EXTREMAL VALUES OF MERRIFIELD-SIMMONS INDEX FOR TREES WITH TWO BRANCHING VERTICES

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ABSTRACT. In this paper we find trees with minimal and maximal Merrifield-Simmons index over the set $\Omega(n, 2)$ of all trees with $n$ vertices and 2 branching vertices, and also over the subset $\Omega^t(n, 2)$ of all trees in $\Omega(n, 2)$ such that the branching vertices are connected by the path $P_t$.

1. Introduction

A topological index is a numerical value associated to a molecular graph of a chemical compound, used for correlation of chemical structure with physical properties, chemical reactivity or biological activity [2, 9, 10]. Among the numerous topological indices considered in chemical graph theory, an important example is the Merrifield-Simmons index, conceived by the chemists Merrifield and Simmons for describing molecular structure by means of finite-set topology [7]. Given a graph $G$, denote by $n(G, k)$ the number of ways in which $k$ mutually independent vertices can be selected in $G$. By definition $n(G, 0) = 1$ for all graphs, and $n(G, 1)$ is the number of vertices of $G$. The Merrifield-Simmons index of $G$ is defined as

$$\sigma = \sigma(G) = \sum_{k \geq 0} n(G, k).$$

For detailed information on the mathematical properties of $\sigma$ we refer to [11].

A fundamental problem in chemical graph theory consists in finding the extremal values of a topological index over a significant set of graphs. For instance, for trees with exactly one branching vertex (i.e. starlike trees), the problem was solved for the

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Wiener index [3], the Hosoya index [4], the Randić index or more generally, for vertex-degree-based topological indices [1]. Moreover, the extremal values of the Hosoya index over trees with exactly 2 branching vertices can be deduced from [6]. See also [5] for the Wiener index.

Let \( \Omega (n,i) \) denote the set of all trees with \( n \) vertices and \( i \) branching vertices. Note that in \( \Omega (n,1) \) (i.e., the set of starlike trees), the star maximizes \( \sigma \) [8] and the starlike tree \( T_{2,2,n-5} \) (two branches of length 2 and one branch of length \( n - 5 \)) minimizes \( \sigma \) [12]. So it is natural to consider the question: which trees in \( \Omega (n,2) \) minimize and maximize \( \sigma \)? Denoting by \( S(a_1,\ldots,a_r; t; b_1,\ldots,b_s) \) the tree with two branching vertices of degrees \( r+1, s+1 > 2 \) connected by the path \( P_t \), and in which the lengths of the pendent paths attached to the two branching vertices are \( a_1,\ldots,a_r \) and \( b_1,\ldots,b_s \) respectively (see Figure 1). We show in Theorems 2.1 and 2.5 that among all trees in \( \Omega (n,2) \), the tree \( S \left( \frac{1,\ldots,1; 2; 1,\ldots,1}{n-4} \right) \) maximizes \( \sigma \) and the tree \( S(n-8,2; 2; 2) \) minimizes \( \sigma \).

![Figure 1. The tree \( S(a_1,\ldots,a_r; t; b_1,\ldots,b_s) \) in \( \Omega (n,2) \).](image)

For each integer \( t \geq 2 \), we also consider the set \( \Omega^t (n,2) \) of all trees in \( \Omega (n,2) \) such that the branching vertices are connected by the path \( P_t \). We show in Theorems 2.6 and 2.7 that among all trees in \( \Omega^t (n,2) \), the tree \( S \left( 1,1; t; \underbrace{1,\ldots,1}_{n-t-2} \right) \) maximizes \( \sigma \) and the tree \( S(2,2; t; 2, n-t-6) \) minimizes \( \sigma \).

2. Extremal Values of the Merrifield-Simmons Index for Trees With Two Branching Vertices

The following relations for the Merrifield-Simmons index are fundamental and can be found in [7]:
a) if \( G_1,\ldots,G_r \) are the connected components of the graph \( G \), then

\[
\sigma (G) = \prod_{i=1}^{r} \sigma (G_i);
\]
b) if \( v \) is a vertex of \( G \), then

\[
\sigma(G) = \sigma(G - v) + \sigma(G - N_G[v])
\]

where \( N_G[v] = \{v\} \cup \{u \in V(G) : uv \in E(G)\} \).

