Extremal Hosoya index and Merrifield–Simmons index of hexagonal spiders

W.C. Shiu

Department of Mathematics, Hong Kong Baptist University, Kowloon Tong, Hong Kong, China

Received 13 July 2007; received in revised form 11 December 2007; accepted 9 January 2008
Available online 4 March 2008

Abstract

For any graph $G$, let $m(G)$ and $i(G)$ be the numbers of matchings (i.e., the Hosoya index) and the number of independent sets (i.e., the Merrifield–Simmons index) of $G$, respectively. In this paper, we show that the linear hexagonal spider and zig-zag hexagonal spider attain the extremal values of Hosoya index and Merrifield–Simmons index, respectively.

Keywords: Hexagonal spider; Hosoya index; Merrifield–Simmons index

1. Introduction and notations

A \textit{hexagonal system} is a 2-connected plane graph whose every interior face is bounded by a regular hexagon. Hexagonal systems are of great importance for theoretical chemistry because they are the natural graph representation of benzenoid hydrocarbons \cite{7}. A considerable amount of research in mathematical chemistry has been devoted to hexagonal systems \cite{7–9}.

Suppose $H$ is a hexagonal system. Denote by $H_C$ the graph whose vertex set is the set of the centers of hexagons in $H$, and edge set is the set of straight lines connecting the centers of any two adjacent hexagons. The graph $H_C$ is called the \textit{centroid-induced graph} of $H$. A hexagonal system $H$ is called a \textit{hexagonal chain} if the graph $H_C$ is a path. Hexagonal chains are the graph representations of an important subclass of benzenoid molecules, unbranched catacondensed benzenoid molecules, which play a distinguished role in the theoretical chemistry of benzenoid hydrocarbons. The extremal graphs with respect to some useful topological indices in chemical applications have been extensively studied, and many results concerning this topic can be found in \cite{2–4,6–10,12,15,16,19–23}. In this paper, we shall consider a subclass of branched catacondensed benzenoid molecules which are called hexagonal spiders.

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. Denote by $N_v$ the set $\{u \in V \mid vu \in E\} \cup \{v\}$. Let $V'$ be a...
Let $G$ be a graph. For each $u \in V$, the subgraph of $G$ induced by $V'$ is denoted by $G[V']$, and $G[V \setminus V']$ is denoted by $G - V'$. Undefined concepts and notations of graph theory are referred to [1].

Two edges of a graph $G$ are said to be independent if they are not adjacent. A subset $M$ of $E(G)$ is called a matching of $G$ if any two edges of $M$ are independent in $G$. Denote by $m(G)$ the number of matchings of $G$. In chemical terminology, $m(G)$ is called the Hosoya index. 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 [18]. Details of chemical applications can be found in [5,12,13].

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. Denote $i(G)$ the number of independent sets of $G$. In chemical terminology, $i(G)$ is called the Merrifield–Simmons index, which was introduced by Merrifield and Simmons [14] in 1989. Details of chemical applications can be found in [5,14,17].

Clearly, the Hosoya index or the Merrifield–Simmons index of a graph is larger than that of its proper subgraphs. These indices can be determined from the values of smaller graphs (please see Lemmas 2.3, 2.4 and 2.6).

Fig. 1. $L_5$ and $Z_5$.

Suppose $v$ is a vertex of a graph $G$ of degree $k$. We called that $v$ is a $k$-vertex (of $G$). We denote by $\mathcal{C}_n$ the set of the hexagonal chains with $n$ hexagons. Let $B_n \in \mathcal{C}_n$. We denote by $V_3 = V_3(B_n)$ the set of all 3-vertices of $B_n$. Thus the subgraph $B_n[V_3]$ is an acyclic graph. If the subgraph $B_n[V_3]$ is a matching with $n - 1$ edges, then $B_n$ is called a linear chain and is denoted by $L_n$. If the subgraph $B_n[V_3]$ is a path, then $B_n$ is called a zig-zag chain and denoted by $Z_n$. Fig. 1 illustrates $L_5$ and $Z_5$, respectively, where $B_5[V_3]$ are indicated by heavy edges.

