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On the Minimal Merrifield-Simmons Index of Trees of Order n with at Least $[\frac{n}{2}]+1$ Pendent Vertices[1]

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Abstract

The Merrifield-Simmons index of a graph is defined as the total number of its independent sets. In this paper, we give the minimal Merrifield-Simmons index of trees of order n with at least $[\frac{n}{2}]+1$ pendent vertices and characterize the extremal trees.

1 Introduction

The Merrifield-Simmons index $i(G)$ of a graph G is one of prominent examples of many topological indices which are of interest in combinatorial chemistry. It is defined as the total number of independent vertex subsets of a graph. The Merrifield-Simmons index was introduced by Merrifield and

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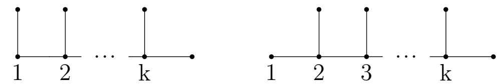
Simmons [1-3], and it turned out to be applicable to several questions of molecular chemistry; in [2] it was shown that $i(G)$ is correlated with boiling points. For further details on the Merrifield-Simmons index, we refer to [2-9]. Similar connections are known for the Hosoya index or Z-index $z(G)$ introduced in [10]. 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 [8-9,12-18].

For the Merrifield-Simmons index, bounds for several classes of graphs were given. For instance, it was observed in [3,8] that the star S_n and the path P_n have the largest and the minimal Merrifield-Simmons index among all trees with n vertices, respectively. [9] gave upper and lower bounds for those two indices in unicyclic graphs in terms of order and characterized the extremal graphs. These results show that typically the graphs of minimal Hosoya index coincide with those of maximal Merrifield-Simmons index and vice versa. In view of the similar definitions, this might not be too surprising; however, the correlations between these two indices are not fully understood yet. [14] determined the extremal graph with the maximal Merrifield-Simmons index among all $(n, n+1)$-graphs. [15] determined the extremal graphs with the maximal and minimal Hosoya index among all $(n, n+1)$-graphs.

Let $G = (V, E)$ be a simple connected graph with vertex set V and edge set E. For any $v \in V$, $N_G(v)$ denotes the neighbors of v, and $d_G(v) = |N(v)|$ is the degree of v, $N_G[v] = \{v\} \cup \{u|uv \in E(G)\}$. A pendent vertex is a vertex of degree one and a pendent edge is an edge incident to a pendent vertex.

Let $\mathcal{T}_n$ be the set of trees of order $n \geq 4$ with at least $[\frac{n}{2}] + 1$ pendent vertices. If $n = 2k$ is even, then $T^{(n)}$ is the tree of order $n \geq 4$ which is obtained from the path P_{k+1} of order $k + 1$ by attaching a pendent edge to every vertex of degree 2 in P_{k+1}; if $n = 2k+1$ is odd, then $T^{(n)}$ is one which is obtained from the path P_{k+1} of order $k+1$ by attaching a pendent edge to every vertex of degree 2 and one of pendent vertices in P_{k+1}, see Figure 1.



(a) $T^{(2k+1)}$ (b) $T^{(2k)}$

Figure 1. The trees $T^{(2k+1)}$ and $T^{(2k)}$.

Recently, Yan and Ye [17] showed that if $T \in \mathcal{T}_n$ then $E(T) \le E(T^{(n)})$ and $z(T) \le z(T^{(n)})$ with two equalities if and only if $T = T^{(n)}$; Using this result, they proved that if T is a tree of order n then $per(L(T)) \le per(L(T^{(n)}))$, a result obtained by Brualdi et al (Discrete Math., 48(1984)1-21), where $E(T)$ is the energy of T and $per(L(T))$ is the permanent of the Laplacian matrix $L(T)$ of T. In this paper, we will also find that $T^{(n)}$ is the tree with the minimal Merrifield-Simmons index in $\mathcal{T}_n$.

2 The tree with the minimal Merrifield-Simmons index in $\mathcal{T}_n$

Let G be a graph and v a vertex of G, $W \subseteq V(G)$, then $G - v$ and $G - W$ denote the subgraphs obtained from G obtained by deleting the vertex v and the vertices of W, respectively. If a graph G has components $G_1, G_2, \cdots, G_t$, then G is denoted by $G_1 \cup G_2 \cup \cdots \cup G_t$.

The following basic results are immediate and will be used.

Lemma 2.1. (i) If v is a vertex of G, then

$$i(G) = i(G - v) + i(G - N_G[v])$$

(ii) If G is a graph with components G_1, G_2, $\cdots$, G_k, then

$$i(G) = \prod_{i=1}^{k} i(G_i)$$

(iii) If G' is a spanning subgraph (resp. a proper spanning subgraph) of a simple graph G, then $i(G) \leq i(G')$ (resp. $i(G) < i(G')$).

