MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **55** (2006) 137-158

ISSN 0340 - 6253

Catacondensed Hexagonal Systems with Large Wiener Numbers *

Liqiong Xu [a, b]   Xiaofeng Guo [a †]

[a] Institute of Mathematics, Xiamen University,
Xiamen Fujian 361005, P. R. China

[b] Institute of Mathematics and computer science, Fujian Normal University,
Fuzhou Fujian 350007, P. R. China

(Received December 27, 2004)

Abstract

In this paper, we consider the catacondensed hexagonal systems (simply $CHSs$) with h hexagons and large Wiener numbers. The length transformations and the length transformation diagraphs of the hexagonal chains containing no nonzigzag segment, or containing exactly one nonzigzag segment, or containing exactly two nonzigzag segments, are introduced. In addition, some algorithms for ordering the hexagonal chains by Wiener numbers are established. A similar length transformation digraph and algorithm for ordering the CHSs with only one branch hexagon and with no kink is also given. Based on the length transformation digraphs and the algorithms, the above several classes of CHS_s with h hexagons can be completely ordered for a given h. Furthermore, the catacondensed hexagonal systems with the second up to the thirty-third largest Wiener numbers are determined.

* The project supported by NSFC.
† Corresponding author . *E-mail:* xfguo@xmu.edu.cn

1 Introduction

The Wiener number W is a well-known distance-based topological index introduced originally for molecular graphs of alkanes (Wiener, 1947 [23]). For a cycle-containing graph G, the Wiener number is defined as the sum of distances between all unordered pairs of its vertices (Hosoya, 1971 [21]):

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

where $d(u,v)$ is the number of edges in a shortest path connecting the vertices u and v. The Wiener number has been found to have interesting applications in organic and polymer chemistry, in studies of crystals, and in drug design. A number of publications, reviews and books in the chemical and mathematical literature are devoted to the Wiener number [15, 16, 17, 22]. In particular, the Wiener number was used in the analysis of physico-chemical properties of benzenoid hydrocarbons.

Hexagonal systems are the natural graph representation of benzenoid hydrocarbons. A hexagonal system without internal vertex is called catacondensed hexagonal system, written as CHS for short. Let CHS_h be the set of $CHSs$ with h hexagons. For $G \in CHS_h$, a hexagon s of G is called a kink of G, if s has exactly two consecutive vertices with degree 2 in G, and s is called a branched hexagon if s has no vertex with degree 2. The set of all kinks of G is denoted by $Kink(G)$. A CHS with no branched hexagon is called a hexagonal chain, simply an HC. Let $HC_h \subseteq CHS_h$ denote the set of all the hexagonal chains with h hexagons. The linear chain L_h with h hexagons is the hexagonal chain without kink. The subgraph S of a CHS G is called a segment of G if it is a maximal linear chain in G, including the kinks and/or terminal hexagons at its ends. The number of hexagons in a segment S is called its length and is denoted by $l(S)$. A segment including a terminal hexagon is called a terminal segment.

Consider a nonterminal segment S embeded into $G \in HC_h$ consisting of an ordered sequence of segments, and draw a line through the centers of the hexagons of S (see Fig. 1). If the subgraphs H_1 and H_2 lie on the same side of the line, then S is called a nonzigzag segment. If H_1 and H_2 lie on the different sides of the line, then S is called a zigzag segment. Assume for convenience that zigzag segments also include both terminal segments. The number of hexagons in the subgraphs H_1 and H_2 of G will be denoted by $h_1 = h_1(S)$ and $h_2 = h_2(S)$, respectively. The set of all nonzigzag segments (resp. zigzag

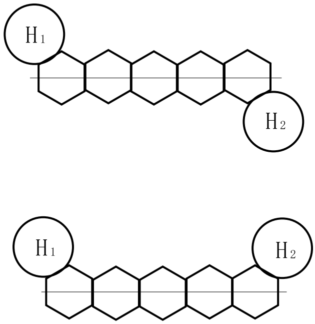

Figure 1: Types of segments.

segments) of a hexagonal chain G is denoted by $\Omega(G)$ (resp. $\bar{\Omega}(G)$).

Let $S_1, S_2, \cdots, S_n$ be the ordered sequence of segments in a hexagonal chain G with h hexagons, and let $l_i = l(S_i), i = 1, 2, \cdots, n$. G can be uniquely determined by a length vector $L(G) = (l_1, l_2, \cdots, \bar{l}_i, \cdots, l_n)$, where the length of any nonzigzag segment S_i is denoted by $\bar{l}_i$. Especially, if $G = L_h$, $L(G) = (h)$. If $L(G) = (l_1, l_2)$, denote G by $L_h(l_1, l_2)$. If $L(G) = (l_1, l_2, \cdots, l_n)$, denote G by $L_h(l_1, l_2, \cdots, l_n)$. If G has exactly one nonzigzag segment, say S_i, we denote G by $L_h(l_1, \cdots, \bar{l}_i, \cdots, l_n)$.

Let $\mathcal{L}_h(l_1, l_2, \cdots, l_n) = \{L_h(l_1, l_2, \cdots, l_n) \mid h = \sum_{i=1}^{n} l_i - n + 1,\ l_i \geq 2,\ 1 \leq n \leq h - 1\}$, and let $\mathcal{L}_h(l_1, l_2, \cdots) = \cup_{n=1}^{h-1} \mathcal{L}_h(l_1, l_2, \cdots, l_n)$. A hexagonal chain with no nonzigzag segment is also called a zigzag hexagonal chain, simply a zigzag HC. Similarly, let $\mathcal{L}_h(l_1, \cdots, \bar{l}_i, \cdots)$ be the set of the hexagonal chains each of which contains exactly one nonzigzag segment and has h hexagons, and $\mathcal{L}_h(l_1, \cdots, \bar{l}_i, \cdots, \bar{l}_j, \cdots)$ the set of the hexagonal chains each of which contains exactly two nonzigzag segments and has h hexagons.

Let $S_h(l_1, l_2, l_3)$ denote a branched CHS consisting of three terminal segments S_1, S_2, S_3 only, where $h = l_1 + l_2 + l_3 - 2$, $l(S_i) = l_i \geq 2$, $i = 1, 2, 3$. By symmetry, without loss of generality, we assume $l_1 \geq l_2 \geq l_3 \geq 2$, and let $\mathcal{S}_h(l_1, l_2, l_3) = \{S_h(l_1, l_2, l_3) \mid h = \sum_{i=1}^{3} l_i - 2,\ l_1 \geq l_2 \geq l_3 \geq 2\}$.

In the theory of the Wiener number, the most basic problems are how to calculate W and to find the correlation between structures and Wiener numbers of graphs. The greatest progress in solving the problems was made for trees and hexagonal systems. The results on the Wiener number of trees and hexagonal systems were summarized in ref

[9, 10, 12] by Dobrynin and Gutman et al. For general hexagonal systems, there is no known recursive method to calculate W of them. However Klavzar and Gutman [11] showed that the complexity of computing the Wiener number of them can be reduced to $O(p)$ and developed a sublinear time algorithm for simple hexagonal systems. For some special classes of hexagonal systems, Dobrynin [8] provided their calculating formulas. Followed from them, the extremal elements of these special classes of hexagonal systems with respect to W were specified in ref [11]. In ref [14], Gutman proved that in CHS_h, L_h have the maximum Wiener number. In ref [5], Dobrynin proved that in CHS_h the serpent S_h have the minimum Wiener numbers, where $S_h \in HC_h$, $L(S_h) = (2, \bar{2}, \bar{2}, 2, \bar{2}, \bar{2}, 2, \cdots, 2)$. In ref [1], Bonchev determined that the CHS_h with the minimum Wiener number which have zigzag segments only is the HC whose segments are of length 2.

A natural generalization of the problem of determining the extremal elements of the $CHSs$ with respect to W is to order $CHSs$ by W. The order of $CHSs$ can uncover the correlation between structures and Wiener numbers of graphs and will be useful in comparing the stability and other properties of molecular graphs. Some results in ordering graphs with respect to some topological indices can be seen in [20, 24, 25]. In the present paper, we introduce the length transformations and the length transformation digraphs of several classes of hexagonal chains, $\mathcal{L}_h(l_1, l_2, \cdots)$, $\mathcal{L}_h(l_1, \cdots, \bar{l}_i, \cdots)$, $\mathcal{L}_h(l_1, \cdots, \bar{l}_i, \cdots, \bar{l}_j, \cdots)$, and $\mathcal{S}_h(l_1, l_2, l_3)$, in which the length transformation digraphs of $\mathcal{L}_h(l_1, l_2, \cdots)$ and $\mathcal{S}_h(l_1, l_2, l_3)$ show partial order relations of the hexagonal chains with respect to their Wiener numbers. In addition, some algorithms for ordering the hexagonal chains by Wiener numbers are established. Based on the length transformation digraphs and the algorithms, the above several classes of CHS_s with h hexagons can be completely ordered for a given h. Furthermore, the catacondensed hexagonal systems with the second up to the thirty-third largest Wiener numbers are determined.

2 Some related results

To obtain our main results we need the following lemmas.

Lemma 1. [8] Let G be an arbitrary element of HC_h with $L(G) = (l_1, l_2, \cdots, l_n)$. Then $W(G) = W(L_h) - 16 \sum_{S \in \Omega(G)} h_1 h_2 - 4(h^2 + n - 1 - \sum_{i=1}^{n} l_i^2)$, where the first summation goes over all nonzigzag segments of G.

Let $r \in Kink(G)$, the subgraph of G induced by all the hexagons of G other than r has two connected components, say G_1 and G_2, the numbers of hexagons of G_1 and G_2 are denoted by $h_3 = h(G_1)$ and $h_4 = h(G_2)$, respectively. The following lemma is a variant of Dobrynin's results.

Lemma 2. [4] Let $G \in HC_h$. Then

$W(G) = W(L_h) - 8(\sum_{r\in Kink(G)} h_3h_4 + \sum_{S\in\Omega(G)} h_1h_2 - \sum_{S\in\bar{\Omega}(G)} h_1h_2)$.

Lemma 3. [4] $W(S_h(l_1, l_2, l_3)) = W(L_h) - 8(4(l_1 - 1)(l_2 - 1)(l_3 - 1) + (l_1 - 1)(l_2 - 1) + (l_1 - 1)(l_3 - 1) + (l_2 - 1)(l_3 - 1))$.

Let G_1, G_1', G_2, G_2' be the $CHSs$ in Fig. 2. We say that G_1' (resp. G_2') is obtained from G_1 (resp. G_2) by the first kink transformation (resp. the second kink transformation). Let $l_1 = l(S_1)$, $l_2 = l(S_2)$, A and B stand for arbitrary fragments, in particular, they may be absent. A and B contains h_A and h_B hexagons, respectively [7].