2. Some useful results

Among hexagonal chains with extremal properties on topological indices, $L_n$ and $Z_n$ play important roles. We list some of them about the Hosoya index and Merrifield–Simmons index as follows.

**Theorem 2.1** ([10,19]). For any $n \geq 1$ and any $B_n \in \mathcal{C}_n$, if $B_n$ is neither $L_n$ nor $Z_n$, then

$$m(L_n) < m(B_n) < m(Z_n).$$

**Theorem 2.2** ([10,19]). For any $n \geq 1$ and any $B_n \in \mathcal{C}_n$, if $B_n$ is neither $L_n$ nor $Z_n$, then

$$i(Z_n) < i(B_n) < i(L_n).$$

Among many properties of $m(G)$ and $i(G)$, we mention the following results which will be used later [11,14].

**Lemma 2.3.** Let $G$ be a graph consisting of two components $G_1$ and $G_2$, i.e., $G = G_1 + G_2$. Then

(a) $m(G) = m(G_1)m(G_2)$;
(b) $i(G) = i(G_1)i(G_2)$.

**Lemma 2.4.** Let $G$ be a graph.

(a) Suppose $uv \in E(G)$. Then $m(G) = m(G - uv) + m(G - u - v)$.
(b) Suppose $u \in V(G)$. Then $i(G) = i(G - u) + i(G - N_u)$.

**Lemma 2.5.** Let $G$ be a graph. For each $uv \in E(G)$,

(a) $m(G) - m(G - u) - m(G - u - v) \geq 0$;
(b) $i(G) - i(G - u) - i(G - u - v) \leq 0$.

Moreover, the equalities hold only if $v$ is the unique neighbor of $u$. 

Suppose $G$ is the union of a graph $A$ and a 6-cycle $C$ in which $A$ and $C$ have only one common edge. Let this common edge be $xy$ and let the cycle $C$ be $abcdxy$ (i.e., $a, b, c, d, x, y$ are vertices of $C$) (see Fig. 2). We shall denote $G$ by $A@^\gamma_3 C$. By Lemmas 2.3 and 2.4 we have the following lemma.

**Lemma 2.6.** Suppose $G = A@^\gamma_3 C$ is defined above. Then

\[
\begin{pmatrix}
m(G) \\
m(G - a) \\
m(G - b) \\
m(G - c) \\
m(G - d) \\
m(G - a - b) \\
m(G - b - c) \\
m(G - c - d)
\end{pmatrix} =
\begin{pmatrix}
5 & 3 & 3 & 2 \\
3 & 0 & 2 & 0 \\
2 & 2 & 1 & 1 \\
2 & 1 & 2 & 1 \\
3 & 2 & 0 & 0 \\
2 & 0 & 1 & 0 \\
1 & 1 & 1 & 1 \\
2 & 1 & 0 & 0
\end{pmatrix}
\begin{pmatrix}
m(A) \\
nm(A - x) \\
nm(A - y) \\
nm(A - x - y)
\end{pmatrix}
\]

(2.1)

and

\[
\begin{pmatrix}
i(G) \\
i(G - a) \\
i(G - b) \\
i(G - c) \\
i(G - d) \\
i(G - a - b) \\
i(G - b - c) \\
i(G - c - d)
\end{pmatrix} =
\begin{pmatrix}
3 & 2 & 2 & 1 \\
3 & 0 & 2 & 0 \\
2 & 2 & 1 & 1 \\
2 & 1 & 2 & 1 \\
3 & 2 & 0 & 0 \\
2 & 0 & 1 & 0 \\
1 & 1 & 1 & 1 \\
2 & 1 & 0 & 0
\end{pmatrix}
\begin{pmatrix}
i(A) \\
ni(A - x) \\
ni(A - y) \\
ni(A - x - y)
\end{pmatrix}
\]

(2.2)

For the detailed computation on obtaining the above relations, one may find a similar computation from [16].

