MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **62** (2009) 621-628

ISSN 0340 - 6253

The Second Largest Hosoya Index of Unicyclic Graphs

Lixin Xu [1]
Department of Science and Information Science, Shaoyang University, Shaoyang, Hunan 422000, P. R. China
Email: lixinxusyu@gmail.com
(Received October 11, 2007)

Abstract

Let $m(G,k)$ be the number of the k-matching of a graph G, $z(G)$ denotes the Hosoya index of the graph G, then the Hosoya index of G is $z(G) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} m(G,k)$, where n denote the number of vertex of G. In this paper, the second largest Hosoya index of unicyclic graphs is determined.

1 Introduction

Let $G = (V, E)$ be a simple connected graph with the vertex set $V(G)$ and the edge set $E(G)$. For any $v \in V$, $N(v)$ denotes the neighbors of v, and

[1] A Project Supported by Hunan Provincial Education Department (06C755).

$N_G[v] = \{v\} \cup \{u|uv \in E(G)\}$, $d_G(v) = |N(v)|$ is the degree of v. A leaf is a vertex of degree one and a stem is a vertex adjacent to at least one leaf, leaves and their stems consisting all pendent edges. The girth of a graph is the smallest cycle length of the graph, if the graph contains no cycle, the girth is defined as $\propto$. If $E' \subseteq E(G)$, we denote by $G - E'$ the subgraph of G obtained by deleting the edges of E'. If $W \subseteq V(G)$, we denote by $G - W$ the subgraph of G obtained by deleting the vertices of W and the edges incident with them. If $W = \{v\}$ and $E' = \{xy\}$, we write $G - v$ and $G - xy$ instead of $G - \{v\}$ and $G - \{xy\}$, respectively. If G has components G_1, G_2, $\cdots$, G_t, then G is denoted by $\bigcup_{i=1}^{t} G_i$. We denote the sequence of fibonacci numbers by $F(n)$, i.e. $F(0) = 0$, $F(1) = 1$, and for $n \geq 2$, the fibonacci number has the recursion formula: $F(n) = F(n-1) + F(n-2)$. The related reviews referred as [2-4].

The Hosoya index $z(G)$ of a graph, proposed by Hosoya in [1], defined as the total number of its matching, namely

$$z(G) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} m(G,k)$$

where $\lfloor \frac{n}{2} \rfloor$ stands for the integer part of $\frac{n}{2}$ and $m(G,k)$ is the number of k-matching of G. A k-matching of graph G is a subset S of its edge set such that $|S| = k$ and that no two different edges of S enjoy a common vertex. It is convenient to see $m(G,0) = 1$ and $m(G,1) = m$, the number of edges of graph G. When $k > n/2$, we have $m(G,k) = 0$. The Hosoya index is well correlated with the boiling points, entropies, calculated bond orders, and for the coding of chemical structures [2,3]. Since then, many authors have investigated the Hosoya index. It was established long ago that the n-vertex path P_n has maximal Hosoya index, which equal to the $(n+1)th$ Fibonacci number $F(n+1)$ and the star S_n has the minimal Hosoya index. In recent, Hou [5] characterized the acyclic graphs that have the first and the second minimal Hosoya indices. Gutman [6] showed that the linear chain is the unique chain with minimal Hosoya index among all hexagonal chain. Zhang [7] determined the unique graphs with minimal and second minimal Hosoya index among all catacondensed systems. Ou [8] characterized the unicyclic molecular graphs with the smallest Hosoya index. Deng and Chen [9] characterized the extremal Hosoya index of unicyclic graphs, and Deng [10] got the smallest Hosoya index of bicyclic graphs.

Let P_n, C_n and S_n (i.e.,$K_{1,n-1}$) be the path, cycle and the star on n vertices.

A graph is called *unicyclic* if it is connected and contains exactly one cycle. A graph is *unicyclic* if and only if it is connected and has size equal to its order.

Let $\mathcal{U}_n$ denote the set of the unicyclic graphs with n vertices.

Let $\mathcal{U}_n^g$ denote the set of the unicyclic graphs with n vertices and girth g.

$H_{n,g}$ be the unicyclic graph that results from identifying one vertex u of C_g with the vertex v_0 of a simple path $v_0 v_1 \cdots v_{n-g}$ of length $n-g$.

In this paper, we shall determine the second largest Hosoya index of unicyclic graphs.

The related graph notations and terminologies undefined will conform to [11].

2 Preliminaries

The following basic results will be used and can be found in the references cited.

(i) If G is a graph with components $G_1, G_2, \cdots, G_k$, then $z(G) = \prod_{i=1}^{k} z(G_i)$.

