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Extremal Merrifield–Simmons Index and Hosoya Index of Polyphenyl Chains[1]

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Abstract: "The polyphenyl chains" is a graph consisting of n benzene rings B_1, $B_2, \cdots, B_n$ with the properties that for any $1 \leq k < j \leq n-1, B_k$ and B_j are linked by a cut edge if and only if $j = k+1$, the common vertex of a benzene ring and a cut edge is a vertex with degree three. *Merrifield-Simmons index* [1] and *Hosoya index* [2] are the two valuable topological indices in chemical graph theory. In this paper, we discuss the Merrifield-Simmons index and Hosoya index of polyphenyl chains and obtain some extremal results: among all polyphenyl chains, the S_n and Z_n attain the extremal values of Merrifield-Simmons index and Hosoya index, respectively.

1. Introduction and notations

For this topic, two or more benzene rings are linked by a cut edge consisting of aromatics called polycyclic aromatic hydrocarbons which is a class of aromatics. A kind of compounds which two or more benzene rings are directly linked by cut edge known as the biphenyl compounds. For example: Ortho-terphenyl, Meta-terphenyl and Pera-terphenyl (see Figure-1).

First, Let us give some basic concepts. The *polyphenyl chains* is a graph consisting of n benzene rings $B_1, B_2, \cdots, B_n$ with the properties that for any $1 \leq k < j \leq$

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$n-1$, B_k and B_j are linked by a cut edge if and only if $j = k+1$, the common vertex of a benzene ring and a cut edge is a vertex with degree three.

The "polyphenyl chains" can be considered as the graph representation of an important subclass of Linear unbranched polyphenyl simplified skeletons molecules. We are trying to find the extremal Merrifield-Simmons index and Hosoya index of polyphenyl chains. This will help study the thermodynamic stability and chemical structure of biphenyl compounds.

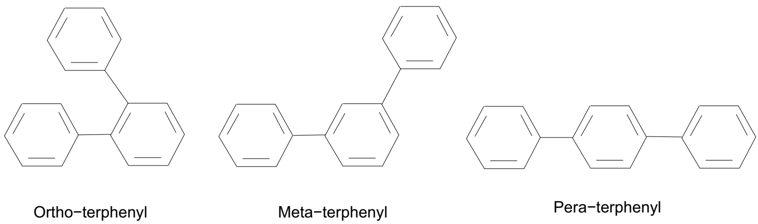

Figure 1

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

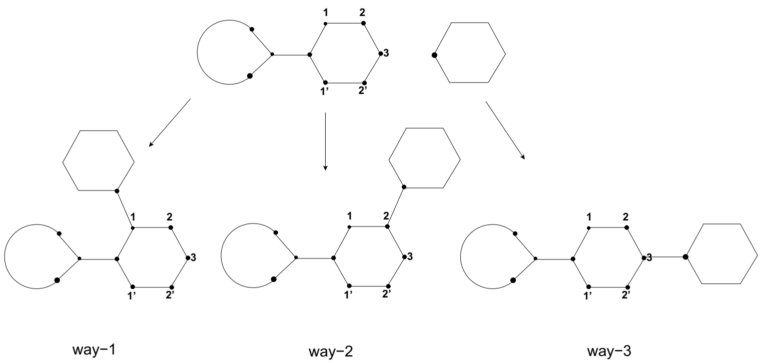

Figure 2

In particular, if every benzene ring in the polyphenyl chains is added by the way-1, then denote by Z_n; if every benzene ring in the polyphenyl chains is added by the way-2, then denote by S_n; if every benzene ring in the polyphenyl chains is added by the way-3, then denote by L_n. Obviously, $\mathscr{G}_1 = \{L_1\} = \{Z_1\} = \{S_1\}$, $\mathscr{G}_2 = \{L_2\} = \{Z_2\} = \{S_2\}$, $\mathscr{G}_3 = \{L_3, Z_3, S_3\}$. Graph L_n, Z_n and S_n of $\mathscr{G}_n$ are shown in Figure-3.

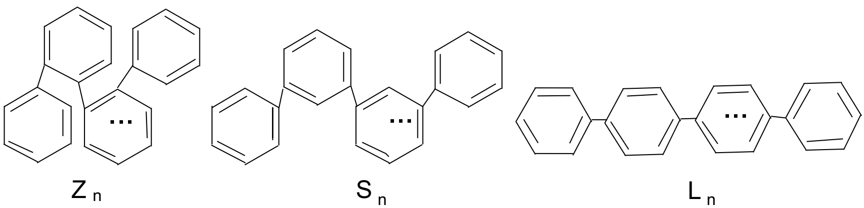

Figure 3

In this paper, we will prove that the S_n and Z_n of polyphenyl chains attain the extremal values of Merrifield-Simmons index and Hosoya index, respectively.

