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The inverse Wiener polarity index problem for chemical trees

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Abstract

The Wiener polarity number (which, nowadays, known as the Wiener polarity index and usually denoted by W_p) was devised by the chemist Harold Wiener, for predicting the boiling points of alkanes. The index W_p of chemical trees (chemical graphs representing alkanes) is defined as the number of unordered pairs of vertices (carbon atoms) at distance 3.
The inverse problems based on some well-known topological indices have already been addressed in the literature. The solution of such inverse problems may be helpful in speeding up the discovery of lead compounds having the desired properties. This paper is devoted to solving a stronger version of the inverse problem based on Wiener polarity index for chemical trees. More precisely, it is proved that for every integer $t \in \{n-3, n-2, \ldots, 3n-16, 3n-15\}$, $n \geq 6$, there exists an n-vertex chemical tree T such that $W_p(T) = t$.

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Introduction

A (chemical) topological index is a real number calculated from chemical graphs (graphs representing chemical compounds, in which vertices represent atoms and edges represent covalent bonds between atoms) such that it remains unchanged under graph isomorphism [1]. Topological indices are usually used in quantitative structure-activity and structure-property relationships studies for predicting the biological activities or physical-chemical properties of chemical compounds [2].

The Wiener polarity number (which, nowadays, known as the Wiener polarity index and usually denoted by W_p) was devised in 1947 by the chemist Harold Wiener [3] for predicting the boiling points of alkanes, and this index is among the oldest topological indices. The index W_p of chemical trees (chemical graphs representing alkanes) is defined as the number of unordered pairs of vertices at distance 3.

Lukovits and Linert [4] extended the definition of W_p for cycle-containing chemical graphs by using a heuristic approach, and used this new definition to demonstrate quantitative structure-property relationships in a series of acyclic and cycle-containing hydrocarbons. Hosoya and Gao [5] found that the relative magnitude of W_p among isomeric alkanes keeps pace with the number of gauche structures in the most probable confirmation, and thus W_p can predict the relative magnitude of liquid density. Miličević and Nikolić [6] used W_p in modeling the

boiling points of lower (C_3–C_8) alkanes. Shafiei and Saeidifar [7] performed quantitative structure-activity relationships studies on 41 sulfonamides for predicting their heat capacity and entropy, using W_p together with some other topological indices. In a recent study [8], some models for predicting the thermal energy, heat capacity and entropy of 19 amino acids were developed and it was found that W_p is a good topological index for modeling thermal energy.

In the last decade, W_p has attracted a considerable attention from researchers, for example, see the recent papers [9–14] and related references listed therein.

In this paper, we are concerned with the possible values of W_p for chemical trees. As usual, denote by uv the edge connecting the vertices u, v in a chemical tree T, and $d_T(u)$ the degree of vertex u in T. The following beautiful result is due to Du *et al.* [15]:

Lemma 1. *Let T be a (chemical) tree. Then*

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

where $E(T)$ denotes the edge set of T.

Here, it should be mentioned that W_p is the same as the reduced second Zagreb index [16–18] in case of (chemical) trees. Deng [19] reported the maximum W_p value of chemical trees. The same authors of this paper [20] characterized all the chemical trees with maximum W_p value. Recently, Ashrafi and Ghalavand [21] determined the first two minimum W_p values of chemical trees and characterized the corresponding chemical trees attaining the first two minimum W_p values. In the reference [22], main extremal results of the paper [21] are re-established in an alternative but shorter way, and all members with the third minimum W_p value are determined from the collection of all n-vertex chemical trees.

The problem of finding chemical structure(s) corresponding to a given value of a topological index TI is known as the inverse problem based on TI [23]. Solutions of such inverse problems may be helpful in designing a new combinatorial library, and speed up the discovery of lead compounds with some desired properties [24].

