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Ordering Trees with Perfect Matchings by Their Wiener Indices*

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Abstract

The Wiener index of a connected graph is the sum of all pairwise distances of vertices of the graph. In this paper, we consider the Wiener indices of trees with perfect matchings, characterizing the eight trees with smallest Wiener indices among all trees of order $2m\ (m \geq 11)$ with perfect matchings.

1. Introduction

The *Wiener index* (also called *Wiener number*) is one of the oldest topological indices of molecular structures. It was put forward by Harold Wiener [1] in 1947. The Wiener index $W(G)$ of a connected graph G is defined by

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d_G(u,v),$$

where $V(G)$ is the vertex set of G, and $d_G(u,v)$ denotes the distance between vertices u and v of G.

As summarized by Dobrynin and Gutman et al. [2], the Wiener index, as a molecular structure descriptor, is extensively used in theoretical chemistry for the design of so-called

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quantitative structure-property relations (QSPR) and quantitative structure activity relations (QSAR). Moreover, note that the *average distance* between the vertices of a graph G, denoted by $\mu(G)$, is given by $\mu(G)=W(G)/\binom{n(G)}{2}$, where $n(G)$ denotes the number of vertices of G. Hence, the Wiener index has also found some applications in interconnected networks [3-6].

Chemists are interested in the extremal Wiener indices of certain trees which represent molecular structures. Many results on Wiener indices of trees can be found in [7]. Throughout the present paper, we denote the set of trees of order n by $\mathcal{T}_n$.

Entringer et al. [8] proved that among the trees in $\mathcal{T}_n$ the Wiener index is maximized by the path P_n and minimized by the star $K_{1,n-1}$. Among all trees in $\mathcal{T}_n$ with a given maximum degree, Liu et. al [9] and Fischermann et. al [10] proved that the dendrimer is the unique tree reaching the minimum Wiener index. Shi [11] and Entringer [12] obtained the maximum of the Wiener index among trees of order n with a fixed number of pendant vertices, and the minimum was obtained by Burns and Entringer [13]. Naturally, ordering trees by their Wiener indices may help us to understand the relationship between the Wiener indices and the structures of trees. In [14] Dong and Guo considered the order of trees in $\mathcal{T}_m$ ($m \geq 24$) by their Wiener indices, and obtained the fifteen trees (shown in Fig. 1) with smallest Wiener indices. The main results of [14] can be restated as below.

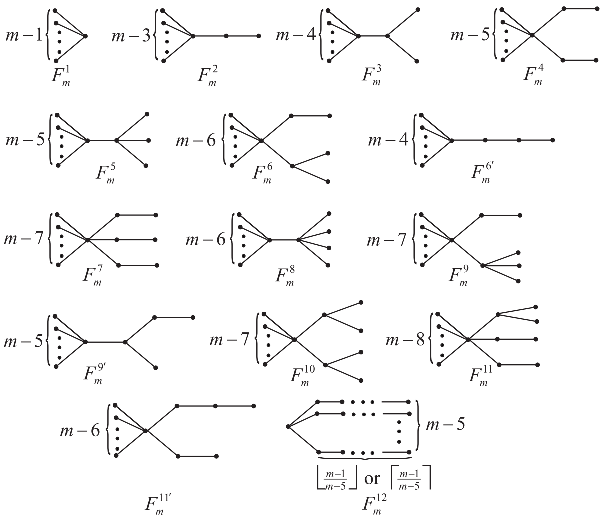

Fig.1. The fifteen trees in $\mathcal{T}_m$ which have smallest Wiener indices.

Lemma 1.1 [14]. Let $T \in \mathcal{F}_m \setminus \{F_m^1, F_m^2, F_m^3, F_m^4, F_m^5, F_m^6, F_m^{6'}, F_m^7, F_m^8, F_m^9, F_m^{9'}, F_m^{10}, F_m^{11}, F_m^{11'}, F_m^{12}\}$ and $m \geq 24$. Then $W(F_m^1) < W(F_m^2) < W(F_m^3) < W(F_m^4) < W(F_m^5) < W(F_m^6) = W(F_m^{6'}) < W(F_m^7)$ $< W(F_m^8) < W(F_m^9) = W(F_m^{9'}) < W(F_m^{10}) < W(F_m^{11}) = W(F_m^{11'}) < W(F_{2m}^{12}) < W(T)$.

