Some Graphs with Minimum Hosoya Index and Maximum Merrifield-Simmons Index

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Abstract

The Hosoya index of a graph is defined as the total number of the matchings of the graph and the Merrifield-Simmons index of a graph is defined as the total number of the independent sets of the graph. In this paper, we obtain the graphs with minimum Hosoya index among the trees with \( n \) vertices and diameter \( d \). The extremal graphs is the same as ones given by X. Li \textit{et al} with maximum Merrifield-Simmons index among such a class of graphs. Also, we give the graphs with both minimum Hosoya index and maximum Merrifield-Simmons index among the trees with \( n \) vertices and \( r \) pendant vertices.

1 Introduction and Results

It is well known that a topological index is a map from the set of chemical compounds represented by molecular graphs to the set of real numbers. There are more than hundred topological indices available in the literature [1]. Many topological indices are closely correlated with some physico-chemical characteristics of the underlying compounds [2]. The Hosoya index is one of the topological indices. It was introduced by Hosoya in 1971 [3] and

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was applied to correlations with boiling points, entropies, calculated bond orders, as well as for coding of chemical structures (see [4,5]). Since 1971, many authors have investigated the Hosoya index and many results are obtained (see [5-13]). Similar to the Hosoya index, the Merrifield and Simmons index is also a topological index whose correlation with the boiling points is shown in [4]. Its mathematical properties were studied in some details [2,13–26]. In particular, Li, Zhao and Gutman [2] gave the graphs with maximum Merrifield-Simmons index among the trees with order \( n \) and diameter \( d \).

Recently, finding the graphs with both minimum Hosoya index and maximum Merrifield-Simmons index attracted the attention of a few researchers and some results are achieved. Among these results, Gutman [27] pointed out the linear hexagonal chain is the unique hexagonal chain with minimum Hosoya index and maximum Merrifield-Simmons index among all the hexagonal chains with \( n \) hexagons. Zhang [13] noticed that the graph with minimum Hosoya index is also the graph with maximum Merrifield-Simmons index in some classes of graphs, such as hexagonal chains and catacondensed systems. Yu and Tian [28] characterized the graphs with minimum Hosoya index and maximum Merrifield-Simmons index among the connected graphs with the given cyclomatic number and edge-independence number.

In this paper, we give two classes of graphs, i.e. trees of \( n \) vertices with diameter \( d \) and trees of \( n \) vertices with \( r \) pendant vertices, in each of which the graph with minimum Hosoya index is also the graph with maximum Merrifield-Simmons index.

All graphs considered here are finite and simple. Undefined terminology and notation may refer to [29]. Let \( G = (V, E) \) be a graph of \( n \) vertices. Two edges of \( G \) are said to be independent if they are not adjacent in \( G \). A \( k \)-matching of \( G \) is a set of \( k \) mutually independent edges. Denote by \( z(G, k) \) the number of the \( k \)-matchings of \( G \). For convenience, let \( z(G, 0) = 1 \) for any graph \( G \). Hosoya index of \( G \), denoted by \( z(G) \), is defined as

\[
z(G) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} z(G, k).
\]

Obviously, \( z(G) \) is equal to the total number of the matchings of the graph \( G \). Similarly, two vertices of \( G \) are said to be independent if they are not adjacent in \( G \). A \( k \)-independent set of \( G \) is a set of \( k \) mutually independent vertices. Denote by \( \sigma(G, k) \) the number of the \( k \)-independent sets of \( G \). For convenience, let \( \sigma(G, 0) = 1 \) for any graph \( G \). Merrifield-Simmons index of \( G \), denoted by \( \sigma(G) \), is defined as

\[
\sigma(G) = \sum_{k=0}^{n} \sigma(G, k).
\]

So \( \sigma(G) \) is equal to the total number of the independent sets of the graph \( G \).
Denoted by $n(G)$ and $D(G)$ the total number of vertices in $G$ and the diameter of $G$, respectively. For a vertex $v$ of $G$, we denote the degree of $v$ by $d(v)$, and define $N_v = \{ v \} \cup \{ u|uv \in E(G) \}$. Let $V' \subset V$, we will use $G - V'$ to denote the graph obtained from $G$ by deleting the vertices in $V'$ together with their incident edges. If $V' = \{ v \}$, we write $G - v$ for $G - \{ v \}$. A pendant vertex is a vertex of degree 1 and a pendant edge is an edge incident to a pendant vertex. Denoted by $PV(G)$ the total number of pendant vertices in $G$. Let $T_{n,d} = \{ T: T$ is a tree with $n$ vertices and diameter $d \}$ and $T^n_{r} = \{ T: T$ is a tree with $n$ vertices and $r$ pendant vertices $\}$. Let $S_{p,q}$ (See Fig 1.) denote the tree obtained from stars $S_{p+1}$ and $S_q$ by identifying a pendant vertex of $S_{p+1}$ with the center of $S_q$. Let $P_{n-d,d}$ (see Fig. 1) denote the tree created from path $P_d$ by adding $n - d$ pendant edges to an end vertex of $P_d$.

