# Ordering Unbranched Catacondensed Benzenoid Hydrocarbons by the Number of Kekulé Structures* 

Yaqian Tang, Yang Zuo, Zikai Tang, Hanyuan Deng ${ }^{\dagger}$<br>College of Mathematics and Statistics, Hunan Normal University, Changsha, Hunan 410081, P. R. China

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#### Abstract

In this paper, we first determine the order of caterpillar trees (Gutman trees) in terms of the Hosoya index, and then by using a connection between the Hosoya index of caterpillar trees and the number of Kekulé structures of hexagonal chains, polyomino chains, square-hexagonal chains and pentagonal chains, we present the first ten hexagonal chains, polyomino chains, square-hexagonal chains and pentagonal chains with the minimal numbers of Kekulé structures, the first five hexagonal chains, polyomino chains, square-hexagonal chains with the maximal numbers of Kekulé structures among all of these polycyclic molecules with given number of polygons, respectively.


## 1 Introduction

Kekulé structures have been used in organic chemistry since Kekulé proposed a hexagonal structure for benzene. In the theory of benzenoid hydrocarbons [2], Kekulé structures play a significant role, and the number of Kekulé structures in benzenoid hydrocarbons is a most important quantity because the stability and many other properties of these hydrocarbons have been found to correlate with the number of Kekulé structures, and is often used for predicting physical properties and chemical behavior thereof. The Kekulé structures and various Kekulé-structure-based properties of benzenoid molecules have

[^0]been extensively studied in the past, and many papers have appeared on the problems of the enumeration of Kekule structures, for details see [1-3, 5-7,12-14].

Kekulé structures of a molecule graph $G=(V, E)$ is a set of pairwise disjoint edges of $G$ that cover all vertices. Denote by $K(G)$ the number of Kekulé structures of a molecule graph $G$. The Kekulé structures are also known as perfect matchings or 1-factors in graph theory. For a general background on matching theory and terminology we refer the reader to the classical monograph by Lovász and Plummer [11].

For a molecule graph $G=(V, E)$, we denote by $m(G, t)$ the number of ways in which $t$ mutually independent edges can be selected in $G$. Thus, $m(G, 1)$ is equal to the number of edges of $G$. If $n=|V|$ is even, then $m\left(G, \frac{n}{2}\right)$ is the number $K(G)$ of Kekulé structures of $G$. The number of matchings of $G$ is called the Hosoya index [8] and be denoted by $Z(G)$, i.e., $Z(G)=\sum_{t=0}^{\left\lfloor\frac{n}{2}\right\rfloor} m(G, t)$, where $m(G, 0)=1$.

In 1977, Gutman [4] discovered a curious relation between the sextet polynomial of a hexagonal chain and the matching polynomial of a caterpillar tree (also named as Gutman tree). This result implied that, for a hexagonal chain $G$, there exists a corresponding caterpillar tree $T$ such that the number of Kekule structures of $G$ is equal to the Hosoya index of $T$. For some related results, see [9,17]. More recently, Li and Yan in [10] proved a similar result for polyomino chains. Xiao and Chen in [15] proved that there exists a caterpillar tree $T$ such that the number of Kekulé structures of square-hexagonal chains is equal to the Hosoya index of $T$. Xiao, Chen and Raigorodskii [16] showed that for a pentagonal chain $G$ with even number of pentagons, there exists a caterpillar tree $T$ such that the number of Kekulé structures of $G$ is equal to the Hosoya index of $T$. This result can be generalized to any polygonal chain with even number of odd polygons.

Based on the relation above between the Hosoya index of a caterpillar tree and the number of Kekulé structures of many polycyclic molecules, we will first order the caterpillar trees with given number of edges by their Hosoya indices, and then present the first few hexagonal chains, polyomino chains, square-hexagonal chains and pentagonal chains with the minimal numbers and the maximal numbers of Kekule structures among all of these polycyclic molecules with given number of polygons, respectively.

## 2 Ordering caterpillar trees by the Hosoya index

In this section, we are concerned with the ordering of caterpillar trees in terms of the Hosoya index, and characterize the extremal caterpillar trees with the first ten minimal Hosoya indices and the first five maximal Hosoya indices among all caterpillar trees with $n$ edges.

A caterpillar tree $C$ with parameters $k_{1}, k_{2}, \cdots, k_{l}$ is obtained by attaching $k_{i}$ pendent vertices to the $i$-th vertex of $P_{l}$ for $i=1,2, \cdots, l$. This caterpillar tree will be denoted by $C_{l}\left(k_{1}, k_{2}, \cdots, k_{l}\right)$. It has $k_{1}+k_{2}+\cdots+k_{l}+l$ vertices and $k_{1}+k_{2}+\cdots+k_{l}+l-1$ edges. Specially, caterpillar trees $C_{n}(0,0, \cdots, 0)$ and $C_{1}(n-1)$ are the path $P_{n}$ and the star $S_{n}$ on $n$ vertices, and their Hosoya indices are $\frac{1}{\sqrt{5}}\left[\left(\frac{1+\sqrt{5}}{2}\right)^{n+1}-\left(\frac{1-\sqrt{5}}{2}\right)^{n+1}\right]$ and $n$, respectively.

The following properties, derived directly from the definition of the Hosoya index, allow us to enumerate the number of matchings of a graph $G$ by recursively reducing it. Here $G-e$ denotes the result of deleting an edge $e$ from $G$ but keeping its end-vertices, while $G-u-v$ denotes the graph obtained from $G$ by deleting vertices $u$ and $v$ and all edges incident with them.

Lemma 1. Let $G$ be a graph and $e$ its edge, connecting the vertices $u$ and $v$. Then $Z(G)=Z(G-e)+Z(G-u-v)$.

Lemma 2. Let $G$ be a graph with components $G_{1}, \cdots, G_{p}$. Then $Z(G)=Z\left(G_{1}\right) \cdots Z\left(G_{p}\right)$.
The following edge-lifting transformation can be easily obtained from Lemmas 1 and 2.

Lemma 3. (Edge-lifting transformation) Let $G_{1}$ and $G_{2}$ be two simple and non-trivial connected graphs. If $G$ is the graph obtained from $G_{1}$ and $G_{2}$ by adding an edge between a vertex $u$ of $G_{1}$ and a vertex $v_{0}$ of $G_{2}, G^{\prime}$ is the graph obtained by identifying $u_{0}$ of $G_{1}$ to $v_{0}$ of $G_{2}$ and adding a pendent edge to $u_{0}\left(v_{0}\right)$, then $Z(G)>Z\left(G^{\prime}\right)$.