In this paper, we focus on the Wiener indices of trees with *perfect matchings*. In quantum chemistry a tree with a perfect matching represents an acyclic Kekulean conjugated hydrocarbon molecule (see [15, 16]). Hence, it is interesting to investigate the Wiener index of a tree with a perfect matching. If $T \in \mathcal{F}_n$ is a tree with a perfect matching, then n should be even, say $n = 2m$, and T has a unique perfect matching. Denote the unique perfect matching of T by $M(T)$. Throughout the present paper, we denote the set of trees of order $2m$ with perfect matchings by $\mathcal{T}_{2m}$. In Section 4 we will determine the eight trees in $\mathcal{T}_{2m}$ with smallest Wiener indices.

2. A tree transformation and a partition of $\mathcal{T}_{2m}$

Firstly, we introduce the so-called *edge-growing transformation* of trees.

Definition 2.1 [17]. Let T be a tree in $\mathcal{F}_m$, and $m \geq 3$. Suppose $e = uv$ is a non-pendant edge of T, and T_1 and T_2 are the two components of $T - e$ with $u \in V(T_1)$ and $v \in V(T_2)$. T_0 is the tree obtained from T in the following way.

(1) Contract the edge $e = uv$;

(2) Add a pendant edge to the vertex $u(= v)$.

The procedures (1) and (2) (as shown in Fig. 2) are called the edge-growing transformation of T (on edge e), or *e.g.t* (on e) for short. If T can be transformed into T_0 by one step of e.g.t, then we write $T \to T_0$.

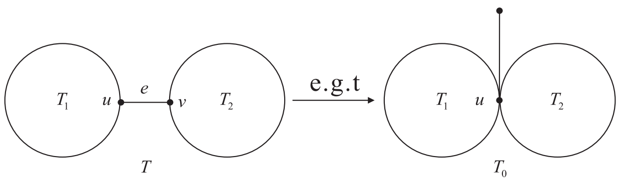

Fig.2. The edge-growing transformation of tree T.

Lemma 2.2 [14]**.** Let $T \in \mathcal{F}_m$ be a tree with non-pendant edges. If $T \to T_0$, then $W(T_0) < W(T)$.

We will use e.g.t to compare the Wiener indices of two trees with perfect matchings. Note that, if $T \in \mathcal{T}_{2m}$ and $T \to T_0$, then T_0 may not have a perfect matching. In fact, $T_0 \in \mathcal{T}_{2m}$ iff the e.g.t is carried out on an (non-pendant) edge in $M(T)$. Hereafter e.g.t will be carried out on edges in $M(T)$ only.

We also need the following partition of $\mathcal{T}_{2m}$ introduced by Chang in [18]. Let X_{2m} be the set of all trees on $2m$ vertices obtained from a tree $\hat{T}$ of order m by adding one pendant edge to each of the m vertices of $\hat{T}$. Then $X_{2m} \subseteq \mathcal{T}_{2m} \subseteq \mathcal{F}_{2m}$. If $T \in X_{2m}$ is obtained from $\hat{T}$, then T is denoted by $C(\hat{T})$. Clearly every pendant edge of a tree T in X_{2m} belongs to $M(T)$, i.e., $M(T)$ consists of the pendant edges of T. Let $X_{2m}^t = \{T \in \mathcal{T}_{2m} \mid$ there are exactly t non-pendant edges which belong to $M(T)$ $\}$. Then $X_{2m}^0 = X_{2m}$, $X_{2m}^{m-2} = \{P_{2m}\}$, and $\mathcal{T}_{2m} = \bigcup_{t=0}^{m-2} X_{2m}^t$. It is not difficult to see that any $T \in X_{2m}^t$ ($t = 1, 2, \ldots, m-2$) can be transformed into a tree T' in X_{2m}^{t-1} by a step of e.g.t on a non-pendant edge in $M(T)$.