(i) If $e = uv$ is an edge of G, then $z(G) = z(G-uv) + z(G - \{u,v\})$.

(iii) If v is a vertex of G, then $z(G) = z(G-v) + \sum_{x \in N_G(v)} z(G - \{v,x\})$.

(iv) $z(P_0) = 0$, $z(P_1) = 1$ and $z(P_n) = F(n+1)$ for $n \geq 2$;

$z(C_n) = F(n-1) + F(n+1)$, $z(K_{1,n-1}) = n$.

From above, if uv be an edge of G, then we have $z(G) > z(G - uv)$; moreover if G is a graph with at least one edge, then $z(G) > z(G - v)$.

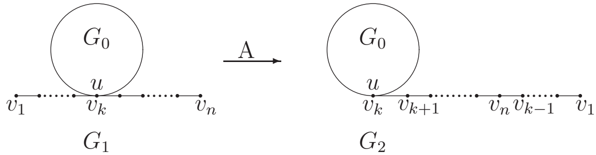

Fig.1. Transformation A

For convenience, we introduce two transformations.

Transformation A. Let $G \neq P_1$ be a simple connected graph, $u \in V(G)$. G_1 be the graph that results from identifying u with the vertex v_k $(1 < k < n)$ of the simple path $v_1v_2 \cdots v_n$; G_2 is obtained from G_1 by deleting the edge $v_{k-1}v_k$ and adding the edge $v_{k-1}v_n$ (see Fig 1.).

Lemma 1 ([9,10]). Let G_1 and G_2 be the graphs depicted above. Then $z(G_2) > z(G_1)$.

Remark 1. Repeating transformation A, an arbitrary tree T_i in G can be changed into the graph P_i (see Fig.2), and the Hosoya index increasing after transformation.

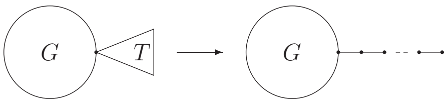

Fig 2.

Transformation B. Let $P = uu_1u_2 \cdots u_tv$ be a path in G, and $G \neq P$. Let G is obtained from identifying u with the vertex v_k of $P_1 = v_1v_2 \cdots v_k$, and identifying v with the vertex v_{k+1} of $P_2 = v_{k+1}v_{k+2} \cdots v_n$; G_1 is obtained from G by deleting the edge $v_{k-1}v_k$ and adding the edge v_nv_{k-1}; G_2 is obtained from G by deleting the edge $v_{k+1}v_{k+2}$ and adding the edge v_1v_{k+2} (see Fig.3).

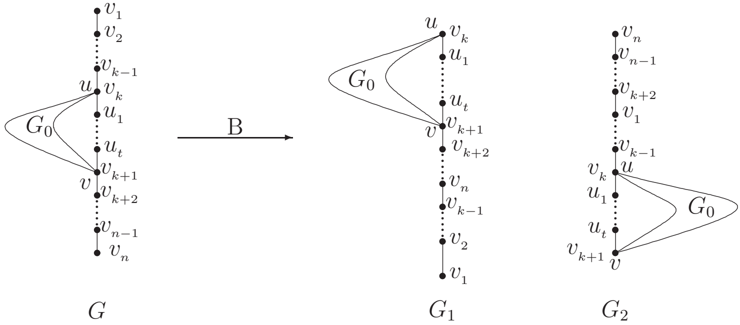

Fig.3. Transformation B

Lemma 2 ([9,10]). Let G_1 and G_2 be the graphs depicted in Fig 3, then $z(G_1) > z(G)$ or $z(G_2) > z(G)$.

Remark 2. After repeating transformation A, if we repeating transformation B, then, any arbitrary unicyclic graph with girth g can be changed into the graph $H_{n,g}$, and the Hosoya index increasing.

3 The unicyclic graphs with the second largest Hosoya index

In this section we shall get the upper bounds of the unicyclic graphs with respect to their Hosoya indices.

Theorem 1 ([9]). $H_{n,g}$ has the largest Hosoya index in $\mathcal{U}_n^g$ $(g \geq 3)$.

Theorem 2 ([9]). C_n (i.e.,$H_{n,n}$) is the unique graph with the largest Hosoya index among all unicyclic graphs of order n.

Theorem 3. $H_{n,4}$ and $H_{n,n-2}$ are the graphs with the second largest Hosoya index among all unicyclic graphs of order n, where $H_{n,4}$ and $H_{n,n-2}$ are shown in Fig.4.

$H_{n,4}$ $H_{n,n-2}$

Fig.4.