Study of the inverse problem based on topological indices was initiated by the Zefirov group in Moscow [25–29]. Gutman [30] studied the inverse problem based on the Wiener index (this index appeared in the same paper [3] where W_p was reported, see the recent survey [31] for more details about Wiener index). Solving the inverse problem based on Wiener index was the subject of several papers, for example see the papers [32–34] and related references listed therein. Li *et al.* [35] addressed the inverse problem based on four other well-known topological indices, introduced in mathematical chemistry. Recently, an inverse problem based on the k-th Steiner Wiener index (a generalized version of Wiener index) was studied in the paper [36]. Further details about inverse problem can be found in the survey [37], recent papers [38, 39] and related references listed therein.

Here we attempt to solve a stronger version of the inverse problem based on Wiener polarity index for chemical trees. We have been able to show that for every integer $t \in \{n - 3, n - 2, \ldots, 3n - 16, 3n - 15\}$, where $n \geq 6$, there exists an n-vertex chemical tree T such that $W_p(T) = t$.

Methods

By Lemma 1, we may get the following two lemmas immediately.

Lemma 2. *Let T and T_1 be the two chemical trees as depicted in Fig 1. Then*

$$W_p(T_1) - W_p(T) = -d_T(u) + 1.$$

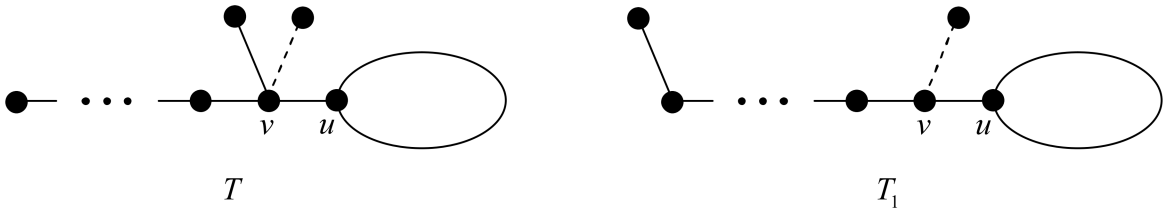

Fig 1. The chemical trees T and T_1 in Lemma 2. (The edges which are represented by dashed lines may or may not occur in the tree).

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In particular, the transformation from T to T_1 depicted in Lemma 2 is called a grafting pendent path transformation at v in T.

A vertex of degree 1 is said to be a pendent vertex.

Lemma 3. *Suppose that v is a pendent vertex with unique neighbor u in the chemical tree T. Let T_1 be another chemical tree obtained from T by attaching a pendent vertex to v. Then*

$$W_p(T_1) - W_p(T) = d_T(u) - 1.$$

Results

Theorem 1. *For every integer $n-3 \leq t \leq 3n-15$, where $n \geq 6$, there exists a chemical tree T of order n such that $W_p(T) = t$, i.e.,*

$$\{W_p(T) : T \text{ is a chemical tree of order } n\} = \{n-3, n-2, \ldots, 3n-16, 3n-15\}.$$

Proof. Clearly, the three chemical trees of order n depicted in Fig 2 have Wiener polarity indices $n-3$, $n-2$ and $n-1$, respectively. So we need only to focus on the existence of chemical trees T of order n with $W_p(T) = t$, where $n \leq t \leq 3n-15$, i.e., $n \geq 8$.

For the case $n = 8$, t can only be 8 or 9. It is easily checked that the chemical tree of order 8 obtained from $P = v_1v_2v_3v_4v_5$ by attaching three pendent vertices each to v_2, v_3, v_4 has Wiener polarity index 8, and the chemical tree of order 8 obtained from $P = v_1v_2v_3v_4v_5$ by attaching a pendent vertex to v_2 and two pendent vertices to v_3 has Wiener polarity index 9.

Suppose in the following that $n \geq 9$. We partition our proof into three cases according to the value n(mod 3).

Case 1. $n = 3k$, where $k \geq 3$.

Since the results for $t = n-3, n-2, n-1$, or equivalently, $t = 3k-3, 3k-2, 3k-1$, follow from Fig 2, we are left to consider $n \leq t \leq 3n-15$, which is equivalent to $3k \leq t \leq 9k-15$.