Using Lemma 3 (i.e., the edge-lifting transformation) repeatedly on a tree with $n$ vertices, we can deduce that the path $P_{n}$ and the star $S_{n}$ are the extremal trees with the maximum Hosoya index and the minimum Hosoya index among all (caterpillar) trees
with $n$ vertices, respectively, i.e.,

$$
\begin{equation*}
n=Z\left(S_{n}\right)<Z\left(C_{l}\left(k_{1}, k_{2}, \cdots, k_{l}\right)\right)<Z\left(P_{n}\right)=\frac{1}{\sqrt{5}}\left[\left(\frac{1+\sqrt{5}}{2}\right)^{n+1}-\left(\frac{1-\sqrt{5}}{2}\right)^{n+1}\right] \tag{1}
\end{equation*}
$$

if $C_{l}\left(k_{1}, k_{2}, \cdots, k_{l}\right)$ is different from $P_{n}$ and $S_{n}$, where $k_{1}+k_{2}+\cdots+k_{l}+l=n$.
In the following, we will consider the ordering of caterpillar trees in terms of the Hosoya index and characterize the extremal trees with smaller Hosoya indices over all caterpillar trees with $n$ edges.
(I) Firstly, we consider the ordering of all caterpillar trees of form $C_{2}(i-1, n-i)$ in terms of the Hosoya index. Note that $C_{l}\left(k_{1}, k_{2}, \cdots, k_{l}\right) \cong C_{l-1}\left(k_{2}+1, k_{3}, \cdots, k_{l}\right)$ for $k_{1}=0$ and $C_{l}\left(k_{1}, k_{2}, \cdots, k_{l}\right) \cong C_{l}\left(k_{l}, k_{l-1}, \cdots, k_{1}\right)$, we may assume that $2 \leq i \leq\left\lfloor\frac{n}{2}\right\rfloor$. By the definition of Hosoya index, we have

$$
Z\left(C_{2}(i-1, n-i)\right)=1+n+(i-1) \times(n-i)=-i^{2}+i \times(n+1)+1 .
$$

Obviously, $g(i)=-i^{2}+i \times(n+1)+1$ is monotonically increasing for $2 \leq i \leq\left\lceil\frac{n}{2}\right\rceil$. So, it achieves the minimum value at $i=2$, and $g(2)=2 n-1, g(3)=3 n-5, g(4)=4 n-11$, $g(5)=5 n-19, g(6)=6 n-29, \cdots$,

$$
\begin{equation*}
g(2)<g(3)<g(4)<g(5)<g(6)<\cdots<g\left(\left\lceil\frac{n}{2}\right\rceil\right) \tag{2}
\end{equation*}
$$

i.e.,

$$
Z\left(C_{2}(1, n-2)\right)<Z\left(C_{2}(2, n-3)\right)<\cdots<Z\left(C_{2}\left(\left\lceil\frac{n}{2}\right\rceil-1, n-\left\lceil\frac{n}{2}\right\rceil\right)\right.
$$

and $C_{2}(1, n-2)$ is the caterpillar tree with the minimum Hosoya index among all caterpillar trees $C_{2}(i-1, n-i)$ with $2 \leq 2 \leq\left\lfloor\frac{n}{2}\right\rfloor$.

From the edge-lifting transformation, we know that the caterpillar tree with the second minimal Hosoya index over all the caterpillar trees with $n$ edges must be the form of $C_{2}(i-1, n-i)$, where $2 \leq 2 \leq\left\lfloor\frac{n}{2}\right\rfloor$. So, $C_{2}(1, n-2)$ is the caterpillar tree with the second minimal Hosoya index over all the caterpillar trees with $n$ edges.
(II) Secondly, we consider the ordering of all caterpillar trees of form $C_{3}(i-1, j-$ $1, n-i-j$ ), where $2 \leq i \leq\left\lfloor\frac{n}{2}\right\rfloor, j \geq 1$ and $i+j \leq\left\lceil\frac{n}{2}\right\rceil$. By Lemmas 1 and 2, we have

$$
Z\left(C_{3}(i-1, j-1, n-i-j)\right)=1+n+i j(n+1-i-j)-j .
$$

Let $f(x, y)=1+n+x y(n+1-x-y)-y$. Then $Z\left(C_{3}(i-1, j-1, n-i-j)\right)=f(i, j)$. $\frac{\partial f}{\partial x}=y(n+1-2 x-y)>0$ and $\frac{\partial f}{\partial y}=x(n+1-2 y-x)-1>0$ since $2 \leq x \leq\left\lfloor\frac{n}{2}\right\rfloor$ and
$x+y \leq\left\lceil\frac{n}{2}\right\rceil$. So, $f(i, j)<f(i+1, j)$ and $f(i, j)<f(i, j+1)$. Note that

$$
\begin{array}{ccc}
f(2,1)=3 n-4, & f(2,2)=5 n-13, & f(2,3)=7 n-26, \\
\cdots \\
f(3,1)=4 n-9, & f(3,2)=7 n-25, & f(3,3)=10 n-47, \\
\cdots(4,1)=5 n-16, & f(4,2)=9 n-41, & \cdots,
\end{array}
$$

we have

$$
\begin{equation*}
f(2,1)<f(3,1)<f(4,1)<f(2,2)<f(2,3)<\cdots \tag{3}
\end{equation*}
$$

and

$$
\begin{aligned}
Z\left(C_{3}(1,0, n-3)\right) & <Z\left(C_{3}(2,0, n-4)\right)<Z\left(C_{3}(3,0, n-5)\right)<Z\left(C_{3}(1,1, n-4)\right) \\
& <Z\left(C_{3}(1,2, n-5)\right)<\cdots
\end{aligned}
$$

From the edge-lifting transformation, we know that the caterpillar tree with the third minimal Hosoya index among all caterpillar trees with $n$ edges must be the form of $C_{2}(i-1, n-i)$ or $C_{3}(i-1, j-1, n-i-j)$. And $Z\left(C_{2}(1, n-2)\right)=2 n-1<Z\left(C_{2}(2, n-3)\right)=$ $3 n-6<Z\left(C_{3}(1,0, n-3)\right)=3 n-4$, it is showed that $C_{2}(2, n-3)$ the caterpillar tree with the third minimal Hosoya index among all caterpillar trees with $n$ edges.
(III) Next, we consider all caterpillar trees of form $C_{4}(x-1, y-1, z-1, n-x-y-z)$, where $2 \leq x \leq\left\lfloor\frac{n-1}{2}\right\rfloor, y \geq 1, z \geq 1$ and $x+y+z \leq\left\lceil\frac{n}{2}\right\rceil$. By Lemmas 1 and 2 , we have

$$
Z\left(C_{4}(x-1, y-1, z-1, n-x-y-z)\right)=1+x y+(x y z+x+z)(n+1-x-y-z) .
$$

Let $\varphi(x, y, z)=1+x y+(x y z+x+z)(n+1-x-y-z)=Z\left(C_{4}(x-1, y-1, z-\right.$ $1, n-x-y-z))=\varphi(x, y, z)$.
(i) If $y=1$ and $z=1$, then $Z\left(C_{4}(x-1, y-1, z-1, n-x-y-z)\right)=\varphi(x, y, z)=$ $\varphi(x, 1,1)=-2 x^{2}+(2 n-2) x+n=\sigma(x) . \sigma^{\prime}(x)=0$ implies $x=\frac{n-1}{2}$. Since $2 \leq x \leq\left\lfloor\frac{n-1}{2}\right\rfloor$, we have $\varphi(2,1,1)=5 n-12<\varphi(x, 1,1)$ for $3 \leq x \leq\left\lfloor\frac{n-1}{2}\right\rfloor$.
(ii) If $y \geq 2$ or $z \geq 2$, then $y+z \geq 3 . \varphi(x, y, z)=Z\left(C_{4}(x-1, y-1, z-1, n-x-y-z)\right)>$ $Z\left(C_{3}(x-1, y+z-1, n-x-y-z)\right)=f(x, y+z) \geq f(2,3)=7 n-26$.

