MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **63** (2010) 789-798

ISSN 0340 - 6253

The extremal $\theta-$graphs with respect to Hosoya index and Merrifield-Simmons index

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(Received July 15, 2009)

Abstract. For a graph G, the Hosoya index and the Merrifield-Simmons index are defined as the total number of its matchings and the total number of its independent sets, respectively. In this paper, we obtain the smallest and the largest Hosoya index and Merrifield-Simmons index of $\theta-$graphs, which are obtained by subdividing the edges of the multigraph consisting of 3 parallel edges, denoted by $\theta(r, s, t)$. At the same time, we characterize the corresponding extremal graphs. Our results show that the graphs of the smallest Merrifield-Simmons index do not coincide with those of the largest Hosoya index among $\theta-$graphs. Surprisedly, they attain their lower bound for at the same graph $\theta(0, 1, n-3)$.

1. Introduction

Let G be a graph with vertex set $V(G)$, edge set $E(G)$. The *Hosoya index* and the *Merrifield-Simmons index* of a graph G are two prominent examples of topological indices which are of interest in combinatorial chemistry. They are defined as the total number of matchings (independent edge subsets), denoted by $z(G)$, and the total number of independent vertex subsets, denoted by $i(G)$, of a graph G, respectively. The *Hosoya index* was introduced by Hosoya [1] in 1971, and it turned out to be applicable to several questions of molecular chemistry. For example, the connections with physico-chemical

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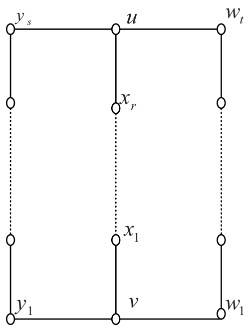
properties such as boiling point, entropy or heat of vaporization are well studied. Similar connections are known for the *Merrifield-Simmons index*, that was introduced by Merrifield and Simmons [2] in 1989. For detailed information on the chemical applications, we refer to [1, 3, 4] and the references therein.

Several papers deal with the characterization of the extremal graphs with respect to these two indices in several given graph classes. Usually, trees, unicyclic graphs and certain structures involving pentagonal and hexagonal cycles are of major interest [5-14].

$\theta-$graphs are obtained by subdividing the edges of the multigraph consisting of 3 parallel edges, and they are denoted by $\theta(r, s, t)$(see Fig.1). Without loss of generality, let $r \leq s \leq t$. In [15], F. Ramezani et.al. have shown that any $\theta-$graph G is determined by the spectrum (the multiset of eigenvalues) except possibly when it contains a unique 4-cycle. In this paper, we consider the extremal Hosoya index and Merrifield-Simmons index of $\theta-$graphs.

In order to present our results, we introduce some notations and terminologies. For other undefined notation we refer to Bollobás [16]. 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. We denote by P_n, C_n the path, the cycle on n vertices, respectively. Let $N(v) = \{u|uv \in E(G)\}$, $N[v] = N(v) \cup \{v\}$.



$\theta(r,s,t)$

Figure 1: $\theta-$graph

We list some results that will be used in this paper.

Lemma 1.1 ([3])**.** *Let $G = (V, E)$ be a graph.*

(i) *If $uv \in E(G)$, then $z(G) = z(G - uv) + z(G - \{u, v\}))$;*

(ii) *If $v \in V(G)$, then $z(G) = z(G - v) + \sum_{u \in N(v)} z(G - \{u, v\})$;*

(iii) *If $G_1, G_2, \dots, G_t$ are the components of the graph G, then $z(G) = \prod_{j=1}^{t} z(G_j)$.*

Lemma 1.2 ([3])**.** *Let $G = (V, E)$ be a graph.*

(i) *If $uv \in E(G)$, then $i(G) = i(G - uv) - i(G - \{N[u] \cup N[v]\}))$;*

(ii) *If $v \in V(G)$, then $i(G) = i(G - v) + i(G - N[v])$;*

(iii) *If $G_1, G_2, \dots, G_t$ are the components of the graph G, then $i(G) = \prod_{j=1}^{t} i(G_j)$.*

Denote by F_n the nth Fibonacci number. Recall that $F_n = F_{n-1} + F_{n-2}$ with initial conditions $F_0 = 1$ and $F_1 = 1$. Then $z(P_n) = F_n, i(P_n) = F_{n+1}$. Note that $F_{n+m} = F_n F_m + F_{n-1} F_{m-1}$. For convenience, we let $F_n = 0$ for $n < 0$.