For the three chemical trees T_1, T_2 and T_3 of order $n = 3k$ in Fig 3, it is easily verified that

$$W_p(T_1) = 9k-15, \quad W_p(T_2) = 9k-16, \quad W_p(T_3) = 9k-17.$$

First, we start with the chemical tree T_1 as depicted in Fig 3, whose Wiener polarity index is $9k-15$. We apply grafting pendent path transformations successively at

$$v_3, v_3, v_4, v_4, \ldots, v_{k-1}, v_{k-1}, v_k,$$

which gives $2k-5$ transformations in total. A detailed illustration can be found in Fig 4.

In particular, for the above series of grafting pendent path transformations, by Lemma 2, the Wiener polarity index would decrease 3 each time. This means that we may construct a

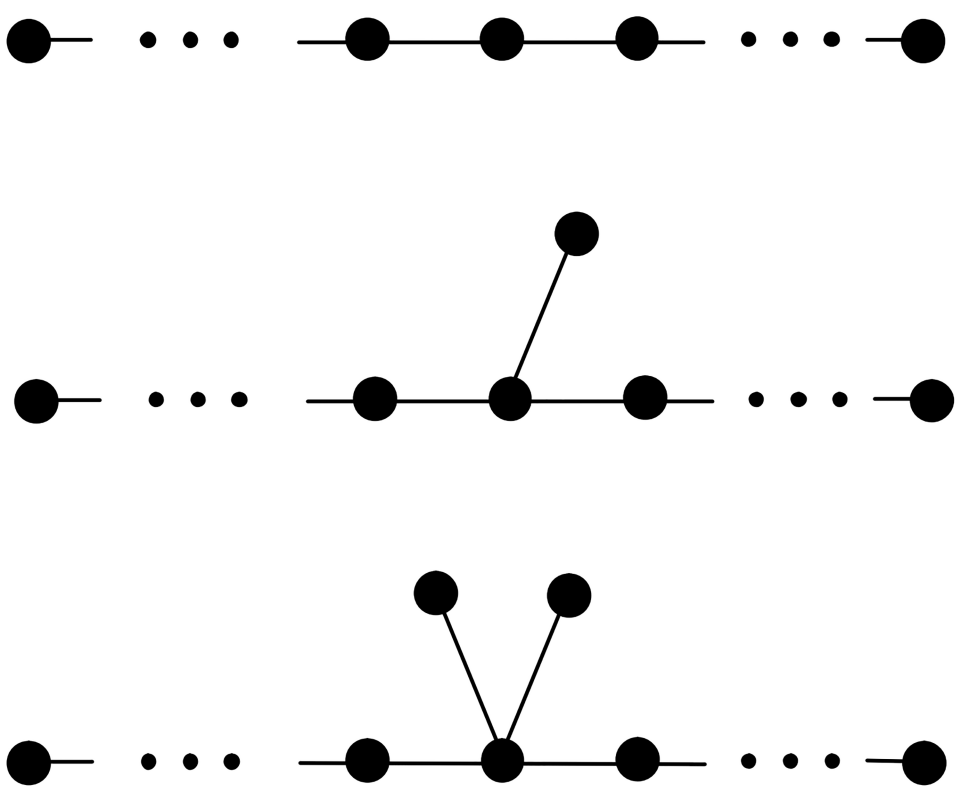

Fig 2. The chemical trees of order n with Wiener polarity indices $n-3$, $n-2$ and $n-1$, respectively.

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series of chemical trees of order $n = 3k$ with Wiener polarity indices

$$9k-15, 9k-18, \ldots, 3k+3, 3k,$$

respectively.

Next, the initial tree is changed as the chemical tree T_2 in Fig 3, its Wiener polarity index is $9k-16$. This time, we will use grafting pendent path transformations successively at

$$v_3, v_3, v_4, v_4, \ldots, v_{k-1}, v_{k-1},$$

totally $2k-6$ times grafting pendent path transformations. The corresponding illustration is shown in Fig 5.

Likewise the Wiener polarity index for the above series of transformations would decrease by 3 each time. Hence we may construct a series of chemical trees of order $n = 3k$ with Wiener polarity indices

$$9k-16, 9k-19, \ldots, 3k+5, 3k+2,$$

respectively.