3. Some order relations of the trees in X_{2m} and X_{2m}^1

Firstly we consider the order of the trees in X_{2m}.

If $T \in X_{2m}$, say $T = C(\hat{T})$, then in fact T is a thorn tree of $\hat{T}$ obtained from T by attaching one new vertex of degree one to each vertex of $\hat{T}$ (see [7]). From Theorem 17 of [7] we have the following result.

Lemma 3.1 [7]**.** Let $T \in X_{2m}$ and $T = C(\hat{T})$. Then $W(T) = 4W(\hat{T}) + m(2m-1)$.

That is, for a tree $T = C(\hat{T}) \in X_{2m}$, $W(T)$ strictly increases with $W(\hat{T})$. From Lemma 1.1 we immediately obtain the fifteen trees in X_{2m} ($m \geq 24$) with smallest Wiener indices.

Theorem 3.2. Let $T \in X_{2m} \setminus \{C(F_m^1), C(F_m^2), C(F_m^3), C(F_m^4), C(F_m^5), C(F_m^6), C(F_m^{6'}), C(F_m^7), C(F_m^8), C(F_m^9), C(F_m^{10}), C(F_m^{11}), C(F_m^{11'}), C(F_m^{12})\}$, where $m \geq 24$. Then

$$W(T_{2m}^1) < W(C(F_m^2)) < W(C(F_m^3)) < W(C(F_m^4)) < W(C(F_m^5)) < W(C(F_m^6)) = W(C(F_m^{6'}) <$$
$$W(C(F_m^7)) < W(C(F_m^8)) < W(C(F_m^9)) = W(C(F_m^{9'})) < W(C(F_m^{10})) < W(C(F_m^{11}))$$
$$= W(C(F_m^{11'})) < W(C(F_m^{12})) < W(T).$$

In fact from the list in [14] of trees of order m $(9 \le m \le 23)$ with smallest Wiener indices, the following conclusion is immediate.

Theorem 3.2'. Let $T \in X_{2m}^{0} \setminus \{C(F_m^1), C(F_m^2), C(F_m^3), C(F_m^4), C(F_m^5)\}$, where $m \ge 10$. Then

$$W(T_{2m}^1) < W(C(F_m^2)) < W(C(F_m^3)) < W(C(F_m^4)) < W(C(F_m^5)) < W(T).$$

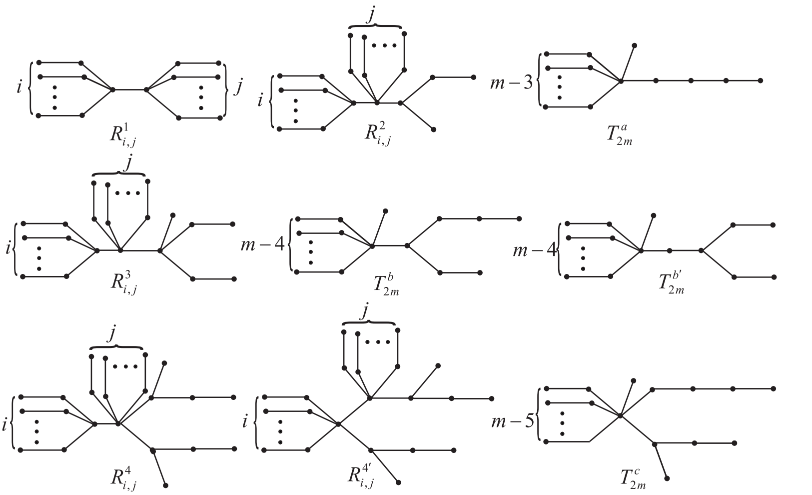

Fig.3. The trees in X_{2m}^1 that can be transformed into $C(F_m^i)$, $i = 1,2,3,4$.