Theorem 2.2. Let T be a tree of order $n \geq 4$ with at least $[\frac{n}{2}] + 1$ pendent vertices, i.e., $T \in \mathcal{T}_n$. Then

$$i(T) \geq i(T^{(n)})$$

with equality if and only if $T = T^{(n)}$.

Proof. We prove the result by induction on n. If $n = 4$, then there is a unique tree $T^{(4)} = S_4$ in $\mathcal{T}_4$, and the result holds. If $n = 5$, then there are two trees $T^{(5)}$ and S_5 in $\mathcal{T}_5$. Obviously, $i(T^{(5)}) = 14 < i(S_5) = 17$, and the result holds. Now we assume inductively that the result holds for a tree in $\mathcal{T}_n$ with $n < m$ and $m \geq 6$. We need to prove that if $T \in \mathcal{T}_m$ and $T \neq T^{(m)}$ then $i(T) > i(T^{(m)})$.

Case 1. $m = 2k$ is even. Then T is a tree of order $2k$ with at least $[\frac{2k}{2}] + 1 = k + 1$ pendent vertices. If T is a star S_{2k}, it is obvious that $i(T) > i(T^{(m)})$ since S_{2k} is the unique tree with the maximal Merrifield-Simmons index among all trees of order $2k$. Hence we may assume that T is not a star. Note that T must have a vertex v such that there are at least two pendent vertices in its neighbors $N(v)$, otherwise T has at most k pendent vertices. Let $v_1, v_2, \cdots, v_r$ ($r \geq 2$) be the pendent vertices in $N(v)$. Also, there must exist a non-pendent vertex $u \in N(v)$ since T is not a star. Hence T has the form showed in Figure 2(a), where $|V(T_3)| > 1$. By Lemma 2.1,

$$i(T) = i(T_1) + i(T_2)$$

$$i(T^{(2k)}) = i(T^{(2k-1)}) + 2i(T^{(2k-3)})$$

where $T_1 = T - v_1$ and $T_2 = T - v_1 - v$. T_1 is a tree of order $m-1 = 2k-1$ with at least $k = [\frac{2k-1}{2}] + 1$ pendent vertices. By induction, $i(T^{(2k-1)}) \leq i(T_1)$.

Now we only need to show that $i(T^{(2k-1)}) \leq i(T_1)$ and $2i(T^{(2k-3)}) < i(T_2)$, or $i(T^{(2k-1)}) < i(T_1)$ and $2i(T^{(2k-3)}) \leq i(T_2)$.

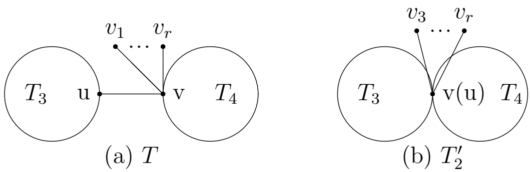


Figure 2. The trees T and T_2'.

Subcase 1.1. $T_1 = T^{(2k-1)}$.

By the definition of T_1 and $T \neq T^{(2k)}$, T must be a tree obtained from $T^{(2k-1)}$ by attaching a pendent edge to some vertex i $(1 < i < k)$ of degree 3, see Figure 3. Then $T_2 = T - v_1 - v = K_1 \cup T' \cup T''$, where K_1, T' and T'' are the components of $T - v_1 - v$. Note that $T' \cup T''$ is a proper spanning subgraph of $T^{(2k-3)}$ since we can obtain $T^{(2k-3)}$ by adding an edge between the vertices $i-1$ and $i+1$ in $T' \cup T''$. By Lemma 2.1, $i(T' \cup T'') > i(T^{(2k-3)})$ and $i(T_2) = i(K_1 \cup T' \cup T'') > 2i(T^{(2k-3)})$. So, we have proved that $i(T^{(2k-1)}) \leq i(T_1)$ and $2i(T^{(2k-3)}) < i(T_2)$.

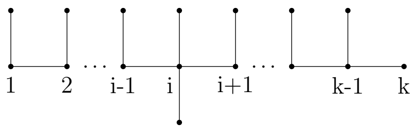


Figure 3. The tree T in the subcase 1.1.

Subcase 1.2. $T_1 \neq T^{(2k-1)}$.