**Corollary 2.7.** Suppose $A_1$ and $A_2$ are two graphs containing a common edge $xy$. Let $G_1 = A_1@^\gamma_3 C$ and $G_2 = A_2@^\gamma_3 C$, where $C$ is the 6-cycle $abcdyx$.

(a) If $m(A_1) > m(A_2)$, $m(A_1 - x) > m(A_2 - x)$, $m(A_1 - y) > m(A_2 - y)$ and $m(A_1 - x - y) > m(A_2 - x - y)$, then $m(G_1) > m(G_2)$, $m(G_1 - u) > m(G_2 - u)$ and $m(G_1 - v - w) > m(G_2 - v - w)$.

(b) If $i(A_1) < i(A_2)$, $i(A_1 - x) < i(A_2 - x)$, $i(A_1 - y) < i(A_2 - y)$ and $i(A_1 - x - y) < i(A_2 - x - y)$, then $i(G_1) < i(G_2)$, $i(G_1 - u) < i(G_2 - u)$ and $i(G_1 - v - w) < i(G_2 - v - w)$.

Here $u \in \{a, b, c, d\}$ and $vw \in \{ab, bc, cd\}$.

3. Attaching process

Let $A$ and $B$ be any graphs and $C$ be a hexagon. Let $G = A@^\gamma_3 C$. Let $r$ and $s$ be two adjacent vertices of $B$ of at least degree two. Denote by $G_rB$ the graph obtained from $G$ and $B$ by identifying the edge $ab$ with $rs$; by $G_B$ from $G$ and $B$ by identifying $bc$ with $rs$; by $G_\xi B$ from $G$ and $B$ by identifying $cd$ with $rs$ (see Fig. 3).

**Lemma 3.1** ([16]). Let $A$, $B$, $G = A@^\gamma_3 C$, $G_\eta B$ and $G_\xi B$ be shown in Fig. 3. We have

(a) if $m(A - x) > m(A - y)$, then $m(G_\xi B) > m(G_\eta B)$;

(b) if $i(A - x) < i(A - y)$, then $i(G_\xi B) < i(G_\eta B)$.
Lemma 3.2. Let $A$, $B$, $G = A \circ \varepsilon C$, $G_\eta B$, $G_\beta B$ and $G_\zeta B$ be shown in Fig. 3. Then $m(G_\eta B) > m(G_\beta B)$, $m(G_\zeta B) > m(G_\beta B)$ and $i(G_\eta B) < i(G_\beta B)$, $i(G_\beta B) < i(G_\zeta B)$.

Proof. Similar to the proof of Lemma 3.2 in [16] we have $m(G_\eta B) - m(G_\beta B) = [m(A) - m(A - x) - m(B - x - y)] [m(B) - m(B - s) - m(B - r - s)]$. By Lemma 2.5 we get that $m(G_\eta B) - m(G_\beta B) > 0$. Similarly, we will get $m(G_\zeta B) > m(G_\beta B)$.

$$i(G_\beta B) - i(G_\eta B) = i(A)[i(B) - i(B - N_r) - 2i(B - r - s)] + i(A - x)[i(B - r) - 2(B - N_r)]$$
$$+ i(A - y)[i(B) - i(B - r - s) - i(B - N_r)]$$
$$+ i(A - x - y)[i(B - r - s) - i(B - N_r)].$$

Since $i(B) = i(B - r) + i(B - N_r)$, $i(B - r) = i(B - r - s) + i(B - N_r)$ and $i(B - s) = i(B - r - s) + i(B - N_r)$, $i(G_\beta B) - i(G_\eta B)$ becomes $[i(B - r - s) - i(B - N_r)] [i(A - x - y) + i(A - x) - i(A)]$. Since $B - N_x$ is a proper subgraph of $B - r - s$, by Lemma 2.5 we have $i(G_\beta B) - i(G_\eta B) > 0$. Similarly, we will get $i(G_\zeta B) < i(G_\beta B)$.