Our main results are stated in the following three theorems.

**Theorem 1.** If $T \in T_{n,d}$, then

$$z(T) \geq (n - d + 1)F_{d-1} + F_{d-2}$$

and the equality holds if and only if $T \cong P_{n-d,d}$.

**Theorem 2.** If $T \in T^n_{r}$, then

$$z(T) \geq rF_{n-r} + F_{n-r-1}$$

and the equality holds if and only if $T \cong P_{r-1,n-r+1}$.

**Theorem 3.** If $T \in T^n_{r}$, then

$$\sigma(T) \leq 2^{r-1}F_{n-r+1} + F_{n-r}$$

and the equality holds if and only if $T \cong P_{r-1,n-r+1}$.

Here, $F_n$ is the $n$-th Fibonacci number which satisfies $F_n = F_{n-1} + F_{n-2}$ with initial conditions $F_0 = 1$ and $F_1 = 1$.

The proofs of the above theorems are given in section 2.
2 Proofs

We only give the proof of Theorem 2. Proofs of Theorems 1 and 3 are similar to that of Theorem 2, so we omitted them here. We use some techniques in [2]. First we give some lemmas.

**Lemma 1** [10]. Let \( v \) be a vertex of \( G \). Then

(i) \( z(G) = z(G - v) + \sum_u z(G - \{u, v\}) \), where the summation extends over all vertices adjacent to \( v \).

(ii) \( \sigma(G) = \sigma(G - v) + \sigma(G - N_v) \).

**Lemma 2** [10]. If \( G_1, G_2, \ldots, G_t \) are the components of a graph \( G \), then

(i) \( z(G) = \prod_{i=1}^t z(G_i) \).

(ii) \( \sigma(G) = \prod_{i=1}^t \sigma(G_i) \).

**Proof of Theorem 2.** It is not difficult to check that \( z(P_{r-1,n-r+1}) = rF_{n-r} + F_{n-r-1} \) by Lemma 1 and \( z(P_n) = F_n \). Now we prove if \( T \in \mathcal{T}_r^n \), then \( z(T) \geq rF_{n-r} + F_{n-r-1} \) with equality only if \( T \cong P_{r-1,n-r+1} \).

Since \( T \in \mathcal{T}_r^n \), we have that \( PV(T) = r \) and \( n \geq r + 1 \). We prove the theorem by double induction on \( r \) and \( n \).

If \( r = 2 \), then \( T \cong P_n \cong P_{1,n-1} \) and the theorem holds obviously for \( r = 2 \).

If \( T \) is a tree with \( PV(T) = r \) and \( n(T) = r + 1 \), then \( T \cong S_{r+1} \cong P_{n-1,2} \) and hence there is nothing to prove. If \( T \) is a tree with \( PV(T) = r \) and \( n(T) = r + 2 \), then \( T \cong S_{p,q} \) with \( p + q = r + 2 \), and \( z(S_{p,q}) = pq + 1 \geq 2r + 1 \) with equality only if \( T \cong P_{r-1,3} \). Thus the theorem holds for \( PV(T) = r \) and \( n(T) = r + 2 \).

In the following, we assume \( r \geq 3 \) and \( n \geq r + 3 \). Suppose that the theorem holds for \( PV(T) \leq r - 1 \) and \( n(T) \geq r + 1 \), and for \( PV(T) = r \) and \( r + 2 \leq n(T) \leq n - 1 \). When \( PV(T) = r \) and \( n(T) = n \), we distinguish the following two cases.

**Case 1.** There is at least one maximal path \( u_1 u_2 u_3 \ldots u_d u_{d+1} \) in \( T \), such that \( d(u_2) = 2 \) or \( d(u_d) = 2 \). Without loss of generality, assume \( d(u_2) = 2 \). From Lemma 1, we have

\[
z(T) = z(T - u_1) + z(T - \{u_1, u_2\}).
\]

(1)

Now, \( n(T - u_1) = n - 1 \) and \( n(T - \{u_1, u_2\}) = n - 2 \). In addition, \( PV(T - u_1) = r \) and
\[ r - 1 \leq PV(T - \{u_1, u_2\}) \leq r. \]

By the induction hypothesis, we have
\[ z(T - u_1) \geq z(P_{r-1,n-r}) = rF_{n-r-1} + F_{n-r-2} \] (2)
with equality only if \( T - u_1 \cong P_{r-1,n-r} \).