Proof. From the theorems 1 and 2, we need only to compare the Hosoya indices of $H_{n,r}$ for $3 \leq r \leq n-1$. By the definition of Hosoya index, it is easy to see that

$z(H_{n,r}) = F(n+1) + F(r-1)F(n+1-r) = z(H_{n,n+2-r})$;

Let $\Delta = z(H_{n,r}) - z(H_{n,r-1})$, $\Delta' = z(H_{n,r}) - z(H_{n,r-2})$.

When $4 \leq r \leq \lfloor \frac{n}{2} \rfloor + 1$, we have

$$\begin{aligned}
\Delta &= F(r-1)F(n+1-r) - F(r-2)F(n+2-r) \\
&= [F(r-2) + F(r-3)][F(n-r+2) - F(n-r)] \\
&\quad -F(r-2)F(n+2-r) \\
&= -[F(r-2)F(n-r) - F(r-3)F(n+1-r)] \\
&= \cdots \\
&= (-1)^{r-2}[F(1)F(n+3-2r) - F(0)F(n+4-2r)] \\
&= (-1)^{r}F(n+3-2r).
\end{aligned}$$

So,

$z(H_{n,3}) < z(H_{n,4}) > H_{n,5}) < z(H_{n,6}) > \cdots$

and $z(H_{n,n-1}) < z(H_{n,n-2}) > H_{n,n-3}) < z(H_{n,n-4}) > \cdots$ since $z(H_{n,r}) = z(H_{n,n+2-r})$.

When $5 \leq r \leq \lfloor \frac{n}{2} \rfloor + 1$,

$$\begin{aligned}
\Delta' &= F(r-1)F(n+1-r) - F(r-3)F(n+3-r) \\
&= [F(r-2) + F(r-3)][F(n+3-r) - F(n+2-r)] \\
&\quad -F(r-2)F(n+3-r) \\
&= -[-F(r-2)F(n+3-r) + F(r-1)F(n+2-r)] \\
&= \cdots \\
&= (-1)^{r-2}[-F(1)F(n+6-2r) + F(2)F(n+5-2r)] \\
&= (-1)^{r-1}F(n+4-2r)
\end{aligned}$$

So, we have

$z(H_{n,3}) < z(H_{n,5}) < \cdots$ and $z(H_{n,n-1}) < z(H_{n,n-3}) < \cdots$;

$z(H_{n,4}) > z(H_{n,6}) > \cdots$ and $z(H_{n,n-2}) > z(H_{n,n-4}) > \cdots$.

We now only need to compare $z(H_{n,4}) = z(H_{n,n-2})$ with $z(H(n, \frac{n}{2} + 1))$ (n is even) or $z(H_{n,\frac{n+1}{2}})$ (n is odd).

Calculating immediately, $z(H_{n,4}) > z(H(n, \frac{n}{2}+1))$ or $z(H_{n,4}) > z(H_{n,\frac{n+1}{2}})$.

Therefore, $H_{n,4}$ and $H_{n,n-2}$ have the second largest Hosoya index among all unicyclic graphs, and $H_{n,4}$ and $H_{n,n-2}$ are the graphs with the second largest Hosoya index among all unicyclic graphs.

The proof of the Theorem is completed.

References

[1] H. Hosoya, Topological index, a newly proposed quantity characterizing the topo- logical nature of structural isomers of saturated hydrocarbons, Bull. Chem. Soc. Japan 44 (1971) 2332-2339.

[2] I. Gutman, O.E. Polansky, Mathematical Concepts in Organic Chemistry, Springer, Berlin, 1986.

[3] R. E. Merrifield and H. E. Simmons, Topological Methods in Chemistry, Wiley, New York, 1989.

[4] J. W. Moon, L. Moser, On cliques in graphs, Israel J. Math. 3 (1965) 23-28.

[5] Y. P. Hou, On acyclic systems with minimal Hosoya index, Discrete Appl. Math. 119 (2002) 251-257.

[6] I. Gutman, Extremal hexagonal chains, J. Math. Chem. 12 (1993) 197-210.

[7] L. Zhang, F. Tian, Extremal catacondensed benzenoids, J. Math. Chem. 34 (2003)111-122.

[8] J. P. Ou, On extremal unicyclic molecular graphs with prescribed girth and minimal Hosoya index, J. Math. Chem. 42 (2007) 423-432.

[9] H. Deng, S. Chen, The extremal unicyclic graphs with respect to Hosoya index and Merrifield-Simmons index, MATCH Commun. Math. Commun. Comput. Chem. 59 (2008) 171-190.

[10] H. Deng, The smallest Hosoya index in (n, n+1)-graphs, J. Math. Chem. (2006), DOI: 10.1007/s10910-006-9186-6.

[11] J. A. Bondy and U. S. R. Murty, Graph Theory with Applications, Macmillan, New York, 1976.