Let \( G \) and \( H \) be two graphs and \( u \in V(G), v \in V(H) \). We denote by \( G(u, v)H \) the coalescence of \( G \) and \( H \) at the vertices \( u \) and \( v \).

Let \( \mathcal{P}_n, \mathcal{S}_n \) and \( \mathcal{T}_n \) be the path, the star and an arbitrary tree with \( n \) vertices respectively and consider arbitrary connected graphs \( X \) and \( A \) with at least two vertices. If \( \{1, 2, \ldots, n\} \) are the vertices of \( \mathcal{P}_n \), \( s \) is the central vertex of \( \mathcal{S}_n \) and \( t, x \) and \( a \) are vertices of \( \mathcal{T}_n, X \) and \( A \) respectively, we define the coalescence graphs \( \mathcal{X} \mathcal{P}_n(X) = \mathcal{P}_n(1, x)X, \mathcal{X} \mathcal{T}_n(X) = \mathcal{T}_n(t, x)X, \mathcal{X} \mathcal{S}_n(X) = \mathcal{S}_n(s, x)X, \mathcal{X} \mathcal{T}_n(X) = \mathcal{T}_n(t, x)X \) and \( \mathcal{A} \mathcal{X} \mathcal{S}_n(X) = A(a, n)\mathcal{X} \mathcal{T}_n(X), \mathcal{X} \mathcal{N}_i(X) = \mathcal{P}_n(i, x)X \) and \( \mathcal{A} \mathcal{X} \mathcal{N}_i(X) = A(a, n)\mathcal{X} \mathcal{N}_i(X) \), where the last two graphs are defined for each \( i = 1, \ldots, n \) (see Figure 2).

**Figure 2.** Some special graphs

The following results plays a major role in the analysis of treelike graphs and will be used in the sequel.

**Lemma 2.1.** [11, Theorem 15] Let \( X \) be a connected graph, \( x \in V(X) \) and \( \mathcal{T}_n \) any tree of order \( n \). Then

\[
\sigma(\mathcal{X} \mathcal{P}_n(X)) \leq \sigma(\mathcal{X} \mathcal{T}_n(X)) \leq \sigma(\mathcal{X} \mathcal{S}_n(X)).
\]

**Lemma 2.2.** [12, Theorem 1] Let \( X \) be a connected graph with at least two vertices and \( x \in V(X) \): Let \( n = 4m + i \) where \( i \in \{1, 2, 3, 4\} \). Then

\[
\sigma(X_{n, 2}) > \sigma(X_{n, 3}) > \cdots > \sigma(X_{n, 2m+2})
\]

\[
> \sigma(X_{n, 2m+1}) > \cdots > \sigma(X_{n, 5}) > \sigma(X_{n, 3}) > \sigma(X_{n, 1}),
\]

where \( l = \lfloor \frac{i-1}{2} \rfloor \).

Our first auxiliary result is of great importance in our work.

**Lemma 2.3.** Let \( A \) and \( X \) be a connected graphs with at least two vertices. Then

\[
\sigma(A \mathcal{X} \mathcal{N}_i(X)) > \sigma(A \mathcal{X} \mathcal{N}_3(X),
\]

for all \( 2 \leq i \leq n - 2 \) and \( i \neq 3 \).
Theorem 2.1. Let $AX_{n,i} = A(a, n)X_{n,i}$ we denote by $x$ the vertex obtained by identifying $a$ and $n$. Then for every $2 \leq i \leq n - 2$ we have
\[
\sigma(AX_{n,i}) - \sigma(AX_{n,3}) = \sigma(A - x) \left[ \sigma(X_{n-1,i}) - \sigma(X_{n-1,3}) \right] + \sigma(A - N_A[x]) \left[ \sigma(X_{n-2,i}) - \sigma(X_{n-2,3}) \right].
\]
The result follows from Lemma 2.2. □

We first consider the problem of finding the tree in $\Omega(n, 2)$ with maximal value of the Merrifield-Simmons index.