Note that the polyphenyl chains considered by us include both geometrially planar (e.g., L_n, Z_n, and S_n) and geometrially non-planar (e.g., L_n, Z_n and S_n) species.

Let e and v be an edge and a vertex of a graph $G(V, E)$, respectively. Denote by $G - e$ and $G - v$ the graph obtained from G by removing e and v, respectively. Undefined concepts and notations of graph theory are referred to [3].

In chemical terminology, the Merrifield-Simmons index of a molecular graph G is defined to be the total number of its independent sets (include empty set), where a independent set is a subset I of the $V(G)$ of G with the property that no two different vertices of I share a common edge, denote by $\sigma(G)$. Details of chemical applications can be found in [1,5,6].

The Hosoya index of a molecular graph G is defined to be the total number of its matchings (include empty set), where a matching is a subset M of the $E(G)$ of G with the property that no two different edges of M share a common vertex, denote by $m(G)$. This index was connected with various physico-chemical properties of alkanes, for example, boiling point, entropy, heat of vaporization. There is an example showing the high correlation between the Hosoya index and the boiling points of acyclic alkanes in [4]. Details of chemical applications can be found in [5,7,8].

There have been numerous other new results on the Hosoya and Merrifield Simmons indices are referred to [10-16].

2. Some useful results

Among polyphenyl chains with extremal properties on topological indices, S_n and Z_n play important roles. In order to obtain the result about the Hosoya index and Merrifield-Simmons index,we need some auxiliary lemmas.

Lemma 2.1 [9] Let G be a graph, suppose $u \in V(G)$, denote by $N_G[u]$ the set $\{u\} \bigcup \{v|uv \in E(G)\}$

(a) Suppose $u \in V(G)$, then $\sigma(G) = \sigma(G-u) + \sigma(G - N_G[u])$ (1)

(b) Suppose $uv \in E(G)$, then $m(G) = m(G-uv) + m(G-u-v)$ (2)

Lemma 2.2 [9] Let G be a graph consisting of two components G_1 and G_2, i.e., $G = G_1 \cup G_2$, we have

(a) $\sigma(G) = \sigma(G_1)\sigma(G_2)$ (3)

(b) $m(G) = m(G_1)m(G_2)$ (4)

3. Main result and proofs

Let A be a polyphenyl chains with $i-1 (i \geq 2)$ benzene rings, B_i is attached in the vertex s of A, and denoted by G_i. Let C be a polyphenyl chains with $n-i$ $(n > i)$ benzene rings, the graph C is added by way-1, way-2 or way-3 in the i-th benzene ring B_i, denoted by $G_n(i,1)$, $G_n(i,2)$ or $G_n(i,3)$ respectively (see Figure-4).

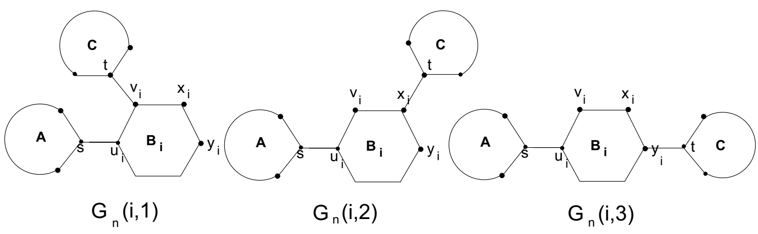

Figure 4

Now we consider to compare the number of independent sets (i.e., the Merrifield-Simmons index) of $G_n(i,1),\ G_n(i,2)$ and $G_n(i,3)$. First, we show Lemma 3.1 followed.

Lemma 3.1 $\sigma(G_i - v_i) \leq \sigma(G_i - y_i) \leq \sigma(G_i - x_i)$, where the vertices $v_i,\ y_i$ and x_i are in the graph B_i (see Figure-4).

Proof: Obviously, $\sigma(G_1 - v_1) = \sigma(G_1 - y_1) = \sigma(G_1 - x_1)$.

Now we suppose that $i \geq 2$.

Applying (1) and (3) to $(G_i - v_i),\ (G_i - y_i)$ and $(G_i - x_i)$, we get

$$\begin{aligned}\sigma(G_i - v_i) &= \sigma(G_i - v_i - s) + \sigma(G_i - v_i - N_{G_i}[s])\\ &= \sigma(A - s)\sigma(P_5) + \sigma(A - N_A[s])\sigma(P_4)\\ &= 13\sigma(A - s) + 8\sigma(A - N_A[s])\end{aligned}$$

$$\begin{aligned}\sigma(G_i - x_i) &= \sigma(G_i - x_i - s) + \sigma(G_i - x_i - N_{G_i}[s])\\ &= \sigma(A - s)\sigma(P_5) + \sigma(A - N_A[s])\sigma(P_1)\sigma(P_3)\\ &= 13\sigma(A - s) + 10\sigma(A - N_A[s])\end{aligned}$$

$$\begin{aligned}\sigma(G_i - y_i) &= \sigma(G_i - y_i - s) + \sigma(G_i - y_i - N_{G_i}[s])\\ &= \sigma(A - s)\sigma(P_5) + \sigma(A - N_A[s])\sigma(P_2)\sigma(P_2)\\ &= 13\sigma(A - s) + 9\sigma(A - N_A[s])\end{aligned}$$

Hence, we have $\sigma(G_i - v_i) - \sigma(G_i - y_i) < 0,\ \ \sigma(G_i - y_i) - \sigma(G_i - x_i) < 0$.

