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Six-membered ring spiro chains with extremal Merrifield-Simmons index and Hosoya index *

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Abstract. For any graph G, let $\sigma(G)$ and $Z(G)$ be the number of independent sets (i.e., the Merrifield-Simmons index) and the number of matchings (i.e., the Hosoya index) of G, respectively. It is well-known that two graph invariants $\sigma(G)$ and $Z(G)$ are important ones in structural chemistry. In this paper, we first definite the "Six-membered ring spiro chains" that can be considered as the graph representations of a subclass of unbranched multispiro molecules, in which every ring is six-membered ring. Next, we determine the six-membered spiro chains having extremal values of Merrifield-Simmons index and Hosoya index.

1. Introduction and notations

Spiro compounds are an important subclass of Cycloalkynes in Organic Chemistry. In Spiro compounds, a 'spiro union' is a linkage between two rings that consists of a single atom common to both rings and 'a free spiro union' is a linkage that consists of the only direct union between the rings. The common atom is designated as the 'spiro atom'. According to the number of spiro atoms present, compounds are distinguished as monospiro, dispiro, trispiro, etc., ring systems. Figure 1 illustrates three linear polyspiro alicyclic hydrocarbons.

In this paper, we consider a subclass of unbranched multispiro molecules, in which

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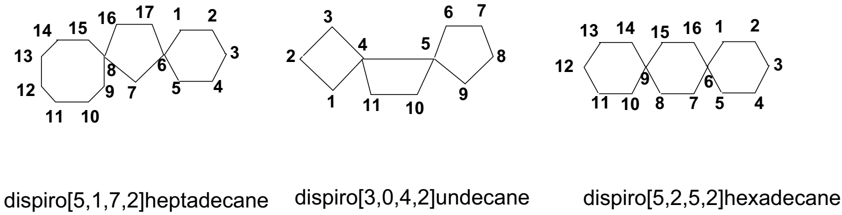

Figure 1:

every ring is six-membered ring, and the graph representations of them are called "six-membered ring spiro chains".

Definition 1: Two six-membered rings are have only one common vertex, this linkage is called *spiro union*, the common vertex is designated as *spiro vertex*.

Definition 2: A *six-membered ring spiro chains* is a graph consisting of n six-membered rings $H_1, H_2, \ldots, H_n$ with the properties that (i) For any $1 \leq k < j \leq n-1$, H_k and H_j are linked by spiro union if and only if j=k+1; (ii) The spiro vertex should be the vertex with degree four in the six-membered ring sprio chains.

We denote by $\mathscr{G}_n$ the set of the six-membered ring spiro chains with n six-membered rings. Any element G_n of $\mathscr{G}_n$ can be obtained from an appropriately chosen graph $G_{n-1} \in \mathscr{G}_{n-1}(n \geq 2)$ by spiro union a six-membered ring to the terminal of G_{n-1}. There are three non-isomorphic adding ways $G_{n-1} \rightarrow [G_{n-1}]_k$=$G_n$, where k=1,2,3 (see Figure 2). we call these three spiro union ways respectively: way-1, way-2, way-3.

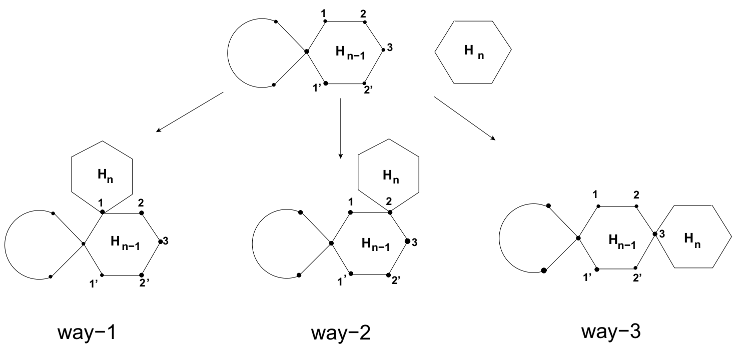

Figure 2:

In particular, if every six-membered ring in the six-membered ring spiro chains is added by the way-1, then denote by R_n; if every six-membered ring in the six-membered ring spiro chains is added by the way-2, then denote by S_n; if every six-membered ring in the six-membered ring spiro chains is added by the way-3, then denote by L_n. It is easy to see that $\mathscr{G}_1 = \{L_1 = S_1 = R_1\}$, $\mathscr{G}_2 = \{L_2 = S_2 = R_2\}$, $\mathscr{G}_3 = \{L_3, S_3, R_3\}$. Figure 3 illustrates R_n, S_n and L_n, respectively.

