MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **55** (2006) 103-118

ISSN 0340 - 6253

A Kind of Graphs with Minimal Hosoya Indices and Maximal Merrifield-Simmons Indices*

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(Received February 2, 2005)

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 characterize the graphs with minimal Hosoya indices and maximal Merrifield-Simmons indices, respectively, among the connected graphs with the given cyclomatic number and edge-independence number.

1. Introduction

Let G be a graph on 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, we regard the empty edge set as a matching. Then $z(G,0) = 1$ for any graph G. The *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 matchings of 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 $i(G,k)$ the number of the k-independent sets of G. For convenience,

*This work is partially supported by National Natural Science Foundation of China. (No. 10431020)

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we regard the empty vertex set as an independent set. Then $i(G,0) = 1$ for any graph G. The *Merrifield-Simmons index* of G, denoted by $i(G)$, is defined as $i(G) = \sum_{k=0}^{n} i(G,k)$. So $i(G)$ is equal to the total number of the independent sets of G.

The Hosoya index of a graph was introduced by Hosoya in 1971 [9] and was applied to correlations with boiling points, entropies, calculated bond orders, as well as for coding of chemical structures ([11, 12]). Since then, many authors have investigated the Hosoya index (e.g., see [2]-[5], [7, 8, 12]). An important direction is to determine the graphs with maximal or minimal Hosoya indices in a given class of graphs. In [6], Gutman showed that linear hexagonal chain is the unique chain with minimal Hosoya index among all hexagonal chains. In [13], Zhang showed that zig-zag hexagonal chain is the unique chain with maximal Hosoya index among all hexagonal chains. In [15], Zhang and Tian gave another proof on Gutman's and Zhang's results above mentioned. In [14], Zhang determined the graph with the second minimal Hosoya index among all hexagonal chains. In [16], Zhang and Tian determined the graphs with minimal and second minimal Hosoya index among catacondensed systems. As for n-vertex trees, it has been shown that the path P_n has the maximal Hosoya index and the star S_n has the minimal Hosoya index (see [7]). Recently, Hou [10] characterized the trees with a given size of matching and having minimal and second minimal Hosoya index, respectively.

In [11], Merrifield and Simmons developed a topological approach to structural chemistry. The cardinality of the topological space in their theory turns out to be equal to $i(G)$ of the respective molecular graph G. In [6], Gutman first use "Merrifield-Simmons index" to name the quantity. The graphs with maximal or minimal Merrifield-Simmons indices in a given class of graphs are also considered. In [16], Zhang noticed that the graph with minimal Hosoya index is also the graph with maximal Merrifield-Simmons indices in some classes of graphs, such as hexagonal chains and catacondensed systems, and proposed the problem whether it is true for other classes of graphs.

In this paper, we characterize the graphs with minimal Hosoya indices and maximal Merrifield-Simmons indices, respectively, among the connected graphs with the given cyclomatic number and edge-independence number. From our results, we find the graphs with minimal Hosoya indices are almost the graphs with maximal Merrifield-Simmons indices for the class of the connected graphs with the given cyclomatic number and edge-independence number.

In order to state our results, we introduce some notation and terminology.

Let M be a matching of G. A vertex v is said to be M-saturated, if some edge of M is incident with v; otherwise, v is M-unsaturated. If every vertex of G is M-saturated, the matching M is perfect. If G has no matching M' with $|M'| > |M|$, then M is a maximum matching; clearly, every perfect matching is a maximum matching. We call the number of edges in a maximum matching of G the edge-independence number of G and denote it by $\alpha'(G)$. Similarly, we can define the maximum independent set and call the number of vertices in a maximum independent set of G the independence number of G and denote it by $\alpha(G)$.

We denote

$$\mathcal{H}(n,q,m) = \{G: \ G \text{ is a connected graph of order } n \text{ and size } q \text{ with } \ \alpha'(G) = m\},$$

where $m \leq \lfloor \frac{n}{2} \rfloor$ and $n-1 \leq q \leq \frac{1}{2}\, n(n-1)$.