Finally, choosing the chemical tree T_3 in Fig 3 with Wiener polarity index $9k-17$. Similarly, $2k-6$ times grafting pendent path transformations will be made, they are successively aimed to

$$v_4, v_4, v_5, v_5, \ldots, v_k, v_k.$$

The process is as seen in Fig 6.

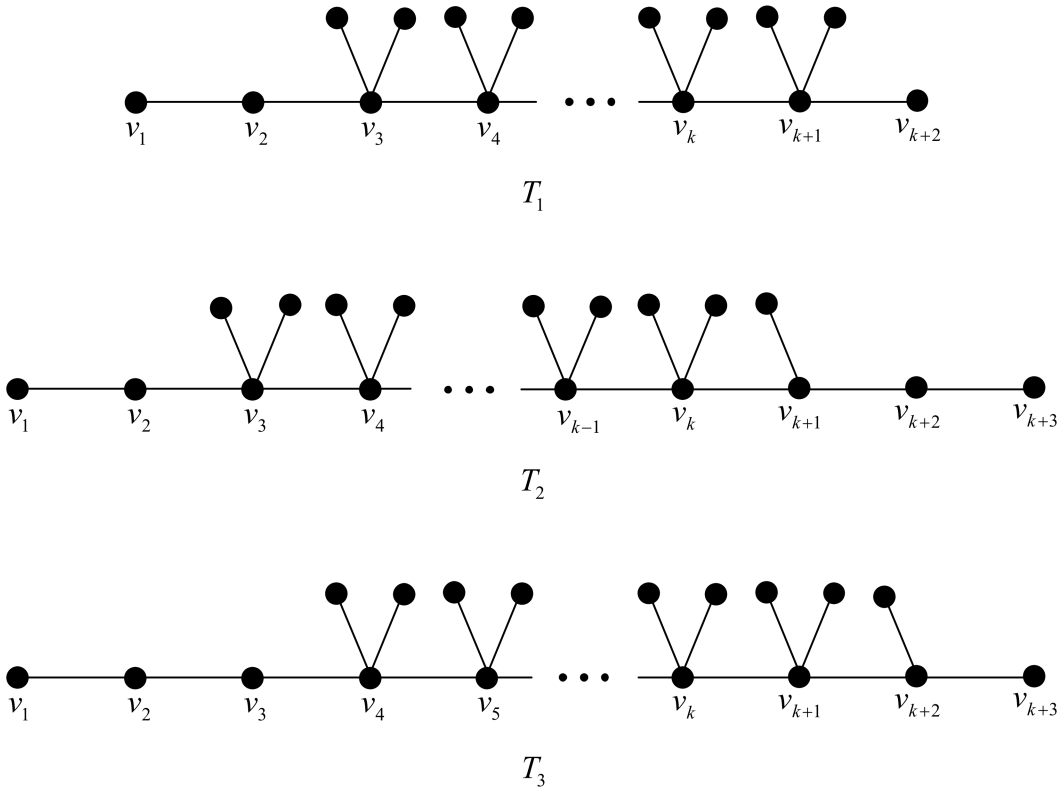

Fig 3. The chemical trees T_1, T_2 and T_3 in the proof of Case 1 in Theorem 1.

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Each time, the Wiener polarity index would decrease by 3. Thus, we may construct a series of chemical trees of order $n = 3k$ with Wiener polarity indices

$$9k - 17, 9k - 20, \ldots, 3k + 4, 3k + 1,$$

respectively.

Combining the above arguments, we get a series of chemical trees of order $n = 3k$ with Wiener polarity indices

$$3k - 3, 3k - 2, \ldots, 9k - 16, 9k - 15,$$

or equivalently,

$$n - 3, n - 2, \ldots, 3n - 16, 3n - 15.$$

Before continuing our proofs for Cases 2 and 3, we first sketch our strategy.

From Case 1, a series of chemical trees of order $3k$ with Wiener polarity indices

$$3k - 3, 3k - 2, \ldots, 9k - 16, 9k - 15$$

have been constructed. Notice that each of the chemical trees of order $3k$ constructed in Case 1 (see Figs 4, 5 and 6) with Wiener polarity indices

$$3k - 1, 3k, \ldots, 9k - 16, 9k - 15$$

has some vertex of degree 4 with two pendent neighbors, say x, y.