In the following we investigate the trees in X_{2m}^1 that can be transformed into $C(F_m^1)$, $C(F_m^2)$, $C(F_m^3)$ or $C(F_m^4)$, which are shown in Fig. 3, i.e., the trees in $\{R_{i,j}^1 \mid i, j \ge 1, i + j = m-1\}$, $\{R_{i,j}^2 \mid i \ge 1, j \ge 0, i + j = m-3\}$ $\{T_{2m}^a\}$, $\{R_{i,j}^3 \mid i \ge 1, j \ge 0, i + j = m-4\}$ $\{T_{2m}^b, T_{2m}^{b'}\}$, and $\{R_{i,j}^4 \mid i \ge 1, j \ge 0, i + j = m-5\}$ $\{R_{i,j}^{4'} \mid i \ge 0, j \ge 0, i + j = m-5\}$ $\{T_{2m}^c\}$. Clearly, $R_{i,j}^1 = R_{j,i}^1$ and $R_{i,j}^{4'} = R_{j,i}^{4'}$, so without loss of generality we assume $i \le j$ for $R_{i,j}^1$ and $R_{i,j}^{4'}$. It is easy to compute their Wiener indices as follows.

Lemma 3.3. $W(R_{i,j}^1) = 6m^2 - 11m + 5 + (2i+1)(2j+1)$;

$$W(R_{i,j}^2) = 6m^2 - 7m - 7 + (2i+1)(2j+5);$$

$$W(R_{i,j}^3) = 6m^2 - 3m - 27 + (2i+1)(2j+7);$$

$$W(R_{i,j}^4) = 6m^2 - 3m - 19 + (2i+1)(2j+9);$$

$$W(R_{i,j}^{4'}) = 6m^2 - 3m - 19 + (2i+5)(2j+5);$$

$$W(T_{2m}^a) = 6m^2 - m - 16;$$

$$W(T_{2m}^{b}) = 6m^2 + 3m - 36\,;$$

$$W(T_{2m}^{b'}) = 6m^2 + 7m - 52\,;$$

$$W(T_{2m}^{c}) = 6m^2 + 3m - 28\,.$$

From Lemma 3.3 the following result follows immediately.

Theorem 3.4. Let $m \geq 3$. Then $W(R_{1,m-2}^{1}) < W(R_{2,m-3}^{1}) < \quad < W(R^{1}_{\lfloor\frac{m-1}{2}\rfloor,\lceil\frac{m-1}{2}\rceil})$.

Theorem 3.5. Let $m \geq 4$. Then $W(R_{1,m-4}^{2}) < W(R_{2,m-5}^{2}) = W(R_{m-3,0}^{2}) < W(R_{3,m-6}^{2}) =$ $W(R_{m-4,1}^{2}) < \quad < W(R^{2}_{\lfloor\frac{m-1}{2}\rfloor,\lceil\frac{m-1}{2}\rceil-2}) = W(R^{2}_{\lceil\frac{m-1}{2}\rceil,\lfloor\frac{m-1}{2}\rfloor-2})$.

Theorem 3.6. Let $m \geq 5$. Then $W(R_{1,m-5}^{3}) < W(R_{2,m-6}^{3}) < W(R_{3,m-7}^{3}) = W(R_{m-4,0}^{3}) <$ $W(R_{4,m-8}^{3}) = W(R_{m-5,1}^{3}) < \quad < W(R^{3}_{\lfloor\frac{m-1}{2}\rfloor,\lceil\frac{m-1}{2}\rceil-3}) = W(R^{3}_{\lceil\frac{m-1}{2}\rceil,\lfloor\frac{m-1}{2}\rfloor-3})$.

Theorem 3.7. Let $m \geq 6$. Then $W(R_{1,m-6}^{4}) < W(R_{2,m-7}^{4}) < W(R_{3,m-8}^{4}) < W(R_{4,m-9}^{4}) =$ $W(R_{m-5,0}^{4}) < W(R_{5,m-10}^{4}) = W(R_{m-6,1}^{4}) < \quad < W(R^{4}_{\lfloor\frac{m-1}{2}\rfloor,\lceil\frac{m-1}{2}\rceil-4}) = W(R^{4}_{\lceil\frac{m-1}{2}\rceil,\lfloor\frac{m-1}{2}\rfloor-4})$.