Recall that $\eta(G) = |E(G)| - |V(G)| + \omega(G)$ is defined as the cyclomatic number of the graph G, where $|E(G)|$, $|V(G)|$ and $\omega(G)$ are the number of the vertices, edges and connected components of G, respectively. Then if we denote

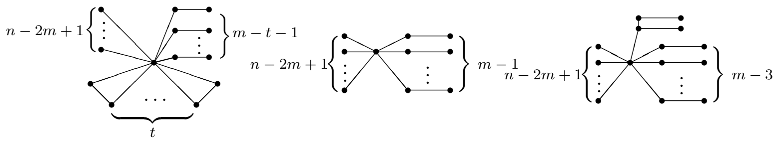
$$\mathcal{G}(n,\eta,m) = \{G: \ G \text{ is a connected graph of order } n \text{ with } \eta(G) = \eta \text{ and } \alpha'(G) = m\},$$

then

$$\mathcal{G}(n,\eta,m) = \mathcal{H}(n, n+\eta-1, m).$$

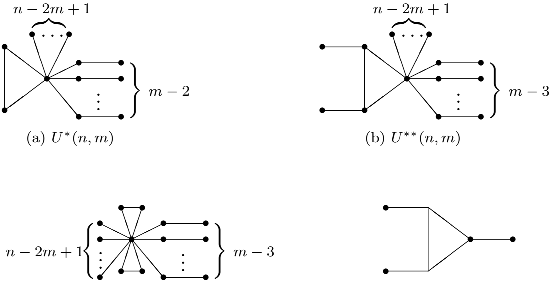
Then $\mathcal{G}(n,0,m)$ is the set of all trees on n vertices with $\alpha' = m$; $\mathcal{G}(n,1,m)$ is the set of all connected unicyclic graphs on n vertices with $\alpha' = m$; $\mathcal{G}(n,2,m)$ is the set of all connected bicyclic graphs on n vertices with $\alpha' = m$. For short, we denote $\mathcal{G}(n,0,m)$, $\mathcal{G}(n,1,m)$, $\mathcal{G}(n,2,m)$ by $\mathcal{T}(n,m)$, $\mathcal{U}(n,m)$, $\mathcal{B}(n,m)$, respectively.

Let $G^*(n,t,m)$ be the graph obtained from t triangles with a common vertex by attaching $m-t-1$ paths of length 2 and $n-2m+1$ pendent edges together to the common vertex (see Fig. 1(a)). For short, we denote $G^*(n,0,m)$, $G^*(n,1,m)$ and $G^*(n,2,m)$ by $T^*(n,m)$, $U^*(n,m)$ and $B^*(n,m)$, respectively (see Fig. 1(b), Fig. 2(a) and (c)).



(a) $G^*(n,t,m)$ (b) $T^*(n,m)$ (c) $T^{**}(n,m)$

Fig. 1



(a) $U^*(n,m)$ (b) $U^{**}(n,m)$ (c) $B^*(n,m)$ (d) $U^{**}(6,3)$

Fig. 2

If $W \subset V(G)$, we denote by $G - W$ the subgraph of G obtained by deleting the vertices of W and the edges incident with them. Similarly, if $E' \subset E(G)$, we denote by $G - E'$ the subgraph of G obtained by deleting the edges of E'. If $W = \{v\}$ and $E' = \{xy\}$, we write $G - v$ and $G - xy$ instead of $G - \{v\}$ and $G - \{xy\}$, respectively. If a graph G has components $G_1,\ G_2, \cdots, G_t$, then G is denoted by $\bigcup_{i=1}^t G_i$. For a vertex of G, we denote $N_v = \{v\} \cup \{\ u \mid uv \in E(G)\}$.

2. Preliminaries

According to the definitions of the Hosoya index and Merrifield-Simmons index, we immediately get the following results.

Lemma 2.1 *Let G be a graph and uv be an edge of G. Then*

(1) **(see [7])** $z(G) = z(G - uv) + z(G - \{u, v\})$,

(2) $i(G) = i(G - uv) - i(G - (N_u \cup N_v))$.

Lemma 2.2 **(see [7])** *Let v be a vertex of G. Then*

(1) $z(G) = z(G-v) + \sum_{u} z(G - \{u, v\})$, where the summation extends over all vertices adjacent to v,

(2) $i(G) = i(G - v) + i(G - N_v)$.