Then $\sigma(G_i - v_i) \leq \sigma(G_i - y_i) \leq \sigma(G_i - x_i)$ is obtained. ∎

Lemma 3.2 $\sigma(G_n(i,1)) \leq \sigma(G_n(i,3)) \leq \sigma(G_n(i,2))$ (see Figure-4).

Proof: It is obvious for $n = 1, 2$.

Applying (1) and (3) to $G_n(i,1),\ G_n(i,2)$ and $G_n(i,3)$ for $n \geq 3$, we get

$$\begin{aligned}\sigma(G_n(i,1)) &= \sigma(G_n(i,1) - t) + \sigma(G_n(i,1) - N_{G_n(i,1)}[t])\\ &= \sigma(G_i)\sigma(C - t) + \sigma(G_i - v_i)\sigma(C - N_C[t])\end{aligned}$$

$$\begin{aligned}\sigma(G_n(i,2)) &= \sigma(G_n(i,2) - t) + \sigma(G_n(i,2) - N_{G_n(i,2)}[t])\\ &= \sigma(G_i)\sigma(C - t) + \sigma(G_i - x_i)\sigma(C - N_C[t])\end{aligned}$$

$$\begin{aligned}\sigma(G_n(i,3)) &= \sigma(G_n(i,3) - t) + \sigma(G_n(i,3) - N_{G_n(i,3)}[t])\\ &= \sigma(G_i)\sigma(C - t) + \sigma(G_i - y_i)\sigma(C - N_C[t])\end{aligned}$$

By Lemma 3.1, we obtain $\sigma(G_n(i,1)) \leq \sigma(G_n(i,3)) \leq \sigma(G_n(i,2))$. ∎

Let G_n be a polyphenyl chains, we denote by G_n the polyphenyl chains that a new benzene ring B is attached to G_{n-1} by way-k, where $k \in \{1,2,3\}$. Obviously, each G_n with $n \geq 3$ 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.

Theorem 3.3 For any $n \geq 1$ and any $G_n \in \mathscr{G}_n$,

(1) If $G_n \neq S_n$, then $\sigma(G_n) < \sigma(S_n)$

(2) If $G_n \neq Z_n$, then $\sigma(Z_n) < \sigma(G_n)$

Proof: (1) Let $G_n \in \mathscr{G}_n$ be the polyphenyl chains with the largest number of independent sets.

When $n = 1, 2$, $G_n = S_n$.

When $n \geq 3$, suppose $G_n \neq S_n$, let k_i be the first element of $k_2, k_3, \cdots, k_{n-1}$ such that $k_i \neq 2$. That is $G_n = 32 \cdots 2k_ik_{i+1} \cdots k_{n-1}$, where $k_i = 1$ or 3. Assume, without loss of generality, that $k_i = 1$.

Let $G_n^{'} = 32 \cdots 2k_{i+1} \cdots k_{n-1}$. By lemma 3.2, we have $\sigma(G_n) < \sigma(G_n^{'})$, this is a contradiction.

(2) Let $G_n \in \mathscr{G}_n$ be the polyphenyl chains with the smallest number of independent sets. By a similar proof of Theorem 3.3 (1), we have the proof of Theorem 3.3 (2). ■

We complete the proof of Theorem 3.3 and obtain the polyphenyl chains with the largest number of independent sets and the smallest number of independent sets.

Now we consider to compare the numbers of matchings (i.e., the Hosoya index) of $G_n(i, 1)$, $G_n(i, 2)$ and $G_n(i, 3)$ respectively.

By a similar argument of lemma 3.1 and lemma 3.2, we have lemma 3.4 and lemma 3.5 followed.

Lemma 3.4 $m(G_i - x_i) \leq m(G_i - y_i) \leq m(G_i - v_i)$, where the vertices v_i, y_i and x_i are in the graph B_i (see Figure-4).

Lemma 3.5 $m(G_n(i, 2)) \leq m(G_n(i, 3)) \leq m(G_n(i, 1))$ (see Figure-4).

Theorem 3.6 For any $n \geq 1$ and any $G_n \in \mathscr{G}_n$,

(1) If $G_n \neq S_n$, then $m(S_n) < m(G_n)$

(2) If $G_n \neq Z_n$, then $m(G_n) < m(Z_n)$

Proof: By a similar proof of Theorem 3.3, we have the proof of Theorem 3.6. ■

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