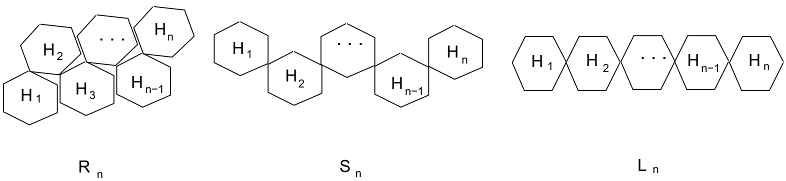

Figure 3:

Let $G = (V, E)$ be a graph with the vertex set $V(G)$ and the edge set $E(G)$. Let e and v be an edge and a vertex in G, respectively. We will denote by $G - e$ the graph obtained form G by removing edge e, and by $G - v$ the graph obtained from G by removing vertex v (and all its incident edges). Let S be a subset of $V(G)$. We denote by $G - S$ the graph obtained from G by removing all the vertices of S. Two vertices of a graph G are said to be independent if they are not adjacent. A subset I of $V(G)$ is called an independent set of G if any two vertices of I are independent in G. Two edges of a graph G are said to be independent if they are not incident. A subset M of $E(G)$ is called a matching of G if any two edges of M are independent in G. Undefined concepts and notations of graph theory are referred to [1].

For any graph G, we denote by $\sigma(G)$ and $Z(G)$ the numbers of independent sets and the numbers of matchings of G, respectively. It is well-known that two graph invariants $\sigma(G)$ and $Z(G)$ are important ones in structural chemistry [2, 3].

In the chemical graph theory, $\sigma(G)$ is called the Merrifield-Simmons index that was introduced by Merrifield and Simmons [2] in 1989. Details of chemical applications can be found in [3,4,5].

In the chemical graph theory, $Z(G)$ is called the Hosoya index that was introduced by Hosoya in 1971. This index was connected with various physico-chemical properties of alkanes, for example, boiling point, entropy and heat of vaporization. About the Hosoya index, there is an example showing the high correlation between the Hosoya index and the boiling points of acyclic alkanes in [6]. Details of chemical applications can be found in [4,7,8].

There have been numerous other new results on the Merrifield Simmons and Hosoya indices referred to [9-15].

2. Main results

In this paper, we show that the R_n and S_n attain the extremal graphs with extremal the Merrifield-Simmons index and the Hosoya index, respectively.

Theorem 2.1 For any $n \geq 1$ and any $G_n \in \mathscr{G}_n$, we have

(1) $\sigma(R_n) \leq \sigma(G_n)$, the equality hold if and only if $G_n = R_n$.

(2) $\sigma(G_n) \leq \sigma(S_n)$, the equality hold if and only if $G_n = S_n$.

Theorem 2.2 For any $n \geq 1$ and any $G_n \in \mathscr{G}_n$, we have

(3) $Z(S_n) \leq Z(G_n)$, the equality hold if and only if $G_n = S_n$.

(4) $Z(G_n) \leq Z(R_n)$, the equality hold if and only if $G_n = R_n$.

3. Proof of theorem 2.1

To complete the proof, we first list some useful results . Let G be a graph, $u \in V(G)$, denote by $N_G[u]$ the set $\{u\} \bigcup \{v|uv \in E(G)\}$.

Lemma 3.1[16] $\sigma(G) = \sigma(G-u) + \sigma(G - N_G[u])$.

Let P_n be a path of n vertices ($n \geq 1$), then $\sigma(P_{n+2}) = \sigma(P_{n+1}) + \sigma(P_n)$, and $\sigma(P_1) = 2$, $\sigma(P_2) = 3$.

Lemma 3.2[16] Let G be a graph consisting of two components G_1 and G_2, i.e., $G = G_1 + G_2$. Then $\sigma(G) = \sigma(G_1) \cdot \sigma(G_2)$.