Theorem 3.8. Let $m \geq 5$. Then $W(R_{0,m-5}^{4'}) < W(R_{1,m-6}^{4'}) < \quad < W(R^{4'}_{\lfloor\frac{m-5}{2}\rfloor,\lceil\frac{m-5}{2}\rceil})$.

4. The eight trees in $\mathcal{T}_{2m}$ with smallest Wiener indices

Now we consider the order of trees in $\mathcal{T}_{2m}$ by their Wiener indices.

Theorem 4.1. Let $T \in \mathcal{T}_{2m} \setminus \{C(F_m^1), C(F_m^2), R_{1,m-2}^{1}, C(F_m^3), C(F_m^4), R_{2,m-3}^{1}, R_{1,m-4}^{2}, T_{2m}^{a}\}$, and $m \geq 11$. Then $W(C(F_m^1)) < W(C(F_m^2)) < W(R_{1,m-2}^{1}) < W(C(F_m^3)) < W(C(F_m^4)) = W(R_{2,m-3}^{1})$ $< W(R_{1,m-4}^{2}) = W(T_{2m}^{a}) < W(T)$.

Proof. From Lemma 3.1 and Lemma 3.3, and simple computations, we have

$$W(C(F_m^1)) = 6m^2 - 9m + 4\,;$$

$$W(C(F_m^2)) = 6m^2 - 5m - 8\,;$$

$$W(R_{1,m-2}^{1}) = 6m^2 - 5m - 4\,;$$

$$W(C(F_m^3)) = 6m^2 - m - 28\,;$$

$$W(C(F_m^4)) = W(R_{2,m-3}^{1}) = 6m^2 - m - 20\,;$$

$$W(R_{1,m-4}^{2}) = W(T_{2m}^{a}) = 6m^2 - m - 16\,.$$

Hence when $m \geq 10$ $W(C(F_m^1)) < W(C(F_m^2)) < W(R_{1,m-2}^{1}) < W(C(F_m^3)) < W(C(F_m^4)) =$

$W(R^1_{2,m-3}) < W(R^2_{1,m-4}) = W(T^a_{2m})$.

It is sufficient to show that $W(T) > W(R^2_{1,m-4}) = W(T^a_{2m}) = 6m^2 - m - 16$. We distinguish the following three cases.

Case 1. $T \in X^0_{2m}$. $W(T) \geq W(C(F^5_m)) = 6m^2 + 3m - 56 > 6m^2 - m - 16$ from Theorem 3.2' .

Case 2. $T \in X^1_{2m}$. If $T \to C(F^1_m)$, since $T \ncong R^1_{1,m-2}$ or $R^1_{2,m-3}$, $T = R^1_{i,j}$, where $3 \leq i \leq j$. From Theorem 3.4 $W(T) \geq W(R^1_{3,m-4}) = 6m^2 + 3m - 44 > 6m^2 - m - 16$.

If $T \to C(F^2_m)$, since $T \ncong R^2_{1,m-4}$ or T^a_{2m}, $T = R^2_{i,j}$, where $i \geq 2$ and $i + j = m - 3$. From Theorem 3.5 $W(T) \geq W(R^2_{2,m-5}) = 6m^2 + 3m - 32 > 6m^2 - m - 16$.

If $T \to C(F^3_m)$, then $T \in \{R^3_{i,j} \mid i \geq 1, j \geq 0, i + j = m - 4\} \quad \{T^b_{2m}, T^{b'}_{2m}\}$. From Theorem 3.6 and Lemma 3.3, $W(T) \geq \min\{W(R^3_{1,m-5}), W(T^b_{2m}), W(T^{b'}_{2m})\} = 6m^2 + 3m - 36 > 6m^2 - m - 16$.