In particular, when v is a pendent vertex of G and u is the unique vertex adjacent to v, we have $z(G) = z(G - v) + z(G - \{u, v\})$ and $i(G) = i(G - v) + i(G - \{u, v\})$.

Lemma 2.3 **(see [7])** *If G_1, $G_2, \cdots, G_t$ are the components of a graph G, we have*

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

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

Lemma 2.4 **[10]** *Let $T \in \mathcal{T}(n, m)$, where $n = 2m$. Then T has a pendent edge which is incident with a vertex of degree 2.*

Lemma 2.5 **[10]** *Let $T \in \mathcal{T}(n, m)$, where $n > 2m$. Then there is an m-matching M and a pendent vertex v such that M does not saturate v.*

In [10], Hou characterized the trees in $\mathcal{T}(n, m)$ having minimal and second minimal Hosoya index, respectively.

Lemma 2.6 **[10]** *Let $T \in \mathcal{T}(n, m)$, where $m \geq 1$. Then*

$$z(T) \geq 2^{m-2}(2n - 3m + 3)$$

with equality if and only if $T \cong T^*(n, m)$ (see Fig. 1(b)).

Lemma 2.7 **[10]** *Let $T \in \mathcal{T}(n, m)$, where $m \geq 3$ and $T \ncong T^*(n, m)$. Then*

$$z(T) \geq 2^{m-4}(10n - 15m + 9)$$

with equality if and only if $T \cong T^{**}(n, m)$, where $T^{**}(n, m)$ is the tree obtained from $T^*(n - 2, m - 1)$ by attaching a path of length 2 to a vertex of degree 2 (as shown in Fig. 1(c)).

3. Main results

First we characterize the graphs in $\mathcal{U}(n,m)$ with minimal and second minimal Hosoya index, respectively.

Theorem 3.1 *Let G be a graph in $\mathcal{U}(n,m)$ $(n \geq 2m, \quad m \geq 2)$. Then*

$$z(G) \geq 2^{m-2}(2n-3m+4)$$

and the equality holds if and only if $G \cong U^*(n,m)$ or $U^{**}(6,3)$ (see Fig. 2(a) and Fig. 2(d)).

Proof. Let G be a graph in $\mathcal{U}(n,m)$ $(n \geq 2m, \ m \geq 2)$ and M an m-matching of G. We always can take an edge uv from the unique cycle of G such that $uv \notin M$. Then $G-uv$ is a n-vertex tree with $\alpha'(G-uv)=m$. (Since $G-uv$ is a subgraph of G, we have $\alpha'(G-uv) \leq \alpha'(G)=m$. Noting that M is an m-matching of $G-uv$, we have $\alpha'(G-uv) \geq m$. Hence $\alpha'(G-uv)=m$.) By Lemma 2.6, we have

$$z(G-uv) \geq 2^{m-2}(2n-3m+3) \tag{1}$$

with equality if and only if $G-uv \cong T^*(n,m)$. Noting that $G-\{u,v\}$ has an $(m-2)$-matching, we have

$$z(G-\{u,v\}) \geq 2^{m-2}. \tag{2}$$

By Lemma 2.1 (1) and inequalities (1) and (2), we have

$$\begin{aligned} z(G) &= z(G-uv)+z(G-\{u,v\}) \\ &\geq 2^{m-2}(2n-3m+3)+2^{m-2} \\ &= 2^{m-2}(2n-3m+4) \\ &= z(U^*(n,m)). \end{aligned} \tag{3}$$

The equality in (3) holds if and only if both the equalities in (1) and (2) hold. The equality in (1) holds if and only if $G-uv \cong T^*(n,m)$. The equality in (2) holds if and only if $G-\{u,v\} \cong (n-2m+2)K_1 \cup (m-2)K_2$. If $G \in \mathcal{U}(n,m)$, $G-uv \cong T^*(n,m)$

and $G - \{u, v\} \cong (n - 2m + 2)K_1 \cup (m - 2)K_2$, by $m \geq 2$, it is easy to see that either one end of uv is the vertex of degree $n - m$ of $T^*(n, m)$ and the other end of uv is the pendent vertex adjacent to a vertex of degree 2 of $T^*(n, m)$, or u, v are the vertices of degree 2 of $T^*(n, m)$ in the case $n = 6$ and $m = 3$. Thus the equality in (3) holds if and only if $G \cong U^*(n, m)$ or $U^{**}(6, 3)$. This completes the proof of Theorem 3.1. ■