Now let $G_i \in \mathscr{G}_i (i \geq 2)$, then G_i is the union of a six-membered ring spiro chains A with $i-1$ six-membered rings and a six-membered ring H_i in which A and H_i have only one common vertex. Let this common vertex be u (or $s = u$,) and $v_i, x_i, y_i, x_i^{'}, v_i^{'}, u$ be six vertices of H_i (see Figure 4). In fact, H_i is the i-th six-membered ring in $G_i (i \geq 2)$.

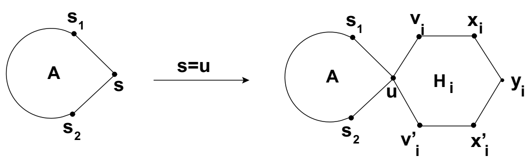

Figure 4: G_i

Next, we will show some lemmas below.

Lemma 3.3 Denote $G_i (i \geq 2)$ and A as above, shown in Figure 4. We have

(1) $\sigma(G_i - v_i) = 8\sigma(A-s) + 5\sigma(A - N_A[s])$

(2) $\sigma(G_i - x_i) = 10\sigma(A-s) + 3\sigma(A - N_A[s])$

(3) $\sigma(G_i - y_i) = 9\sigma(A-s) + 4\sigma(A - N_A[s])$.

Proof: By Lemma 3.1 and Lemma 3.2, we can compute

(1) $\sigma(G_i - v_i) = \sigma(G_i - v_i - u) + \sigma(G_i - v_i - N_{G_i}[u]))$
$= \sigma(A - s) \cdot \sigma(p_4) + \sigma(A - N_A[s]) \cdot \sigma(p_3)$
$= 8\sigma(A - s) + 5\sigma(A - N_A[s])$.

(2) $\sigma(G_i - x_i) = \sigma(G_i - x_i - u) + \sigma(G_i - x_i - N_{G_i}[u])$
$=\sigma(A - s) \cdot \sigma(p_1) \cdot \sigma(p_3) + \sigma(A - N_A[s]) \cdot \sigma(p_2)$
$=10\sigma(A - s) + 3\sigma(A - N_A[s])$.

(3) $\sigma(G_i - y_i) = \sigma(G_i - y_i - u) + \sigma(G_i - y_i - N_{G_i}[u])$
$=\sigma(A - s) \cdot \sigma(p_2) \cdot \sigma(p_2) + \sigma(A - N_A[s]) \cdot \sigma(p_1) \cdot \sigma(p_1)$
$=9\sigma(A - s) + 4\sigma(A - N_A[s])$.

So the proof is completed. ■

Lemma 3.4 Denote $G_i (i \geq 2)$ and A as above, shown in Figure 4. We have that $\sigma(G_i - v_i) < \sigma(G_i - y_i) < \sigma(G_i - x_i)$.

Proof: By Lemma 3.3 and Lemma 3.1, we have

$\sigma(G_i - y_i) - \sigma(G_i - v_i) = \sigma(A - s) - \sigma(A - N_A[s]) > 0$

$\sigma(G_i - x_i) - \sigma(G_i - y_i) = \sigma(A - s) - \sigma(A - N_A[s]) > 0$

Hence, we obtain that $\sigma(G_i - v_i) < \sigma(G_i - y_i) < \sigma(G_i - x_i)$. ■

Let $A \in \mathscr{G}_{i-1}$, $B \in \mathscr{G}_{n-i}$, and H_i be a six-membered ring. G_i is the union of the six-membered ring spiro chain with $i - 1$ six-membered rings A and a six-membered ring H_i in which A and H_i have only one common vertex. Let this common vertex be u (or s, $s = u$) and $v_i, x_i, y_i, x_i^{'}, v_i^{'}, u$ be six vertices of H_i. Denote by $G_n(i, k) \in \mathscr{G}_n (n \geq 3)$ obtained from G_i and B in which spiro union B to H_i by way-k (k=1,2,3), furthermore, when k=1,2,3, $t = v_i, x_i, y_i$, respectively(see Figure 5). In fact, H_i is the i-th six-membered ring in $G_n (n \geq 3)$.