2. Extremal $\theta-$graphs with respect to the Hosoya index

We first consider the extremal θ-graphs with respect to the Hosoya index.

Lemma 2.1. *Let $\theta(r, s, t)$ be the graph in Fig. 1,*

(i)[17] If $r = 0$, then $z(\theta(0, s, t)) = F_{s+t+2} + F_{s+t} + F_s F_t$;

(ii)If $r > 0$, then $z(\theta(r, s, t)) = F_r F_{s+t+2} + F_r F_{s+t} + 2F_{r-1} F_{s+t+1} + F_{r-2} F_s F_t$.

Proof. By Lemma 1.1, we have

(i) For $r = 0$,

$$\begin{aligned} z(\theta(0, s, t)) &= z(\theta(0, s, t) - uv) + z(\theta(0, s, t) - u - v) \\ &= F_{s+t+2} + F_{s+t} + F_s F_t; \end{aligned}$$

(ii) For $r > 0$,

$$\begin{aligned} z(\theta(r, s, t)) &= z(\theta(r, s, t) - ux_r) + z(\theta(r, s, t) - u - x_r) \\ &= z(\theta(r, s, t) - ux_r - vx_1) + z(\theta(r, s, t) - ux_r - v - x_1) \\ &\quad + z(\theta(r, s, t) - u - x_r - vx_1) + z(\theta(r, s, t) - u - x_r - v - x_1) \\ &= F_r F_{s+t+2} + F_r F_{s+t} + 2F_{r-1} F_{s+t+1} + F_{r-2} F_s F_t. \end{aligned}$$

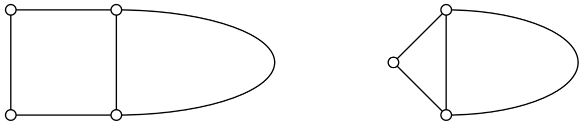


Figure 2: (a) $\theta(0, 2, n-4)$, (b) $\theta(0, 1, n-3)$

This completes the proof. $\square$

Lemma 2.2. *([17]) Let $\theta(r, s, t)$ be the graph in Fig. 1, $\theta(0, 2, n-4)$ be the graph in Fig.2(a), where $r+s+t = n-2$. $z(\theta(r, s, t)) \leq z(\theta(0, 2, n-4))$, with the equality holds if and only if $\theta(r, s, t) \cong \theta(0, 2, n-4)$ or $\theta(r, s, t) \cong \theta(1, 1, 1)$.*

Lemma 2.3. *Let $\theta(r, s, t)$ be the graph in Fig. 1, $\theta(0, 1, n-3)$ be the graph in Fig.2(b), where $r+s+t = n-2, 0 \leq r \leq s \leq t$, we have $z(\theta(r, s, t)) \geq F_{n+1}$, with the equality if and only if $\theta(r, s, t) \cong \theta(0, 1, n-3)$, or $r = 1$ in $\theta(r, s, t)$.*

Proof. By Lemma 2.1(i), we have

$$z(\theta(0, 1, n-3)) \quad = \quad F_{n+1} = F_{r+s+t+3}. \tag{2.1}$$

Case 1. $r = 0$.

Then $1 \leq s \leq t$, if $s = 1$, $\theta(0, s, t)) \cong \theta(0, 1, n-3)$; if $s \geq 2$, by Lemma 2.1(i) and (2.1), we have

$$\begin{aligned} z(\theta(0, s, t)) - z(\theta(0, 1, n-3)) &= F_{s+t+2} + F_{s+t} + F_s F_t - F_{n+1} \\ &= F_{s-2} F_{t-2} > 0 \end{aligned}$$

Case 2. $r > 0$.

If $r = 1$, by Lemma 2.1(ii) , we have $z(\theta(r, s, t)) = F_{n+1}$, then

$$z(\theta(r, s, t)) = z(\theta(0, 1, n-3))$$

.

If $r \geq 2$, by Lemma 2.1(ii) and (2.1), we have

$$\begin{aligned} z(\theta(r, s, t)) - z(\theta(0, 1, n-3)) &= F_r F_{s+t+2} + F_r F_{s+t} + 2F_{r-1} F_{s+t+1} \\ &\quad + F_{r-2} F_s F_t - F_{r+s+t+3} \\ &= F_{r-2} F_{s-2} F_{t-2} > 0 \end{aligned}$$

So, $z(\theta(r,s,t)) \geq z(\theta(0,1,n-3))$.