From (i)-(ii), we know that $\varphi(x, y, z)>\varphi(2,1,1)$ for $(x, y, z) \neq(2,1,1)$, i.e., $Z\left(C_{4}(x-\right.$ $1, y-1, z-1, n-x-y-z))>Z\left(C_{4}(1,0,0, n-4)\right)$ for $(x, y, z) \neq(2,1,1)$. So, $C_{4}(1,0,0, n-4)$ is the caterpillar tree with the minimum Hosoya index among all caterpillar trees of form $C_{4}(x-1, y-1, z-1, n-x-y-z)$.

Moreover, by the edge-lifting transformation, $Z\left(C_{l}\left(k_{1}, k_{2}, \cdots, k_{l}\right)\right)>Z\left(C_{4}\left(k_{1}, k_{2}, k_{3}\right.\right.$, $\left.k_{4}+\cdots+k_{l}+n-4\right)$ ) for $l \geq 5$. So, we can obtain the following result from Equations (1) and (3).

Theorem 4. Let $G$ be a caterpillar tree with $n \geq 9$ edges, and it does not belong to $\left\{C_{1}(n), C_{2}(1, n-2), C_{2}(2, n-3), C_{3}(1,0, n-3), C_{2}(3, n-4), C_{3}(2,0, n-4), C_{2}(4, n-\right.$ 5), $\left.C_{3}(3,0, n-5), C_{3}(1,1, n-4), C_{4}(1,0,0, n-4)\right\}$. Then $Z\left(C_{1}(n)\right)<Z\left(C_{2}(1, n-1)\right)<$ $Z\left(C_{2}(2, n-3)\right)<Z\left(C_{3}(1,0, n-3)\right)<Z\left(C_{2}(3, n-4)\right)<Z\left(C_{3}(2,0, n-4)\right)<Z\left(C_{2}(4, n-\right.$ $5))<Z\left(C_{3}(3,0, n-5)\right)<Z\left(C_{3}(1,1, n-4)\right)<Z\left(C_{4}(1,0,0, n-4)\right)<Z(G)$.

Theorem 4 characterizes the caterpillar trees with the first ten minimal Hosoya index among all caterpillar trees with $n$ edges.

Next, we will characterize the caterpillar trees with larger Hosoya index over all caterpillar trees with $n$ edges. From Equation (1), the path $P_{n+1}$ with $n$ edges has the maximum Hosoya index among all caterpillar trees with $n$ edges, this number $Z\left(P_{n+1}\right)$ is equal to the $(n+2)$-th Fibonacci number.

The Fibonacci sequence is the sequence of integers $F_{1}, F_{2}, F_{3}, \cdots$, defined by means of the recurrence relation

$$
F_{n+2}=F_{n+1}+F_{n}
$$

and by means of the initial conditions $F_{1}=F_{2}=1$.
Lemma 5. For the Fibonacci sequence $F_{n}$, we have
(i) $F_{1}+F_{2}+\cdots+F_{n}=F_{n+2}-F_{2}$;
(ii) $F_{2 t} \times F_{n-2 t+1}=F_{n-1}+F_{n-5}+F_{n-9}+\cdots+F_{n-4(t-1)-1}$;
(iii) $F_{2 t+1} \times F_{n-2 t}=F_{n-1}+F_{n-5}+F_{n-9}+\cdots+F_{n-4(t-1)-1}+F_{n-4 t}$.

Proof. (i) It can be easily proved and can be found in pertinent books.
We prove (ii)-(iii) by the inductive method.
For $t=1, F_{2} \times F_{n-1}=F_{n-1}$ and $F_{3} \times F_{n-2}=2 F_{n-2}=F_{n-1}+F_{n-4}$.
For $t=2, F_{4} \times F_{n-3}=3 F_{n-1}=F_{n-1}+F_{n-5}$ and $F_{5} \times F_{n-4}=5 F_{n-4}=F_{n-1}+F_{n-5}+$ $F_{n-8}$.

Now, we assume that it is true for $t$. Then

$$
\begin{aligned}
F_{2 t+2} \times F_{n-2 t-1}= & \left(F_{2 t+1}+F_{2 t}\right) \times F_{n-2 t-1} \\
= & F_{2 t+1} \times F_{(n-1)-2 t}+F_{2 t} \times F_{(n-2)-2 t+1} \\
= & F_{n-2}+F_{n-6}+F_{n-10}+\cdots+F_{(n-1)-4(t-1)-1}+F_{(n-1)-4 t} \\
& +F_{n-3}+F_{n-7}+F_{n-11}+\cdots+F_{(n-2)-4(t-1)-1} \\
& (\text { by the inductive assumption }) \\
= & F_{n-1}+F_{n-5}+F_{n-9}+\cdots+F_{n-4(t-1)-1}+F_{n-4 t-1}
\end{aligned}
$$

and

$$
\begin{aligned}
F_{2 t+3} \times F_{n-2 t-2}= & \left(F_{2 t+1}+F_{2 t+2}\right) \times F_{n-2 t-2} \\
= & F_{2 t+1} \times F_{(n-2)-2 t}+F_{2 t+2} \times F_{(n-1)-2 t-1} \\
= & F_{n-3}+F_{n-7}+F_{n-11}+\cdots+F_{(n-2)-4(t-1)-1}+F_{(n-2)-4 t} \\
& +F_{n-2}+F_{n-6}+F_{n-10}+\cdots+F_{(n-1)-4(t-1)-1}+F_{(n-1)-4 t-1}
\end{aligned}
$$

(by the inductive assumption)

$$
=F_{n-1}+F_{n-5}+F_{n-9}+\cdots+F_{n-4(t-1)-1}+F_{n-4 t-1}+F_{n-4(t+1)} .
$$

The proof is complete by the mathematical induction.

In order to find the caterpillar trees with larger Hosoya indices, we should focus on the caterpillar trees with less leaves.
(I) We consider the ordering of all caterpillar trees with $n \geq 14$ edges and exactly three leaves in terms of the Hosoya index. Let $k_{1}=\cdots=k_{i-1}=k_{i+1}=\cdots=k_{n}=0$ and $k_{i}=1$, where $2 \leq i \leq\left\lceil\frac{n}{2}\right\rceil . C_{n}\left(k_{1}, k_{2}, \cdots, k_{l}\right)=C_{n}(0, \cdots, 0,1,0, \cdots, 0)$ is a caterpillar tree with $n$ edges and exactly three leaves. By Lemmas 1 and 2, we have

$$
Z\left(C_{n}(0, \ldots, 0,1,0, \ldots, 0)\right)=Z\left(P_{n}\right)+Z\left(P_{i-1}\right) Z\left(P_{n-i}\right)=F_{n+1}+F_{i} \times F_{n-i+1} .
$$

