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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 σ 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 σ [8] and the starlike tree $T_{2,2,n-5}$ (two branches of length 2 and one branch of length $n-5$) minimizes σ [12]. So it is natural to consider the question: which trees in $\Omega(n,2)$ minimize and maximize σ? Denoting by $S(a_1,\ldots,a_r;\mathbf{t};b_1,\ldots,b_s)$ 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 $S\left(\underbrace{1,\ldots,1}_{n-4};\mathbf{2};1,1\right)$ maximizes σ and the tree $S(n-8,2;\mathbf{2};2,2)$ minimizes σ.

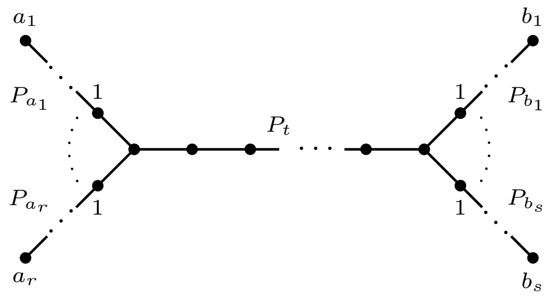

FIGURE 1. The tree $S(a_1,\ldots,a_r;\mathbf{t};b_1,\ldots,b_s)$ in $\Omega(n,2)$.

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 $S\left(1,1;\mathbf{t};\underbrace{1,\ldots,1}_{n-t-2}\right)$ maximizes σ and the tree $S(2,2;\mathbf{t};2,n-t-6)$ minimizes σ.

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

$$\sigma(G)=\prod_{i=1}^{r}\sigma(G_i); \tag{2.1}$$

b) if v is a vertex of G, then

$$\sigma(G) = \sigma(G - v) + \sigma(G - N_G[v]) \tag{2.2}$$

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 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).

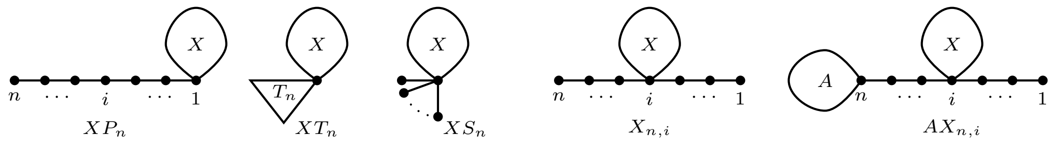

FIGURE 2. Some special graphs

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*

$$\sigma(X_{n,2}) > \sigma(X_{n,4}) > \cdots > \sigma(X_{n,2m+2l}) > \sigma(X_{n,2m+1}) > \cdots > \sigma(X_{n,5}) > \sigma(X_{n,3}) > \sigma(X_{n,1}),$$

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*

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

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 $2 \le i \le n-2$ we have

$$\begin{aligned}\sigma(AX_{n,i}) - \sigma(AX_{n,3}) =& \,\sigma(A-x)\left[\sigma(X_{n-1,i}) - \sigma(X_{n-1,3})\right]\\ &+ \sigma(A - N_A[x])\left[\sigma(X_{n-2,i}) - \sigma(X_{n-2,3})\right].\end{aligned}$$

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 $t,p,q \ge 2$ be integers such that $p \le q$. Then*

$$\sigma(S(\underbrace{1,\dots,1}_{p};\mathbf{t};\underbrace{1,\dots,1}_{q})) < \sigma(S(\underbrace{1,\dots,1}_{p-1};\mathbf{t};\underbrace{1,\dots,1}_{q+1})).$$

Proof. Let $U = S(\underbrace{1,\dots,1}_{p};\mathbf{t};\underbrace{1,\dots,1}_{q})$ and $V = S(\underbrace{1,\dots,1}_{p-1};\mathbf{t};\underbrace{1,\dots,1}_{q+1})$.