Hence $z(\theta(r,s,t)) \geq F_{n+1}$, with the equality if and only if $\theta(r,s,t) \cong \theta(0,1,n-3)$, or $r=1$ in $\theta(r,s,t)$. $\square$

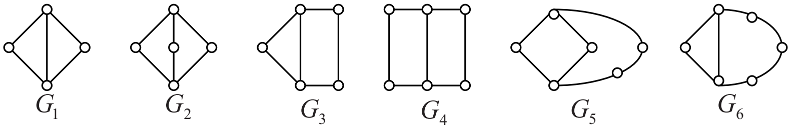


Figure 3: $\theta-$graphs with order of 4, 5 and 6

$\theta-$graphs with order of 4 and 5 are shown in Fig. 3, by Lemma 1.1, $z(G_1)=8$, and $z(G_2)=z(G_3)=13$. Furthermore, $z(\theta(0,2,n-4)) = F_n + F_{n-2} + 2F_{n-4}$, by Lemma 2.2, 2.3, we have

Theorem 2.4. *For any $\theta-$graph $\theta(r,s,t)$, where $r+s+t+2=n$, $0 \leq r \leq s \leq t$, we have*

(i)If $n=4$, $z(\theta(0,1,1))=8$;

(ii)If $n=5$, $z(\theta(0,1,2))=z(\theta(1,1,1))=13$;

(iii)If $n \geq 6$, $F_{n+1} \leq z(\theta(r,s,t)) \leq F_n + F_{n-2} + 2F_{n-4}$, with the first equality holds if and only if $r=1$ or $\theta(r,s,t) \cong \theta(0,1,n-3)$ in $\theta(r,s,t)$, and the last equality holds if and only if $\theta(r,s,t) \cong \theta(0,2,n-4)$.

3. Extremal $\theta-$graphs with respect to the Merrifield-Simmons index

Now we study the extremal $\theta-$graphs with respect to the Merrifield-Simmons index.

Lemma 3.1. *Let $\theta(r,s,t)$ be the graph in Fig. 1,*

(i)If $r=0$, then $i(\theta(0,s,t)) = F_{s+t+3} - F_{s+t-1} - F_{s-1}F_{t-1}$;

(ii)If $r>0$, then $i(\theta(r,s,t)) = F_{s+1}F_{r+1}F_{t+1} + 2F_sF_rF_t + F_{s-1}F_{r-1}F_{t-1}$.

Proof. By Lemma 1.1, we have

$$\begin{aligned} i(\theta(0,s,t)) &= i(\theta(0,s,t)-uv) - i(\theta(0,s,t)-N[u]-N[v]) \\ &= i(C_{s+t+2}) - i(P_{s-2} \cup P_{t-2}) \\ &= F_{s+t+3} - F_{s+t-1} - F_{s-1}F_{t-1}; \end{aligned}$$

$$\begin{aligned}
i(\theta(r,s,t)) &= i(\theta(r,s,t)-u)+i(\theta(r,s,t)-N[u]) \\
&= i(\theta(r,s,t)-u-v)+i(\theta(r,s,t)-u-N[v])+i(\theta(r,s,t)-N[u]-v) \\
&\quad +i(\theta(r,s,t)-N[u]-N[v]) \\
&= i(P_s\cup P_r\cup P_t)+2i(P_{s-1}\cup P_{r-1}\cup P_{t-1})+i(P_{s-2}\cup P_{r-2}\cup P_{t-2}) \\
&= F_{s+1}F_{r+1}F_{t+1}+2F_sF_rF_t+F_{s-1}F_{r-1}F_{t-1}.
\end{aligned}$$

□

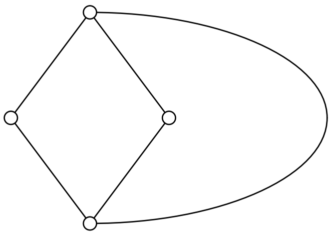


Figure 4: $\theta(1,1,n-4)$

Lemma 3.2. *For any $\theta-$graph $\theta(r,s,t)$, where $r+s+t=n-2$, $0\le r\le s\le t, n\ge 7$, $i(\theta(r,s,t))\le i(\theta(1,1,n-4))$, with the equality if and only if $\theta(r,s,t)\cong\theta(1,1,n-4)$(see Fig. 4).*

Proof. By Lemma 3.1(ii), we have

$$i(\theta(1,1,n-4)) = F_{n-1}+3F_{n-3}. \tag{3.2}$$

$$\begin{aligned}
i(\theta(0,2,n-4)) &= F_{n+1}-F_{n-3}-F_{n-5}=3F_{n-2}+F_{n-4}; \\
i(\theta(0,1,n-3)) &= F_n+F_{n-3}.
\end{aligned}$$

Case 1. $r=0$.

