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The Wiener polarity index of molecular graphs of alkanes with a given number of methyl groups

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Abstract: The Wiener polarity index of a graph G is the number of unordered pairs of vertices $\{u,v\}$ of G such that the distance between u and v is equal to 3. In this paper, the maximum Wiener polarity index of molecular graphs of alkanes with a given number of methyl groups is studied.

Keywords: topological index; Wiener polarity index; distance; alkane with k methyl groups.

INTRODUCTION

Among various topological indices considered in chemical graph theory, only a few have been widely studied in mathematical and chemical literatures. However, it seems that less attention has been paid to the Wiener polarity index. It was introduced by Harold Wiener[1] for acyclic molecules in 1947. The Wiener polarity index of an organic molecule the molecular graph of which is $G = (V,E)$ is defined as:[2,3]

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

which is the number of unordered pairs of vertices $\{u,v\}$ of G such that $d_G(u,v) = 3$, where $d_G(u,v)$ is the distance between two vertices u and v in G.

Using the Wiener polarity index, Lukovits and Linert[4] demonstrated quantitative structure–property relationships in a series of acyclic and cycle-containing hydrocarbons. Hosoya[5] found a physico-chemical interpretation of $W_p(G)$. Very recently, Du, Li and Shi[2] described a linear time algorithm APT for computing the index of trees and characterized the trees maximizing the index among all trees of a given order. Deng *et al*.[3] characterized the extremal trees with respect to this index among all trees of order n and diameter k. Deng[6] gave the extremal Wiener polarity indices of all chemical trees of order n.

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In this paper, the Wiener polarity index of molecular graphs of alkanes with k methyl groups will be studied. For an alkane with k methyl groups, its graph representation can be considered as a chemical tree with k pendents in which a pendent vertex corresponds to a methyl group. Thus, the maximum Wiener polarity index of chemical trees with n and k pendents will be discussed.

SOME PROPERTIES OF THE WIENER POLARITY INDEX

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

A path P in T is called an i-degree pendent chain if all of its internal vertices are of degree 2 and its ends of degree 1 and I, respectively, where $i \geq 3$. In particular, P is called an i-degree pendent edge if P is an edge. Here, only chemical trees are considered.

For convenience, let $\mathbf{C}_n$ be the set of chemical trees (*i.e.*, trees for which every vertex has a degree at most of 4) of order n and $\mathbf{C}_{n,k}$ the set of chemical trees of order n with k pendents.

The degree sequence (n_1, n_2, n_3, n_4) is associated to $T\in \mathbf{C}_{n,}$ where n_i denotes the number of vertices of T with degree i $(1 \leq i \leq 4)$. In particular, n_1 is the number of pendents. Recall the relations:

$$n_1 + n_2 + n_3 + n_4 = n \text{ and } n_1 + 2n_2 + 3n_3 + 4n_4 = 2n - 2$$

which implies

$$n_3 + 2n_4 + 2= n_1 \text{ and } n = 2 +n_1 + n_2 + 2n_3 + 3n_4$$

First, a formula for computing the Wiener polarity index of trees is given.

Lemma 1.[2,3] Let $T = (V,E)$ be a tree. Then

$$W_{\mathrm{p}}(T) = \sum_{uv\in E} (d_T(u)-1)(d_T(v)-1)$$

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

$$W_{\mathrm{p}}(T) = \sum_{uv\in E} (d_T(u)-1)(d_T(v)-1) = \sum_{1\leq i\leq j\leq 4} (i-1)(j-1)m_{ij}$$

Especially, if T is a chemical tree, then

$$W_{\mathrm{p}}(T) = m_{22} + 2m_{23} + 3m_{24} + 4m_{33} + 6m_{34} + 9m_{44}$$

Now, two graph transformations are introduced, which will be used in the next section.

An edge $e = uv$ is said to be subdivided when it is deleted and replaced by a path of length two connecting u and v, the internal vertex w of this path being a new vertex. The converse of subdividing is called smoothing the vertex w of degree 2. This is illustrated in Fig. 1.

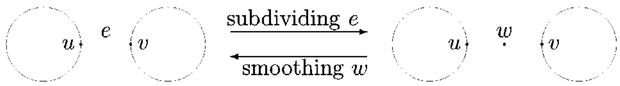

Fig. 1. The operations in subdividing and smoothing.

The following two lemmas can be proved by immediately computing from Lemma 1.