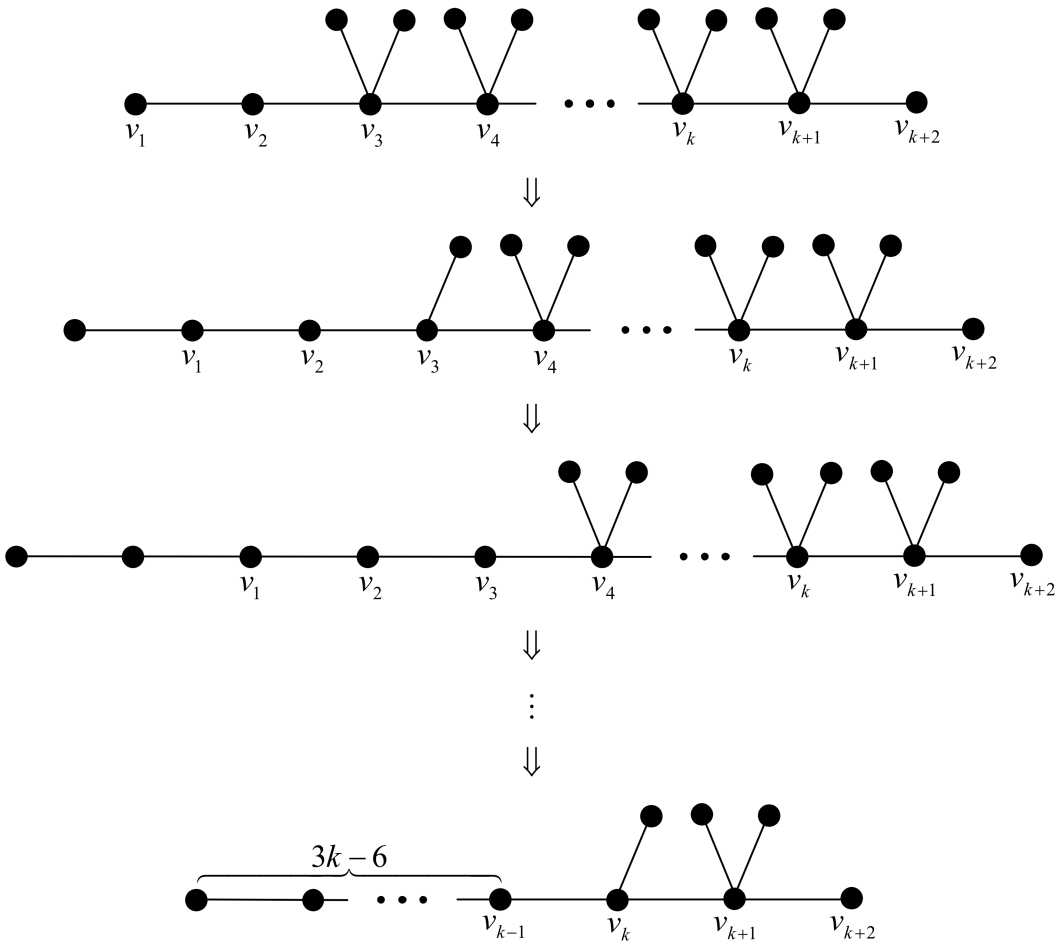

Fig 4. A series of chemical trees of order $3k$ with Wiener polarity indices $9k-15, 9k-18, \ldots, 3k$, respectively.

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For Case 2, since the order is $3k + 1$, adding one more pendent vertex to x is enough for us to form chemical trees of order $3k + 1$ with desired Wiener polarity indices. While in Case 3, note that the order is $3k + 2$, we need to attach a pendent vertex to x and a pendent vertex to y to obtain our desired chemical trees.

Case 2. $n = 3k + 1$, where $k \geq 3$.

