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

ROBERTO CRUZ\(^1\), CARLOS ALBERTO MARÍN\(^2\), AND JUAN RADA\(^3\)

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...
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 pendant 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 \( S \left( \frac{1, \ldots, 1}{n-4}; 2; 1, \ldots, 1 \right) \) maximizes \( \sigma \) and the tree \( S \left( 2, 2; 2; 2, 2 \right) \) 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 \( \Omega'(n,2) \) 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 \( \Omega'(n,2) \), the tree \( S \left( 1, 1; t; 1, \ldots, 1 \right) \) maximizes \( \sigma \) and the tree \( S \left( 2, 2; t; 2, n-t-6 \right) \) 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

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

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 \( G(u, v) \) the coalescence of \( G \) and \( H \) at the vertices \( u \) and \( v \).

Let \( P_n \), \( S_n \) and \( T_n \) 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 \( P_n \), \( s \) is the central vertex of \( S_n \) and \( t, x \) and \( a \) are vertices of \( T_n \), \( X \) and \( A \) respectively, we define the coalescence graphs \( XP_n = P_n(1, x)X \), \( XT_n = T_n(t, x)X \), \( XS_n = S_n(s, x)X \), \( X_{n,i} = P_n(i, x)X \) and \( AX_{n,i} = A(a, n)X_{n,i} \), where the last two graphs are defined for each \( i = 1, \ldots, n \) (see Figure 2).

\[\text{Figure 2. Some special graphs}\]

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 \( T_n \) any tree of order \( n \). Then

\[\sigma(XP_n) \leq \sigma(XT_n) \leq \sigma(XS_n).\]

**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

\[
\begin{align*}
\sigma(X_{n,2}) > \sigma(X_{n,4}) & > \cdots > \sigma(X_{n,2m+2i}) \\
& > \sigma(X_{n,2m+1}) > \cdots > \sigma(X_{n,5}) > \sigma(X_{n,3}) > \sigma(X_{n,1}),
\end{align*}
\]

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

\[\sigma(AX_{n,i}) > \sigma(AX_{n,3}),\]

for all \( 2 \leq i \leq n - 2 \) and \( i \neq 3 \).
Proof. For \( AX_n,i = A(a, n)X_n,i \) we denote by \( x \) the vertex obtained by identifying \( a \) and \( n \). Then for every \( 2 \leq i \leq n - 2 \) we have
\[
\sigma (AX_n,i) - \sigma (AX_n,3) = \sigma (A - x) [\sigma (X_{n-1,i}) - \sigma (X_{n-1,3})] \\
+ \sigma (A - N_A[x]) [\sigma (X_{n-2,i}) - \sigma (X_{n-2,3})].
\]
The result follows from Lemma 2.2. \( \square \)

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

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.

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 class \( \Omega(n, 2) \), it is enough 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.

\[\]
Lemma 2.5. 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
\[ \sigma(A) = \sigma(S(w, 2; t; 1, 2)) + \sigma(T_{w,t+1}) \]
\[ \sigma(B) = \sigma(S(w, 2; t; 1, 2)) + \sigma(S(w - 1, 2; t; 1, 2)) \]
\[ \geq \sigma(S(w, 2; t; 1, 2)) + \sigma(T_{w+t+1,1}) \]
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
\[ \sigma(B) - \sigma(A) \geq \sigma(T_{w+t+1,2,1}) - \sigma(T_{w,t+1}) > 0 \]
by Lemma 2.2. □

Lemma 2.6. Let $t, w, y$ be integers such that $t \geq 2$ and $w \geq y \geq 2$. 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
\[ \sigma(B) - \sigma(A) = (-1)^{y-2}[\sigma(S(w, 2; t; y - 2, 2)) - \sigma(S(w - 1, 2; t; y - 1, 2))]. \]
Repeating this argument $y - 2$ times we deduce
\[ \sigma(B) - \sigma(A) = (-1)^{y-2}[\sigma(S(w - y + 3, 2; t; 1, 2)) - \sigma(S(w - y + 2, 2; t; 2, 2))]. \]
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. □

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 $G(P_a, P_b) = S(a, 2; b; 2)$, 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).
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
\[
\sigma(A) - \sigma(B) = (-1) \left[ \sigma(G(P_{a-2}, P_{b+1})) - \sigma(G(P_{a-1}, P_{b})) \right]
\]
and so
\[
\sigma(A) - \sigma(B) = (-1)^b \left[ \sigma(G(P_{a-b-1}, P_2)) - \sigma(G(P_{a-b}, P_1)) \right]
\]
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
\[
\sigma(S(w, x; 2; 1, 1)) > \sigma(S(n-8, 2; 2; 2, 2)).
\]
Proof. Let $A = S(w, x; 2; 1, 1)$ and $B = S(n-8, 2; 2; 2, 2)$. Since $n > 10$ we have that $w + x > 6$ and by Lemma 2.2 we can construct a tree $A_1 = S(n-6, 2; 2; 1, 1) \in \Omega(n, 2)$ 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

$$\sigma(T) \leq \sigma(S(n - 8, 2; 2; 2)).$$

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

$$\sigma(A) = 81\sigma(P_{n-10}) + 72\sigma(P_{n-11}) + 16\sigma(P_{n-12})$$

$$= 41\sigma(P_{n-8}) + 15\sigma(P_{n-9}),$$

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 $T = S(p, q, 1, \ldots, 1)$. We may assume that $p \leq q$. Now, a repeated application of Lemma 2.4 gives that $\sigma(T) < \sigma(S(1, 1; 1, \ldots, 1))$. \hfill $\square$

**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 $T_1 = S(r, 2; s, 2)$ 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. \hfill $\square$

**REFERENCES**


1 Instituto de Matemáticas, Universidad de Antioquia
Medellín, Colombia.
E-mail address: roberto.cruz@udea.edu.co

2 Instituto de Matemáticas
Universidad de Antioquia
Medellín, Colombia.
E-mail address: calberto.marin@udea.edu.co

3 Instituto de Matemáticas
Universidad de Antioquia
Medellín, Colombia.
E-mail address: pablo.rada@udea.edu.co