If $B$ is a hexagon, then we shall use $G_\eta$, $G_\beta$ and $G_\zeta$ to instead of $G_{\eta B}$, $G_{\beta B}$ and $G_{\zeta B}$, respectively. Also, the common edge of $B$ and $C$ is denoted by $x' y'$ so that the distance between $x$ and $x'$ is 2. The other vertices of $B$ are denoted by $a', b', c'$ and $d'$ so that $x' = a' b' c' d' y' = B$.

Suppose $B_n \in \mathcal{C}_n$, $n \geq 2$. Then $B_n$ can be written as $\left(\left(\left(\left(\left(L_2\right)\theta_2\right)\theta_3\right)\cdots\right)\theta_{n-1}\right)$, where $\theta_j \in \{\eta, \beta, \zeta\}$. We denote $B_n = \theta_2 \theta_3 \cdots \theta_{n-1}$ for short. Notice that, this notation is different from the notation introduced in [16] (the $\beta$ at the beginning of the sequence is omitted from that notation. The main difference is the distance of $x$ and $x'$ is always 2 in this paper. Consequently, $Z_n = \eta \eta \eta \eta \eta \zeta \zeta$ is the zig-zag chain in this paper (see Fig. 5), but in [16] $H_4 = \beta \alpha \alpha \alpha \alpha \beta \gamma \gamma \gamma$ is the helicene (chain).

Note that if all the $\theta_j$ are $\beta$, then $B_n = L_n$. Its centroid-induced graph is a straight line. If all the $\theta_j \in \{\eta, \zeta\}$ and $\theta_j \neq \theta_{j-1}$, then $B_n = H_n$ is a helicene chain. Its centroid-induced graph is a helix curve. If all $\theta_j$ are $\eta$ or all $\theta_j$ are $\zeta$, then $B_n = Z_n$ is a zig-zag chain. Its centroid-induced graph is a zig-zag curve.

Suppose $B_n \in \mathcal{C}_n$. Let $C_1, C_2, \ldots, C_n$ be the $n$ hexagons of $B_n$ such that $C_{k-1}$ and $C_k$ are adjacent for $k = 2, \ldots, n$. We use $x_{k-1}, y_{k-1}, a_k, b_k, c_k$ and $d_k$ to denote the vertices of $C_k$ such that $x_{k-1} y_{k-1}$ is the common edge of $C_k$ and $C_{k-1}$, and $y_{k-1} d_k a_k b_k c_k d_k$ and $d_k y_{k-1}$ are edges of $C_k$. Moreover, we request that $x_k$ and $x_{k-1}$ have the distance two. Sometimes, $B_n$ is denoted by $C_1 \cdots C_n$. So that when $B_n = L_n$, then $x_k = b_k$ and $y_k = c_k$. When $B_n = Z_n$, then either $x_k = d_k$ and $y_k = c_k$ for all $k$ or $x_k = b_k$ and $y_k = a_k$ for all $k$. For the last case, we can exchange the labeling of $x_1$ and $y_1$, then the resulting labels become $x_k = d_k$ and $y_k = c_k$ for all $k$. So up to isomorphic we may assume that $Z_n = \underbrace{\zeta \zeta \cdots \zeta}_{n-2 \text{ times}}$.