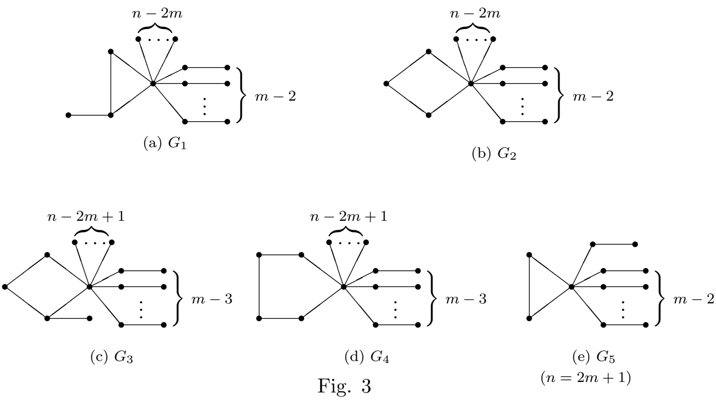


Fig. 3

Theorem 3.2 *Let G be a graph in $\mathcal{U}(n, m)$ $(n \geq 2m,\ \ m \geq 3)$ and $G \ncong U^*(n, m)$. Then*

$$z(G) \geq 2^{m-4}(10n - 15m + 13)$$

and the equality holds if and only if $G \cong U^{**}(n, m)$ (see Fig. 2(b)).

Proof. Let G be a graph in $\mathcal{U}(n, m)$ $(n \geq 2m,\ m \geq 3)$ such that $G \ncong U^*(n, m)$ and M be an m-matching of G. We always can take an edge uv from the unique cycle of G such that $uv \notin M$. Then $G - uv$ is a n-vertex tree with $\alpha'(G - uv) = m$. (Since $G - uv$ is a subgraph of G, we have $\alpha'(G - uv) \leq \alpha'(G) = m$. Noting that M is an m-matching of $G - uv$, we have $\alpha'(G - uv) \geq m$. Hence $\alpha'(G - uv) = m$.) Now we distinguish the following two cases:

Case 1. $G - uv \ncong T^*(n, m)$.

In this case, by Lemma 2.7, we have

$$z(G-uv) \geq 2^{m-4}(10n-15m+9) \tag{4}$$

with equality if and only if $G-uv \cong T^{**}(n,m)$. Noting that $G-\{u,v\}$ has an $(m-2)$-matching, we have

$$z(G-\{u,v\}) \geq 2^{m-2}. \tag{5}$$

By Lemma 2.1 (1) and inequalities (4) and (5), we have

$$\begin{aligned} z(G) &= z(G-uv)+z(G-\{u,v\}) \\ &\geq 2^{m-4}(10n-15m+9)+2^{m-2} \qquad (6) \\ &= 2^{m-4}(10n-15m+13) \\ &= z(U^{**}(n,m)). \end{aligned}$$

The equality in (6) holds if and only if both the equalities in (4) and (5) hold. The equality in (4) holds if and only if $G-uv \cong T^{**}(n,m)$. The equality in (5) holds if and only if $G-\{u,v\} \cong (n-2m+2)K_1 \cup (m-2)K_2$. Note that if $G \in \mathcal{U}(n,m)$, $G \ncong U^*(n,m)$, $G-uv \cong T^{**}(n,m)$ and $G-\{u,v\} \cong (n-2m+2)K_1 \cup (m-2)K_2$, by $m \geq 3$, it is easy to see that either u or v must be the vertex of degree $n-m-1$ of $T^{**}(n,m)$ and $G \cong U^{**}(n,m)$. So the equality in (6) holds if and only if $G \cong U^{**}(n,m)$.

Case 2. $G-uv \cong T^*(n,m)$.

In this case, by that $G-uv \cong T^*(n,m)$ and $G \ncong U^*(n,m)$, it is easy to see that $G \in \{U^{**}(n,m),\ G_1,\ G_2,\ G_3,\ G_4,\ G_5\}$ (see Fig. 2 and Fig. 3).