Then $1\le s\le t$, if $s=1$, $\theta(0,s,t))\cong\theta(0,1,n-3)$, we have

$$i(\theta(1,1,n-4))-i(\theta(0,1,n-3)) = F_{n-5}>0.$$

If $s=2$, $\theta(0,s,t)\cong\theta(0,2,n-4)$, we have

$$i(\theta(1,1,n-4))-i(\theta(0,2,n-4))) = F_{n-7}>0.$$

If $s > 2$

$$\begin{aligned} i(\theta(1,1,n-4)) - i(\theta(0,s,t)) &= F_{n-1} + 3F_{n-3} - (F_{s+t+3} - F_{s+t-1} - F_{s-1}F_{t-1}) \\ &= F_{s-2}F_{t-3} + F_{s-3}F_{t-2} > 0 \end{aligned}$$

So, $i(\theta(1,1,n-4)) \geq i(\theta(0,s,t))$.

Case 2. $r = 1$.

Then $1 \leq s \leq t$, if $s = 1$, then $\theta(r,s,t)) \cong \theta(1,1,n-4)$;

If $s \geq 2$, by Lemma 3.1(ii) and (3.2), we have

$$\begin{aligned} i(\theta(1,1,n-4)) - i(\theta(1,s,t)) &= F_{n-1} + 3F_{n-3} \\ &- (F_2F_{s+1}F_{t+1} + 2F_sF_1F_t + F_{s-1}F_{1-1}F_{t-1}) \\ &= F_{n-1} + 3F_{n-3} - 2F_{s+t+2} - F_{s-1}F_{t-1} \\ &= F_{n-5} - F_{s-1}F_{t-1} \\ &= F_{s+t-2} - F_{s-1}F_{t-1} \\ &= F_{s-2}F_{t-2} > 0. \end{aligned}$$

Case 3. $r \geq 2$.

By Lemma 3.1(ii) and (3.2), we have

$$\begin{aligned} & i(\theta(1,1,n-4)) - i(\theta(r,s,t)) \\ = \ & F_{n-1} + 3F_{n-3} - (F_{s+1}F_{r+1}F_{t+1} + 2F_sF_rF_t + F_{s-1}F_{r-1}F_{t-1}) \\ = \ & F_{r+s+t+1} + 3F_{r+s+t-1} - (F_{s+1}F_{r+1}F_{t+1} + 2F_sF_rF_t + F_{s-1}F_{r-1}F_{t-1}) \\ = \ & F_rF_{s+t+1} + F_{r-1}F_{s+t} + 3F_rF_{s+t-1} + 3F_{r-1}F_{s+t-2} \\ & -(F_{s+1}F_{r+1}F_{t+1} + 2F_sF_rF_t + F_{s-1}F_{r-1}F_{t-1}) \\ = \ & F_rF_sF_{t+1} + F_rF_{s-1}F_t + F_{r-1}F_sF_t + F_{r-1}F_{s-1}F_{t-1} \\ & +3F_rF_sF_{t-1} + 3F_rF_{s-1}F_{t-2} + 3F_{r-1}F_{s-1}F_{t-1} + 3F_{r-1}F_{s-2}F_{t-2} \\ & -(F_{s+1}F_{r+1}F_{t+1} + 2F_sF_rF_t + F_{s-1}F_{r-1}F_{t-1}) \\ = \ & F_rF_s(F_{t+1} + 2F_{t-1} - 3F_t) + F_rF_{s-1}(3F_{t-2} - F_{t-1}) \\ & +F_{r-1}F_{s-1}(2F_{t-1} - F_t) + 3F_{r-1}F_{s-2}F_{t-2} - F_{r-1}F_sF_{t-1} \\ = \ & F_{r-2}F_{s-1}F_{t-2} + F_{r-1}F_{s-2}F_{t-2} - F_{r-2}F_{s-2}F_{t-4} \\ = \ & F_{r-2}F_{s-1}F_{t-2} + F_{r-2}F_{s-2}F_{t-3} + F_{r-3}F_{s-2}F_{t-2} > 0 \end{aligned}$$

Hence, $i(\theta(r,s,t)) \leq i(\theta(1,1,n-4))$, with the equality if and only if $\theta(r,s,t) \cong \theta(1,1,n-4)$. $\square$

Lemma 3.3. *Let $\theta(r,s,t)$ be a $\theta-$graph on n vertices. Then $i(\theta(r,s,t)) \geq F_n + F_{n-3}$, where the equality holds if and only if $\theta(r,s,t) \cong \theta(0,1,n-3)$.*

Proof. By Lemma 3.1(i), we have

$$i(\theta(0,1,n-3)) \quad = \quad F_n + F_{n-3}. \tag{3.3}$$

Case 1. $r = 0$.