Let $h(i)=F_{n+1}+F_{i} \times F_{n-i+1}$ for a given $n$. By Lemma 5 , we have

$$
\begin{aligned}
& h(2)=F_{n+1}+F_{n-2}+F_{n-3}=F_{n+1}+F_{n-1} \\
& h(4)=F_{n+1}+F_{n-2}+F_{n-3}+F_{n-6}+F_{n-7}=F_{n+1}+F_{n-1}+F_{n-5} \\
& h(6)=F_{n+1}+F_{n-2}+F_{n-3}+F_{n-6}+F_{n-7}+F_{n-10}+F_{n-11}=F_{n+1}+F_{n-1}+F_{n-5}+F_{n-9} \\
& h(8)=F_{n+1}+F_{n-1}+F_{n-5}+F_{n-9}+F_{n-13}
\end{aligned}
$$

and

$$
h(2 r+2)-h(2 r)=F_{n-4 r-2}+F_{n-4 r-3}=F_{n-4 r-1} .
$$

Thus,

$$
h(2 i)=F_{n+1}+F_{n-1}+F_{n-5}+\cdots+F_{n-4 i+3} .
$$

$$
\begin{aligned}
& h(3)=F_{n+2}-F_{n-3}=F_{n+1}+F_{n-1}+F_{n-4} \\
& h(5)=F_{n+2}-F_{n-3}-F_{n-7}=F_{n+1}+F_{n-1}+F_{n-5}+F_{n-8} \\
& h(7)=F_{n+2}-F_{n-3}-F_{n-7}-F_{n-11}=F_{n+1}+F_{n-1}+F_{n-5}+F_{n-9}+F_{n-12}
\end{aligned}
$$

and

$$
h(2 r+1)-h(2 r-1)=-F_{n-4 r}-F_{n-4 r-1}=-F_{n-4 r+1} .
$$

Thus,

$$
h(2 i+1)=F_{n+1}+F_{n-1}+F_{n-5}+\cdots+F_{n-4 i+3}+F_{n-4 i} .
$$

So,

$$
\begin{gathered}
h(2)<h(4)<h(6)<h(8)<\cdots<h\left(2\left\lfloor\frac{n+1}{4}\right\rfloor\right), \\
h(3)>h(5)>h(7)>\cdots>h\left(2\left\lfloor\frac{n-1}{4}\right\rfloor+1\right) .
\end{gathered}
$$

Since $h\left(2\left\lfloor\frac{n-1}{4}\right\rfloor+1\right)>h\left(2\left\lfloor\frac{n+1}{4}\right\rfloor\right)$, we have

$$
h(3)>h(5)>h(7)>\cdots>h(6)>h(4)>h(2)
$$

and we can obtain the ordering of all caterpillar trees with $n$ edges and exactly three leaves

$$
\begin{align*}
& Z\left(C_{n}(0,0,1,0, \cdots, 0)\right)>Z\left(C_{n}(0,0,0,0,1,0, \cdots, 0)\right)>Z\left(C_{n}(0,0,0,0,0,0,1,0, \cdots, 0)\right)> \\
& \quad \cdots>Z\left(C_{n}(0,0,0,0,0,1,0, \cdots, 0)\right)>Z\left(C_{n}(0,0,0,0,1,0, \cdots, 0)\right)>Z\left(C_{n}(0,1,0, \cdots, 0)\right) . \tag{4}
\end{align*}
$$

So, $C_{n}(0,0,1,0, \cdots, 0)$ is the caterpillar tree with the maximum Hosoya index among all caterpillar trees with $n$ edges and exactly three leaves.

Note that the caterpillar tree with the second maximal Hosoya index among all the caterpillar trees with $n$ edges must contain exactly three leaves from the edge-lifting transformation, $C_{n}(0,0,1,0, \cdots, 0)$ is the caterpillar tree with the second maximal Hosoya index among all caterpillar trees with $n$ edges.
(II) We consider the ordering of caterpillar trees with $n$ edges and exactly four leaves in terms of the Hosoya index. In the following, we will show that $Z(G)<h(9)$ for any caterpillar tree $G$ with $n \geq 17$ edges and at least four leaves.

Let $G=C_{n-1}\left(k_{1}, k_{2}, \cdots, k_{n-1}\right)$ be a caterpillar tree with $n \geq 17$ edges and exactly four leaves, where $k_{1}+\cdots+k_{n-1}=k_{i}+k_{j}=2,2 \leq i \leq\left\lfloor\frac{n}{2}\right\rfloor$ and $j \geq i$.
(i) If $j \geq 8$, then by the edge-lifting transformation,

$$
Z(G)<Z\left(C_{n}\left(0, \cdots, 0, k_{j+1}^{\prime}, 0, \cdots, 0\right)\right)=h(j+1) \leq h(9)
$$

where $k_{j+1}^{\prime}=1$.
(ii) If $i=j \leq 7$, then by the edge-lifting transformation,

$$
Z(G)<Z\left(C_{n}\left(0, \cdots, 0, k_{i}^{\prime}, 0, \cdots, 0\right)\right)=h(i), \quad \text { where } k_{i}^{\prime}=1
$$

and $Z(G)<Z\left(C_{n}\left(0, \cdots, 0, k_{i+1}^{\prime}, 0, \cdots, 0\right)\right)=h(i+1), \quad$ where $k_{i+1}^{\prime}=1$
So, $Z(G)<\min \{h(i), h(i+1)\} \leq h(8)<h(9)$ since $i$ or $i+1$ is even.
(iii) If $i \neq j \leq 7, i$ is even or $j$ is odd, then by the edge-lifting transformation,

$$
Z(G)<Z\left(C_{n}\left(0, \cdots, 0, k_{i}^{\prime}, 0, \cdots, 0\right)\right)=h(i) \leq h(8)<h(9)
$$

or

$$
Z(G)<Z\left(C_{n}\left(0, \cdots, 0, k_{j+1}^{\prime}, 0, \cdots, 0\right)\right)=h(j+1) \leq h(8)<h(9) .
$$

(iv) If $i \neq j \leq 7, i$ is odd and $j$ is even, then $(i, j) \in\{(3,4),(3,6),(5,6)\}$.

If $i=3$ and $j=4$, then by Lemmas 1 and $2, Z(G)=Z\left(C_{n-1}(0,0,1,1,0, \cdots, 0)\right)=$ $Z\left(P_{4}\right) Z\left(P_{n-3}\right)+Z\left(P_{2}\right) Z\left(P_{n-5}\right)=F_{5} \times F_{n-2}+F_{3} \times F_{n-4}=5 F_{n-2}+2 F_{n-4}$. It can be showed easily by the Fibonacci recurrence relation that $5 F_{n-2}+2 F_{n-4}<F_{n+1}+F_{n-1}+$ $F_{n-5}+F_{n-9}+F_{n-13}+F_{n-16}=h(9)$. So, $Z(G)<h(9)$.

If $i=3$ and $j=6$, then by Lemmas 1 and $2, Z(G)=Z\left(C_{n-1}(0,0,1,0,0,1,0, \cdots, 0)\right)=$ $Z\left(C_{n-2}(0,0,1,0, \cdots, 0)\right)+Z\left(C_{5}(0,0,1,0,0)\right) \times Z\left(P_{n-7}\right)=\left(F_{n-1}+F_{n-3}+F_{n-6}\right)+\left(F_{6}+\right.$ $\left.F_{4}+F_{1}\right) \times F_{n-6}=F_{n-1}+F_{n-3}+12 F_{n-6}$. By the Fibonacci recurrence relation, we can show that $F_{n-1}+F_{n-3}+12 F_{n-6}<F_{n+1}+F_{n-1}+F_{n-5}+F_{n-9}+F_{n-13}+F_{n-16}=h(9)$. So, $Z(G)<h(9)$.