By Lemmas 2.1 (1) and 2.6, it is not difficult to get

$$\begin{aligned} z(G_1) &= 2^{m-2}(2n-3m+3)+2^{m-3}(2n-3m) \\ z(G_2) &= 2^{m-2}(2n-3m+3)+2^{m-3}(2n-3m+2), \\ z(G_3) &= 2^{m-2}(2n-3m+3)+2^{m-4}(2n-3m+3), \\ z(G_4) &= 2^{m-2}(2n-3m+3)+2^{m-4}(2n-3m+5), \\ z(G_5) &= 2^{m-2}(2m+6). \end{aligned}$$

By the simple calculation, we have $z(G_i) > z(U^{**}(n,m))$ for $1 \leq i \leq 5$. This completes the proof of Theorem 3.2. ■

By the similar argument to the proof of Theorem 3.1, we can prove the following result.

Theorem 3.3 *Let G be a graph in $\mathcal{B}(n,m)$ $(n \geq 2m, \quad m \geq 3)$. Then*

$$z(G) \geq 2^{m-2}(2n-3m+5)$$

and the equality holds if and only if $G \cong B^*(n,m)$ (see Fig. 2(c)).

Proof. Let G be a graph in $\mathcal{B}(n,m)$ $(n \geq 2m, \quad m \geq 3)$ and M an m-matching of G. We always can take an edge uv from a cycle of G such that $uv \notin M$. Then $G-uv$ is a connected unicyclic graph. Furthermore, $\alpha'(G-uv) = m$. (Since $G-uv$ is a subgraph of G, we have $\alpha'(G-uv) \leq \alpha'(G) = m$. Noting that M is an m-matching of $G-uv$, we have $\alpha'(G-uv) \geq m$. Hence $\alpha'(G-uv) = m$.) So $G-uv \in U(n,m)$. From Theorem 3.1, we have

$$z(G-uv) \geq 2^{m-2}(2n-3m+4), \tag{7}$$

and the equality in (7) holds if and only if $G \cong U^*(n,m)$ or $U^{**}(6,3)$. Noting that $G-\{u,v\}$ has an $(m-2)$-matching, we have

$$z(G-\{u,v\}) \geq 2^{m-2}. \tag{8}$$

By Lemma 2.1 (1) and inequalities (7) and (8), we have

$$\begin{aligned} z(G) &= z(G-uv) + z(G-\{u,v\}) \\ &\geq 2^{m-2}(2n-3m+4) + 2^{m-2} \\ &= 2^{m-2}(2n-3m+5) \\ &= z(B^*(n,m)). \end{aligned} \tag{9}$$

The equality in (9) holds if and only if both the equalities in (7) and (8) hold. The equality in (7) holds if and only if $G-uv \cong U^*(n,m)$ or $U^{**}(6,3)$. The equality in (8) holds if and only if $G-\{u,v\}\cong(n-2m+2)K_1\cup(m-2)K_2$. Note that if $G\in\mathcal{B}(n,m)$, $G-uv\cong U^*(n,m)$ or $U^{**}(6,3)$ and $G-\{u,v\}\cong(n-2m+2)K_1\cup(m-2)K_2$, by $m\geq 3$, it is easy to see that $G-uv\cong U^*(n,m)$, one end of uv is the vertex of degree of $n-m+1$ of $U^*(n,m)$, and the other end of uv is the pendent vertex adjacent to a vertex of degree 2 of $U^*(n,m)$. So the equality in (9) holds if and only if $G\cong B^*(n,m)$. ∎

Now we generalize Lemma 2.6 and Theorems 3.1 and 3.3 to $\mathcal{G}(n,t,m)$.

Theorem 3.4 *Let G be a graph in $\mathcal{G}(n,t,m)$, where $n\geq 2m$ and $0\leq t\leq m-1$. Then*

$$z(G)\geq 2^{m-2}(2n-3m+t+3).$$

When $n=6$, $m=3$ and $t=1$, the equality holds if and only if $G\cong U^*(6,3)$ or $U^{**}(6,3)$. In other cases, the equality holds if and only if $G\cong G^*(n,t,m)$ (see Fig. 1(a)).