In this case, as previous arguments, starting from the chemical trees of order $3k$ with Wiener polarity indices

$$3k-1, 3k, \ldots, 9k-16, 9k-15,$$

after adding one more pendent vertex to x, from Lemma 3, such operation increases the Wiener polarity index by 3, so we would get a series of chemical trees of order $n = 3k + 1$ with Wiener polarity indices

$$3k+2, 3k+3, \ldots, 9k-13, 9k-12,$$

or equivalently,

$$n+1, n+2, \ldots, 3n-16, 3n-15.$$

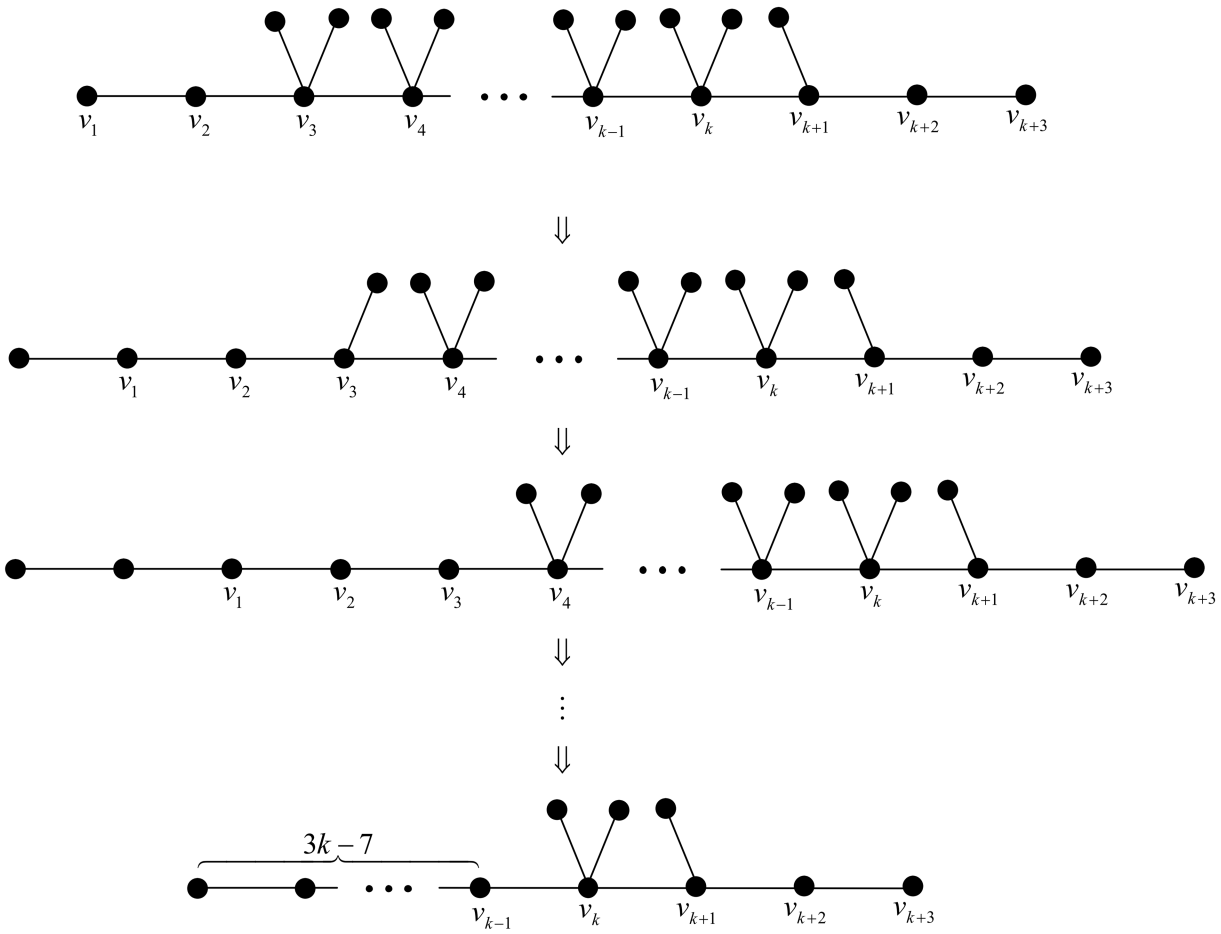

Fig 5. A series of chemical trees of order $3k$ with Wiener polarity indices $9k-16$, $9k-19$,. . .,$3k+2$, respectively.