Lemma 2. Let $T\in \mathbf{C}_n$. $e = uv$ is an edge of T with $d_T(u)\le d_T(v)$. T' is the tree obtained by subdividing e. Then:

$$W_p(T')-W_p(T)=\begin{cases} 1, & d_T(u)=1, \quad d_T(v)=2;\\ 2, & d_T(u)=1, \quad d_T(v)=3;\\ 3, & d_T(u)=1, \quad d_T(v)=4;\\ 1, & d_T(u)=2, \quad d_T(v)=2,3,4;\\ 0, & d_T(u)=3, \quad d_T(v)=3;\\ -1, & d_T(u)=3, \quad d_T(v)=4;\\ -3, & d_T(u)=4, \quad d_T(v)=4; \end{cases}$$

Lemma 3. Let $T\in \mathbf{C}_n$. w is a vertex of degree 2 of T with the neighbors u and v, $d_T(u)\le d_T(v)$. T' is the tree obtained by smoothing w. Then

$$W_p(T')-W_p(T)=\begin{cases} -1, & d_T(u)=1, \quad d_T(v)=2;\\ -2, & d_T(u)=1, \quad d_T(v)=3;\\ -3, & d_T(u)=1, \quad d_T(v)=4;\\ -1, & d_T(u)=2, \quad d_T(v)=2,3,4;\\ 0, & d_T(u)=3, \quad d_T(v)=3;\\ 1, & d_T(u)=3, \quad d_T(v)=4;\\ 3, & d_T(u)=4, \quad d_T(v)=4; \end{cases}$$

Lemma 4. Let $T\in \mathbf{C}_{n,k}$ ($n \ge 7$) with the degree sequence (n_1, n_2, n_3, n_4), and all the vertices of degree 2 in T are on the pendent chains. If $n_3 \ge 2$, then there exists $T'\in \mathbf{C}_{n,k}$ with the degree sequence (n_1, n_2+1, n_3-2, n_4+1) such that $W_p(T')\ge W_p(T)$.

Proof. $x,y\in V(T)$ can be chosen such that $d_T(x) = d_T(y) = 3$ and there is neither a vertex of degree 3 nor a vertex of degree 2 between them since all the vertices of degree 2 in T are on the pendent chains. Let $T' = T - xa + ya$. Obviously, $T'\in \mathbf{C}_{n,k}$ has the degree sequence (n_1, n_2+1, n_3-2, n_4+1).

i) If $x,y\in E(T)$, see Fig. 2i. Without loss of generality, it is assumed that $d_T(a)\ge d_T(b)$ and $d_T(a)+d_T(b)\le d_T(c)+d_T(d)$. By Lemma 1:

$$W_p(T')-W_p(T) = [3(d_T(a)-1)+(d_T(b)-1)+3+3(d_T(c)-1)+3(d_T(d)-1)] -$$
$$- [2(d_T(a)-1)+2(d_T(b)-1)+4+2(d_T(c)-1)+2(d_T(d)-1)] =$$
$$= (d_T(a)-1)-(d_T(b)-1)-1+(d_T(c)-1)+(d_T(d)-1) =$$
$$= (d_T(a)-d_T(b))+(d_T(c)+d_T(d)-3)$$

If $d_T(a) > 1$, then $d_T(c)+d_T(d) \geq d_T(a)+d_T(b) \geq 3$; thus $W_p(T') \geq W_p(T)$. 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 $n \geq 7$; thus, $W_p(T') \geq W_p(T)$.

ii) Otherwise, x,y may be chosen as in Fig. 2ii. Notice that $x_1 = y_1$ is possible. Without loss of generality, it is assumed that $d_T(a) \geq d_T(b)$. By Lemma 1:

$$W_p(T') - W_p(T) = [3(d_T(a)-1)+(d_T(b)-1)+3+9+3(d_T(c)-1)+3(d_T(d)-1)] -$$
$$- [2(d_T(a)-1)+2(d_T(b)-1)+6+6+2(d_T(c)-1)+2(d_T(d)-1)] =$$
$$= (d_T(a)-1)-(d_T(b)-1)+(d_T(c)-1)+(d_T(d)-1) =$$
$$= (d_T(a)-d_T(b))+(d_T(c)+d_T(d)-2) \geq 0$$

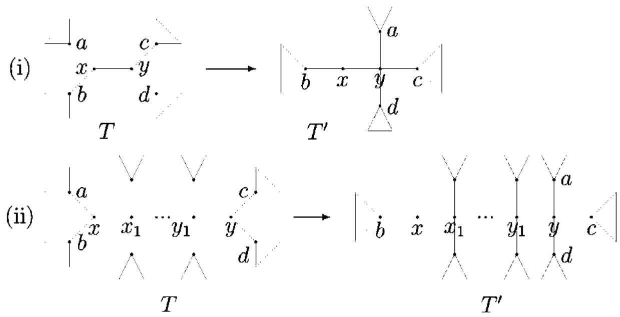

Fig. 2. Proof cases of Lemma 4.