If $i=5$ and $j=6$, then by Lemmas 1 and $2, Z(G)=Z\left(P_{6}\right) Z\left(P_{n-5}\right)+Z\left(P_{4}\right) Z\left(P_{n-7}\right)=$ $F_{7} \times F_{n-4}+F_{5} \times F_{n-6}=13 F_{n-4}+5 F_{n-6}$. From the Fibonacci recurrence relation, it is easily to prove that $13 F_{n-4}+5 F_{n-6}<F_{n+1}+F_{n-1}+F_{n-5}+F_{n-9}+F_{n-13}+F_{n-16}=h(9)$. So, $Z(G)<h(9)$.

From (i)-(iv), we know that $Z(G)<h(9)$ for any caterpillar tree $G$ with $n \geq 17$ edges and exactly four leaves.

Moreover, for a caterpillar tree $G$ with $n \geq 17$ edges and at least five leaves, by the edge-lifting transformation, there is a caterpillar tree $G^{\prime}$ with $n$ edges and exactly four leaves such that $Z(G)<Z\left(G^{\prime}\right)$.

So, we can obtain the following result from Equation (4).
Theorem 6. Let $G$ be a caterpillar tree with $n \geq 17$ edges, different from $C_{n+1}(0, \cdots, 0)$, $C_{n}(0,0,1,0, \cdots, 0), C_{n}(0,0,0,0,1,0, \cdots, 0), C_{n}(0,0,0,0,0,0,1,0, \cdots, 0)$ and $C_{n}(0,0,0,0,0,0,0,0,1,0, \cdots, 0)$. Then

$$
\begin{aligned}
& Z\left(C_{n+1}(0, \cdots, 0)\right)>Z\left(C_{n}(0,0,1,0, \cdots, 0)\right)>Z\left(C_{n}(0,0,0,0,1,0, \cdots, 0)\right) \\
> & Z\left(C_{n}(0,0,0,0,0,0,1,0, \cdots, 0)\right)>Z\left(C_{n}(0,0,0,0,0,0,0,0,1,0, \cdots, 0)\right)>Z(G)
\end{aligned}
$$

Theorem 6 characterizes the caterpillar trees with the first five Hosoya indices among all caterpillar trees with $n \geq 17$ edges.

## 3 Applications

In this section, by using Theorems 4 and 6 and a connection between the Hosoya index of caterpillar trees and the number of Kekulé structures of hexagonal chains, polyomino chains, square-hexagonal chains and pentagonal chains, we will present the first ten hexagonal chains, polyomino chains, square-hexagonal chains and pentagonal chains with the minimal numbers of Kekulé structures, the first five hexagonal chains, polyomino chains, square-hexagonal chains with the maximal numbers of Kekulé structures among all of these polycyclic molecules with given number of polygons, respectively.

### 3.1 Ordering unbranched catacondensed benzenoid hydrocarbons by the number of Kekulé structures

A hexagonal chain or unbranched catacondensed benzenoid hydrocarbon is a benzenoid system in which no hexagon has more than two neighbors.

As in $[4,9]$, the Kekulé structure count of a hexagonal chain was shown to be equal to the Hosoya index of the corresponding caterpillar tree.

For a hexagonal chain $G$ with $n$ hexagons $c_{1}, c_{2}, \cdots, c_{n}$, where the hexagons are numbered successively. That is, the hexagon $c_{i}(1<i<n)$ is neighbouring to the hexagons $c_{i-1}$ and $c_{i+1}$. Then it is easy to see that a hexagon in $G$ with exactly two neighbours is concatenated in one of the two modes: (i) a linear mode-a hexagon adjacent to two hexagons in which the common edges are parallel, called linearly annelated (L-mode); (ii) an angular mode-a hexagon adjacent to two hexagons in which the common edges
are not parallel, called angularly annelated (A-mode). With a hexagonal chain $G$ having $n$ hexagons, we associate a $n$-tuple $\left(S_{1}, S_{2}, \cdots, S_{n}\right)$ of symbols $L$ and $A$, called the $\{\mathrm{L}, \mathrm{A}\}$-sequence of the hexagonal chain $G$ as follows. We define $S_{1}=S_{n}=L$ and for $1<i<n, S_{i}=L$ if the $i$-th hexagon of $G$ is linearly annelated and $S_{i}=A$ if the $i$-th hexagon of $G$ is angularly annelated. We often use the $\{\mathrm{L}, \mathrm{A}\}$-sequence of a hexagonal chain $G$ instead of the graph $G$.

The general form of the $\{\mathrm{L}, \mathrm{A}\}$-sequence of a hexagonal chain with $n$ hexagon in which there are $t-1$ angularly annelated hexagons is

$$
L^{k_{1}} A L^{k_{2}} A L^{k_{3}} A \cdots L^{k_{t-1}} A L^{k_{t}}
$$

where $k_{i}$ is the number of L-mode hexagons lying between the $(i-1)$-th and $i$-th angularly annelated hexagon, $i=2, \cdots, t-1$, whereas $k_{1}$ and $k_{t}$ are, respectively, the number of the L-mode hexagons before the first and after the last A-mode hexagon. Therefore, $k_{1}, k_{t} \geq 1, k_{2}, \cdots, k_{t-1} \geq 0$ and

$$
k_{1}+k_{2}+\cdots+k_{t}+(t-1)=n
$$

The corresponding caterpillar tree is $C_{t}\left(k_{1}, k_{2}, \cdots, k_{t}\right)$.
A result obtained in $[4,9]$ is the following:
Lemma 7. [4, 9] If $G$ is a hexagonal chain whose $\{L, A\}$-sequence is $L^{k_{1}} A L^{k_{2}} A \cdots L^{k_{t-1}} A L^{k_{t}}$, then the number $K(G)$ of its Kekulé structures is equal to the Hosoya index of the caterpillar tree $C_{t}\left(k_{1}, k_{2}, \cdots, k_{t}\right)$.

By Lemma 7, Theorems 4 and 6, we can characterize the first ten hexagonal chains with the minimal numbers of Kekulé structures and the first five hexagonal chains with the maximal numbers of Kekulé structures among all of hexagonal chains with given number of hexagons, respectively.

Theorem 8. Let $G$ be a hexagonal chain with $n \geq 9$ hexagons, and its $\{L, A\}$-sequence is different from $L^{n}, L A L^{n-2}, L^{2} A L^{n-3}, L A^{2} L^{n-3}, L^{3} A L^{n-4}, L^{2} A^{2} L^{n-4}, L^{4} A L^{n-5}, L^{3} A^{2} L^{n-5}$, $L A L A L^{n-4}, L A^{3} L^{n-4}$. Then $K\left(L_{n}\right)<K\left(L A L^{n-2}\right)<K\left(L^{2} A L^{n-3}\right)<K\left(L A^{2} L^{n-3}\right)<$ $K\left(L^{3} A L^{n-4}\right)<K\left(L^{2} A^{2} L^{n-4}\right)<K\left(L^{4} A L^{n-5}\right)<K\left(L^{3} A^{2} L^{n-5}\right)<K\left(L A L A L^{n-4}\right)<$ $K\left(L A^{3} L^{n-4}\right)<K(G)$.