Proof. By Lemma 2.6 and Theorem 3.1, it is sufficient to show that the result holds for $2\leq t\leq m-1$. We show it by induction on t. When $t=2$, the result holds immediately by Theorem 3.3. Now we suppose the result holds for $t=k$ $(k\geq 3)$. Let G be a graph in $\mathcal{G}(n,k+1,m)$ $(n\geq 2m,\ \ 3\leq k\leq m-2)$ and M an m-matching of G. We always can take an edge uv from a cycle of G such that $uv\notin M$. It is easy to see that $G-uv\in\mathcal{G}(n,k,m)$ $(n\geq 2m,\ \ 3\leq k\leq m-2)$. (Since $G-uv$ is a subgraph of G, we have $\alpha'(G-uv)\leq\alpha'(G)=m$. Noting that M is an m-matching of $G-uv$, we have $\alpha'(G-uv)\geq m$. Hence $\alpha'(G-uv)=m$.) By the induction hypothesis, we have

$$z(G-uv)\geq 2^{m-2}(2n-3m+k+3) \tag{10}$$

with equality if and only if $G-uv\cong G^*(n,k,m)$. Noting that $G-\{u,v\}$ has an $(m-2)$-matching, we have

$$z(G-\{u,v\})\geq 2^{m-2}. \tag{11}$$

By Lemma 2.1 (1) and inequalities (10) and (11), we have

$$\begin{aligned} z(G) &= z(G-uv)+z(G-\{u,v\}) \\ &\geq 2^{m-2}(2n-3m+k+3)+2^{m-2} \qquad (12) \\ &= 2^{m-2}(2n-3m+k+4) \\ &= z(G^*(n,k+1,m)). \end{aligned}$$

The equality in (12) holds if and only if both the equalities in (10) and (11) hold. The equality in (10) holds if and only if $G-uv \cong G^*(n,k,m)$. The equality in (11) holds if and only if $G-\{u,v\} \cong (n-2m+2)K_1 \cup (m-2)K_2$. Note that if $G \in \mathcal{G}(n,k+1,m)$, $G-uv \cong G^*(n,k,m)$, $G-\{u,v\} \cong (n-2m+2)K_1 \cup (m-2)K_2$, by $3 \leq k \leq m-2$, it is easy to see that one end of uv must be the vertex of degree of $n-m+t$ of $G^*(n,k,m)$, and the other end of uv must be the pendent vertex adjacent to a vertex of degree 2 of $G^*(n,k,m)$. So the equality in (12) holds if and only if $G \cong G^*(n,k+1,m)$. This completes the proof of Theorem 3.4. ■

Now we consider the graphs with maximal Merrifield-Simmons indices among the connected graphs with the given cyclomatic number and edge-independence number.

Lemma 3.1 *Let G be a graph with $\alpha'(G) = m$. Then $i(G) \leq 2^{n-2m} \cdot 3^m$, and the equality holds if and only if $G \cong (n-2m)K_1 \cup mK_2$.*

Proof. By Lemma 2.3, it is easy to see that $i((n-2m)K_1 \cup mK_2) = 2^{n-2m} \cdot 3^m$. Let M be an m-matching of G. If $e = uv \notin M$, then $i(G) < i(G-uv)$ by Lemma 2.1(2). Hence $i(G) \leq 2^{n-2m} \cdot 3^m$, and the equality holds if and only if $G \cong (n-2m)K_1 \cup mK_2$.■

Theorem 3.5 *Let $T \in \mathcal{T}(n,m)$. Then*

$$i(T) \leq 2^{n-2m+1} \cdot 3^{m-1} + 2^{m-1}$$

with equality if and only if $T \cong T^*(n,m)$ (see Fig. 1(b)).

Proof. Let $T \in \mathcal{T}(n,m)$. First we show the theorem holds for $n = 2m$, that is

$$i(T) \leq 2 \cdot 3^{m-1} + 2^{m-1}$$

with equality if and only if $T \cong T^*(2m,m)$, by induction on m. Obviously, in this case T is a tree with perfect matching. If $m = 1,\ 2$ and 3, the results hold immediately. We suppose the result holds when $m = k-1$. For $T \in \mathcal{T}(2k,k)$, by Lemma 2.4, T has a pendent vertex v adjacent to a vertex u of degree 2. Let $w\ (\neq v)$ be the vertex adjacent to u. By Lemma 2.1 (2),

$$i(T) \;=\; i(T-uw) - i(T-(N_u \cup N_w))$$

$$
\begin{aligned}
&= i((T-\{u,v\})\cup K_2) - i(T-(N_u\cup N_w)) \\
&= 3\cdot i(T-\{u,v\}) - i(T-(N_u\cup N_w)). \qquad (13)
\end{aligned}
$$