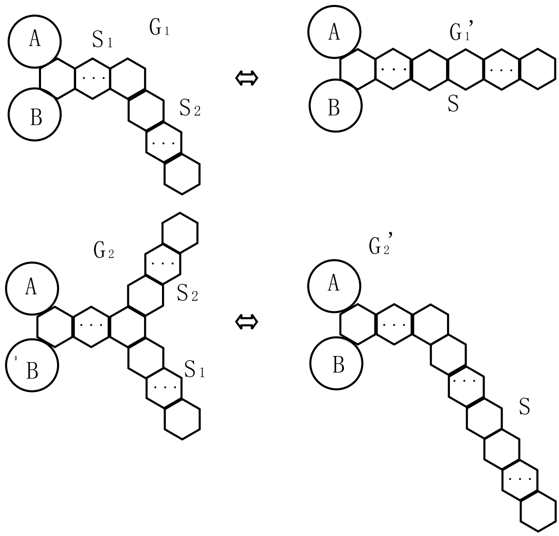

Figure 2: kink transformations of hexagonal systems.

Lemma 4. [7] Let G_1' (resp. G_2') be the CHS obtained from a CHS G_1 (resp. G_2) by the first kink transformation (resp. the second kink transformation). Then

$W(G_1') - W(G_1) = 16(l_2 - 1)h_B + 8(l_1 - 1)(l_2 - 1)$,

$W(G_2') - W(G_2) = 16(l_2-1)[2(l_1-1)(h_G-l_1)+h_A-h_B] + 8(l_1-1)(l_2-1).$

Following from Lemma 1, Lemma 2, we have

Corollary 5. $W(L_h(l_1,l_2)) = W(L_h) - 4(h^2+1) + 4(l_1^2+l_2^2) = W(L_h) - 8(l_1-1)(l_2-1),$

$W(L_h(l_1,l_2,l_3)) = W(L_h) - 4(h^2+2) + 4(l_1^2+l_2^2+l_3^2) = W(L_h) - 8((l_1-1)(l_3-1) + (l_1-1)(l_2-1) + (l_2-1)(l_3-1)),$

$W(L_h(l_1,\bar{l_2},l_3)) = W(L_h) - 8(3(l_1-1)(l_3-1) + (l_1-1)(l_2-1) + (l_2-1)(l_3-1)),$

$W(L_h(l_1,l_2,l_3,l_4)) = W(L_h) - 4(h^2+3) + 4(l_1^2+l_2^2+l_3^2+l_4^2) = W(L_h) - 8((l_1-1)(l_2-1) + (l_1-1)(l_3-1) + (l_1-1)(l_4-1) + (l_2-1)(l_3-1) + (l_2-1)(l_4-1) + (l_3-1)(l_4-1)),$

$W(L_h(l_1,l_2,\cdots,\bar{l_i},\cdots,l_n)) = W(L_h) - 4(h^2+n-1) + 4(l_1^2+l_2^2+\cdots+l_n^2) - 16(l_1 + l_2 + \cdots + l_{i-1} - i + 1)(l_{i+1} + \cdots + l_n - n + i),$

$W(L_h(l_1,\bar{l_2},\bar{l_3},l_4)) = W(L_h) - 8((l_1-1)(l_2-1) + 3(l_1-1)(l_3-1) + 5(l_1-1)(l_4-1) + (l_2-1)(l_3-1) + 3(l_2-1)(l_4-1) + (l_3-1)(l_4-1)).$

3 Some order relations in $\mathcal{L}_h(l_1,l_2,\cdots)$, $\mathcal{L}_h(l_1,\cdots,\bar{l_i},\cdots)$, $\mathcal{L}_h(l_1,\cdots,\bar{l_i},\cdots,\bar{l_j},\cdots)$, and $\mathcal{S}_h(l_1,l_2,l_3)$ on Wiener numbers

By Lemma 1, l_1, l_2, $\cdots$, l_n are symmetric in the formula $W(L_h(l_1,l_2,\cdots,l_n))$. In other words, let $(l_1',l_2',\cdots,l_n')$ be a permutation of $(l_1,l_2,\cdots,l_n)$, then $W(L_h(l_1',l_2',\cdots,l_n')) = W(L_h(l_1,l_2,\cdots,l_n))$. In this sense, we may assume without generality $l_1 \geq l_2 \geq \cdots \geq l_n \geq 2$, and let $L_h(l_1,l_2,\cdots,l_n)$ be the representative of the set of all the HCs consisting of any ordered sequences of n zigzag segments S_1, S_2, $\cdots$, S_n, where $l_i = l_i(S_i)$, $i = 1, 2, \cdots, n$. Let $\mathcal{L}_h^*(l_1,l_2,\cdots,l_n) = \{L_h(l_1,l_2,\cdots,l_n) \mid l_1 \geq l_2 \geq \cdots \geq l_n \geq 2,\ h = \sum_{i=1}^n l_i - n + 1\} \subset \mathcal{L}_h(l_1,l_2,\cdots,l_n)$. Let $\mathcal{L}_h^*(l_1,l_2,\cdots) = \cup_{n=1}^{h-1}\mathcal{L}_h^*(l_1,l_2,\cdots,l_n) = \{L_h(l_1,\cdots,l_{h-1}) \mid l_1 \geq l_2 \geq \cdots \geq l_{h-1} \geq 0,\ l_i \neq 1, i = 1,2,\cdots,h-1\}$.

It is clear that, for ordering the HCs in $\mathcal{L}_h(l_1,l_2,\cdots)$, we need only to order the HCs in $\mathcal{L}_h^*(l_1,l_2,\cdots)$. Now we will establish an algorithm for ordering the HCs in $\mathcal{L}_h^*(l_1,l_2,\cdots)$. To do this, we first introduce some operations called length transformations.

Definition 6. Let $G = L_h(x_1,x_2,\cdots,x_{h-1}) \in \mathcal{L}_h^*(l_1,l_2,\cdots)$. Let G' be obtained from G by one of the following three operations: (1) if there exists some $i < h-1$

such that $x_i - 2 \geq x_{i+1} \geq 2$, then $G' = L_h(x_1, \cdots, x_i - 1, x_{i+1} + 1, \cdots, x_{h-1})$; (2) if there exists some $i < h - 1$ such that $x_i \geq 3$, $x_{i+1} < 3$, $x_j = 0$, $x_{j-1} > 0$, then $G' = L_h(x_1, \cdots, x_i - 1, 2, \cdots, 2, x_{j+1}, \cdots)$; (3) if there exists $i + 1 < j < h$ such that $x_i - 1 = x_{i+1} = \cdots = x_{j-1} = x_j + 1$, then $G' = L_h(x_1, \cdots, x_i - 1, \cdots, x_j + 1, \cdots, x_{h-1})$. Then G' is said to be obtained from G by an kth length transformation (or a LT_k-transformation), denoted by $G' = LT_k(G)$, where $k = 1, 2, 3$.

By Lemma 1, we have the following lemma.

Lemma 7. Let $G = L_h(x_1, x_2, \cdots, x_n) \in \mathcal{L}_h^*(l_1, l_2, \cdots)$, and let G' be obtained from G by a length transformation. Then (1) if $G' = LT_1(G)$, $W(G) - W(G') = 8(x_i - x_{i+1} - 1)$; (2) if $G' = LT_2(G)$, $W(G) - W(G') = 8(x_i - 2)$; (3) if $G' = LT_3(G)$, $W(G) - W(G') = 8(x_i - x_j - 1) = 8$.

For any $G = L_h(l_1, l_2, \cdots, l_n) \in \mathcal{L}_h^*(l_1, l_2, \cdots)$, where $l_n \geq 2$, G can be uniquely determined by the $(h-1)$-dimension vector $L(G) = (l_1, l_2, \cdots, l_n, 0, \cdots)$, or simply by the n-dimension vector $L(G) = (l_1, l_2, \cdots, l_n)$. The length transformations between two zigzag hexagonal chains $G' = LT_k(G)$ may be expressed as the transformations between the corresponding $(h-1)$-dimension vectors $L(G') = LT_k(L(G))$, where $k = 1$, 2, 3.

We define an order relation of $(h-1)$-dimension vectors $(x_1, x_2, \cdots, x_{h-1})$ as follows: $(x_1, x_2, \cdots, x_{h-1}) \succ (x'_1, x'_2, \cdots, x'_{h-1}) \Leftrightarrow \exists\, j \leq h - 1$ such that $x_j > x'_j$ and $x_i = x'_i$ for $i = 1, 2, \cdots, j - 1$.

Lemma 8. Let $G = L_h(x_1, x_2, \cdots, x_n) \in \mathcal{L}_h^*(l_1, l_2, \cdots)$ be any zigzag HC with h hexagons and $n \geq 2$. Then G can be obtained from L_h by a sequence of length transformations, and also from $L_h(h-1, 2)$ by a sequence of length transformations in which all the second length transformations are taken only for $x_i = 3$.

Proof. $L_h(h-1, 2)$ can be obtained from L_h by the second length transformation. So, if $G \neq L_h(h-1, 2)$, we need only to prove that G can be obtained from $L_h(h-1, 2)$ by a sequence of length transformations in which all the second length transformations are taken only for $x_i = 3$.

If there is some $i < n$ such that $x_i = x_{i+1} > 2$, we may assume that i is minimal and j is maximal such that $x_i = x_{i+1} = \cdots = x_j$, $x_{i-1} > x_i$ if $i > 1$, and $x_j > x_{j+1}$ if $j < n$. Then G can be obtained from $L_h(x_1, \cdots, x_i + 1, \cdots, x_j - 1, \cdots, x_n)$ by either the first length transformation if $j = i + 1$, or the third length transformation if $j > i + 1$.

If there is some $i < n$ such that $x_i = x_{i+1} = 2$, we may assume that i is minimal such that $x_i = x_{i+1} = \cdots = x_n = 2$, $x_{i-1} > x_i$ if $i > 1$. Then G can be obtained from $L_h(x_1, \cdots, x_{i-1}, 3, 2, \cdots, 2, 0)$ by the second length transformation.

Otherwise, $x_1 > x_2 > \cdots > x_n$. If $n \geq 3$, then G can be obtained from $L_h(x_1+1, x_2-1, \cdots, x_n)$ by the first length transformation. If $n = 2$, since $G \neq L_h(h-1, 2)$, then $x_2 > 2$ and G can be obtained from $L_h(x_1+1, x_2-1)$ by the first length transformation.

Now we can assume $G = LT_k(G_1)$, $k = 1, 2, 3$. Clearly, $L(G_1) \succ L(G)$.