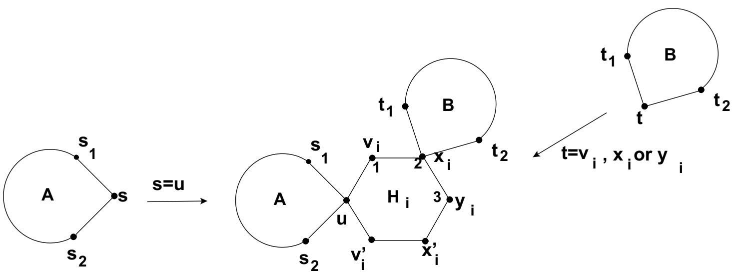

Figure 5: $G_n = G_n(i, k)$

Now we consider to compare $\sigma(G_n(i, 1)), \sigma(G_n(i, 2)), \sigma(G_n(i, 3))$.

Lemma 3.5 Let $G_n = G_n(i,k) \in \mathscr{G}_n(n \geq 3)$, denote $G_n(i,k)$, A and B as above, shown in Figure 5. We have that $\sigma(G_n(i,1)) < \sigma(G_n(i,3)) < \sigma(G_n(i,2))$.

Proof: By computing, we have

$\sigma(G_n(i,1)) = \sigma(G_n(i,1) - t_1) + \sigma(G_n(i,1) - N_{G_n}[t_1])$

$=\sigma(G_n(i,1) - t_1 - t_2) + \sigma(G_n(i,1) - t_1 - N_{G_n}[t_2]) + \sigma(G_n(i,1) - N_{G_n}[t_1])$

$=\sigma(G_i) \cdot \sigma(B - N_B[t]) + \sigma(G_i - v_i) \cdot \sigma(B - t_1 - N_B[t_2]) + \sigma(G_i - v_i) \cdot \sigma(B - N_B[t_1])$

$=\sigma(G_i) \cdot \sigma(B - N_B[t]) + \sigma(G_i - v_i)[\sigma(B - t_1 - N_B[t_2]) + \sigma(B - N_B[t_1])]$

$\sigma(G_n(i,2)) = \sigma(G_n(i,2) - t_1) + \sigma(G_n(i,2) - N_{G_n}[t_1])$

$=\sigma(G_n(i,2) - t_1 - t_2) + \sigma(G_n(i,2) - t_1 - N_{G_n}[t_2]) + \sigma(G_n(i,2) - N_{G_n}[t_1])$

$=\sigma(G_i) \cdot \sigma(B - N_B[t]) + \sigma(G_i - x_i) \cdot \sigma(B - t_1 - N_B[t_2]) + \sigma(G_i - x_i) \cdot \sigma(B - N_B[t_1])$

$=\sigma(G_i) \cdot \sigma(B - N_B[t]) + \sigma(G_i - x_i)[\sigma(B - t_1 - N_B[t_2]) + \sigma(B - N_B[t_1])]$

$\sigma(G_n(i,3)) = \sigma(G_n(i,3) - t_1) + \sigma(G_n(i,3) - N_{G_n}[t_1])$

$=\sigma(G_n(i,3) - t_1 - t_2) + \sigma(G_n(i,3) - t_1 - N_{G_n}[t_2]) + \sigma(G_n(i,3) - N_{G_n}[t_1])$

$=\sigma(G_i) \cdot \sigma(B - N_B[t]) + \sigma(G_i - y_i) \cdot \sigma(B - t_1 - N_B[t_2]) + \sigma(G_i - y_i) \cdot \sigma(B - N_B[t_1])$

$=\sigma(G_i) \cdot \sigma(B - N_B[t]) + \sigma(G_i - y_i)[\sigma(B - t_1 - N_B[t_2]) + \sigma(B - N_B[t_1])]$

By Lemma 3.4, we get that $\sigma(G_n(i,3)) - \sigma(G_n(i,1)) > 0$ and $\sigma(G_n(i,2)) - \sigma(G_n(i,3)) > 0$. Hence, we obtain that $\sigma(G_n(i,1)) < \sigma(G_n(i,3)) < \sigma(G_n(i,2))$.■