It is easy to see that $T-\{u,v\}\in \mathcal{T}(2k-2,k-1)$. By the induction hypothesis,

$$i(T-\{u,v\}) \le 2\cdot 3^{k-2}+2^{k-2}, \qquad (14)$$

and the equality holds if and only if $T-\{u,v\}\cong T^*(2k-2,k-1)$.

For $T-(N_u\cup N_w)$, we have the following fact.

Fact A. $\alpha(T-(N_u\cup N_w))=k-2$.

Proof of Fact A. It is well known that for a bipartite graph, the edge-independence number is equal to the vertex-covering number (König's Theorem), and for any graph, the sum of independence number and vertex-covering number of a graph is equal to the order of the graph (see [1]). Noting that $T-(N_u\cup N_w)$ is a bipartite graph of order $2k-d(w)-2$ with $\alpha'=k-d(w)$, we have $\alpha(T-(N_u\cup N_w))=(2k-d(w)-2)-(k-d(w))=k-2$.■

By Fact A,

$$i(T-(N_u\cup N_w)) \ge 2^{k-2}, \qquad (15)$$

and the equality holds if and only if $T-(N_u\cup N_w)\cong(k-2)K_1$. Therefore, by equality (13) and inequalities (14) and (15), we have

$$
\begin{aligned}
i(T) &\le 3(2\cdot 3^{k-2}+2^{k-2})-2^{k-2} \qquad (16)\\
&= 2\cdot 3^{k-1}+2^{k-1}\\
&= i(T^*(2k,k)).
\end{aligned}
$$

The equality in (16) holds if and only if both the equalities in (14) and (15) hold. When the equalities in (14) and (15) hold, we have $T-uw\cong T^*(2k-2,k-1)\cup K_2$ and $T-(N_u\cup N_w)\cong(k-2)K_1$, and then $T\cong T^*(2k,k)$. Thus the equality in (16) holds if and only if $T\cong T^*(2k,k)$. This completes the proof of Theorem 3.5 when $n=2m$.

Now we suppose $n>2m$ and proceed by induction on n. By Lemma 2.5, T have an m-matching M and a pendent vertex v such that v is M-unsaturated. Let u be the unique vertex adjacent to v, then u must be M-saturated. Since $T - v \in \mathcal{T}(n-1, m)$, by the induction hypothesis,

$$i(T - v) \leq 2^{n-2m} \cdot 3^{m-1} + 2^{m-1}, \tag{17}$$

and the equality holds if and only if $T - v \cong T^*(n-1, m)$. By Lemma 2.2 (2), we have

$$i(T) = i(T - v) + i(T - \{u, v\}). \tag{18}$$

Noting that $\alpha'(T - \{u, v\}) = m - 1$, by Lemma 3.1 we get

$$i(T - \{u, v\}) \leq 2^{n-2m} \cdot 3^{m-1}, \tag{19}$$

and the equality holds if and only if $T - \{u, v\} \cong (n-2m)K_1 \cup (m-1)K_2$. So by equality (18) and inequalities (17) and (19),

$$\begin{aligned} i(T) &\leq 2^{n-2m} \cdot 3^{m-1} + 2^{m-1} + 2^{n-2m} \cdot 3^{m-1} \\ &= 2^{n-2m+1} \cdot 3^{m-1} + 2^{m-1} \\ &= i(T^*(n, m)). \end{aligned} \tag{20}$$

The equality in (20) holds if and only if both the equalities in (17) and (19) hold. When the equalities in (17) and (19) hold, we have $T - v \cong T^*(n-1, m)$ and $T - \{u, v\} \cong (n-2m)K_1 \cup (m-1)K_2$, and then $T \cong T^*(n, m)$. Thus the equality in (20) holds if and only if $T \cong T^*(n, m)$. This completes the proof of Theorem 3.5. ■