If $t=2$, using relations (2.1) and (2.2) we have

$$\sigma(U) = \sigma(S(\underbrace{1,\dots,1}_{p-1};\mathbf{2};\underbrace{1,\dots,1}_{q})) + 2^{p-1}\sigma(S_{q+1}),$$
$$\sigma(V) = \sigma(S(\underbrace{1,\dots,1}_{p-1};\mathbf{2};\underbrace{1,\dots,1}_{q})) + 2^{q}\sigma(S_{p}),$$

where as usual S_n denotes the star graph of order n. Therefore

$$\sigma(V) - \sigma(U) = 2^q\sigma(S_p) - 2^{p-1}\sigma(S_{q+1}) = 2^q(2^{p-1}+1) - 2^{p-1}(2^q+1) = 2^q - 2^{p-1} > 0.$$

If $t \ge 3$, using relations (2.1) and (2.2) we obtain

$$\sigma(U) = \sigma(S(\underbrace{1,\dots,1}_{p-1};\mathbf{t};\underbrace{1,\dots,1}_{q})) + 2^{q+p-1}\sigma(P_{\mathbf{t}-2}) + 2^{p-1}\sigma(P_{\mathbf{t}-3});$$
$$\sigma(V) = \sigma(S(\underbrace{1,\dots,1}_{p-1};\mathbf{t};\underbrace{1,\dots,1}_{q})) + 2^{q+p-1}\sigma(P_{\mathbf{t}-2}) + 2^{q}\sigma(P_{\mathbf{t}-3}).$$

Therefore, $\sigma(V) - \sigma(U) = (2^q - 2^{p-1})\sigma(P_{\mathbf{t}-3}) > 0$. □

Theorem 2.1. *Let $n \ge 7$ and $T = S(a_1,\dots,a_r;\mathbf{t};b_1,\dots,b_s) \in \Omega(n,2)$ where $\mathbf{t} \ge 2$. Then*

$$\sigma(T) \le \sigma(S(\underbrace{1,\dots,1}_{n-4};\mathbf{2};1,1)).$$

Proof. By Lemma 2.1 we have that

$$\sigma(T) \le \sigma(S(a_1,\dots,a_r;\mathbf{2};\underbrace{1,\dots,1}_{s'})) \le \sigma(S(\underbrace{1,\dots,1}_{r'};\mathbf{2};\underbrace{1,\dots,1}_{s'})),$$

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

$$\sigma(S(\underbrace{1,\ldots,1}_{r'};\mathbf{2};\underbrace{1,\ldots,1}_{s'})) \leq \sigma(S(\underbrace{1,\ldots,1}_{n-4};\mathbf{2};1,1))$$

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 $T = S(a_1,\ldots,a_r;\mathbf{t};b_1,\ldots,b_s)$ in $\Omega\,(n,2)$. By Lemma 2.1

$$\sigma(S(a_1,\ldots,a_r;\mathbf{t};b_1,\ldots,b_s)) \geq \sigma(S(a_1,\ldots,a_r;\mathbf{t};s'',b_s)) \geq \sigma(S(r'',a_r;\mathbf{t};s'',b_s)),$$

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 $T = S(w,x;\mathbf{t};y,z)$, 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 $S(w,x;\mathbf{t};y,z)$ with $\mathbf{t} > 2$.

Theorem 2.2. *Let $n > 10$ and $T = S(w,x;\mathbf{t};y,z)$ where $\mathbf{t} > 2$. Then*

$$\sigma(T) \geq \sigma\left(S(2,2;\mathbf{n-8};2,2)\right).$$

Proof. Assume first that $w+x \geq 4$. Then by Lemma 2.2 we obtain

$$\sigma(T) \geq \sigma(S\,(w+x-2,2;\mathbf{t};y,z)).$$

Moreover $\mathbf{t} > 2$ implies that $w+x-2+\mathbf{t} > 4$ then we can use Lemma 2.3 to obtain

$$\sigma(S\,(w+x-2,2;\mathbf{t};y,z)) \geq \sigma(S\,(2,2;\mathbf{t+w+x-4};y,z)).$$

Now if $y+z \geq 4$, then a similar argument ends the proof (see Figure 3). Otherwise $y+z \leq 3$ which implies that $S\,(2,2;\mathbf{t+w+x-4};y,z)$ is the tree $S\,(2,2;\mathbf{n-7};1,2)$ or the tree $S\,(2,2;\mathbf{n-6};1,1)$. 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 $\mathbf{t} > 4$ and the result follows using Lemma 2.3. □