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Until now, all the chemical trees with desired Wiener polarity indices are constructed, except when $t = n(= 3k + 1)$. Aimed to this remaining case, we review the chemical tree of order $3k$ constructed in Case 1 with Wiener polarity index $3k$ (i.e., the last chemical tree in Fig 4), obviously it consists of a vertex of degree 2 with pendent neighbor, say u. By Lemma 3, attaching a pendent vertex to u would increase its Wiener polarity index by 1, i.e., we may construct a chemical tree of order $n = 3k + 1$ with Wiener polarity index $n = 3k + 1$.

Case 3. $n = 3k + 2$, where $k \geq 3$.

Similar to Case 2, we also start from the chemical trees of order $3k$ with Wiener polarity indices

$$3k-1, 3k, \ldots, 9k-16, 9k-15.$$

But this time, we need add two more vertices. After attaching a pendent vertex to x and a pendent vertex to y, and using Lemma 3 twice, this operation increase the Wiener polarity index by 6, which implies that it results in a series of chemical trees of order $n = 3k + 2$ with Wiener polarity indices

$$3k+5, 3k+6, \ldots, 9k-10, 9k-9,$$

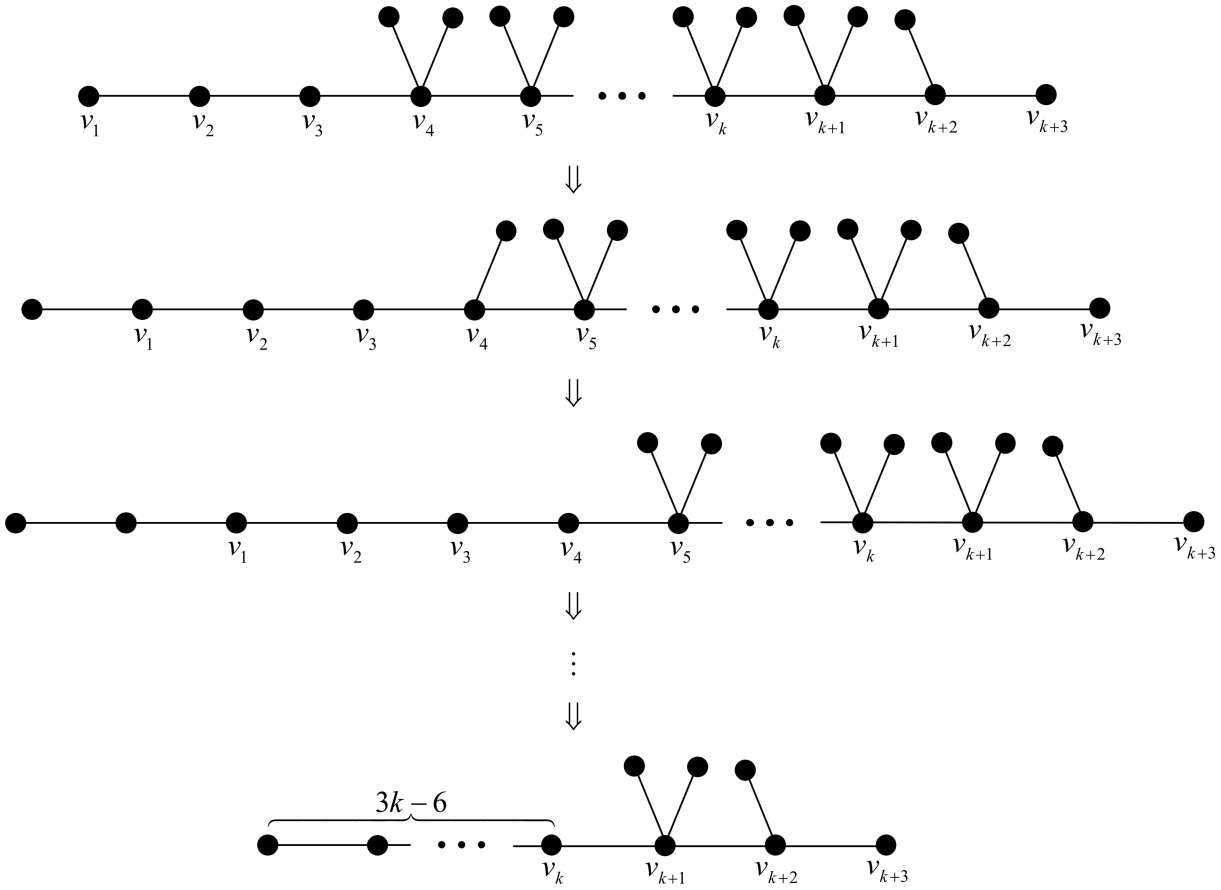

Fig 6. A series of chemical trees of order $3k$ with Wiener polarity indices $9k-17, 9k-20, \ldots, 3k+1$, respectively.

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or equivalently,

$$n+3, n+4, \ldots, 3n-16, 3n-15.$$

For the remaining cases $t = n(= 3k+2)$, $n+1(= 3k+3)$ and $n+2(= 3k+4)$, recall that each of the chemical trees of order $3k$ constructed in Case 1 with Wiener polarity indices $3k$, $3k+1$, $3k+2$ (i.e., the last chemical trees in Figs 4, 5 and 6) contains a vertex of degree 2 with pendent neighbor, say z. Here by applying Lemma 3 twice, attaching a path on two vertices to z would increase the Wiener polarity index by 2. Therefore we may construct three chemical trees of order $n = 3k+2$ with Wiener polarity indices $n = 3k+2$, $n+1 = 3k+3$ and $n+2 = 3k+4$, respectively.