Following ref.[17], we denote by $[G]_k$ the six-membered ring spiro chain obtained from G by way-k attaching to it a new six-membered ring H, where $k \in \{1,2,3\}$. Obviously, every $G_n(n \geq 2)$ can be written as $[\cdots[[[L_2]_{k_2}]_{k_3}]\cdots]_{k_{n-1}}$, where $k_i \in \{1,2,3\}(i = 2,3,\cdots,n-1)$, we set $G_n = 3k_2k_3\cdots k_{n-1}$ for short. For every i, if $k_i = 3$ then $G_n = L_n$, $k_i = 1$ then $G_n = Z_n$, and $k_i = 2$ then $G = S_n$.

Proof of theorem 2.1

(1) Let $G_n \in \mathscr{G}_n$ be the six-membered ring spiro chain with the smallest number of independent. We show that $G_n = R_n$. Since $G_1 = R_1$, $G_2 = R_2$, we may assume that $n \geq 3$. Let $G_n = 3k_2k_3\cdots k_{n-1}$ and $R_n = \underbrace{31\cdots1}_{n-1}$.

Suppose that $G_n \neq R_n$, let k_i be the first element of $k_2, k_3, \cdots, k_{n-1}$, such that $k_i \neq 1$. We discuss the following two cases.

Case 1: If $k_i = 2$, i.e., $G_n = \underbrace{31\cdots1}_{i-1}2k_{i+1}\cdots k_{n-1}$, let $G_n' = \underbrace{31\cdots1}_{i-1}1k_{i+1}\cdots k_{n-1}$, by lemma 3.5, $\sigma(G_n') < \sigma(G_n)$. This produces a contradiction, so that $G_n = \underbrace{31\cdots1}_{n-1}$, i.e., $G_n = R_n$.

Case 2: If $k_i = 3$, by a similar way of proof in case 1 we obtain it.

(2) By a similar method of proof in part (1), we have the second part of theorem 2.1.

The proof of theorem 2.1 is completed.■

4. Proof of theorem 2.2

We note that the method of the proof of theorem 2.1 is also applicable to prove

Theorem 2.2. It is interesting that the frames of the proofs are just same as that in theorem 2.1. First, we list some useful results.

Lemma 4.1[16] Let G be a graph. Suppose $uv \in E(G)$. Then $Z(G) = Z(G-uv) + Z(G-u-v)$

Let P_n be a path of n vertices ($n \geq 1$), then $Z(P_{n+2}) = Z(P_{n+1}) + Z(P_n)$, and $Z(P_1) = 1$, $Z(P_2) = 2$.

Lemma 4.2[16] Let G be a graph consisting of two components G_1 and G_2, i.e., $G = G_1 + G_2$. Then $Z(G) = Z(G_1) \cdot Z(G_2)$

Next, we show some lemmas below.

Lemma 4.3 Denote $G_i (i \geq 2)$ and A as above, shown in Figure 4. We have

(1) $Z(G_i - v_i) = 8Z(A-s) + 5[Z(A-s-s_2) + Z(A-s-s_1)]$

(2) $Z(G_i - x_i) = 8Z(A-s) + 3[Z(A-s-s_2) + Z(A-s-s_1)]$

(3) $Z(G_i - y_i) = 8Z(A-s) + 4[Z(A-s-s_2) + Z(A-s-s_1)]$.

Proof: By Lemma 4.1 and Lemma 4.2, we can compute

(1) $Z(G_i - v_i) = Z(G_i - v_i - us_1) + Z(G_i - v_i - u - s_1)$

$=Z(G_i - v_i - us_1 - us_2) + Z(G_i - v_i - us_1 - u - s_2) + Z(G_i - v_i - u - s_1)$

$=Z(A-s) \cdot Z(p_5) + Z(A-s-s_2) \cdot Z(p_4) + Z(A-s-s_1) \cdot Z(p_4)$

$=8Z(A-s) + 5[Z(A-s-s_2) + Z(A-s-s_1)]$

(2) $Z(G_i - x_i) = Z(G_i - x_i - us_1) + Z(G_i - x_i - u - s_1)$

$=Z(G_i - x_i - us_1 - us_2) + Z(G_i - x_i - us_1 - u - s_2) + Z(G_i - x_i - u - s_1)$