Lemma 3.3. Keeping the notations as in Lemma 3.1. Suppose $B$ is a hexagon (see Fig. 4). We have

(a) if $m(A - x) \geq m(A - y)$, then $m(G_\zeta - d) > m(G_\zeta - c)$ and $m(G_\zeta) \geq m(G_\eta)$, moreover the equality holds only if $m(A - x) = m(A - y)$,
(b) if $i(A - x) \leq i(A - y)$, then $i(G_\zeta - d) < i(G_\zeta - c)$ and $i(G_\zeta) \leq i(G_\eta)$, moreover the equality holds only if $i(A - x) = i(A - y)$.
By a similar proof of Lemma 3.2 in [16] we have the second parts of (a) and (b).

\[ m(G_\xi - d) = m(G_\xi - d - ax) + m(G_\xi - d - a - x) \]
\[ = m(A)m(P_2) + m(A - x)m(P_6) = 21m(A) + 13m(A - x), \]

where \( P_n \) is the path of order \( n \). Also we can get,

\[ m(G_\xi - c) = 16m(A) + 10m(A - y) + 8m(A - x) + 5m(A - x - y). \]

So \( m(G_\xi - d) - m(G_\xi - c) = 5([m(A) - m(A - y) - m(A - x - y)] + [m(A - x) - m(A - y)]) > 0 \) and (a) is proved. To prove (b) we compute

\[
\begin{align*}
i(G_\xi - c) &= i(G_\xi - c - d) + i(G_\xi - c - N_d) \\
&= i(G_\xi - c - d - a) + i(G_\xi - c - d - N_a) + i(G_\xi - c - N_d - a) + i(G_\xi - c - N_d - N_a) \\
&= i(A)i(P_1)i(P_4) + i(A - x)i(P_4) + i(A - y)i(P_1)i(P_3) + i(A - x - y)i(P_1) \\
&= 16i(A) + 5i(A - y) + 5i(A - x - y). \\
\end{align*}
\]

\[
\begin{align*}
i(G_\xi - d) &= i(G_\xi - d - a) + i(G_\xi - d - N_a) \\
&= i(A)i(P_6) + i(A - x)i(P_6) = 21i(A) + 13i(A - x). \\
\end{align*}
\]

So \( i(G_\xi - d) - i(G_\xi - c) = 5[i(A) - i(A - y) - i(A - x - y)] + 5[i(A - x) - i(A - y)] < 0. \]

**Remark 3.4.** For integer \( k \geq 1 \), since \( Z_{k+1} = (Z_k)_\xi \), by using Lemma 3.3 repeatedly we have \( m(Z_{k+1} - d_{k+1}) > m(Z_{k+1} - c_{k+1}) \) and \( i(Z_{k+1} - d_{k+1}) < i(Z_{k+1} - c_{k+1}) \).

4. Hexagonal spiders

A graph \( G \) is called a spider (or spider graph) if it is a tree and contains only one vertex of degree greater than 2. Such vertex is called the center of the spider. A hexagonal system \( H \) is called a hexagonal spider if the centroid-induced graph \( H_C \) of \( H \) is a spider with maximum degree 3, (i.e., the degree of the center of \( H_C \) is 3). Fig. 8 shows some hexagonal spiders and their centroid-induced graphs.

Suppose \( S \) is a spider with maximum degree 3. Let \( c \) be the center of \( S \). Then \( S - c \) consists of three components. Each component is called a leg of \( S \). Suppose \( H \) is a hexagonal spider. Let \( H_C \) be the centroid-induced graph of \( H \). The hexagonal chains correspond to the legs of \( H_C \) are called the legs of \( H \). The number of hexagons containing in a leg is called the length of the leg. The hexagon corresponds to the center of \( S \) is called the central hexagon.

For positive integers \( n_1, n_2, n_3 \), we use \( S(n_1, n_2, n_3) \) to denote a hexagonal spider with three legs of lengths \( n_1, n_2 \) and \( n_3 \), respectively (see Fig. 6). Note that non-isomorphic hexagonal spiders may correspond isomorphic centroid-induced graph.
Theorem 4.1. Suppose \( S(n_1, n_2, n_3) \in \mathscr{F}(n_1, n_2, n_3) \) has the maximum Hosoya index among all the hexagonal spiders in \( \mathscr{F}(n_1, n_2, n_3) \). Then \( S(n_1, n_2, n_3) \) is a zig-zag hexagonal spider.