Repeating the above reasoning, we can obtain a series of graphs $G_1, G_2, \cdots, G_t$ such that $G_i = LT_k(G_{i+1})$ for $i = 1, 2, \cdots, t-1$, $L(G_{i+1}) \succ L(G_i)$, and $G_t = L_h(h-1, 2)$.

The proof is thus completed. $\square$

By Lemma 7, if $G = L_h(x_1, x_2, \cdots, x_n) \in \mathcal{L}_h^*(l_1, l_2, \cdots)$ and $G' = LT_k(G)$, then $\frac{1}{8}(W(G) - W(G'))$ is equal to either $(x_i - x_{i+1} - 1) > 0$ for $k = 1$, or $x_i - 2 > 0$ for $k = 2$, or $1 > 0$ for $k = 3$. Based on Lemmas 7,8, we can define the length transformation digraph of all the zigzag hexagonal chains in $\mathcal{L}_h^*(l_1, l_2, \cdots)$ as follows.

Definition 9. Let $D_h^{(0)} = (V(D_h^{(0)}), A(D_h^{(0)}))$ be the digraph, called the length transformation digraph (simply LT-digraph) of all the zigzag hexagonal chains with h hexagons, where $V(D_h^{(0)}) = \mathcal{L}_h^*(l_1, l_2, \cdots)$, and between two vertices $G_i = L_h(x_1, x_2, \cdots)$ and $G_j = L_h(y_1, y_2, \cdots)$ there is an arc $(G_i, G_j) \in A(D_h^{(0)})$ if and only if $LT_k(G_i) = G_j$ for some $k \in \{1, 2, 3\}$ where if $G_i \neq L_h$ the second length transformation is taken only for $x_i = 3$.

By Lemmas 7,8, we have the following.

Theorem 10. Let $D_h^{(0)}$ be the length transformation digraph of the zigzag hexagonal chains with h hexagons. Then, for any vertex $G^* = L_h(x_1, x_2, \cdots)$ in $D_h^{(0)}$ different from L_h and $L_h(h-1, 2)$, there is a directed path $G_0G_1G_2\cdots G_t$ such that $G_0 = L_h$, $G_1 = L_h(h-1, 2)$, $G_t = G^*$, and $W(G_0) > W(G_1) > W(G_2) > \cdots > W(G_t)$ (that is, a complete order of $G_0, G_1, G_2, \cdots, G_t$ with respect to Wiener numbers).

In the LT-digraph $D_h^{(0)}$ of zigzag hexagonal chains with h hexagons, there are some vertices G_i and G_j which are not connected by a directed path, and so $W(G_i)$ and $W(G_j)$ are not comparable by the LT-digraph $D_h^{(0)}$. Hence the LT-digraph $D_h^{(0)}$ gives a partial order relation of zigzag hexagonal chains with h hexagons with respect to Wiener numbers.

For ordering all zigzag hexagonal chains by Wiener numbers, we need to introduce a number for any zigzag hexagonal chain G^* with h hexagons. By Theorem 10, there are a series of graphs $G_0 = L_h,\ G_1 = L_h(h-1, 2),\ G_2, \cdots,\ G_t = G^*$ such that $G_i = LT_k(G_{i-1})$ for $i = 1, 2, \cdots, t$. Let $\Delta_i = \frac{1}{8}(W(G_{i-1}) - W(G_i))$. For every G_i, we assign a number $n(G_i)$ so that $n(G_1) = 0,\ n(G_2) = -\Delta_2,\ n(G_3) = n(G_2) - \Delta_3 = -\Delta_2 - \Delta_3, \cdots,\ n(G) = n(G_{t-1}) - \Delta_t$. Particularly let $n(L_h) = h - 2$ because $\Delta_1 = \frac{1}{8}(W(L_h) - W(G_0)) = h - 2$. Obviously, $W(G_i) \geq W(G_j)$ if and only if $n(G_i) \geq n(G_j)$. If we can establish an algorithm for generating the LT-digraph $D_h^{(0)}$ of zigzag hexagonal chains with h hexagons and assigning the number $n(G_i)$ to any graph G_i in $\mathcal{L}_h^*(l_1, l_2, \cdots)$ by the above method, the zigzag hexagonal chains in $\mathcal{L}_h^*(l_1, l_2, \cdots)$ will can be ordered by the numbers $n(G_i)$. For convenience, we denote a graph $G = L_h(x_1, x_2, \cdots, x_n)$ in $\mathcal{L}_h^*(l_1, l_2, \cdots)$ by the vector $X = (x_1, x_2, \cdots, x_n)$, $n(G)$ by $n(X)$, and $LT_k(G)$ by $LT_k(X)$. In particular, the linear chain L_h is denoted by the vector (h). If $X \neq (h)$, the second length transformation $LT_2(X)$ is taken only for $x_i = 3$.

Algorithm 11. Let $X_0 = (h)$ and $X_1 = (h-1, 2)$, $n(X_0) = h - 2$, $n(X_1) = 0$, $V_0 = \{X_0\}$, $V_1 = \{X_1\}$, $A_1 = \{(X_0, X_1)\}$, and $i = 1$.

1. For every vector X_j in V_i, find the set $N(X_j) = \{X_r \mid X_r = LT_k(X_j),\ X_r \notin V_i\}$, and let $n(X_r) = n(X_j) - \Delta(X_r)$ for every X_r. Set $V_{i+1} = \cup_{X_j \in V_i} N(X_j)$. Set $A_{i+1} = \{(X_j, X_r) \mid X_r = LT_k(X_j),\ X_j \in V_i \cup V_{i+1},\ X_r \in V_{i+1}\}$.

2. If V_{i+1} has only the vector $(2, 2, \cdots, 2)$, go to step 3. Otherwise, set $i + 1 \to i$, go to step 1.

3. Let $i + 1 = t$, $V(D_h^{(0)}) = \cup_{i=0}^t V_i$, $A(D_h^{(0)}) = \cup_{i=1}^t A_i$. If h is a given constant, order elements in $V(D_h^{(0)}) = \cup_{i=0}^t V_i$ by $n(X_i)$.

By Lemma 8, it is not difficult to see that Algorithm 11 can generate all vectors corresponding to all graphs in $\mathcal{L}_h^*(l_1, l_2, \cdots)$, and the LT-digraph $D_h^{(0)}$ can be determined by $V(D_h^{(0)})$ and $A(D_h^{(0)})$. In addition, for a given value of h, the graphs in $\mathcal{L}_h^*(l_1, l_2, \cdots)$ can be completely ordered by the numbers $n(X_i)$. For example, if $h = 9$, the LT-digraph $D_9^{(0)}$ with the numbers $n(X_i)$ below each vector X_i can be given in Fig. 3.

By the numbers $n(X_i)$, the graphs in $\mathcal{L}_9^*(l_1, l_2, \cdots)$ are completely ordered. Note that the order relation is not a complete order on $\mathcal{L}_9^*(l_1, l_2, \cdots)$, since $n(5, 2, 2, 2, 2) = n(4, 4, 2, 2)$, but $L_9(5, 2, 2, 2, 2) \neq L_9(4, 4, 2, 2)$.

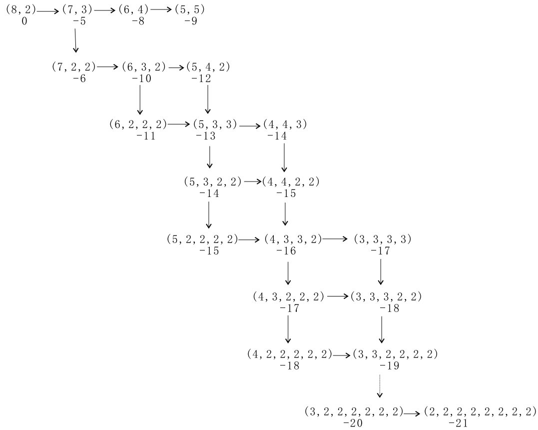

Figure 3: The LT-digraph $D_9^{(0)}$ of $\mathcal{L}_9^*(l_1, l_2, \cdots)$

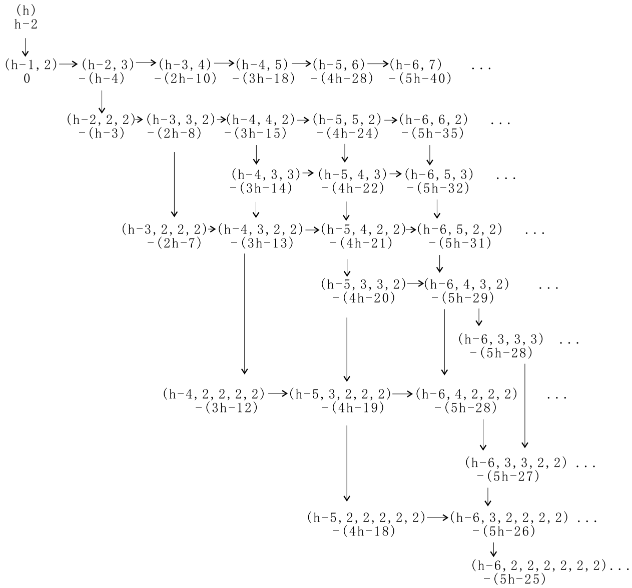

Figure 4: The LT-digraph $D_h^{(0)}$ of $\mathcal{L}_h^*(l_1, l_2, \cdots)$

If h is a unknown number, $n(X_i)$ is a linear function of h and the order relation of some graphs in $\mathcal{L}_h^*(l_1, l_2, \cdots)$ with respect to W should depend on the value of h. The LT-digraph $D_h^{(0)}$ in general cases with the numbers $n(X_i)$ below vectors can be expressed in Fig.4.

Property 12. Let V_i be the subset of $V(D_h^{(0)})$, each vector of which has the first component equal to $h-i$. Then, if $1 \leq i \leq \lfloor \frac{h-1}{2} \rfloor$,
(i) the subgraph of $D_h^{(0)}$ induced by V_i together with a new arc $((h-i, i+1), (h-i, i, 2))$, $D_h^{(0)}[V_i] + ((h-i, i+1), (h-i, i, 2))$, is isomorphic to $D_{i+1}^{(0)}$, and
$LT_k(h-i, x_2, x_3, \cdots) = (h-i, y_2, y_3, \cdots)$ if and only if $LT_k(x_2, x_3, \cdots) = (y_2, y_3, \cdots)$ where $k = 1, 2, 3$;
(ii) the maximum element $max\{V_i\}$ in $D_h^{(0)}[V_i] + ((h-i, i+1), (h-i, i, 2))$ is $(h-i, i+1)$ with $n(h-i, i+1) = -((i-1)h - (i+2)(i-1))$, and the minimum element $min\{V_i\}$ in $D_h^{(0)}[V_i] + ((h-i, i+1), (h-i, i, 2))$ is $(h-i, 2, \cdots, 2)$ with $n(h-i, 2, \cdots, 2)$
$= -((i-1)h - (i+4)(i-1)/2)$;
(iii) $n(h-i+1, 2, \cdots, 2) - n(h-i, i+1) = h - \frac{i(i+1)}{2} - 1$;
(iv) if $h \geq \frac{i(i+1)}{2} + 1$, then $n(min\{V_{i-1}\}) \geq n(max\{V_i\})$ and $n(min\{V_{j-1}\}) > n(max\{V_j\})$ for $1 < j < i$.