$=Z(A-s) \cdot Z(p_5) + Z(A-s-s_2) \cdot Z(p_3) \cdot Z(p_1) + Z(A-s-s_1) \cdot Z(p_1) \cdot Z(p_3)$

$=8Z(A-s) + 3[Z(A-s-s_2) + Z(A-s-s_1)]$

(3) $Z(G_i - y_i) = Z(G_i - y_i - us_1) + Z(G_i - y_i - u - s_1)$

$=Z(G_i - y_i - us_1 - us_2) + Z(G_i - y_i - us_1 - u - s_2) + Z(G_i - y_i - u - s_1)$

$=Z(A-s) \cdot Z(p_5) + Z(A-s-s_2) \cdot Z(p_2) \cdot Z(p_2) + Z(A-s-s_1) \cdot Z(p_2) \cdot Z(p_2)$

$=8Z(A-s) + 4[Z(A-s-s_2) + Z(A-s-s_1)]$

The lemma is completed.■

By Lemma 4.3 and lemma 4.1, we have that

Lemma 4.4 Denote $G_i (i \geq 2)$ and A as above, shown in Figure 4. Then $Z(G_i - x_i) < Z(G_i - y_i) < Z(G_i - v_i)$.

Lemma 4.5 Let $G_n = G_n(i,k) \in \mathscr{G}_n (n \geq 3)$, denote $G_n(i,k)$, A and B as above, shown in Figure 5. Then $Z(G_n(i,2)) < Z(G_n(i,3)) < Z(G_n(i,1))$.

Proof: We can compute,

$$
\begin{aligned}
Z(G_n(i,1)) &= Z(G_n(i,1) - v_i t_1) + Z(G_n(i,1) - v_i - t_1) \\
&= Z(G_n(i,1) - v_i t_1 - v_i t_2) + Z(G_n(i,1) - v_i t_1 - v_i - t_2) + Z(G_n(i,1) - v_i - t_1) \\
&= Z(G_i) \cdot Z(B-t) + Z(G_i - v_i) \cdot Z(B-t-t_2) + Z(G - v_i) \cdot Z(B-t-t_1) \\
&= Z(G_i) \cdot Z(B-t) + Z(G_i - v_i)[Z(B-t-t_2) + Z(B-t-t_1)]
\end{aligned}
$$

$Z(G_n(i,2)) = Z(G_n(i,2) - x_i t_1) + Z(G_n(i,2) - x_i - t_1)$

$$
\begin{aligned}
&= Z(G_n(i,2)-x_it_1-x_it_2)+Z(G_n(i,2)-x_it_1-x_i-t_2)+Z(G_n(i,2)-x_i-t_1)\\
&= Z(G_i)\cdot Z(B-t)+Z(G_i-x_i)\cdot Z(B-t-t_2)+Z(G-x_i)\cdot Z(B-t-t_1)\\
&= Z(G_i)\cdot Z(B-t)+Z(G_i-x_i)[Z(B-t-t_2)+Z(B-t-t_1)]\\
Z(G_n(i,3)) &= Z(G_n(i,3)-y_it_1)+Z(G_n(i,3)-y_i-t_1)\\
&= Z(G_n(i,3)-y_it_1-y_it_2)+Z(G_n(i,3)-y_it_1-y_i-t_2)+Z(G_n(i,3)-y_i-t_1)\\
&= Z(G_i)\cdot Z(B-t)+Z(G_i-y_i)\cdot Z(B-t-t_2)+Z(G-y_i)\cdot Z(B-t-t_1)\\
&= Z(G_i)\cdot Z(B-t)+Z(G_i-y_i)[Z(B-t-t_2)+Z(B-t-t_1)]
\end{aligned}
$$

By lemma 4.4, we get $Z(G_n(i,3))-Z(G_n(i,2))>0$ and $Z(G_n(i,1))-Z(G_n(i,3))>0$. Hence, $Z(G_n(i,2))<Z(G_n(i,3))<Z(G_n(i,1))$.

This completes the proof of lemma 4.5. ■

By similar means of proof of theorem 2.1, we can prove theorem 2.2.

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