THE MAXIMUM WIENER POLARITY INDEX OF CHEMICAL TREES WITH *n* VERTICES AND *k* PENDENTS

In this section, maximum Wiener polarity index of chemical trees with n vertices and k pendents will be discussed.

First, some special cases are considered. Let T be a chemical tree with n vertices and k pendents.

If $k = 2$, then T is the path P_n of length $n-1$, and $W_p(P_2) = 0$, $W_p(P_n) = n-3$ for $n \geq 3$.

If $k = 3$, then $n_3 = 1$, $n_4 = 0$ and $m_{14} = m_{24} = m_{33} = m_{34} = m_{44} = 0$, $0 \leq m_{23} \leq$ ≤ 3. Since

$$\sum_{j=1}^{4} m_{1j} = n_1 = k \text{ and } \sum_{i=1}^{4}\sum_{j=i}^{4} m_{ij} = n-1, \; m_{22} + m_{23} = n-1-k = n-4$$

and

$$W_p(T) = m_{22} + 2m_{23} = n - 4 + m_{23} \leq \begin{cases} 0, n = 4; \\ 2, n = 5; \\ 4, n = 6; \\ n-1, n \geq 7. \end{cases}$$

with equality if and only if T is one of the graphs in Fig. 3.

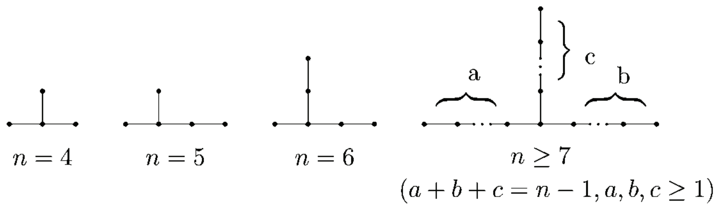

Fig. 3. The extremal tree with 3 pendents.

If $k = 4$ and $n = 5$, then T is a star with 5 vertices and $W_p(T) = 0$. If $k = 4$ and $n = 6$, then there are only two chemical trees with 6 vertices and 4 pendents. One can immediately obtain that $W_p(\mathrm{T}) = 3$ or $W_p(\mathrm{T}) = 4$.

In the following, it is assumed that $k \geq 4$ and $n \geq 7$.

Let $\mathbf{C}^{*}_{n,k}$ be the set of chemical trees T with n vertices and k pendents satisfying the following conditions:

i) there is at most one vertex of degree 3 in T;

ii) all the vertices of degree 2 in T are on the pendent chains;

iii) if P is a path in T with ends of degree 4, then all internal vertices of P are of degree 4;

iv) if $n_2 \geq k$, then there is neither a 4-degree pendent edge nor a 3-degree pendent edge.

Remark. Let $T \in \mathbf{C}^{*}_{n,k}$ with a degree sequence (n_1, n_2, n_3, n_4).

I) If k is even, then $n_3 = 0$, the induced subgraph T' by the vertices of degree 4 in T is also a tree, and $m_{44} = n_4 - 1$. By the relations:

$$\begin{cases} k + n_2 + n_4 = n, \\ k + 2n_2 + 4n_4 = 2n - 2 \end{cases}$$

one has $n_2 = n + 1 - 3k/2$ and $n_4 = k/2 - 1$.

i) If $n_2 \leq k$, *i.e.*, $k \geq 2(n+1)/5$, then $m_{24} = n_2$, $m_{22} = 0$ and

$$W_p(T) = 3m_{24} + 9m_{44} = 3n_2 + 9(n_4 - 1) = 3n - 15$$

ii) If $n_2 \geq k$, *i.e.*, $k \leq 2(n+1)/5$, then $m_{24} = k$, $m_{22} = n - 1 - (k + m_{24} + m_{44}) = n + 1 - 5k/2$ and $W_p(T) = m_{22} + 3m_{24} + 9m_{44} = n + 5k - 17$.