Theorem 9. Let $G$ be a hexagonal chain with $n \geq 17$ hexagons, and its $\{L, A\}$-sequence is different from $L A^{n-2} L, L A L A^{n-4} L, L A^{3} L A^{n-6} L, L A^{5} L A^{n-8} L, L A^{7} L A^{n-10} L$. Then

$$
K\left(L A^{n-2} L\right)>K\left(L A L A^{n-4} L\right)>K\left(L A^{3} L A^{n-6} L\right)>K\left(L A^{5} L A^{n-8} L\right)>
$$

$K\left(L A^{7} L A^{n-10} L\right)>K(G)$.

### 3.2 Ordering polyomino chains by the number of Kekulé structures

A polyomino system is a finite 2-connected plane graph such that each interior face is surrounded by a regular square of length one. A polyomino chain is a polyomino system in which no square has more than two neighbors.

As in [10], the Kekulé structure count of a polyomino chain was shown to be equal to the Hosoya index of the corresponding caterpillar tree.

A squares of a polyomino chain with $n$ squares may be annelated in only three ways: Each chain possesses exactly two terminal squares whereas all other squares are annelated either linearly (L) or angularly (A). With a polyomino chain $G$ having $n$ squares, we can also associate a $n$-tuple $\left(S_{1}, S_{2}, \cdots, S_{n}\right)$ of symbols $L$ and $A$, called the $\{\mathrm{L}, \mathrm{A}\}$-sequence of the polyomino chain $G$ as follows. We define $S_{1}=S_{n}=L$ and for $1<i<n, S_{i}=L$ if the $i$-th square of $G$ is linearly annelated and $S_{i}=A$ if the $i$-th square of $G$ is angularly annelated.

The general form of the $\{\mathrm{L}, \mathrm{A}\}$-sequence of a polyomino chain $G$ with $n$ squares in which there are $t+1$ linearly annelated squares is

$$
L A^{k_{1}} L A^{k_{2}} L A^{k_{3}} L \cdots A^{k_{t}} L
$$

where $k_{i}$ is the number of A-mode squares lying between the $i$-th and $i+1$-th linearly annelated square, $k_{i} \geq 0, i=1,2, \cdots, t$ and

$$
k_{1}+k_{2}+\cdots+k_{t}+t+1=n .
$$

The corresponding caterpillar tree $C_{t}\left(k_{1}+1, k_{2}, \cdots, k_{t-1}, k_{t}\right)$ from the construction method in [10], and the result obtained in [10] is the following:

Lemma 10. [10] If $G$ is a polyomino chain whose $\{L, A\}$-sequence is $L A^{k_{1}} L A^{k_{2}} \cdots L A^{k_{t}} L$, then the number $K(G)$ of its Kekulé structures is equal to the Hosoya index of the caterpillar tree $C_{t}\left(k_{1}+1, k_{2}, \cdots, k_{t-1}, k_{t}\right)$.

By Lemma 10, Theorems 4 and 6, we can characterize the first ten polyomino chains with the minimal numbers of Kekule structures and the first five polyomino chains with the maximal numbers of Kekulé structures among all of polyomino chains with given number of squares, respectively.

Theorem 11. Let $G$ be a polyomino chain with $n \geq 9$ squares, and its $\{L, A\}$-sequence is different from $L A^{n-2} L, L^{2} A^{n-3} L, L A L A^{n-4} L, L^{3} A^{n-4} L, L A^{2} L A^{n-5} L, L A L^{2} A^{n-5} L$, $L A^{3} L A^{n-6} L, L A^{2} L^{2} A^{n-6} L, L^{2} A L A^{n-5} L, L^{4} A^{n-5} L$. Then

$$
\begin{aligned}
& \quad K\left(L A^{n-2} L\right)<K\left(L^{2} A^{n-3} L\right)<K\left(L A L A^{n-4} L\right)<K\left(L^{3} A^{n-4} L\right)<K\left(L A^{2} L A^{n-5} L\right)< \\
& K\left(L A L^{2} A^{n-5} L\right)<K\left(L A^{3} L A^{n-6} L\right)<K\left(L A^{2} L^{2} A^{n-6} L\right)<K\left(L^{2} A L A^{n-5} L\right) \\
& <K\left(L^{4} A^{n-5} L\right)<K(G)
\end{aligned}
$$

Theorem 12. Let $G$ be a polyomino chain with $n \geq 17$ squares, and its $\{L, A\}$-sequence is different from $L^{n}, L^{3} A L^{n-4}, L^{5} A L^{n-6}, L^{7} A L^{n-8}, L^{9} A L^{n-10}$. Then

$$
K\left(L^{n}\right)>K\left(L^{3} A L^{n-4}\right)>K\left(L^{5} A L^{n-6}\right)>K\left(L^{7} A L^{n-8}\right)>K\left(L^{9} A L^{n-10}\right)>K(G)
$$

### 3.3 Ordering square-hexagonal chains by the number of Kekulé structures

By a square-hexagonal chain with $n$ cells (where each cell can be either a square or a hexagon), we mean a finite graph obtained by concatenating $n$ cells in such a way that any two adjacent cells have exactly one edge in common, and each cell is adjacent to exactly two other cells, except the first and last cells which are adjacent to exactly one other cell each. It is clear that different square-hexagonal chains will result, not only according to the manner in which the cells are concatenated, but also the celli ${ }^{-}$s type. Specially, we have hexagonal chains if all the cells are hexagons, polyomino chains if all the cells are squares, and phenylene chains if hexagons and squares are concatenated alternately.

As in [15], the Kekulé structure count of a square-hexagonal chain was shown to be equal to the Hosoya index of the corresponding caterpillar tree.

For a square-hexagonal chain $G$ with $n$ cells $c_{1}, c_{2}, \cdots, c_{n}$, where the cells are numbered successively. Then a cell in $G$ with exactly two neighbours is concatenated in one of the four modes: $a, b, c, d$ (see [15]). A function $f$ from the cells to the symbols $L$ and $A$ is defined as follows:

$$
f\left(c_{i}\right)= \begin{cases}L, & i=1,2 \\ L, & \text { if } i \geq 3 \text { and the concatenating mode of } c_{i-1} \text { is ' }^{\prime} a^{\prime} \text { or ' } d^{\prime} \\ A, & \text { otherwise. }\end{cases}
$$

Thus a unique $\{\mathrm{L}, \mathrm{A}\}$-sequence $f\left(c_{1}\right) f\left(c_{2}\right) \cdots f\left(c_{n}\right)$ is associated with $G$.
The general form of the $\{\mathrm{L}, \mathrm{A}\}$-sequence of a square-hexagonal chain $G$ with $n$ cells is

$$
L^{l_{1}} A^{a_{1}} L^{l_{2}} A^{a_{2}} \cdots L^{l_{t}} A^{a_{t}}
$$

where $l_{1} \geq 2, l_{i} \geq 1$ for $i=2, \cdots, t ; a_{i} \geq 1$ for $i=1, \cdots, t-1, a_{t} \geq 0$ and

$$
l_{1}+a_{1}+l_{2}+a_{2}+\cdots+l_{t}+a_{t}=n .
$$

From the construction method in [15], the corresponding caterpillar tree is

$$
C_{m}\left(k_{1}, k_{2}, \cdots, k_{m}\right)
$$

where $m=l_{1}+\cdots+l_{t}, k_{l_{1}}=a_{1}, \cdots, k_{l_{1}+\cdots+l_{t-1}}=a_{t-1}, k_{m}=a_{t}+1$ and $k_{i}=0$ for $i \neq l_{1}, l_{1}+l_{2}, \cdots, l_{1}+l_{2}+\cdots+l_{t}$. And the result obtained in [15] is the following:

Lemma 13. [15] If $G$ is a square-hexagonal chain whose $\{L, A\}$-sequence is

$$
L^{l_{1}} A^{a_{1}} L^{l_{2}} A^{a_{2}} \cdots L^{l_{t}} A^{a_{t}},
$$

then the number $K(G)$ of its Kekulé structures is equal to the Hosoya index of the caterpillar tree $C_{m}\left(k_{1}, k_{2}, \cdots, k_{m}\right)$, where $m=l_{1}+\cdots+l_{t}, k_{l_{1}}=a_{1}, \cdots, k_{l_{1}+\cdots+l_{t-1}}=a_{t-1}$, $k_{m}=a_{t}+1$ and $k_{i}=0$ for $i \neq l_{1}, l_{1}+l_{2}, \cdots, l_{1}+l_{2}+\cdots+l_{t}$.

By Lemma 13, Theorems 4 and 6, we can characterize the first ten square-hexagonal chains with the minimal numbers of Kekulé structures and the first five square-hexagonal chains with the maximal numbers of Kekulé structures among all of hexagonal chains with given number of hexagons, respectively.

Theorem 14. Let $G$ be a square-hexagonal chain with $n \geq 9$ hexagons, and its $\{L, A\}$-sequence is different from $L^{2} A^{n-2}, L^{3} A^{n-3}, L^{2} A L A^{n-4}, L^{4} A^{n-4}, L^{2} A^{2} L A^{n-5}, L^{2} A L^{2} A^{n-5}$, $L^{2} A^{3} L A^{n-6}, L^{2} A^{2} L^{2} A^{n-6}, L^{3} A L A^{n-5}, L^{5} A^{n-5}$. Then
$K\left(L^{2} A^{n-2}\right)<K\left(L^{3} A^{n-3}\right)<K\left(L^{2} A L A^{n-4}\right)<K\left(L^{4} A^{n-4}\right)<K\left(L^{2} A^{2} L A^{n-5}\right)<$ $K\left(L^{2} A L^{2} A^{n-5}\right)<K\left(L^{2} A^{3} L A^{n-6}\right)<K\left(L^{2} A^{2} L^{2} A^{n-6}\right)<K\left(L^{3} A L A^{n-5}\right)<K\left(L^{5} A^{n-5}\right)<$ $K(G)$.

Theorem 15. Let $G$ be a square-hexagonal chain with $n \geq 17$ hexagons, and its $\{L, A\}$-sequence is different from $L^{n}, L^{3} A L^{n-4}, L^{5} A L^{n-6}, L^{7} A L^{n-8}, L^{9} A L^{n-10}$. Then

$$
K\left(L^{n}\right)>K\left(L^{3} A L^{n-4}\right)>K\left(L^{5} A L^{n-6}\right)>K\left(L^{7} A L^{n-8}\right)>K\left(L^{9} A L^{n-10}\right)>K(G) .
$$

### 3.4 Ordering pentagonal chains by the number of Kekulé structures

A pentagonal chain with $n$ cells (regular pentagons) is a finite graph obtained by concatenating $n$ cells in such a way that any two adjacent cells have exactly one edge in common, each cell is adjacent to exactly two other cells, except the first and last cells which are adjacent to exactly one other cell each, and each vertex is incident to at most three cells.

As in [16], the Kekule structure count of a pentagonal chain was shown to be equal to the Hosoya index of the corresponding caterpillar tree.

For a pentagonal chain $G_{2 n}$ with $2 n$ cells $c_{1}, c_{2}, \cdots, c_{2 n}$, where the cells are numbered successively, $G_{2 n}$ can be formed inductively. Starting from the first two cells $c_{1} c_{2}$, in each step we attach two new cells to the previous one. More clearly, let $G_{2 i}(i=1, \cdots, n)$ be the part of $G_{2 n}$ with the first $2 i$ pentagons, then $G_{2 i}$ is obtained from $G_{2 i-2}$ by attaching to it the $(2 i-1)$-th pentagon $c_{2 i-1}$ and the $2 i$-th pentagon $c_{2 i}$. There are seven ways to attach cells $c_{2 i-1} c_{2 i}$ to an edge of the end pentagon in $G_{2 i-2}: a, b, a, d, e, f, g$ (see [16]). So, using this construction method, each pentagonal chain $G_{2 n}$ can be obtained by attaching $n-1$ times new two cells to the previous one on the basis of $c_{1} c_{2}$.

Let $a_{i}$ denote the $(i-1)$-th time attaching type for $i \geq 2$ and $a_{1}$ denote the attaching way of the first two cells $c_{1} c_{2}$. A function $f$ from the attaching types to the symbols $L$ and $A$ is defined as follows:

$$
f\left(a_{i}\right)= \begin{cases}L, & i=1,2 \\ L, & \text { if } i \geq 3 \text { and the concatenation type of } c_{2 i-1}, c_{2 i-2}, c_{2 i-3}, c_{2 i-4} \\ \text { is ' } a^{\prime},{ }^{\prime} c^{\prime},{ }^{\prime} d^{\prime} \text { or ' } f^{\prime} ; \\ A, & \text { otherwise. }\end{cases}
$$

Thus a unique $\{\mathrm{L}, \mathrm{A}\}$-sequence $f\left(a_{1}\right) f\left(a_{2}\right) \cdots f\left(a_{n}\right)$ is associated with $G_{2 n}$.
The general form of the $\{\mathrm{L}, \mathrm{A}\}$-sequence of a pentagonal chain $G_{2 n}$ with $2 n$ cells is

$$
L^{l_{1}} A^{a_{1}} L^{l_{2}} A^{a_{2}} \cdots L^{l_{t}} A^{a_{t}}
$$

where $l_{1} \geq 2, l_{i} \geq 1$ for $i=2, \cdots, t ; a_{i} \geq 1$ for $i=1, \cdots, t-1, a_{t} \geq 0$ and

$$
l_{1}+a_{1}+l_{2}+a_{2}+\cdots+l_{t}+a_{t}=n
$$

From the construction method in [16], the corresponding caterpillar tree is

$$
C_{m}\left(k_{1}, k_{2}, \cdots, k_{m}\right)
$$

where $m=l_{1}+\cdots+l_{t}, k_{l_{1}}=a_{1}, \cdots, k_{l_{1}+\cdots+l_{t-1}}=a_{t-1}, k_{m}=a_{t}+1$ and $k_{i}=0$ for $i \neq l_{1}, l_{1}+l_{2}, \cdots, l_{1}+l_{2}+\cdots+l_{t}$. And the result obtained in [16] is the following:

Lemma 16. [15] If $G$ is a pentagonal chain whose $\{L, A\}$-sequence is $L^{l_{1}} A^{a_{1}} L^{l_{2}} A^{a_{2}} \ldots$ $L^{l_{t}} A^{a_{t}}$, then the number $K(G)$ of its Kekulé structures is equal to the Hosoya index of the caterpillar tree $C_{m}\left(k_{1}, k_{2}, \cdots, k_{m}\right)$, where $m=l_{1}+\cdots+l_{t}, k_{l_{1}}=a_{1}, \cdots, k_{l_{1}+\cdots+l_{t-1}}=a_{t-1}$, $k_{m}=a_{t}+1$ and $k_{i}=0$ for $i \neq l_{1}, l_{1}+l_{2}, \cdots, l_{1}+l_{2}+\cdots+l_{t}$.