Property 12 holds immediately by Lemmas 7,8, Definition 9 and Algorithm 11. Let $\mathcal{L}_h^*(h-i, l_2, \cdots)$ be the set of all the zigzag hexagonal chains in $\mathcal{L}_h^*(l_1, l_2, \cdots)$ with $l_1 = h-i$. Since, for a given value of h, say a constant k, graphs in $\mathcal{L}_k^*(l_1, l_2, \cdots)$ can be completely ordered by Algorithm 11, we have the following Corollary by Property 12.

Corollary 13. Let $1 \leq i \leq \lfloor \frac{h-1}{2} \rfloor$. Then
(i) the graphs in $\mathcal{L}_h^*(h-i, l_2, \cdots)$ can be completely ordered by Algorithm 11 and the order relation of graphs in $\mathcal{L}_{i+1}^*(l_1, l_2, \cdots)$;
(ii) if $h \geq \frac{i(i+1)}{2} + 1$, the graphs of $\cup_{j=1}^{i-1} \mathcal{L}_h^*(h-j, l_2, ...) \cup \{L_h(h-i, i+1)\}$ can be completely ordered with respect to their Wiener numbers, and any other graph in $\mathcal{L}_h^*(l_1, l_2, \cdots)$ has Wiener number smaller than $L_h(h-i, i+1)$.

Note that if $\frac{k(k+1)}{2} + 1 \leq h < \frac{i(i+1)}{2} + 1$, the order of $\cup_{j=k}^{i-1} \mathcal{L}_h^*(h-j, l_2, ...) \cup \{L_h(h-i, i+1)\}$ will have some change dependent on values of h.

By Theorem 10, Corollary 13, Property 12 and Fig. 4, we also have the following.

Corollary 14. The elements of $\mathcal{L}_h^*(l_1, l_2)$, can be ordered by their Wiener numbers as follows: $W(L_h(h-1, 2)) > W(L_h(h-2, 3)) > \cdots > W(L_h(\lfloor h/2 \rfloor + 1, \lceil h/2 \rceil))$.

Corollary 15. For $h \geq 22$, the hexagonal chains in $\mathcal{L}_h^*(l_1, l_2, \cdots)$ can be ordered by their Wiener numbers as follows:
$W(L_h(h-1,2)) > W(L_h(h-2,3)) > W(L_h(h-2,2,2)) > W(L_h(h-3,4)) >$
$W(L_h(h-3,3,2)) > W(L_h(h-3,2,2,2)) > W(L_h(h-4,5)) > W(L_h(h-4,4,2)) >$
$W(L_h(h-4,3,3)) > W(L_h(h-4,3,2,2)) > W(L_h(h-4,2,2,2,2)) > W(L_h(h-5,6)) >$
$W(L_h(h-5,5,2)) > W(L_h(h-5,4,3)) > W(L_h(h-5,4,2,2)) > W(L_h(h-5,3,3,2)) >$
$W(L_h(h-5,3,2,2,2)) > W(L_h(h-5,2,2,2,2,2)) \geq W(L_h(h-6,7)) > \cdots$.

We now consider to order the HCs in $\mathcal{L}_h(l_1, \cdots, \bar{l_i}, \cdots)$.

Let $\mathcal{L}_h^*(l_1, \cdots, \bar{l_i}, \cdots) = \{L_h(l_1, \cdots, \bar{l_i}, \cdots) \mid l_1 \geq l_2 \geq \cdots \geq l_{i-1} \geq 2,\ l_i \geq 2,\ l_{i+1} \geq 2,\ l_{i+1} \geq l_{i+2} \geq \cdots \geq l_{h-1} \geq 0,\ \sum_{j=1}^{i-1} l_j - (i-1) = h_1(S_i) \geq h_2(S_i) = h - h_1(S_i) - l_i\} \subset \mathcal{L}_h(l_1, \cdots, \bar{l_i}, \cdots)$. Let $\mathcal{L}_h^*(l_1, \cdots, \bar{l_i}, \cdots, l_n) = \{L_h(l_1, \cdots, \bar{l_i}, \cdots, l_n) \mid l_1 \geq l_2 \geq \cdots \geq l_{i-1} \geq 2,\ l_i \geq 2,\ l_{i+1} \geq l_{i+2} \geq \cdots \geq l_n \geq 2,\ \sum_{j=1}^{i-1} l_j - (i-1) \geq \sum_{j=i+1}^{n} l_j - (n-i)\}$. By Lemma 1, if $(l'_1, l'_2, \cdots, l'_{i-1})$ and $(l'_{i+1}, l'_{i+2}, \cdots, l'_{h-1})$ are permutations of $(l_1, l_2, \cdots, l_{i-1})$ and $(l_{i+1}, l_{i+2}, \cdots, l_{h-1})$, respectively, then $W(L_h(l_1, \cdots, \bar{l_i}, \cdots)) = W((l'_1, \cdots, \bar{l_i}, l'_{i+1}, \cdots))$. So we need only to order HCs in $\mathcal{L}_h^*(l_1, \cdots, \bar{l_i}, \cdots)$.

Definition 16. Let $G = L_h(l_1, \bar{l_2}, l_3) \in \mathcal{L}_h^*(l_1, \bar{l_2}, l_3)$. If $l_2 \geq 3$, let $G' = L_h(l_1 + 1, \overline{l_2 - 1}, l_3)$, if $l_2 \geq 3$ and $l_1 > l_3$, let $G'' = L_h(l_1, \overline{l_2 - 1}, l_3 + 1)$. Then G' (resp. G'') is said to be obtained from G by the first length transformation (resp. the second length transformation), denoted by $G' = \overline{LT}_1(G)$ (resp. $G'' = \overline{LT}_2(G)$).

Lemma 17. Let $G = L_h(l_1, \bar{l_2}, l_3)$, $G' = \overline{LT}_1(G)$, and $G'' = \overline{LT}_2(G)$. Then
$\Delta(G') = \frac{1}{8}(W(G) - W(G')) = (l_2 - l_1 - 1) + 2(l_3 - 1)$,
$\Delta(G'') = \frac{1}{8}(W(G) - W(G'')) = (l_2 - l_3 - 1) + 2(l_1 - 1)$.

It is easy to see that any HC in $\mathcal{L}_h^*(l_1, \bar{l_2}, l_3)$ can be obtained from $L_h(2, \overline{h-2}, 2)$ by a sequence of $\overline{LT}_k$-transformations for $k = 1$ or 2. Specially, we say that $L_h(2, \overline{h-2}, 2)$ can be obtained from $L_h(h-1, 2)$ by a $\overline{LT}$-transformation. Note that, by Lemma 17, if $G' = \overline{LT}_1(G)$ and $G'' = \overline{LT}_2(G)$, $\Delta(G') = \frac{1}{8}(W(G) - W(G')) = (l_2 - l_1 - 1) + 2(l_3 - 1)$ may be less than or equal to zero, and so does $\Delta(G'') = (l_2 - l_3 - 1) + 2(l_1 - 1)$. Thus, the length transformation digraph of HCs in $\mathcal{L}_h^*(l_1, \bar{l_2}, l_3)$ can be defined in the following method different from $D_h^{(0)}$.

Definition 18. Let $D_h^{(1)} = (V(D_h^{(1)}), A(D_h^{(1)}))$ be the digraph, called the length transformation digraph (simply $\overline{LT}$-digraph) of all the hexagonal chains in $\mathcal{L}_h^*(l_1, \bar{l_2}, l_3)$, where $V(D_h^{(1)}) = \mathcal{L}_h^*(l_1, \bar{l_2}, l_3)$, and between two vertices $G_i = L_h(x_1, \bar{x_2}, x_3)$ and $G_j =$

$L_h(y_1, \bar{y_2}, y_3)$ there is an arc $(G_i, G_j) \in A(D_h^{(1)})$ if and only if either $\overline{LT}_k(G_i) = G_j$ for some $k \in \{1,2\}$ and $\Delta(G_j) = \frac{1}{8}(W(G_i) - W(G_j)) \geq 0$, or $\overline{LT}_k(G_j) = G_i$ for some $k \in \{1,2\}$ and $\Delta(G_i) = \frac{1}{8}(W(G_j) - W(G_i)) \leq 0$.

Clearly, if $\overline{LT}_k(G_i) = G_j$ for some $k \in \{1,2\}$ and $\Delta(G_j) = \frac{1}{8}(W(G_i) - W(G_j)) = 0$, then there will be two arcs (G_i, G_j) and (G_j, G_i) in $A(D_h^{(1)})$, called an edge or an arc with two directions, and $W(G_i) = W(G_j)$. Hence $D_h^{(1)}$ does not show a partial relation of HCs in $\mathcal{L}_h^*(l_1, \bar{l_2}, l_3)$. However, for a directed path each arc on which is not an arc with two directions, the vertices on the directed path have a complete order with respect to their Wiener numbers.

Before continuing, we give the following Lemmas.

Lemma 19. Let $V_j = \{L_h(j, \overline{h-2j+2}, j),\ L_h(j+1, \overline{h-2j+1}, j),\ L_h(j+2, \overline{h-2j}, j),\ L_h(j+3, \overline{h-2j-1}, j), \cdots,\ L_h(h-j, \overline{2}, j)\}$, $j = 2, 3, \cdots, \lfloor \frac{h}{2} \rfloor$, and let $y = h-j-1$. Then (i) $\Delta(L_h(j+i, \overline{h-2j+2-i}, j)) = \frac{1}{8}(W(L_h(j+i-1, \overline{h-2j+3-i}, j)) - W(L_h(j+i, \overline{h-2j+2-i}, j))) = y - 2(i-1)$ for $i = 1, 2, \cdots, h-2j$; (ii) if $\lfloor \frac{y}{2} \rfloor - j + 3 > 2$, then $W(L_h(j + \lfloor \frac{y}{2} \rfloor - i, \overline{\lceil \frac{y}{2} \rceil - j + 3 + i}, j)) = W(L_h(j + \lceil \frac{y}{2} \rceil + 1 + i, \overline{\lfloor \frac{y}{2} \rfloor - j + 2 - i}, j))$ for $i = 0, 1, \cdots, \lfloor \frac{y}{2} \rfloor - j$.