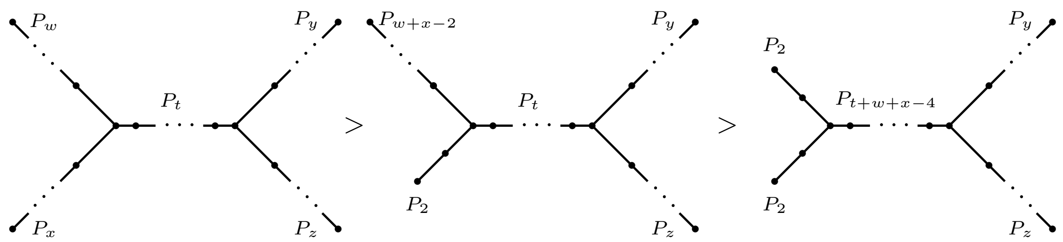

FIGURE 3. Graphs in the proof of Theorem 2.2

Lemma 2.5. *Let* $\mathbf{t}, w \geq 2$ *be integers. Then*

$$\sigma\left(S(w,2;\mathbf{t};2,2)\right) < \sigma\left(S(w+1,2;\mathbf{t};1,2)\right).$$

Proof. Let $A = S(w,2;\mathbf{t};2,2)$ and $B = S(w+1,2;\mathbf{t};1,2)$. Using relations (2.1), (2.2) and Lemma 2.1 we have

$$\begin{aligned}\sigma(A) &= \sigma\left(S(w,2;\mathbf{t};1,2)\right) + \sigma\left(T_{w,2,\mathbf{t+1}}\right),\\ \sigma(B) &= \sigma\left(S(w,2;\mathbf{t};1,2)\right) + \sigma\left(S(w-1,2;\mathbf{t};1,2)\right)\\ &\geq \sigma\left(S(w,2;\mathbf{t};1,2)\right) + \sigma\left(T_{w+\mathbf{t+1},\mathbf{2},\mathbf{1}}\right),\end{aligned}$$

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

$$\sigma(B) - \sigma(A) \geq \sigma\left(T_{w+\mathbf{t+1},\mathbf{2},\mathbf{1}}\right) - \sigma\left(T_{w,2,\mathbf{t+1}}\right) > 0$$

by Lemma 2.2. □

Lemma 2.6. *Let* $\mathbf{t}, w, y$ *be integers such that* $\mathbf{t} \geq 2$ *and* $w \geq y \geq 2$. *If* y *is odd then*

$$\sigma\left(S(w,2;\mathbf{t};y,2)\right) > \sigma\left(S(w+1,2;\mathbf{t};y-1,2)\right).$$

If y *is even then*

$$\sigma\left(S(w,2;\mathbf{t};y,2)\right) < \sigma\left(S(w+1,2;\mathbf{t};y-1,2)\right).$$

Proof. Let $A = S(w,2;\mathbf{t};y,2)$ and $B = S(w+1,2;\mathbf{t};y-1,2)$. Using relations (2.1) and (2.2) we have

$$\sigma(A) = \sigma\left(S(w,2;\mathbf{t};y-1,2)\right) + \sigma\left(S(w,2;\mathbf{t};y-2,2)\right)$$

and

$$\sigma(B) = \sigma\left(S(w,2;\mathbf{t};y-1,2)\right) + \sigma\left(S(w-1,2;\mathbf{t};y-1,2)\right).$$

Hence

$$\sigma(B) - \sigma(A) = (-1)[\sigma\left(S(w,2;\mathbf{t};y-2,2)\right) - \sigma\left(S(w-1,2;\mathbf{t};y-1,2)\right)].$$

Repeating this argument $y-2$ times we deduce

$$\sigma(B) - \sigma(A) = (-1)^{y-2}[\sigma\left(S(w-y+3,2;\mathbf{t};1,2)\right) - \sigma\left(S(w-y+2,2;\mathbf{t};2,2)\right)].$$

By Lemma 2.5 we know that $\sigma\left(S(w-y+3,2;\mathbf{t};1,2)\right) > \sigma\left(S(w-y+2,2;\mathbf{t};2,2)\right)$ and the result follows. □

Theorem 2.3. *Let* $M = 4k+i$, *where* $i \in \{0,1,2,3\}$. *Then*

$$\begin{aligned}\sigma\left(G\left(P_{M-2},P_2\right)\right) < \cdots < \sigma\left(G\left(P_{M-2k},P_{2k}\right)\right) \leq \sigma\left(G\left(P_{M-(2k+1)},P_{2k+1}\right)\right)\\ < \sigma\left(G\left(P_{M-(2k-1)},P_{2k-1}\right)\right) < \cdots < \sigma\left(G\left(P_{M-1},P_1\right)\right),\end{aligned}$$

where $G(P_a,P_b) = S(a,2;\mathbf{t};b,2)$, *that is* $G(P_a,P_b)$ *is the tree obtained from the path* $P_{\mathbf{t}+4} = v_1 v_2 \cdots v_{\mathbf{t}+4}$ *by joining the path* P_a *to the vertex* v_3 *and joining the path* P_b *to the vertex* $v_{\mathbf{t}+2}$ (*see Figure* 4).