By induction, $i(T_1) > i(T^{(2k-1)})$. Let T_2' be the tree obtained from T by deleting vertices v_1 and v_2 and contracting the edge uv, see Figure 2(b). Then T_2' is a tree of order $2k-3$ with at least $k-1 = [\frac{2k-3}{2}] + 1$ pendent vertices. By induction, $i(T_2') \geq i(T^{(2k-3)})$. Note that $T_2 = T - v_1 - v =$

$T_3 \cup (T_4 - v) \cup (r-1)K_1$ is a spanning subgraph of $K_1 \cup T_2'$. By Lemma 2.1, $i(T_2) \geq 2i(T_2') \geq 2i(T^{(2k-3)})$. Hence we have proved that $i(T^{(2k-1)}) < i(T_1)$ and $2i(T^{(2k-3)}) \leq i(T_2)$.

Case 2. $m = 2k+1$ is odd. $T \in \mathcal{T}_m$.

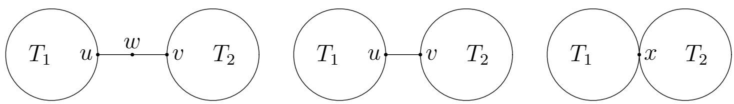
If T has at least $k+2$ pendent vertices, then we can prove that $i(T) > i(T^{(2k+1)})$ by the same reason as in Case 1.

If T has exactly $k+1$ pendent vertices, then T has at least one vertex with degree 2. Hence T has the form showed in Figure 4(a). Let T' be the tree from T by contracting the edge uw and T'' the tree from T' by contracting the edge uv, showed in Figure 4. We have $T' \in \mathcal{T}_{m-1}$ and $T'' \in \mathcal{T}_{m-2}$. By Lemma 2.1,

$$\begin{aligned}
i(T) &= i(T-w) + i(T - N_T[w]) \\
&= i(T_1 \cup T_2) + i((T_1 - u) \cup (T_2 - v)) \\
&= (i(T') + i((T_1 - N_{T_1}[u]) \cup (T_2 - N_{T_2}[v]))) + i((T_1 - u) \cup (T_2 - v)) \\
&= i(T') + (i((T_1 - u) \cup (T_2 - v)) + i((T_1 - N_{T_1}[u]) \cup (T_2 - N_{T_2}[v]))) \\
&= i(T') + [i(T'' - x) + i(T'' - N_{T''}[x])] \\
&= i(T') + i(T'') \\
&\geq i(T^{(2k)}) + i(T^{(2k-1)}) \qquad \text{(by induction)} \\
&= i(T^{(2k+1)}).
\end{aligned}$$

with the equality if and only if $T' = T^{(2k)}$ and $T'' = T^{(2k-1)}$, i.e., $T = T^{(2k+1)}$.

Thus, the theorem follows.



(a) T (b) T' (c) T''

Figure 4. The trees T, T' and T'' in the case 2.

3 The minimal Merrifield-Simmons index in $\mathcal{T}_n$

In the following, we give the minimal Merrifield-Simmons index in $\mathcal{T}_n$, i.e., the Merrifield-Simmoms index of the tree $T^{(n)}$.

Theorem 3.1. $i(T^{(2k+1)}) = \frac{1}{2}(2+\sqrt{3})(1+\sqrt{3})^k + \frac{1}{2}(2-\sqrt{3})(1-\sqrt{3})^k$
$i(T^{(2k)}) = \frac{1}{2}(3+2\sqrt{3})(1+\sqrt{3})^{k-1} + \frac{1}{2}(3-2\sqrt{3})(1-\sqrt{3})^{k-1}$.

Proof. By Lemma 2.1, we have

$$i(T^{(2k+1)}) = i(T^{(2k)}) + i(T^{(2k-1)})$$

$$i(T^{(2k)}) = i(T^{(2k-1)}) + i(K_1 \cup T^{(2k-3)}) = i(T^{(2k-1)}) + 2i(T^{(2k-3)}).$$

Let $f(k) = i(T^{(2k+1)})$. Then $\{f(k)\}$ satisfies the following recurrence relation

$$\begin{cases} f(k) = 2f(k-1) + 2f(k-2); \\ f(1) = 5; \\ f(2) = 14. \end{cases}$$

The solution $f(k)$ of the recurrence relation above is

$$f(k) = \frac{1}{2}(2+\sqrt{3})(1+\sqrt{3})^k + \frac{1}{2}(2-\sqrt{3})(1-\sqrt{3})^k.$$

And

$$\begin{aligned} i(T^{(2k+1)}) &= \tfrac{1}{2}(2+\sqrt{3})(1+\sqrt{3})^k + \tfrac{1}{2}(2-\sqrt{3})(1-\sqrt{3})^k \\ i(T^{(2k)}) &= f(k) - f(k-1) \\ &= \tfrac{1}{2}(3+2\sqrt{3})(1+\sqrt{3})^{k-1} + \tfrac{1}{2}(3-2\sqrt{3})(1-\sqrt{3})^{k-1}. \end{aligned}$$

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