Then $1 \leq s \leq t$, if $s = 1$, $\theta(0,s,t)) \cong \theta(0,1,n-3)$; if $s \geq 2$, by Lemma 3.1(i), we have

$$\begin{aligned} m(\theta(0,s,t)) - m(\theta(0,1,n-3)) &= F_{s+t+3} - F_{s+t-1} - F_{s-1}F_{t-1} - (F_n + F_{n-3}) \\ &= F_{s-2}F_{t-2} > 0 \end{aligned}$$

Case 2. $r > 0$.

By Lemma 3.1(ii) and (3.2), we have

$$\begin{aligned} & i(\theta(r,s,t)) - i(\theta(0,1,n-3)) \\ = \; & (F_{s+1}F_{r+1}F_{t+1} + 2F_sF_rF_t + F_{s-1}F_{r-1}F_{t-1}) - (F_{r+s+t+2} + F_{r+s+t-1}) \\ = \; & (F_{s+1}F_{r+1}F_{t+1} + 2F_sF_rF_t + F_{s-1}F_{r-1}F_{t-1}) \\ & -(F_rF_{s+t+2} + F_{r-1}F_{s+t+1} + F_rF_{s+t-1} + F_{r-1}F_{s+t-2}) \\ = \; & F_{s+1}F_{r-1}F_{t+1} + F_sF_rF_{t-2} \\ & -F_sF_{r-1}F_{t+1} - F_{s-1}F_{r-1}F_t - F_{s-1}F_rF_{t-2} - F_{s-2}F_{r-1}F_{t-2} \\ = \; & F_{s-1}F_{r-1}F_{t+1} + F_{s-2}F_rF_{t-2} - F_{s-1}F_{r-1}F_t - F_{s-2}F_{r-1}F_{t-2} \\ = \; & F_{s-1}F_{r-1}F_{t-1} + F_{s-2}F_{r-2}F_{t-2}. \end{aligned}$$

Since $1 \leq r \leq s \leq t$, so $F_{s-1}F_{r-1}F_{t-1} + F_{s-2}F_{r-2}F_{t-2} > 0$.

Hence, $i(\theta(r,s,t)) \geq F_n + F_{n-3}$, with the equality if and only if $\theta(r,s,t) \cong \theta(0,1,n-3)$. $\square$

$\theta-$graphs with order of 4, 5 and 6 are shown in Fig.3, by Lemma 2.1, $i(G_1) = 6$, $i(G_2) = i(G_3) = 10$, $i(G_4) = 17$, $i(G_5) = 17$, $i(G_6) = 16$. Furthermore, by Lemma 3.2, 3.3, we have

Theorem 3.4. *For any $\theta-$graph $\theta(r, s, t)$, where $r + s + t + 2 = n$, $0 \leq r \leq s \leq t$, we have*

(i) If $n = 4$, $i(\theta(0, 1, 1)) = 6$;

(ii) If $n = 5$, $i(\theta(0, 1, 2)) = i(\theta(1, 1, 1)) = 10$;

(iii) If $n = 6$, $i(\theta(0, 1, 3)) = 16$, $i(\theta(0, 2, 2)) = 17$, $i(\theta(1, 1, 2)) = 17$;

(iv) If $n \geq 7$, $F_n + F_{n-3} \leq i(\theta(r, s, t)) \leq F_{n-1} + 3F_{n-3}$, with the first equality if and only if $\theta(r, s, t) \cong \theta(0, 1, n-3)$, and the last $\theta(r, s, t) \cong \theta(1, 1, n-4)$.

Remark: From Theorems 2.4 and 3.4, we find that, among the θ-graphs of order n, the graphs achieving the maximum Merrifield-Simmons index are not equal to those achieving the maximum Hosoya index. Surprisingly, the graph $\theta(0; 1; n-3)$ achieves the minimum of both Hosoya and Merrifield- Simmons indices.

Acknowledgement: The authors are grateful to Professor Ivan Gutman for providing reprints of papers and his helpful comments. They are also thankful to the referees for their valuable comments, corrections and suggestions, which led to an improved version of the original manuscript.

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