Lemma 2.4. Let $t, p, q \geq 2$ be integers such that $p \leq q$. Then
\[
\sigma(S(1, \ldots, 1; t; 1, \ldots, 1)) < \sigma(S(1, \ldots, 1; t; 1, \ldots, 1)).
\]

Proof. Let $U = S(1, \ldots, 1; t; 1, \ldots, 1)$ and $V = S(1, \ldots, 1; t; 1, \ldots, 1)$. If $t = 2$, using relations (2.1) and (2.2) we have
\[
\sigma(U) = \sigma(S(1, \ldots, 1; 2; 1, \ldots, 1)) + 2^{p-1}\sigma(S_{q+1}),
\]
\[
\sigma(V) = \sigma(S(1, \ldots, 1; 2; 1, \ldots, 1)) + 2^q\sigma(S_q),
\]
where as usual $S_n$ denotes the star graph of order $n$. Therefore
\[
\sigma(V) - \sigma(U) = 2^q\sigma(S_q) - 2^{p-1}\sigma(S_{q+1}) = 2^q(2^{p-1} + 1) - 2^{p-1}(2^q + 1) = 2^q - 2^{p-1} > 0.
\]
If $t \geq 3$, using relations (2.1) and (2.2) we obtain
\[
\sigma(U) = \sigma(S(1, \ldots, 1; t; 1, \ldots, 1)) + 2^{q+p-1}\sigma(P_{t-2}) + 2^{p-1}\sigma(P_{t-3});
\]
\[
\sigma(V) = \sigma(S(1, \ldots, 1; t; 1, \ldots, 1)) + 2^{q+p-1}\sigma(P_{t-2}) + 2^q\sigma(P_{t-3}).
\]
Therefore, $\sigma(V) - \sigma(U) = (2^q - 2^{p-1})\sigma(P_{t-3}) > 0$. □

Theorem 2.1. Let $n \geq 7$ and $T = S(a_1, \ldots, a_r; t; b_1, \ldots, b_s) \in \Omega(n, 2)$ where $t \geq 2$. Then
\[
\sigma(T) \leq \sigma(S(1, \ldots, 1; 2; 1, 1)).
\]

Proof. By Lemma 2.1 we have that
\[
\sigma(T) \leq \sigma(S(a_1, \ldots, a_r; 2; 1, \ldots, 1)) \leq \sigma(S(1, \ldots, 1; 2; 1, \ldots, 1)),
\]
where \( s' = t - 2 + \sum_{j=1}^{s} b_j \geq 2 \) and \( r' = \sum_{i=1}^{r} a_i \geq 2 \). Applying Lemma 2.4 we deduce that
\[
\sigma(S(1, \ldots, 1; 2; 1, \ldots, 1)) \leq \sigma(S(1, \ldots, 1; 2; 1, 1))
\]
and the result follows. \( \Box \)

In what follows we will consider the problem of finding the tree in \( \Omega(n, 2) \) with minimal Merrifield-Simmons index.

Let \( n > 10 \) and \( T = S(a_1, \ldots, a_r; t; b_1, \ldots, b_s) \) in \( \Omega(n, 2) \). By Lemma 2.1
\[
\sigma(S(a_1, \ldots, a_r; t; b_1, \ldots, b_s)) \geq \sigma(S(a_1, \ldots, a_r; t; s''; b_s)) \geq \sigma(S(r'', a_r; t; s''; b_s)),
\]
where \( s'' = \sum_{j=1}^{s-1} b_j \) and \( r'' = \sum_{i=1}^{r-1} a_i \). Therefore, in order to find the tree with minimal Merrifield-Simmons index for the subclass of \( \Omega(n, 2) \) consisting of all trees of the form \( T = S(w, x; t; y, z) \), where \( w, x, y, z \geq 1 \) are integers.

Next we find the tree with minimal Merrifield-Simmons index over the sets of trees of the form \( S(w, x; t; y, z) \) with \( t > 2 \).