If \( T - \{u_1, u_2\} \in \mathcal{T}_{r-1}^{n-2} \), by the induction hypothesis and \( n \geq r + 3 \), we have
\[ z(T - \{u_1, u_2\}) \geq z(P_{r-2,n-r}) = (r - 1)F_{n-r-1} + F_{n-r-2} \]
\[ > rF_{n-r-2} + F_{n-r-3} = z(P_{r-1,n-r-1}). \] (3)

If \( T - \{u_1, u_2\} \in \mathcal{T}_r^{n-2} \), by the induction hypothesis, we have
\[ z(T - \{u_1, u_2\}) \geq z(P_{r-1,n-r-1}) = rF_{n-r-2} + F_{n-r-3}. \] (4)

Hence, by (1)~(4), we have
\[
z(T) = z(T - u_1) + z(T - \{u_1, u_2\}) \]
\[ \geq z(P_{r-1,n-r}) + z(P_{r-1,n-r-1}) \]
\[ = rF_{n-r-1} + F_{n-r-2} + rF_{n-r-2} + F_{n-r-3} \]
\[ = rF_{n-r} + F_{n-r-1} \]
with equality only if \( T \cong P_{r-1,n-r+1} \).

**Case 2.** \( d(u_2) \geq 3 \) and \( d(u_d) \geq 3 \) for each longest path \( u_1u_2u_3 \ldots u_d u_{d+1} \) in \( T \). Suppose that \( d(u_2) = t + 1 \geq 3 \). From Lemma 1, we have
\[ z(T) = z(T - u_1) + z(T - \{u_1, u_2\}). \] (5)

Now, \( T - u_1 \) is an \((n - 1)\)-vertex tree with \( r - 1 \) pendant vertices. Then, by the induction hypothesis,
\[ z(T - u_1) \geq z(P_{r-2,n-r+1}) = (r - 1)F_{n-r} + F_{n-r-1} \] (6)
with equality only if \( T - u_1 \cong P_{r-2,n-r+1} \). On the other hand, there is a tree \( H \) such that \( T - \{u_1, u_2\} = (t - 1)K_1 \cup H \) (otherwise, we can obtain a contradiction to that \( u_1u_2u_3 \ldots u_d u_{d+1} \) is a longest path in \( T \)). Obviously, \( 2 \leq t \leq r - 2 \), \( n(H) = n - t - 1 < n \) and \( r - t \leq PV(H) \leq r - t + 1 \).
If $PV(H) = r - t$, by the induction hypothesis, $t \leq r - 2$ and $n \geq r + 3$, then
\[
 z(H) \geq z(P_{r-t-1,n-r}) = (r-t)F_{n-r-1} + F_{n-r-2} \\
> (r-t+1)F_{n-r-2} + F_{n-r-3}.
\] (7)

If $PV(H) = r - t + 1$, by the induction hypothesis, then
\[
 z(H) \geq z(P_{r-t,n-r-1}) = (r-t+1)F_{n-r-2} + F_{n-r-3}
\] (8)
with equality only if $H \cong P_{r-t,n-r-1}$.

By (5)~(8), Lemma 2, $t \leq r - 2$ and $n \geq r + 3$, we have
\[
z(T) = z(T - u_1) + z(T - \{u_1, u_2\}) \\
= z(T - u_1) + z(H) \\
\geq (r-1)F_{n-r} + F_{n-r-1} + (r-t+1)F_{n-r-2} + F_{n-r-3} \\
\geq (r-1)F_{n-r} + F_{n-r-1} + 3F_{n-r-2} + F_{n-r-3} \\
= (r+1)F_{n-r} \\
> rF_{n-r} + F_{n-r-1}.
\]

This completes the proof of Theorem 2.

3 Conclusion

By Theorem 1 in this paper and Theorem 1 in [2], $P_{n-d,d}$ has both minimum Hosoya index and maximum Merrifield-Simmons index among the trees of $n$ vertices and diameter $d$. Similarly, by Theorems 2 and 3, $P_{r-1,n-r+1}$ has the two extremal indices just mentioned among the trees of $n$ vertices with $r$ pendant vertices.

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References