The proof is completed.

To illustrate our main result, let us consider an example for $n = 9$.

Example 1. *If* $n = 9$, *then from* Fig 7, *it is clear that for every integer* $n-3 = 6 \leq t \leq 12 = 3n-15$, *there exists a chemical tree* T *of order* 9 *such that* $W_p(T) = t$, *and hence*

$$\{W_p(T) : T \text{ is a chemical tree of order } 9\} = \{6, 7, \ldots, 12\}.$$

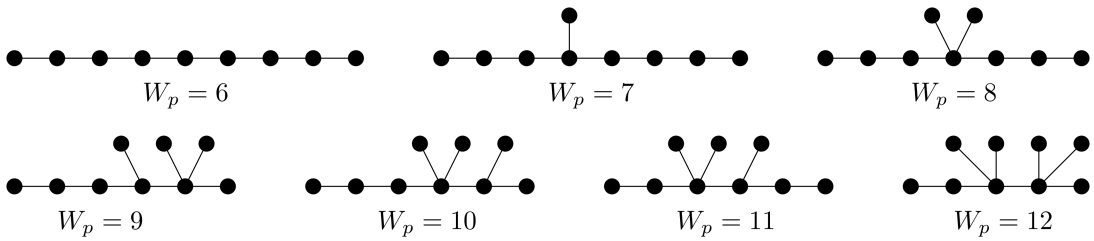

Fig 7. A supporting example for the main result (Theorem 1) when $n = 9$.

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Discussion

In this paper, we prove that the Wiener polarity indices of chemical trees are continuous, that is to say, there is no gap between the minimum value $n - 3$ and the maximum value $3n - 15$ for the Wiener polarity indices of n-vertex chemical trees. As a consequence, we may get a full ordering for the Wiener polarity indices of chemical trees, which extends the ordering about the first three minimum Wiener polarity indices of chemical trees obtained in [21, 22], and the maximum Wiener polarity index of chemical trees obtained in [19, 20].

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Author Contributions

Conceptualization: Zhibin Du, Akbar Ali.

Data curation: Zhibin Du.

Formal analysis: Zhibin Du.

Funding acquisition: Zhibin Du.

Investigation: Zhibin Du, Akbar Ali.

Methodology: Zhibin Du.

Project administration: Zhibin Du.

Resources: Zhibin Du.

Software: Zhibin Du.

Supervision: Akbar Ali.

Validation: Akbar Ali.

Visualization: Akbar Ali.

Writing – original draft: Zhibin Du.

Writing – review & editing: Akbar Ali.

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