**Theorem 2.2.** Let \( n > 10 \) and \( T = S(w, x; t; y, z) \) where \( t > 2 \). Then
\[
\sigma(T) \geq \sigma(S(2, 2; n - 8; 2, 2)).
\]

**Proof.** Assume first that \( w + x \geq 4 \). Then by Lemma 2.2 we obtain
\[
\sigma(T) \geq \sigma(S(w + x - 2; 2; t; y, z)).
\]
Moreover \( t > 2 \) implies that \( w + x - 2 + t > 4 \) then we can use Lemma 2.3 to obtain
\[
\sigma(S(w + x - 2; 2; t; y, z)) \geq \sigma(S(2, 2; t + w + x - 4; y, z)).
\]
Now if \( y + z \geq 4 \), then a similar argument ends the proof (see Figure 3). Otherwise \( y + z \leq 3 \) which implies that \( S(2, 2; t + w + x - 4; y, z) \) is the tree \( S(2, 2; n - 7; 1, 2) \) or the tree \( S(2, 2; n - 6; 1, 1) \). Since \( n > 10 \), we have that \( n - 6 > n - 7 > 3 \) and in both cases the result follows using Lemma 2.3.

The only case left to consider is when \( w + x \leq 3 \) and \( y + z \leq 3 \), but in this situation we note that necessarily \( t > 4 \) and the result follows using Lemma 2.3. \( \Box \)

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure3.png}
\caption{Graphs in the proof of Theorem 2.2}
\end{figure}
Theorem 2.3. Let \( t, w \geq 2 \) be integers. Then
\[
\sigma (S(w, 2; t; 2, 2)) < \sigma (S(w + 1, 2; t; 1, 2)).
\]

Proof. Let \( A = S(w, 2; t; 2, 2) \) and \( B = S(w + 1, 2; t; 1, 2) \). Using relations (2.1), (2.2) and Lemma 2.1 we have
\[
\sigma(A) = \sigma(S(w, 2; t; 1, 2)) + \sigma(T_{w,2,t+1}),
\]
\[
\sigma(B) = \sigma(S(w, 2; t; 1, 2)) + \sigma(S(w - 1, 2; t; 1, 2))
\geq \sigma(S(w, 2; t; 1, 2)) + \sigma(T_{w+t+1,2,1}),
\]
where \( T_{a,b,c} \) is a starlike tree with branches of length \( a, b \) and \( c \) respectively and \( a + b + c + 1 = n \). Hence
\[
\sigma(B) - \sigma(A) \geq \sigma(T_{w+t+1,2,1}) - \sigma(T_{w,2,t+1}) > 0
\]
by Lemma 2.2. \( \square \)

Lemma 2.5. Let \( t, w \geq 2 \) be integers such that \( t \geq 2 \) and \( w \geq 2 \). If \( y \) is odd then
\[
\sigma(S(w, 2; t; y, 2)) > \sigma(S(w + 1, 2; t; y - 1, 2)).
\]
If \( y \) is even then
\[
\sigma(S(w, 2; t; y, 2)) < \sigma(S(w + 1, 2; t; y - 1, 2)).
\]

Proof. Let \( A = S(w, 2; t; y, 2) \) and \( B = S(w + 1, 2; t; y - 1, 2) \). Using relations (2.1) and (2.2) we have
\[
\sigma(A) = \sigma(S(w, 2; t; y - 1, 2)) + \sigma(S(w, 2; t; y - 2, 2))
\]
and
\[
\sigma(B) = \sigma(S(w, 2; t; y - 1, 2)) + \sigma(S(w - 1, 2; t; y - 1, 2)).
\]
Hence
\[
\sigma(B) - \sigma(A) = (-1)[\sigma(S(w, 2; t; y - 2, 2)) - \sigma(S(w - 1, 2; t; y - 1, 2))].
\]
Repeating this argument \( y - 2 \) times we deduce
\[
\sigma(B) - \sigma(A) = (-1)^y[\sigma(S(w - y + 2, 2; t; 2, 2)) - \sigma(S(w - y + 2, 2; t; 2, 2))].
\]
By Lemma 2.5 we know that \( \sigma(S(w - y + 3, 2; t; 1, 2)) > \sigma(S(w - y + 2, 2; t; 2, 2)) \) and the result follows. \( \square \)