By Lemma 16, Theorems 4 and 6, we can characterize the first ten pentagonal chains with the minimal numbers of Kekulé structures and the first five pentagonal chains with the maximal numbers of Kekulé structures among all of pentagonal chains with given number of pentagons, respectively.

Theorem 17. Let $G$ be a pentagonal chain with $2 n \geq 18$ hexagons, and its $\{L, A\}$-sequence is different from $L^{2} A^{n-2}, L^{3} A^{n-3}, L^{2} A L A^{n-4}, L^{4} A^{n-4}, L^{2} A^{2} L A^{n-5}, L^{2} A L^{2} A^{n-5}$, $L^{2} A^{3} L A^{n-6}, L^{2} A^{2} L^{2} A^{n-6}, L^{3} A L A^{n-5}, L^{5} A^{n-5}$. Then
$K\left(L^{2} A^{n-2}\right)<K\left(L^{3} A^{n-3}\right)<K\left(L^{2} A L A^{n-4}\right)<K\left(L^{4} A^{n-4}\right)<K\left(L^{2} A^{2} L A^{n-5}\right)<$ $K\left(L^{2} A L^{2} A^{n-5}\right)<K\left(L^{2} A^{3} L A^{n-6}\right)<K\left(L^{2} A^{2} L^{2} A^{n-6}\right)<K\left(L^{3} A L A^{n-5}\right)<K\left(L^{5} A^{n-5}\right)<$ $K(G)$.

Theorem 18. Let $G$ be a pentagonal chain with $2 n \geq 34$ hexagons, and its $\{L, A\}$-sequence is different from $L^{n}, L^{3} A L^{n-4}, L^{5} A L^{n-6}, L^{7} A L^{n-8}, L^{9} A L^{n-10}$. Then

$$
K\left(L^{n}\right)>K\left(L^{3} A L^{n-4}\right)>K\left(L^{5} A L^{n-6}\right)>K\left(L^{7} A L^{n-8}\right)>K\left(L^{9} A L^{n-10}\right)>K(G)
$$

The results above can summarized as the following tables.
Table 1. Extremal graphs with the first ten minimal values.

| c-trees $(\mathrm{n})$ | h-chains (n) | po-chains (n) | s-h-chains (n) | pe-chains (2n) |
| :--- | :--- | :--- | :--- | :--- |
| $C_{1}(n)$ | $L^{n}$ | $L A^{n-2} L$ | $L^{2} A^{n-2}$ | $L^{2} A^{n-2}$ |
| $C_{2}(1, n-2)$ | $L A L^{n-2}$ | $L^{2} A^{n-3} L$ | $L^{3} A^{n-3}$ | $L^{3} A^{n-3}$ |
| $C_{2}(2, n-3)$ | $L^{2} A L^{n-3}$ | $L A L A^{n-4} L$ | $L^{2} A L A^{n-4}$ | $L^{2} A L A^{n-4}$ |
| $C_{3}(1,0, n-3)$ | $L A^{2} L^{n-3}$ | $L^{3} A^{n-4} L$ | $L^{4} A^{n-4}$ | $L^{4} A^{n-4}$ |
| $C_{2}(3, n-4)$ | $L^{3} A L^{n-4}$ | $L A^{2} L A^{n-5} L$ | $L^{2} A^{2} L A^{n-5}$ | $L^{2} A^{2} L A^{n-5}$ |
| $C_{3}(2,0, n-4)$ | $L^{2} A^{2} L^{n-4}$ | $L A L^{2} A^{n-5} L$ | $L^{2} A L^{2} A^{n-5}$ | $L^{2} A L^{2} A^{n-5}$ |
| $C_{2}(4, n-5)$ | $L^{4} A L^{n-5}$ | $L A^{3} L A^{n-6} L$ | $L^{2} A^{3} L A^{n-6}$ | $L^{2} A^{3} L A^{n-6}$ |
| $C_{3}(3,0, n-5)$ | $L^{3} A^{2} L^{n-5}$ | $L A^{2} L^{2} A^{n-6} L$ | $L^{2} A^{2} L^{2} A^{n-6}$ | $L^{2} A^{2} L^{2} A^{n-6}$ |
| $C_{3}(1,1, n-4)$ | $L A L A L^{n-4}$ | $L^{2} A L A^{n-5} L$ | $L^{3} A L A^{n-5}$ | $L^{3} A L A^{n-5}$ |
| $C_{4}(1,0,0, n-4)$ | $L A^{3} L^{n-4}$ | $L^{4} A^{n-5} L$ | $L^{5} A^{n-5}$ | $L^{5} A^{n-5}$ |

Table 2. Extremal graphs with the first five maximal values.

| c-trees (n) | h-chains (n) | po-chains (n) | s-h-chains (n) | pe-chains (2n) |
| :--- | :--- | :--- | :--- | :--- |
| $T_{1}$ | $L A^{n-2} L$ | $L^{n}$ | $L^{n}$ | $L^{n}$ |
| $T_{2}$ | $L A L A^{n-4} L$ | $L^{3} A L^{n-4}$ | $L^{3} A L^{n-4}$ | $L^{3} A L^{n-4}$ |
| $T_{3}$ | $L A^{3} L A^{n-6} L$ | $L^{5} A L^{n-6}$ | $L^{5} A L^{n-6}$ | $L^{5} A L^{n-6}$ |
| $T_{4}$ | $L A^{5} L A^{n-8} L$ | $L^{7} A L^{n-8}$ | $L^{7} A L^{n-8}$ | $L^{7} A L^{n-8}$ |
| $T_{5}$ | $L A^{7} L A^{n-10} L$ | $L^{9} A L^{n-10}$ | $L^{9} A L^{n-10}$ | $L^{9} A L^{n-10}$ |

where (1) c-trees (n): caterpillar trees with $n$ edges; (2) h-chains (n): hexagonal chains with $n$ hexagons; (3) po-chains (n): polyomino chains with $n$ squares; (4) s-h-chains (n): square-hexagonal chains with $n$ cells; (5) pe-chains (2n): pentagonal chains with $2 n$ pentagons. $T_{1}=C_{n+1}(0, \cdots, 0), T_{2}=C_{n}(0,0,1,0, \cdots, 0), T_{3}=C_{n}(0,0,0,0,1,0, \cdots, 0)$, $T_{4}=C_{n}(0,0,0,0,0,0,1,0, \cdots, 0)$ and $T_{5}=C_{n}(0,0,0,0,0,0,0,0,1,0, \cdots, 0)$.

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    ${ }^{\dagger}$ Corresponding author: hydeng@hunnu.edu.cn