Proof. (i) By Lemma 17, it is easy to verify that $\Delta(L_h(j+1, \overline{h-2j+1}, j))$
$= \frac{1}{8}(W(L_h(j, \overline{h-2j+2}, j)) - W(L_h(j+1, \overline{h-2j+1}, j))) = h-j-1 = y$,
$\Delta(L_h(j+2, \overline{h-2j}, j)) = \frac{1}{8}(W(L_h(j+1, \overline{h-2j+1}, j)) - W(L_h(j+2, \overline{h-2j}, j)))$
$= y-2$, $\cdots$, $\Delta(L_h(j+i, \overline{h-2j+2-i}, j)) = \frac{1}{8}(W(L_h(j+i-1, \overline{h-2j+3-i}, j))$
$- W(L_h(j+i, \overline{h-2j+2-i}, j))) = y - 2(i-1)$ for $i = 1, 2, \cdots, h-2j$.

(ii) If $\lfloor \frac{y}{2} \rfloor - j + 3 > 2$, then $\Delta(L_h(j + \lceil \frac{y}{2} \rceil, \overline{h - 2j + 2 - \lceil \frac{y}{2} \rceil}, j))$
$= \Delta(L_h(j + \lceil \frac{y}{2} \rceil, \overline{\lfloor \frac{y}{2} \rfloor - j + 3}, j)) = 1$ (if y is odd), or 2 (if y is even), and $\Delta(L_h(j + \lceil \frac{y}{2} \rceil + 1, \overline{\lfloor \frac{y}{2} \rfloor - j + 2}, j)) = -1$ (if y is odd), or 0 (if y is even). Hence we have that $W(L_h(j + \lfloor \frac{y}{2} \rfloor - i, \overline{\lceil \frac{y}{2} \rceil - j + 3 + i}, j)) = W(L_h(j + \lceil \frac{y}{2} \rceil + 1 + i, \overline{\lfloor \frac{y}{2} \rfloor - j + 2 - i}, j))$ for $i = 0, 1, \cdots, \lfloor \frac{y}{2} \rfloor - j$. □

Lemma 20. Let $V^* = \{L_h(l_1, \bar{l_2}, l_3) \mid L_h(l_1, \bar{l_2}, l_3) \subset \mathcal{L}_h^*(l_1, \bar{l_2}, l_3)$, and $l_1 = l_3$ or $l_3 + 1\}$. Then the hexagonal chains in V^* can be ordered by their Wiener numbers as follows: $W(L_h(2, \overline{h-2}, 2)) > W(L_h(3, \overline{h-3}, 2)) > W(L_h(3, \overline{h-4}, 3)) > W(L_h(4, \overline{h-5}, 3)) > W(L_h(4, \overline{h-6}, 4)) > \cdots > W(L_h(\lceil \frac{h}{2} \rceil, \bar{2}, \lfloor \frac{h}{2} \rfloor)$, where $\Delta(W(L_h(3, \overline{h-3}, 2))), \Delta(W(L_h(3, \overline{h-4}, 3))), \Delta(W(L_h(4, \overline{h-5}, 3))), \Delta(W(L_h(4, \overline{h-6}, 4))), \cdots$, are equal to $h-3, h-2, h-4, h-3, h-5, h-4, h-6, \cdots$, respectively.

By Lemma 20, the induced subgraph $D_h^{(1)}[V^*]$ in $D_h^{(1)}$ is a directed path having no arc with two directions, and the number $n(G_i)$ of a vertex G_i on the path can be easily given.

From the proof of Lemma 19, if $\lfloor \frac{y}{2} \rfloor - j + 3 > 2$ where $y = h - j - 1$, $\Delta(L_h(j + \lceil \frac{y}{2} \rceil, \overline{h - 2j + 2 - \lceil \frac{y}{2} \rceil}, j)) = \Delta(L_h(j + \lceil \frac{y}{2} \rceil, \overline{\lfloor \frac{y}{2} \rfloor - j + 3}, j)) = 1$ (if y is odd), or 2 (if y is even). So the induced subgraph $D_h^{(1)}[V_j]$ in $D_h^{(1)}$ consists of either two directed paths $P_j^{(1)}$, $P_j^{(2)}$ with one common terminal vertex $L_h(j + \lceil \frac{y}{2} \rceil, \overline{\lfloor \frac{y}{2} \rfloor - j + 3}, j)$ (if y is odd), or two directed paths $P_j^{(1)}$, $P_j^{(2)}$ together with one arc with two directions connecting $L_h(j + \lceil \frac{y}{2} \rceil, \overline{\lfloor \frac{y}{2} \rfloor - j + 3}, j)$ and $L_h(j + \lceil \frac{y}{2} \rceil + 1, \overline{\lfloor \frac{y}{2} \rfloor - j + 2}, j)$ (if y is even), where $P_j^{(1)}$ contains the vertex $L_h(j, \overline{h - 2j + 2}, j)$. In addition, for any vertex G_i on $P_j^{(2)}$, there is a vertex G_k on $P_j^{(1)}$ such that $n(G_i) = n(G_k)$.

Note that $P_j^{(1)}$, $P_j^{(2)}$ are maximal directed paths in $D_h^{(1)}[V_j]$ containing no arc with two directions, respectively. If $\cup_{j=2}^{\lfloor \frac{h}{2} \rfloor} P_j^{(1)}$ and $D_h^{(1)}[V^*]$ together with the numbers $n(G_i)$ of their vertices are given, we will be able to order all HCs in $\mathcal{L}_h^*(l_1, \bar{l_2}, l_3)$.

For convenience, we denote a graph $G = L_h(x_1, \bar{x_2}, x_3)$ in $\mathcal{L}_h^*(l_1, \bar{l_2}, l_3)$ by the 3-dimension vector $X = (x_1, \bar{x_2}, x_3)$, $n(G)$ by $n(X)$, and $\overline{LT}_k(G)$ by $\overline{LT}_k(X)$. By Lemma 1, we have that $\Delta(L_h(2, \overline{h-2}, 2)) = \frac{1}{8}(W(L_h(h-1, 2)) - W(L_h(2, \overline{h-2}, 2))) = h - 1$. Now we can give the following algorithm.

Algorithm 21. Let $V_j = \{(j, \overline{h - 2j + 2}, j),\ (j+1, \overline{h - 2j + 1}, j),\ (j+2, \overline{h - 2j}, j), (j + 3, \overline{h - 2j - 1}, j), \cdots,\ (h - j, \overline{2}, j)\}$, $j = 2, 3, \cdots, \lfloor \frac{h}{2} \rfloor$, and let $y = h - j - 1$. Let $X_0 = (h - 1, 2)$, $X_1 = (2, \overline{h-2}, 2)$, $n(X_0) = 0$, $n(X_1) = -(h - 1)$.

1. By Lemma 20, let $X_2 = (3, \overline{h-3}, 2)$, $X_3 = (3, \overline{h-4}, 3)$, $X_4 = (4, \overline{h-5}, 3)$, $X_5 = (4, \overline{h-6}, 4), \cdots$, $X_{h-3} = (\lceil \frac{h}{2} \rceil, \overline{2}, \lfloor \frac{h}{2} \rfloor)$, and let $n(X_2) = n(X_1) - \Delta(X_2) = -(h-1) - (h - 3) = -(2h - 4)$, $n(X_3) = n(X_2) - \Delta(X_3) = -(2h - 4) - (h - 2) = -(3h - 6)$, $n(X_4) = n(X_3) - \Delta(X_4) = -(3h - 6) - (h - 4) = -(4h - 10), \cdots$.

2. By Lemma 19, for $\forall j \in \{2, 3, \cdots, \lfloor \frac{h}{2} \rfloor\}$, let $\Delta((j + i, \overline{h - 2j + 2 - i}, j)) = y - 2(i - 1) = h - j - 1 - 2(i - 1)$ and $n((j+i, \overline{h - 2j + 2 - i}, j)) = n((j+i-1, \overline{h - 2j + 3 - i}, j)) - (h - j - 1 - 2(i - 1))$ for $i = 1, 2, \cdots, h - 2j$.

3. If h is a given constant, order elements in $\cup_{j=2}^{\lfloor \frac{h}{2} \rfloor} V_j$ by the numbers $n((j + i, \overline{h - 2j + 2 - i}, j))$ for $i = 1, 2, \cdots, h - 2j$ and $j = 2, 3, \cdots, \lfloor \frac{h}{2} \rfloor$.

The $\overline{LT}$-digraph $D_h^{(1)}$ and $\cup_{j=2}^{\lfloor \frac{h}{2} \rfloor} V_j$ with the numbers $n(X_i)$ below vectors can be expressed in Fig.5.

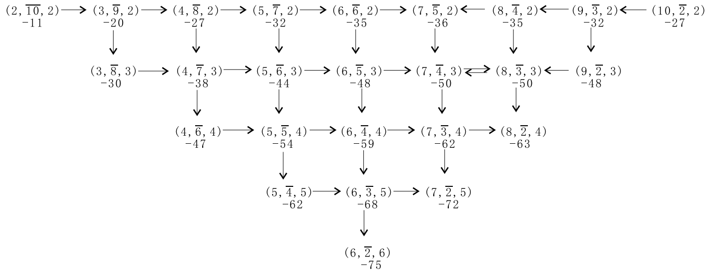

Figure 5: The $\overline{LT}$-digraph $D_{14}^{(1)}$ of $\mathcal{L}_{14}^*(l_1,\bar{l_2},l_3)$

For $G = L_h(l_1,\cdots,\bar{l_i},\cdots,l_n) \in \mathcal{L}_h^*(l_1,\cdots,\bar{l_i},\cdots)$, $n>3$, $h_1 = h_1(S_i)$ and $h_2 = h_2(S_i)$, the $(i-1)$-dimension vector $(l_1,\cdots,l_{i-1})$ and the $(n-i)$-dimension vector $(l_{i+1},\cdots,l_n)$ can be obtained from (h_1+1) and (h_2+1) by a sequence of length transformations respectively. So G can be obtained from $L_h(h_1+1,\bar{l_2},h_2+1)$ by a sequence of length transformations. Let $N_h(h_1,h_2) = \{L_h(l_1,\cdots,\bar{l_i},\cdots,l_n) \mid L_h(l_1,\cdots,\bar{l_i},\cdots,l_n) \in \mathcal{L}_h^*(l_1,\cdots,\bar{l_i},\cdots), h_1(S_i) = h_1,\ h_2(S_i) = h_2,\ l_n \geq 2,\ n = 3,4,5,\cdots\}$. Similarly, we can define the length transformation digraph $D_h^{(1)}$ of all the hexagonal chains in $\mathcal{L}_h^*(l_1,\cdots,\bar{l_i},\cdots)$ by both $\overline{LT}_k$-transformations and LT_k-transformations. By Algorithms 11,21, we can give the following algorithm for ordering the HCs in $\mathcal{L}_h^*(l_1,\cdots,\bar{l_i},\cdots)$.