If $T \to C(F^4_m)$, then $T \in \{R^4_{i,j} \mid i \geq 1, j \geq 0, i + j = m - 5\} \quad \{R^{4'}_{i,j} \mid i \geq 0, j \geq 0, i + j = m - 5\} \quad \{T^c_{2m}\}$. From Theorem 3.7, Theorem 3.8, and Lemma 3.3, $W(T) \geq \min\{W(R^4_{1,m-6}), W(R^{4'}_{0,m-5}), W(T^c_{2m})\} = 6m^2 + 3m - 28 > 6m^2 - m - 16$.

Otherwise, $T \to T_0 \in X_{2m} \setminus \{C(F^1_m), C(F^2_m), C(F^3_m), C(F^4_m)\}$, and from Lemma 2.2, Theorem 3.2', and Case 1 $W(T) > W(T_0) \geq W(F^5_m) > 6m^2 - m - 16$.

Case 3. $T \in X^t_{2m}$, $t \geq 2$. Noting that by e.g.t no trees can be transformed into $R^1_{1,m-2}$ or $R^1_{2,m-3}$, by exactly $t-1$ steps of e.g.t T will be transformed into some tree $T_1 \in X^1_{2m} \setminus \{R^1_{1,m-2}, R^1_{2,m-3}\}$. If $T_1 \cong R^2_{1,m-4}$ or $T_1 \cong T^a_{2m}$, then from Lemma 2.2 $W(T) > W(R^2_{1,m-4}) = W(T^a_{2m}) = 6m^2 - m - 16$. Otherwise from Case 2 and Lemma 2.2 $W(T) > W(T_1) > 6m^2 - m - 16$.

The proof is thus completed. □

Finally, we list the trees in $\mathcal{T}_{2m}$ with smallest Wiener indices for $m \leq 10$.

(1) When $m = 1, 2$, $\mathcal{T}_{2m} = \{C(F^1_m)\}$;

(2) When $m = 3$, $W(C(F^1_3)) < W(R^1_{1,1})$;

(3) When $m = 4$, $W(C(F^1_4)) < W(C(F^2_4)) < W(R^1_{1,2}) < W(R^2_{1,0}) < W(P_8)$;

(4) When $m = 5$, $W(C(F^1_5)) < W(C(F^2_5)) < W(R^1_{1,3}) < W(C(F^4_5)) = W(R^1_{2,2})) <$;

(5) When $m = 6$, $W(C(F^1_6)) < W(C(F^2_6)) < W(C(F^3_6)) = W(R^1_{1,4}) < W(C(F^4_6)) =$

$W(R^1_{2,3}) < W(C(F^5_6)) = W(R^2_{1,2}) = W(T^a_{12}) <$;

(6) When $m = 7$, $W(C(F^1_7)) < W(C(F^2_7)) < W(R^1_{1,5}) < W(C(F^3_7)) < W(C(F^4_7)) =$

$W(R^1_{2,4}) < W(R^1_{3,3}) = W(R^2_{1,3}) = W(T^a_{14}) < W(C(F^6_7)) = W(C(F^{6'}_7)) <$;

(7) When $m = 8$, $W(C(F^1_8)) < W(C(F^2_8)) < W(R^1_{1,6}) < W(C(F^3_8)) < W(C(F^5_8)) <$

$W(C(F^4_8)) = W(R^1_{2,5}) <$;

(8) When $m = 9$, $W(C(F^1_9)) < W(C(F^2_9)) < W(R^1_{1,7}) < W(C(F^3_9)) < W(C(F^4_9)) =$

$W(C(F^5_9)) = W(R^1_{2,6}) <$;

(9) When $m = 10$, $W(C(F^1_{10})) < W(C(F^2_{10})) < W(R^1_{1,8}) < W(C(F^3_{10})) < W(C(F^4_{10})) =$

$W(R^1_{2,7}) < W(C(F^5_{10})) = W(R^2_{1,6}) = W(T^a_{20}) <$.

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