Theorem 2.3. Let \( M = 4k + i \), where \( i \in \{0, 1, 2, 3\} \). Then
\[
\sigma(G(P_{M-2}, P_2)) < \cdots < \sigma(G(P_{M-2k}, P_{2k})) \leq \sigma(G(P_{M-(2k+1)}, P_{2k+1}))
\]
\[
< \sigma(G(P_{M-(2k-1)}, P_{2k-1})) < \cdots < \sigma(G(P_{M-1}, P_1)),
\]
where \( G(P_a, P_b) = S(a, 2; t; b, 2) \), that is \( G(P_a, P_b) \) is the tree obtained from the path \( P_{k+4} = v_1v_2 \cdots v_{k+4} \) by joining the path \( P_a \) to the vertex \( v_3 \) and joining the path \( P_b \) to the vertex \( v_{k+2} \) (see Figure 4).
Figure 4. Trees $G(a,b)$.

Proof. Let $A = G(P_a, P_b)$ and $B = G(P_{a-2}, P_{b+2})$, where $2 \leq b \leq a - 4$. Using relations (2.1) and (2.2) we have

$$\sigma(A) = \sigma(G(P_{a-1}, P_b)) + \sigma(G(P_{a-2}, P_b))$$

and

$$\sigma(B) = \sigma(G(P_{a-2}, P_{b+1})) + \sigma(G(P_{a-2}, P_b)).$$

Consequently

$$\sigma(A) - \sigma(B) = (-1) [\sigma(G(P_{a-2}, P_{b+1})) - \sigma(G(P_{a-1}, P_b))]$$

and so

$$\sigma(A) - \sigma(B) = (-1)^b [\sigma(G(P_{a-6}, P_2)) - \sigma(G(P_{a-b}, P_1))].$$

By Lemma 2.5, if $b$ is even then $\sigma(A) < \sigma(B)$ and if $b$ is odd then $\sigma(A) > \sigma(B)$. Only remains to prove that $\sigma(G(P_{M-2k}, P_{2k})) \leq \sigma(G(P_{M-(2k+1)}, P_{2k+1}))$, but this is a direct consequence of Lemma 2.6.

Lemma 2.7. Let $n > 10$ and let $w, x$ be positive integers. Then

$$\sigma(G_S(w, x; 2; 1, 1)) > \sigma(G_S(n-8, 2; 2; 2, 2)).$$

Proof. Let $A = G_S(w, x; 2; 1, 1)$ and $B = G_S(n-8, 2; 2; 2, 2)$. Since $n > 10$ we have that $w+x > 6$ and by Lemma 2.2 we can construct a tree $A_1 = G_S(n-6, 2; 2; 1, 1) \in \Omega(n, 2)$ such that $\sigma(A) > \sigma(A_1)$. By a direct computation using relations (2.1) and (2.2) we obtain

$$\sigma(A_1) = 8\sigma(P_{n-7}) + 15\sigma(P_{n-6}),$$

and

$$\sigma(B) = 18\sigma(P_{n-9}) + 39\sigma(P_{n-8}).$$

Therefore

$$\sigma(A_1) - \sigma(B) = 4\sigma(P_{n-9}) + \sigma(P_{n-10}) > 0,$$

and the result follows.
Next we find the tree with minimal Merrifield-Simmons index over the sets of trees of the form $S(w, x; 2; y, z)$.

**Theorem 2.4.** Let $n > 10$ and $T = S(w, x; 2; y, z)$. Then
\[
\sigma(T) \leq \sigma(S(n-8, 2; 2; 2, 2)).
\]

**Proof.** Note that $w+x+y+z > 8$. Therefore we may assume without losing generality that $w+x \geq 4$. Then by Lemma 2.2 there exists a tree $T_1 = S(w+x-2, 2; y, z)$ such that $\sigma(T) \leq \sigma(T_1)$.