Corollary 3.1 *Let T be a n-vertex tree ($n \geq 2$). Then $i(T) \leq 2^{n-1} + 1$ and the equality holds if and only if $T \cong T^*(n, 1)$. (Obviously, $T^*(n, 1)$ is isomorphic to n-vertex star.)*

Proof. By elementary calculation, we have

$$\begin{aligned} & i(T^*(n, m)) - i(T^*(n, m+1)) \\ = \; & 2^{n-2m+1} \cdot 3^{m-1} + 2^{m-1} - (2^{n-2m-1} \cdot 3^m + 2^m) \\ = \; & 2^{n-2m-1} \cdot 3^{m-1} - 2^{m-1}. \end{aligned}$$

Since $n \geq 2(m+1)$ and $m \geq 1$, we have $i(T^*(n,m)) > i(T^*(n,m+1))$. By Theorem 3.5, we have $i(T) \leq i(T^*(n,1)) = 2^{n-1}+1$ and the equality holds if and only if $T \cong T^*(n,1)$. ■

By the similar argument to Theorem 3.5, we can get the following results on Merrifield-Simmons index corresponding to Lemma 2.7 and Theorems 3.2-3.4.

Theorem 3.6 *Let $T \in \mathcal{T}(n,m)$, where $m \geq 3$ and $T \ncong T^*(n,m)$. Then*

$$i(T) \leq 8 \cdot 2^{n-2m+1} \cdot 3^{m-3} + 3 \cdot 2^{m-2}$$

with equality if and only if $T \cong T^{**}(n,m)$ (as shown in Fig. 1(c)).

Theorem 3.7 *Let G be a graph in $\mathcal{U}(n,m)$ $(n \geq 2m, \quad m \geq 2)$. Then*

$$i(G) \leq 2^{n-2m+1} \cdot 3^{m-1} + 2^{m-2}.$$

When $G \in \mathcal{U}(4,2)$, the equality holds if and only if $G \cong U^*(4,2)$ or G_2; When $G \in \mathcal{U}(6,3)$, the equality holds if and only if $G \cong U^*(6,3)$, $U^{**}(6,3)$ or G_3; In other cases, the equality holds if and only if $G \cong U^*(n,m)$ (see Fig. 2(a), Fig. 2(d), Fig. 3(b) and Fig. 3 (c)).

Theorem 3.8 *Let G be a graph in $\mathcal{U}(n,m)$ $(n \geq 2m, \quad m \geq 3)$ and $G \ncong U^*(n,m)$. Then*

$$i(G) \leq 8 \cdot 2^{n-2m+1} \cdot 3^{m-3} + 2^{m-1}$$

and the equality holds if and only if $G \cong U^{**}(n,m)$ or G_3 (see Fig. 2(b) and Fig. 3(c)).

Theorem 3.9 *Let G be a graph in $\mathcal{G}(n,t,m)$, where $n \geq 2m$ and $2 \leq t \leq m-1$. Then $i(G) \leq 2^{n-2m+1} \cdot 3^{m-1} + 2^{m-t-1}$ and the equality holds if and only if $G \cong G^*(n,t,m)$ (see Fig. 1(a)).*

4. Question

In this paper, we characterize the graphs with minimal Hosoya indices and maximal Merrifield-Simmons indices , respectively, in $\mathcal{G}(n,t,m)$ when $n \geq 2m$ and $0 \leq t \leq m-1$. Then it is natural to ask:

Which graphs have minimal Hosoya indices and maximal Merrifield-Simmons indices, respectively, in $\mathcal{G}(n,t,m)$ *when* $n \geq 2m$ *and* $m \leq t \leq \frac{1}{2}n(n-1)-(n-1)$*?*

Obviously, in this case, $G^*(n,t,m)$ is no more the graph with minimal Hosoya index and maximal Merrifield-Simmons index in $\mathcal{G}(n,t,m)$, since $G^*(n,t,m) \notin \mathcal{G}(n,t,m)$, when $n \geq 2m$ and $m \leq t \leq \frac{1}{2}n(n-1)-(n-1)$. Moreover, with the growth of t, it seems more and more difficult to determine the graphs with minimal Hosoya indices and maximal Merrifield-Simmons indices, respectively, in $\mathcal{G}(n,t,m)$.

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