II) If k is odd, then T has only a vertex v of degree 3, *i.e.*, $n_3 = 1$. The induced subgraph T' by the vertices of degree 3 or 4 in T is also a tree and v is a pendent of T'. Thus, $m_{44} = n_4 - 1$, $m_{34} = 1$ and $m_{33} = 0$. By the relations:

$$\begin{cases} k + n_2 + n_3 + n_4 = k + n_2 + n_4 = n, \\ k + 2n_2 + 3n_3 + 4n_4 = k + 2n_2 + 3 + 4n_4 = 2n - 2 \end{cases}$$

one has $n_2 = n + 1/2 - 3k/2$ and $n_4 = k/2 - 3/2$.

i) If $n_2 \le k - 2$, *i.e.*, $k \ge 2n/5 + 1$, then $m_{24} = n_2$, $m_{23} = m_{22} = 0$ and

$$W_p(T) = 3m_{24} + 6m_{34} + 9m_{44} = 3n_2 + 6 + 9(n_4 - 1) = 3n - 15$$

ii) If $n_2 = k - 1$, *i.e.*, $k = 2n/5 + 3/5$, then $m_{23} = 1$, $m_{24} = n_2 - 1 = k - 2$, $m_{22} = 0$ and

$$W_p(T) = 2m_{23} + 3m_{24} + 6m_{34} + 9m_{44} = 3n - 16$$

iii) If $n_2 \ge k$, *i.e.*, $k \le 2n/5 + 1/5$, then $m_{23} = 2$, $m_{24} = k - 2$,

$$m_{22} = n - 1 - (k + m_{23} + m_{24} + m_{34} + m_{44}) = n + 1 - 5/2k$$

and

$$W_p(T) = m_{22} + 2m_{23} + 3m_{24} + 6m_{34} + 9m_{44} = n + 5k - 18$$

Hence, for any $T \in \mathbf{C}^{\ast}_{n,k}$, one has:

$$W_p(T) = \begin{cases} n + 5k - 17, & k \text{ is even and } 4 \le k \le \frac{2}{5}(n+1); \\ 3n - 15, & k \text{ is even and } k \le \max\{4, \frac{2}{5}(n+1)\}; \\ n + 5k - 18, & k \text{ is odd and } 5 \le k \le \frac{2}{5}n + \frac{1}{5}; \\ 3n - 16, & k \text{ is odd and } k = \frac{2}{5}n + \frac{3}{5} \ge 5; \\ 3n - 15, & k \text{ is odd and } k \ge \max\{5, \frac{2}{5}n + 1\} \end{cases}$$

Theorem 1. For any $T \in \mathbf{C}^{\ast}_{n,k}$, there is $T^{\ast} \in \mathbf{C}^{\ast}_{n,k}$ such that $W_p(T^{\ast}) \ge W_p(T)$.

Proof. *i*) First, if there is a vertex of degree 2 in T which is not on any pendent chain. Let Q be the set of all vertices of degree 2 in T which are not on any pendent chain. T_1 is obtained from T by smoothing the vertices in Q, then $W_p(T_1) - W_p(T) \ge -|Q|$ by Lemma 3. Now, let T_2 be obtained from T_1 by subdividing a pendent edge $|Q|$ times, then $T_2 \in \mathbf{C}^{\ast}_{n,k}$ and $W_p(T_2) - W_p(T_1) \ge |Q|$ by Lemma 2, and $W_p(T_2) \ge W_p(T)$, *i.e.*, there is $T_2 \in \mathbf{C}^{\ast}_{n,k}$ such that all its vertices of degree 2 are on the pendent chains and $W_p(T_2) \ge W_p(T)$.

ii) Secondly, if there are at least two vertices of degree 3 in T_2, then, by Lemma 4, there exists a tree $T_3 \in \mathbf{C}^{\ast}_{n,k}$ with at the most one vertex of degree 3 such that $W_p(T_3) \ge W_p(T)$. Furthermore, it can be assumed that all the vertices of degree 2 in T_3 are on the pendent chains since process *i*) can be repeated without changing its degree sequence.

iii) Next, we consider $T_3 \in \mathbf{C}^{*}_{n,k}$ with exactly one vertex of degree 3 and with all its vertices of degree 2 on the pendent chains. If there is a path *P* in T_3 with ends of degree 4 and one of its internal vertices is of degree 3, see Fig. 4 (case 1), where $d_{T_3}(v) = 3$, it may be assumed that *P* is maximal, then

$$d_{T_3}(a), d_{T_3}(b), d_{T_3}(c) < 4 \text{ and } d_{T_3}(a), d_{T_3}(b), d_{T_3}(c) \le 2$$

since *v* is the unique vertex of degree 3. Let $T_4 = T_3 - ya + va$, see Fig. 4 (case 2), then $T_4 \in \mathbf{C}^{*}_{n,k}$. Notice that $z = y$ is possible. By Lemma 1, one obtains:

$$W_p(T_4) - W_p(T_3) = [3(d_{T_3}(u)-1) + 3(d_{T_3}(x)-1) + 3(d_{T_3}(z)-1) + 3(d_{T_3}(a)-1) +$$
$$+ 2(d_{T_3}(w)-1) + 2(d_{T_3}(b)-1) + 2(d_{T_3}(c)-1)] - [2(d_{T_3}(u)-1) + 2(d_{T_3}(x)-1) +$$
$$+ 2(d_{T_3}(z)-1) + 3(d_{T_3}(a)-1) + 3(d_{T_3}(w)-1) + 3(d_{T_3}(b)-1) + 3(d_{T_3}(c)-1)] =$$
$$= [9 + 3(d_{T_3}(x)-1) + 9 + 3(d_{T_3}(a)-1) + 6 + 2(d_{T_3}(b)-1) + 2(d_{T_3}(c)-1)] -$$
$$- [6 + 2(d_{T_3}(x)-1) + 6 + 3(d_{T_3}(a)-1) + 9 + 3(d_{T_3}(b)-1) + 3(d_{T_3}(c)-1)] =$$
$$= 4 + d_{T_3}(x) - d_{T_3}(b) - d_{T_3}(c) > 0$$

and $W_p(T_4) > W_p(T_3)$.

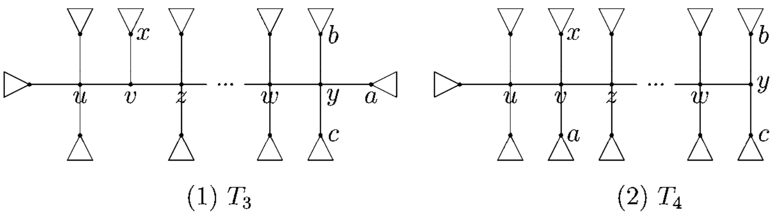

Fig. 4. Proof cases for Theorem 1.

iv) Finally, if $n \ge k$ and there is an *i*-degree pendent edge *e* in T_4 ($i = 3$ or 4), then there is a pendent chain *P* with length at least 3. Let T_5 be the tree obtained from T_5 by smoothing a vertex of degree 2 on the path *P* and subdividing the edge *e*. By Lemmas 2–3, $W_p(T_5) > W_p(T_4)$.

Hence, there is $T^{*} \in \mathbf{C}^{*}_{n,k}$ such that $W_p(T^{*}) \ge W_p(T)$ for any $T \in \mathbf{C}^{*}_{n,k}$.

In order to obtain the maximum Wiener polarity index of trees in $\mathbf{C}_{n,k}$, one only needs to find the Wiener polarity index of trees in $\mathbf{C}^{*}_{n,k}$. By Theorem 1 and the Remark, one has

Theorem 2. Among all chemical trees with $n \ge 7$ vertices and $k \ge 2$ pendents, the maximum Wiener polarity index is $W_p(T)_{max}$, where:

$$W_p(T)_{max} = \begin{cases} n-3, & k=2; \\ n-1, & k=3; \\ n+5k-17, & k \text{ is even and } 4 \le k \le \frac{2}{5}(n+1); \\ 3n-15, & k \text{ is even and } k \ge \max\{4, \frac{2}{5}(n+1)\}; \\ n+5k-18, & k \text{ is odd and } 5 \le k \le \frac{2}{5}n + \frac{1}{5}; \\ 3n-16, & k \text{ is odd and } k = \frac{2}{5}n + \frac{3}{5} \ge 5; \\ 3n-15, & k \text{ is odd and } k \ge \max\{5, \frac{2}{5}n+1\}. \end{cases}$$

From Theorem 2 and the result in the literature,[6] an interesting fact is found, *i.e.*, the maximum Wiener polarity index of chemical trees with $n \ge 7$ vertices and $k \ge 4$ pendents is the same as that of chemical trees with n vertices when $k \ge 2n/5+1$.

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И З В О Д

WIENER-ОВ ИНДЕКС ПОЛАРНОСТИ МОЛЕКУЛСКИХ ГРАФОВА АЛКАНА СА ЗАДАНИМ БРОЈЕМ МЕТИЛ ГРУПА

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Wiener-ов индекс поларности графа G је број парова чворова $\{u,v\}$ графа G таквих да је растојање између u и v једнако 3. У раду је испитан максимални Wiener-ов индекс поларности молекулских графова алкана са заданим бројем метал група.

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