If $y+z \geq 4$, by Lemma 2.2 we construct a tree $T_2 = S(w+x-2, 2; y+z-2, 2)$ such that $\sigma(T_1) > \sigma(T_2)$ and the result follows from Theorem 2.3.

If $y+z \leq 3$ then $T_1 = S(w+x-2, 2; 1, 2)$ or $T_1 = S(w+x-2, 2; 1, 1)$. If $T_1 = S(w+x-2, 2; 1, 2)$ the result follows from Theorem 2.3. On the other hand, if $T_1 = S(w+x-2, 2; 1, 1)$ the result follows from Lemma 2.7. 

In our next result we find the minimal tree with respect to Merrifield-Simmons index over $\Omega(n, 2)$.

**Theorem 2.5.** For every $n \geq 11$, $S(n-8, 2; 2; 2, 2)$ is the tree with minimal Merrifield-Simmons index in $\Omega(n, 2)$.

**Proof.** Bearing in mind Theorems 2.2 and 2.4 to obtain the result it is enough to compare the Merrifiel-Simmons index for the trees $S(2, 2; n-8; 2, 2)$ and $S(n-8, 2; 2; 2, 2)$. Indeed, let $A = S(2, 2; n-8; 2, 2)$ and let $B = S(n-8, 2; 2; 2, 2)$. By a direct computation, using relations (2.1) and (2.2), we obtain
\[
\begin{align*}
\sigma(A) &= 81\sigma(P_{n-10}) + 72\sigma(P_{n-11}) + 16\sigma(P_{n-12}) \\
&= 41\sigma(P_{n-8}) + 15\sigma(P_{n-9}),
\end{align*}
\]
and
\[
\sigma(B) = 39\sigma(P_{n-8}) + 18\sigma(P_{n-9}).
\]
Hence
\[
\sigma(A) - \sigma(B) = 2\sigma(P_{n-10}) - \sigma(P_{n-9}) > 0;
\]
and the result follows.

To end this section we consider the problem of finding extremal values of the Merrifield-Simmons index for trees with two branching vertices at a fixed distance. Consider the set $\Omega^t(n, 2)$ of all trees in $\Omega(n, 2)$ such that the two branching vertices are connected by the path $P_t$, that is, the distance between the two branching vertices is $t-1$. We next find the extremal trees in $\Omega^t(n, 2)$ with respect to the Merrifield-Simmons index.

**Theorem 2.6.** Let $n \geq t+4$ and $T \in \Omega^t(n, 2)$, $T \neq S(1, 1; t; 1, \ldots, 1)$. Then
\[
\sigma(T) < \sigma(S(1, 1; t; 1, \ldots, 1)).
\]
Proof. By Lemma 2.1 it is sufficient to consider trees in \( \Omega^t(n, 2) \) of the form \( T = S(\underbrace{1, \ldots, 1}_p; 1, \ldots, 1) \). We may assume that \( p \leq q \). Now, a repeated application of Lemma 2.4 gives that \( \sigma(T) < \sigma(S(1, 1; 1, \ldots, 1)) \).

\[ \square \]

Theorem 2.7. Let \( n \geq t + 7 \) and \( T \in \Omega^t(n, 2) \), \( T \neq S(2, 2; t; 2, n-t-6) \). Then

\[ \sigma(T) > \sigma(S(2, 2; t; 2, n-t-6)) \]

Proof. Bearing in mind Theorem 2.4 and Lemma 2.1, it is clear that in order to obtain the result it is enough to consider the case \( t \geq 3 \) and trees in \( \Omega^t(n, 2) \) of the form \( T = S(w, x; t; y, z) \).

Note that \( w + x + y + z \geq 7 \). Therefore as in the proof of Theorem 2.2, there exists a tree \( T_1 \in \Omega^t(n, 2) \) of the form \( T_1 = S(r, 2; t; s, 2) \) such that \( \sigma(T) > \sigma(T_1) \), where \( r + s = n - t - 4 \). Note that \( T_1 = G(P_r, P_s) \), therefore the result follows from Theorem 2.3.

\[ \square \]

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