Algorithm 22. Let $\mathcal{L}_h^*(l_1,\cdots,\bar{l_i},\cdots) = \cup_{L_h(h_1+1,\bar{l_2},h_2+1)\in\mathcal{L}_h^*(l_1,\bar{l_2},l_3)} N_h(h_1,h_2)$.

1. Attach the number $n(X)$ to all X in $\mathcal{L}_h^*(l_1,\bar{l_2},l_3)$ by Algorithm 21.

2. For every $L_h(h_1+1,\bar{l_2},h_2+1)$ in $\mathcal{L}_h^*(l_1,\bar{l_2},l_3)$, by Algorithm 11, generate all the HCs in $N_h(h_1,h_2)$ from $L_h(h_1+1,\bar{l_2},h_2+1)$ and obtain the correspond numbers $n(X)$ to them.

3. If h is a given constant, order the HCs in
$\mathcal{L}_h^*(l_1,\cdots,\bar{l_i},\cdots) = \cup_{L_h(h_1+1,\bar{l_2},h_2+1)\in\mathcal{L}_h^*(l_1,\bar{l_2},l_3)} N_h(h_1,h_2)$ by the numbers $n(X)$.

By lemmas 17,18,19 and algorithms 21,22, we have the following:

Corollary 23. For $h \geq 30$, the hexagonal chains in $\mathcal{L}_h^*(l_1,\cdots,\bar{l_i},\cdots)$ can be ordered by their Wiener numbers as follows (where the number $n(G_i)$ of every hexagonal chain G_i is attached after $W(G_i)$):
$W(L_h(2,\overline{h-2},2))\ \ (-(h-1)) > W(L_h(3,\overline{h-3},2))\ \ (-(2h-4))$
$> W(L_h(2,2,\overline{h-3},2))\ \ (-(2h-3)) > W(L_h(4,\overline{h-4},2))\ \ (-(3h-9)) = W(L_h(h-2,\overline{2},2))$

$> W(L_h(3,2,\overline{h-4},2))\ \ (-(3h-7)) > W(L_h(2,2,2,\overline{h-4},2))\ \ (-(3h-6))$
$= W(L_h(3,\overline{h-4},3)) > W(L_h(2,2,\overline{h-4},3))\ \ (-(3h-5))$
$> W(L_h(2,2,\overline{h-4},2,2))\ \ (-(3h-4)) > W(L_h(5,\overline{h-5},2))\ \ (-(4h-16))$
$= W(L_h(h-3,\bar{3},2)) > W(L_h(4,2,\overline{h-5},2))\ \ (-(4h-13))$
$> W(L_h(3,3,\overline{h-5},2))\ \ (-(4h-12)) > W(L_h(3,2,2,\overline{h-5},2))\ \ (-(4h-11))$
$> W(L_h(2,2,2,2,\overline{h-5},2))\ \ (-(4h-10)) = W(L_h(4,\overline{h-5},3))$
$> W(L_h(4,\overline{h-5},2,2))\ \ (-(4h-9)) > W(L_h(3,2,\overline{h-5},3))\ \ (-(4h-8))$
$> W(L_h(3,2,\overline{h-5},2,2))\ \ (-(4h-7)) = W(L_h(2,2,2,\overline{h-5},3))$
$> W(L_h(2,2,2,\overline{h-5},2,2))\ \ (-(4h-6)) > W(L_h(6,\overline{h-6},2))\ \ (-(5h-25))$
$= W(L_h(h-4,\bar{4},2)) > W(L_h(5,2,\overline{h-6},2))\ \ (-(5h-21))$
$> W(L_h(4,3,\overline{h-6},2))\ \ (-(5h-19)) > W(L_h(4,2,2,\overline{h-6},2))\ \ (-(5h-18))$
$> W(L_h(3,3,2,\overline{h-6},2))\ \ (-(5h-17)) > W(L_h(3,2,2,2,\overline{h-6},2))\ \ (-(5h-16))$
$= W(L_h(5,\overline{h-6},3)) > W(L_h(2,2,2,2,2,\overline{h-6},2))\ \ (-(5h-15)) = W(L_h(5,\overline{h-6},2,2))$
$> W(L_h(4,2,\overline{h-6},3))\ \ (-(5h-13)) = W(L_h(4,\overline{h-6},4))$
$> W(L_h(3,3,\overline{h-6},3))\ \ (-(5h-12)) = W(L_h(4,2,\overline{h-6},2,2))$
$> W(L_h(3,2,2,\overline{h-6},3))\ \ (-(5h-11)) = W(L_h(3,3,\overline{h-6},2,2))$
$= W(L_h(3,2,\overline{h-6},4)) > W(L_h(3,2,2,\overline{h-6},2,2))\ \ (-(5h-10))$
$= W(L_h(2,2,2,2,\overline{h-6},3)) = W(L_h(2,2,2,\overline{h-6},4)) = W(L_h(4,\overline{h-6},2,2,2))$
$> W(L_h(2,2,2,2,\overline{h-6},2,2))\ \ (-(5h-9)) = W(L_h(3,2,\overline{h-6},3,2))$
$> W(L_h(2,2,2,\overline{h-6},3,2))\ \ (-(5h-8)) = W(L_h(3,2,\overline{h-6},2,2,2))$
$> W(L_h(2,2,2,\overline{h-6},2,2,2))\ \ (-(5h-7)) > W(L_h(7,\overline{h-7},2)\ \ (-(6h-36))$
$= W(L_h(h-5,\bar{5},2)) > \cdots.$

Similar to the case of $\mathcal{L}_h^*(l_1,l_2,\cdots,l_n)$, we can also define the length transformations and the length transformation digraph for $\mathcal{S}_h(l_1,l_2,l_3)$, and give an algorithm for ordering $\mathcal{S}_h(l_1,l_2,l_3)$ with respect to Wiener numbers.

Definition 24. Let $G = S_h(x_1,x_2,x_3) \in \mathcal{S}_h(l_1,l_2,l_3)$, let G' be obtained from G by one of the following three operations:
(1) If $x_1 - 2 \geq x_2 \geq 2$, let $G' = S_h(x_1-1,x_2+1,x_3)$; (2) if $x_2 - 2 \geq x_3 \geq 2$, let $G' = S_h(x_1,x_2-1,x_3+1)$; (3) if $x_1 - 1 = x_2 = x_3 + 1$, let $G' = S_h(x_1-1,x_2,x_3+1)$. Then G' is said to be obtained from G by an kth length transformation , denoted by $G' = LT_k(G)$, where $k = 1,2,3$.

Lemma 25. Let $G = S_h(x_1,x_2,x_3) \in \mathcal{S}_h(l_1,l_2,l_3)$, and let G' be obtained from G by a length transformation. Then (1) if $G' = LT_1(G)$, $\Delta(G') = \frac{1}{8}(W(G) - W(G')) =$

$(4x_3-3)(x_1-x_2-1)) > 0$; (2) if $G' = LT_2(G)$, $\Delta(G') = \frac{1}{8}(W(G)-W(G')) = (4x_1-3)(x_2-x_3-1) > 0$; (3) if $G' = LT_3(G)$, $\Delta(G') = \frac{1}{8}(W(G) - W(G')) = (4x_2 - 3)(x_1 - x_3 + 1) = 3(4x_3 + 1) > 0$.

It is easy to see that any CHS in $\mathcal{S}_h(l_1, l_2, l_3)$ can be obtained from $S_h(h-2, 2, 2)$ by a sequence of LT_k-transformations for $k = 1, 2, 3$, and $\frac{1}{8}(W(L_h(h-1, 2) - W(S_h(h-2, 2, 2))) = 5h - 15$. Similarly we can define the length transformation digraph of $\mathcal{S}_h(l_1, l_2, l_3)$. Now we can give the following algorithm.

Algorithm 26. Let $X_0 = (h-2, 2, 2)$, $n(X_0) = -(5h-15)$, $V_0 = \{X_0\}$ and $i = 0$.

1. For every vector X_j in V_i, find the set $N(X_j) = \{X_r \mid X_r = LT_k(X_j),\ X_r \notin V_i\}$, and let $n(X_r) = n(X_j) - \Delta(X_r)$ for every X_r. Set $V_{i+1} = \cup_{X_j \in V_i} N(X_j)$.

2. If V_{i+1} has only the vector (k, k, k) when $h = 3k-2$, $(k+1, k, k)$ when $h = 3k-1$ or $(k+1, k+1, k)$ when $h = 3k$, go to step 3. Otherwise, set $i + 1 \to i$, go to step 1.

3. Let $i + 1 = t$. Order all vectors in $\cup_{i=0}^{t} V_i$ by the numbers $n(X_j)$ for a definite value of h.

By the above algorithm, the length transformation digraph with the numbers $n(X_i)$ below vectors similar to Fig. 3 can be obtained. Thus we have the following:

Corollary 27. For $h \geq 37$, the $CHSs$ in $\mathcal{S}_h(l_1, l_2, l_3)$ can be ordered by their Wiener numbers as follows:
$W(S_h(h-2, 2, 2)) > W(S_h(h-3, 3, 2)) > W(S_h(h-4, 4, 2)) > W(S_h(h-4, 3, 3)) \geq W(S_h(h-5, 5, 2)) > W(S_h(h-6, 6, 2)) > W(S_h(h-5, 4, 3)) \geq W(S_h(h-7, 7, 2)) > W(S_h(h-8, 8, 2)) \geq W(S_h(h-6, 5, 3)) > \cdots$. If $30 \leq h \leq 37$, the only change in the above order is $W(S_h(h-5, 4, 3)) \geq W(S_h(h-7, 7, 2))$. If $26 \leq h \leq 30$, the changes in the above order are $W(S_h(h-5, 4, 3)) \geq W(S_h(h-7, 7, 2))$ and $W(S_h(h-8, 8, 2)) \geq W(S_h(h-6, 5, 3))$. If $h \leq 26$, the changes in the above order are $W(S_h(h-5, 4, 3)) \geq W(S_h(h-7, 7, 2))$, $W(S_h(h-8, 8, 2)) \geq W(S_h(h-6, 5, 3))$ and $W(S_h(h-4, 3, 3)) \geq W(S_h(h-5, 5, 2))$.

