24} + 9m_{44} = 3 + 9m_{44}.$$

Because $m_{12}+m_{14}+m_{24}+m_{44}=n-1$ and $m_{12}+m_{14}=n_1$, $m_{44}=n-2-n_1$. Also, $n=n_1+n_2+n_4=n_1+1+n_4$ and $2n-2=n_1+2n_2+4n_4=n_1+2+4n_4$, we have $n_1=\frac{2n}{3}$ and $m_{44}=\frac{n-6}{3}$. So,

$$W_P(T)=3n-15.$$

(ii) $m_{12}=0$. Then $m_{24}=2$, and

$$W_P(T)=3m_{24}+9m_{44}=6+9m_{44}.$$

Because $m_{14}+m_{24}+m_{44}=n-1$ and $m_{14}=n_1$, $m_{44}=n-3-n_1$. Also, $n=n_1+n_2+n_4=n_1+1+n_4$ and $2n-2=n_1+2n_2+4n_4=n_1+2+4n_4$, we have $n_1=\frac{2n}{3}$ and $m_{44}=\frac{n-9}{3}$. So,

$$W_P(T)=3n-21.$$

By Theorem 3 and the cases I-III above, we have

Theorem 4. The maximum Wiener polarity index of chemical trees with order $n\geq 7$ is $3n-15$.

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References

[1] H. Wiener, Structural determination of paraffin boiling points, *J. Amer. Chem. Soc.* **69** (1947) 17–20.

[2] I. Lukovits, W. Linert, Polarity–numbers of cycle–containing structures, *J. Chem. Inf. Comput. Sci.* **38** (1998) 715–719.

[3] H. Hosoya, Mathematical and chemical analysis of Wiener's polarity number, in: D. H. Rouvray, R. B. King (Eds.), *Topology in Chemistry–Discrete Mathematics of Molecules*, Horwood, Chichester, 2002, pp. 57.

[4] W. Du, X. Li, Y. Shi, Algorithms and extremal problem on Wiener polarity index, *MATCH Commun. Math. Comput. Chem.* **62** (2009) 235–244.

[5] H. Deng, H. Xiao, F. Tang, On the extremal Wiener polarity index of trees with a given diameter, *MATCH Commun. Math. Comput. Chem.* **63** (2010) 257–264.