Proof. Suppose not, there is a leg of \( S(n_1, n_2, n_3) \) combining with the central hexagon \( C \) which is not a zig-zag chain. Let this chain be \( B = C_1C_2 \cdots C_nC \), and \( n \in \{n_1, n_2, n_3\} \). That is, \( B = \theta_2 \theta_3 \cdots \theta_n \) and not all \( \theta_j \) are \( \zeta \). In this case \( n \geq 2 \). Let \( k \) be the least integer such that \( \theta_k \neq \zeta \), \( 2 \leq k \leq n \). Let \( K = S(n_1, n_2, n_3) - (C_1 \cup \cdots \cup C_{k-1}) - \{d_k, v\} \), where \( v = c_k \) or \( a_k \) for \( \theta_k = \eta \) or \( \beta \), respectively (see Fig. 7).

Let \( Z_k \) be the zig-zag chain with \( k \) hexagons. Then \( S(n_1, n_2, n_3) = (Z_k)_\theta K \). By Lemmas 3.1 and 3.2 and Remark 3.4, we have \( m((Z_k)_\zeta K) > m(S(n_1, n_2, n_3)) \). Since \( (Z_k)_\zeta K \in \mathscr{F}(n_1, n_2, n_3) \), there is a contradiction. 

By using Lemma 3.2 and a similar argument of Theorem 4.1 we have

Theorem 4.2. Suppose \( S(n_1, n_2, n_3) \in \mathscr{F}(n_1, n_2, n_3) \) has the minimum Hosoya index among all the hexagonal spiders in \( \mathscr{F}(n_1, n_2, n_3) \). Then \( S(n_1, n_2, n_3) \) is a linear hexagonal spider.

By a similar argument of Theorems 4.1 and 4.2 we have

Theorem 4.3. Suppose \( S(n_1, n_2, n_3) \in \mathscr{F}(n_1, n_2, n_3) \). If \( S(n_1, n_2, n_3) \) is neither \( L(n_1, n_2, n_3) \) nor \( Z(n_1, n_2, n_3) \), then

\[
i(Z(n_1, n_2, n_3)) < i(S(n_1, n_2, n_3)) < i(L(n_1, n_2, n_3)).
\]
In general there may have eight non-isomorphic zig-zag hexagonal spiders with the same parameter \((n_1, n_2, n_3)\) (see Fig. 8). We shall introduce another notation to distinguish these zig-zag hexagonal spiders. Suppose \(S\) is a zig-zag hexagonal spider. We draw it as a plane graph. Suppose one of its leg is of length \(n\). Consider the hexagonal chain formed by the central hexagon and the first two hexagons of this leg. If this chain turns anticlockwise, then we call this leg a positive leg of length \(n^+\), otherwise a negative leg of length \(n^-\). Thus a zig-zag hexagonal spider will be denoted as \(Z(n_1^a, n_2^b, n_3^c)\), where \(a, b, c \in \{+,-\}\). If \(a = b = c\), then such zig-zag hexagonal spider is called regular and denoted by \(RZ(n_1, n_2, n_3)\).

Note that \(Z(2^-, 4^-, 3^-) \cong Z(2^+, 3^+, 4^+) = RZ^+(2, 3, 4), Z(2^-, 4^+, 3^-) \cong Z(2^+, 3^+, 4^-), Z(2^-, 4^-, 3^+) \cong Z(2^+, 3^-, 4^+), Z(2^-, 4^-, 3^+) \cong Z(2^+, 3^-, 4^-).\) Up to isomorphic, we may always assume that \(n_1\) is the smallest integer among \(n_1, n_2\) and \(n_3\) and the orientation of the leg which is of length \(n_1\) is positive.

There is a question for further study: Which zig-zag hexagonal spiders will attach the maximum Hosoya index and which will attach the minimum Merrifield–Simmons index?

References

<table>
<thead>
<tr>
<th>Reference</th>
</tr>
</thead>
</table>