From the above, we can see that the orders of $\mathcal{S}_h(l_1, l_2, l_3)$ are much different from $\mathcal{L}_h(l_1, l_2, l_3)$.

Now we consider to order the HCs in $\mathcal{L}_h(l_1, \cdots, \bar{l_i}, \cdots, \bar{l_j}, \cdots)$ by Wiener number.

Let $\mathcal{L}_h^*(l_1, \cdots, \bar{l_i}, \cdots, \bar{l_j}, \cdots) = \{L_h(l_1, \cdots, \bar{l_i}, \cdots, \bar{l_j}, \cdots) \mid l_1 \geq l_2 \geq \cdots \geq l_{i-1} \geq 2,\ l_i, l_j, l_{j+1} \geq 2,\ l_{i+1} \geq l_{i+2} \geq \cdots \geq l_{j-1} \geq 0,\ l_{j+1} \geq l_{j+2} \geq \cdots \geq l_{h-1} \geq 0,\ h_1(S_i) =$

$(\sum_{t=1}^{i-1} l_t) - i + 1 \geq h_2(S_j)\} \subset \mathcal{L}_h(l_1, \cdots, \bar{l_i}, \cdots, \bar{l_j}, \cdots)$. Let $\mathcal{L}_h^*(l_1, \cdots, \bar{l_i}, \cdots, \bar{l_j}, \cdots, l_n) = \{L_h(l_1, \cdots, \bar{l_i}, \cdots, \bar{l_j}, \cdots, l_n) \mid l_1 \geq l_2 \geq \cdots \geq l_{i-1} \geq 2,\ l_i, l_j, l_{j+1} \geq 2,\ l_{i+1} \geq l_{i+2} \geq \cdots \geq l_{j-1} \geq 0,\ l_{j+1} \geq l_{j+2} \geq \cdots \geq l_n \geq 2,\ h_1(S_i) \geq h_2(S_j)\} \subset \mathcal{L}_h^*(l_1, \cdots, \bar{l_i}, \cdots, \bar{l_j}, \cdots)$. By Lemma 1, if $(l'_1, l'_2, \cdots, l'_{i-1})$, $(l'_{i+1}, l'_{i+2}, \cdots, l'_{j-1})$ and $(l'_{j+1}, l'_{j+2}, \cdots, l'_{h-1})$ are permutations of $(l_1, l_2, \cdots, l_{i-1})$, $(l_{i+1}, l_{i+2}, \cdots, l_{j-1})$ and $(l_{j+1}, l_{j+2}, \cdots, l_{h-1})$ respectively, then $W(L_h(l_1, \cdots, \bar{l_i}, l_{i+1}, \cdots, \bar{l_j}, \cdots)) = W(L_h(l'_1, \cdots, \bar{l_i}, l'_{i+1}, \cdots, \bar{l_j}, l'_{j+1}, \cdots))$. So we need only to order HCs in $\mathcal{L}_h^*(l_1, \cdots, \bar{l_i}, \cdots, \bar{l_j}, \cdots)$.

Definition 28. Let $G = L_h(l_1, \bar{l_2}, l_3, \bar{l_4}, l_5) \in \mathcal{L}_h^*(l_1, \bar{l_2}, l_3, \bar{l_4}, l_5)$ where $l_1 \geq l_5$ and if $l_1 = l_5$ we may assume $l_2 \geq l_4$. For $l_3 \neq 0$, if $l_2 \geq 3$, let $G^{(1)} = L_h(l_1 + 1, \overline{l_2 - 1}, l_3, \bar{l_4}, l_5)$, let $G^{(2)} = L_h(l_1, \overline{l_2 - 1}, l_3 + 1, \bar{l_4}, l_5)$ where if $l_1 = l_5$ let $l_2 > l_4$, and let $G^{(3)} = L_h(l_1, \overline{l_2 - 1}, l_3, \overline{l_4 + 1}, l_5)$ where if $l_1 = l_5$ let $l_2 - l_4 \geq 2$; if $l_4 \geq 3$ and $l_1 > l_5$, let $G^{(4)} = L_h(l_1, \bar{l_2}, l_3, \overline{l_4 - 1}, l_5 + 1)$. Then $G^{(k)},\ k = 1, 2, 3, 4$, are said to be obtained from G by a $\overline{\overline{LT}}_k$-transformation, denoted by $G^{(k)} = \overline{\overline{LT}}_k(G)$. For $l_3 = 0$, similarly, if $l_2 \geq 3$, let $G^{(1')} = L_h(l_1 + 1, \overline{l_2 - 1}, \bar{l_4}, l_5)$, let $G^{(2')} = L_h(l_1, \overline{l_2 - 1}, 2, \bar{l_4}, l_5)$ where if $l_1 = l_5$ let $l_2 > l_4$, and let $G^{(3')} = L_h(l_1, \overline{l_2 - 1}, \overline{l_4 + 1}, l_5)$ where if $l_1 = l_5$ let $l_2 - l_4 \geq 2$; if $l_4 \geq 3$ and $l_1 > l_5$, let $G^{(4')} = L_h(l_1, \bar{l_2}, \overline{l_4 - 1}, l_5 + 1)$. Then $G^{(k')},\ k = 1, 2, 3, 4$, are said to be obtained from G by a $\overline{\overline{LT}}_{k'}$-transformation, denoted by $G^{(k')} = \overline{\overline{LT}}_{k'}(G)$.

By Lemma 1, we have the following.

Lemma 29. Let $G = L_h(l_1, \bar{l_2}, l_3, \bar{l_4}, l_5)$. For $l_3 \neq 0$, let $G^{(k)} = \overline{\overline{LT}}_k(G),\ k = 1, 2, 3, 4$. Then

$\Delta(G^{(1)}) = \frac{1}{8}(W(G) - W(G^{(1)})) = l_2 - l_1 + 2l_3 + 2l_4 + 2l_5 - 7$,
$\Delta(G^{(2)}) = \frac{1}{8}(W(G) - W(G^{(2)})) = 2l_1 + l_2 - l_3 - 3$,
$\Delta(G^{(3)}) = \frac{1}{8}(W(G) - W(G^{(3)})) = 2l_1 + l_2 - l_4 - 2l_5 - 1$,
$\Delta(G^{(4)}) = \frac{1}{8}(W(G) - W(G^{(4)})) = 2l_1 + 2l_2 + 2l_3 + l_4 - l_5 - 7$.
For $l_3 = 0$, let $G^{(k')} = \overline{\overline{LT}}_{k'}(G),\ k = 1, 2, 3, 4$. Then
$\Delta(G^{(1')}) = \frac{1}{8}(W(G) - W(G^{(1')})) = l_2 - l_1 + 2l_4 + 2l_5 - 5$,
$\Delta(G^{(2')}) = \frac{1}{8}(W(G) - W(G^{(2')})) = 2l_1 + l_2 - 4$,
$\Delta(G^{(3')}) = \frac{1}{8}(W(G) - W(G^{(3')})) = 2l_1 + l_2 - l_4 - 2l_5 - 1$,
$\Delta(G^{(4')}) = \frac{1}{8}(W(G) - W(G^{(4')})) = 2l_1 + 2l_2 + l_4 - l_5 - 5$.

It is easy to see that any HC_h in $\mathcal{L}_h^*(l_1, \bar{l_2}, l_3, \bar{l_4}, l_5)$ can be obtained from $L_h(2, \overline{h-4}, \bar{2}, 2)$ by a sequence of $\overline{\overline{LT}}_k$-transformations and $\overline{\overline{LT}}_{k'}$-transformations for $k = 1, 2, 3, 4$, and any HC_h in $\mathcal{L}^*{}_h(l_1, \cdots, \bar{l_i}, \cdots, \bar{l_j}, \cdots)$ can be obtained from $L_h(2, \overline{h-4}, \bar{2}, 2)$ by a sequence of

$\overline{\overline{LT}}_k$-transformations and $\overline{\overline{LT}}_{k'}$-transformations for $k = 1, 2, 3, 4$ and LT_k-transformations for $k = 1, 2, 3$.

Similar to the discussion for $\mathcal{L}^*{}_h(l_1, \bar{l_2}, l_3)$ and $\mathcal{L}^*{}_h(l_1, \cdots, \bar{l_j}, \cdots)$, we can define the length transformation digraph and design analogous algorithm to order HCs in $\mathcal{L}^*{}_h(l_1, \bar{l_2}, l_3, \bar{l_4}, l_5)$ and $\mathcal{L}^*{}_h(l_1, \cdots, \bar{l_i}, \cdots, \bar{l_j}, \cdots)$ with respect to their Wiener numbers, and give the following.

Corollary 30. For $h > 19$, the HC_h in $\mathcal{L}^*{}_h(l_1, \cdots, \bar{l_i}, \cdots, \bar{l_j}, \cdots)$ can be ordered by their Wiener numbers as follows (where the number $n(G_i)$ of every hexagonal chain G_i is attached after $W(G_i)$):
$W(L_h(2, \overline{h-3}, \overline{2}, 2))$ $(-(4h-9))$ $> W(L_h(2, \overline{h-4}, \overline{3}, 2))$ $(-(5h-15))$
$> W(L_h(2, \overline{h-4}, 2, \overline{2}, 2))$ $(-(5h-12))$ $> W(L_h(3, \overline{h-4}, \overline{2}, 2))$ $(-(5h-11))$
$> W(L_h(2, \overline{h-5}, \overline{4}, 2))$ $(-(6h-23))$ $> W(L_h(2, \overline{h-5}, 2, \overline{3}, 2))$ $(-(6h-19))$
$> W(L_h(2, \overline{h-5}, 3, \overline{2}, 2))$ $(-(6h-17))$ $> W(L_h(3, \overline{h-5}, \overline{3}, 2))$ $(-(6h-16))$
$> W(L_h(4, \overline{h-5}, \overline{2}, 2))$ $(-(6h-15))$ $> W(L_h(3, \overline{h-5}, 2, \overline{2}, 2))$ $(-(6h-13))$
$> W(L_h(2, \overline{h-6}, \overline{5}, 2))$ $(-(7h-33))$ $> \cdots$. Furthermore, for $h \geq 5$, $W(L_h(2, \overline{h-3}, \overline{2}, 2))$ is the HC in $\mathcal{L}^*_h(l_1, \cdots, \bar{l_i}, \cdots, \bar{l_j}, \cdots)$ with the maximum Wiener number, and
$\Delta(L_h(2, \overline{h-3}, \overline{2}, 2)) = \frac{1}{8}(W(L_h(h-1, 2)) - W(L_h(2, \overline{h-3}, \overline{2}, 2))) = 4h - 9$.

4 The $CHSs$ with the second up to thirty-second larger Wiener number

Lemma 31. The hexagonal chain in HC_h with at least two nonzigzag segments and with the maximum Wiener number is $L_h(2, \overline{h-3}, \overline{2}, 2)$ for $h > 6$.

Proof: Let G be a hexagonal chain in HC_h with at least two nonzigzag segments and with the maximum Wiener number. If G has more than two nonzigzag segments, suppose $G = L_h(l_1, \cdots, \bar{l}_{i_1}, \cdots, \bar{l}_{i_2}, \cdots, \bar{l}_{i_3}, \cdots, \bar{l}_{i_k}, \cdots, l_n)$, let
$G' = L_h(l_1, \cdots, \bar{l}_{i_1}, \cdots, \bar{l}_{i_2}, \cdots, l_{i_3}, \cdots, l_{i_k}, \cdots, l_n)$, by Lemma 1, $W(G) < W(G')$, a contradiction. Hence G has exactly two non-zigzag segments. and so by Corollary 30, $G = L_h(2, \overline{h-3}, \overline{2}, 2)$ for $h > 6$. $\square$

Lemma 32. The branched CHS with the maximum Wiener number is $S_h(h-2, 2, 2)$.

Proof: Let G be a branched CHS with the maximum Wiener number. If $G \notin \mathcal{S}_h(l_1, l_2, l_3)$, then either G contains at least two branched hexagons or G contains exactly one branched hexagon and at least one kink. Then either G has a terminal segment such that an end hexagon r of S is a kink of G, or there are two terminal segments with a common end hexagon r which is a branched hexagon of G. By Lemma 4. there is a branched CHS in $\mathcal{S}_h(l_1, l_2, l_3)$, say G_t, such that G_t is obtained from G by a series of the first or the second kink transformations, and $W(G_t) > W(G)$, a contradiction. Hence $G \in \mathcal{S}_h(l_1, l_2, l_3)$. By Corollary 27, G can only be $S_h(h-2, 2, 2)$. □

Now, from the results in Section 2 and 3, we can obtain the following result:

Theorem 33. Let W_i, $i = 1, 2, \cdots$, be the CHS with the ith largest Wiener number. Then, for $h \geq 31$, $W_1 = L_h$, $W_2 = L_h(h-1, 2)$, $W_3 = L_h(h-2, 3)$, $W_4 = L_h(h-2, 2, 2)$, $W_5 = L_h(2, \overline{h-2}, 2)$, $W_6 = L_h(h-3, 4)$, $W_7 = L_h(h-3, 3, 2)$, $W_8 = L_h(h-3, 2, 2, 2)$, $W_9 = L_h(3, \overline{h-3}, 2)$, $W_{10} = L_h(2, 2, \overline{h-3}, 2)$, $W_{11} = L_h(h-4, 5)$, $W_{12} = L_h(h-4, 4, 2)$, $W_{13} = L_h(h-4, 3, 3)$, $W_{14} = L_h(h-4, 3, 2, 2)$, $W_{15} = L_h(h-4, 2, 2, 2, 2)$, $W_{16} = L_h(h-2, \overline{2}, 2)$ or $L_h(4, \overline{h-4}, 2)$, $W_{17} = L_h(3, 2, \overline{h-4}, 2)$, $W_{18} = L_h(2, 2, 2, \overline{h-4}, 2)$ or $L_h(3, \overline{h-4}, 3)$, $W_{19} = L_h(2, 2, \overline{h-4}, 3)$, $W_{20} = L_h(2, 2, \overline{h-4}, 2, 2)$, $W_{21} = L_h(h-5, 6)$, $W_{22} = L_h(h-5, 5, 2)$, $W_{23} = L_h(h-5, 4, 3)$, $W_{24} = L_h(h-5, 4, 2, 2)$, $W_{25} = L_h(h-5, 3, 3, 2)$, $W_{26} = L_h(h-5, 3, 2, 2, 2)$, $W_{27} = L_h(h-5, 2, 2, 2, 2, 2)$, $W_{28} = L_h(5, \overline{h-5}, 2)$, $W_{29} = L_h(4, 2, \overline{h-5}, 2)$, $W_{30} = L_h(3, 3, \overline{h-5}, 2)$; $W_{31} = L_h(3, 2, 2, \overline{h-5}, 2)$, $W_{32} = L_h(2, 2, 2, 2, \overline{h-5}, 2)$, $W_{33} = L_h(4, \overline{h-5}, 2, 2)$ or $L_h(2, \overline{h-3}, \overline{2}, 2)$.

Proof. By Corollary 30 and Algorithm 26, $n(L_h(2, \overline{h-3}, \overline{2}, 2)) = -(4h-9) > n(S_h(h-2, 2, 2)) = -(5h-15)$ for $h > 6$. Then , by Lemmas 31,32, for any $H \in CHS_h$ with $W(H) > W(L_h(2, \overline{h-3}, \overline{2}, 2))$, H must be a hexagonal chain with at most one nonzigzag segment.

For $h \geq 31$, $n(L_h(2, \overline{h-3}, \overline{2}, 2)) = -(4h-9) \geq n(L_h(h-6, 7)) = -(5h-40) > n(L_h(6, \overline{h-6}, 2)) = -(5h-25)$. Now, by Corollaries 15,23, $W_1, W_2, \cdots, W_{33}$ can be determined as shown in the theorem.

The proof is thus completed. □

Remark. For $h \leq 30$, all the CHSs with Wiener numbers greater than or equal to $W(L_h(2, \overline{h-3}, \overline{2}, 2))$ can also be determined by Corollaries 15,23, the order of which will be different from the order in Theorem 33. For a given $h \leq 30$, the first changed HC in the order in Theorem 33 can be listed as follows:
(i) if $h \in \{28, 29, 30\}$, then $L_h(h-6, 7) = W_{(h+2)}$;
(ii) if $h \in \{25, 26, 27\}$, then $L_h(h-6, 7) = W_{29}$;

(iii) if $h \in \{22, 23, 24\}$, then $L_h(h-5, 6) = W_{(h-4)}$;
(iv) if $h \in \{20, 21\}$, then $L_h(h-5, 6) = W_{17}$;
(v) if $h \in \{17, 18, 19\}$, then $L_h(h-5, 6) = W_{16}$;
(vi) if $h = 16$, then $L_h(h-5, 6) = W_{15}$;
(vii) if $h = 15$, then $L_h(h-4, 5) = W_{10}$;
(viii) if $h \in \{12, 13, 14\}$, then $L_h(h-4, 5) = W_9$.

References

[1] D. Bonchev, O. Mekenyan, N. Trinajstic, Topological characterization of cyclic structures, *Int. J. Quantum Chem.* 17(1980) 845-893.

[2] V. Chepoi, S. Klavzar, Distances in benzenoid systems: further development, *Discr.Math.* 192(1998) 27-39.

[3] J. S. Deogun, Xiaofeng Guo, Wandi Wei, Fuji Zhang, Catacondense hexagonal systems with smaller numbers of Kekule structures, *THEOCHEM J. Mol. Struct.* 639 (2003) 101-108.

[4] A. A. Dobrynin, Formula for calculating the Wiener index of catacondensed benzenoid graphs, *J. Chem. Inf. Comput. Sci.* 38 (1998) 811-814.

[5] A. A. Dobrynin, Graph distance numbers of nonbranched hexagonal systems, *Siberian Adv. Math.* 2 (1992) 121-134.

[6] A. A. Dobrynin, A new formula for the calculation of the Wiener index of hexagonal chains, *MATCH Commun. Math. Comput. Chem.* 35 (1997) 75-90.

[7] A. A. Dobrynin, New congruence relations for the Wiener index of catacondensed benzenoid graphs, *J. Chem. Inf. Comput. Sci.* 38 (1998) 405-409.

[8] A. A. Dobrynin, A simple formula for the calculation of the Wiener index of hexagonal chains, *Comput.Chem.* 23(1) (1999) 43-48.

[9] A. A. Dobrynin, R. C. Entringer, I. Gutman, Wiener index of trees: theory and applications, *Acta Appl. Math.* 66 (2001) 211-249.

[10] A. A. Dobrynin, I. Gutman, The Wiener index for trees and graphs of hexagonal systems, *Diskretn. Anal. Issled. Oper. Ser. 2* 5(2) (1998) 34-60 (in Russian).

[11] A. A. Dobrynin, I. Gutman, S. Klavzar, P. Zigert, Wiener index of Hexagonal Systems, *Acta. Appl. Math.* 72 (2002) 247-294.

[12] R. C. Entringer, Distance in graphs: trees, *J. Combin. Math. Combin. Comput.* 24 (1997) 65-84.

[13] R. C. Entringer, D. E. Jackson, D. A. Snyder, Distance in graphs, *Czechoslovak Math. J.* 26 (1976) 283-296.

[14] I. Gutman, Calculating the Wiener numbers of benzenoid hydrocarbons: two theorems, *Chem. Phys. Lett.* 136 (1987) 134-136.

[15] I. Gutman, O. E. Polansky, *Mathematical Concepts in Organic Chemistry*, Springer-Verlag: Berlin, 1986.

[16] I. Gutman, J. H. Potgieter, Wiener index and intermolecular forces, *J. Serb. Chem. Soc.* 62 (1997) 185-192.

[17] I. Gutman, Y. N. Yeh, S. L. Lee, Y. L. Luo, Some results in the theory of the Wiener number, *Indian J. Chem.* 32A (1993) 651-661.

[18] I. Gutman, O. E. Polansky, Wiener numbers of polyacenes and related benzenoid molecules, *MATCH Commun. Math. Comput. Chem.* 20 (1986) 115-123.

[19] I. Gutman, Y. N. Yeh, S. L. Lee, Y. L. Luo, Some recent results in the theory of the Wiener number, *Indian J. Chem.* 32(A) (1993) 651-661.

[20] I. Gutman, Fuji Zhang, On the ordering of graphs with respect to their matching numbers, *Discr. Appl. Math.* 15 (1986) 25-33.

[21] H. Hosoya, Topological index. A newly proposed quantity characterizing the topological nature of structural isomers of saturated hydrocarbons, *Bull. Chem. Soc. Jpn.* 4 (1971) 2332-2339.

[22] S. Nikolic, N. Trinajstic, Z. Mihalic, The Wiener index:developments and applications, *Croat. Chem. Acta.* 68 (1995) 105-129.

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

[24] Lianzhu Zhang, On the ordering of a class of hexagonal chains with respect to Merrifield-Simmons index systems science and mathematical sciences, *J. Sys. Sci. Math. Sci.* 2 (2000) 219-224.

[25] Lianzhu Zhang, The proof of Gutman's conjectures concerning extremal hexagonal chains, *Adv. Math.* 28 (1999) 465-466.