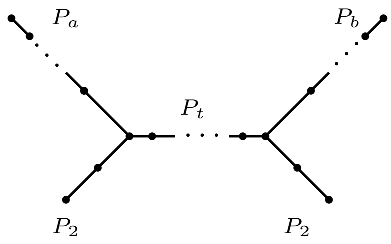

FIGURE 4. Trees $G(a,b)$.

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

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

and

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

Consequently

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

and so

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

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 $\sigma\left(G(P_{M-2k}, P_{2k})\right) \leq \sigma\left(G(P_{M-(2k+1)}, P_{2k+1})\right)$, but this is a direct consequence of Lemma 2.6. ☐

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

$$\sigma(S\,(w, x; \mathbf{2}; 1, 1)) > \sigma(S\,(n-8, 2; \mathbf{2}; 2, 2)).$$

Proof. Let $A = S\,(w, x; \mathbf{2}; 1, 1)$ and $B = S\,(n-8, 2; \mathbf{2}; 2, 2)$. Since $n > 10$ we have that $w+x > 6$ and by Lemma 2.2 we can construct a tree $A_1 = S\,(n-6, 2; \mathbf{2}; 1, 1) \in \Omega(n, 2)$ 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 $S(w, x; \mathbf{2}; y, z)$.

Theorem 2.4. *Let $n > 10$ and $T = S(w, x; \mathbf{2}; y, z)$. Then*

$$\sigma(T) \leq \sigma\left(S(n-8, 2; \mathbf{2}; 2, 2)\right).$$

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 $T_1 = S\left(w + x - 2, 2; \mathbf{2}; y, z)\right)$ such that $\sigma(T) \leq \sigma(T_1)$.

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

If $y + z \leq 3$ then $T_1 = S\left(w + x - 2, 2; \mathbf{2}; 1, 2\right)$ or $T_1 = S\left(w + x - 2, 2; \mathbf{2}; 1, 1\right)$. If $T_1 = S\left(w + x - 2, 2; \mathbf{2}; 1, 2\right)$ the result follows from Theorem 2.3. On the other hand, if $T_1 = S\left(w + x - 2, 2; \mathbf{2}; 1, 1\right)$ 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 $n \geq 11$, $S(n-8, 2; \mathbf{2}; 2, 2)$ 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 enought to compare the Merrifiel-Simmons index for the trees $S(2, 2; \mathbf{n-8}; 2, 2)$ and $S(n-8, 2; \mathbf{2}; 2, 2)$. Indeed, let $A = S(2, 2; \mathbf{n-8}; 2, 2)$ and let $B = S(n-8, 2; \mathbf{2}; 2, 2)$. By a direct computation, using relations (2.1) and (2.2), we obtain

$$\begin{aligned}\sigma(A) &= 81\sigma(P_{n-10}) + 72\sigma(P_{n-11}) + 16\sigma(P_{n-12}) \\ &= 41\sigma(P_{n-8}) + 15\sigma(P_{n-9}),\end{aligned}$$

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 $\Omega^{\mathbf{t}}(n, 2)$ 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 $\Omega^{\mathbf{t}}(n, 2)$ with respect to the Merrifield-Simmons index.

Theorem 2.6. *Let $n \geq \mathbf{t} + 4$ and $T \in \Omega^{\mathbf{t}}(n, 2)$, $T \neq S(1, 1; \mathbf{t}; \underbrace{1, \ldots, 1}_{n-\mathbf{t}-2})$. Then*

$$\sigma(T) < \sigma(S(1, 1; \mathbf{t}; \underbrace{1, \ldots, 1}_{n-\mathbf{t}-2})).$$

Proof. By Lemma 2.1 it is sufficient to consider trees in $\Omega^{\mathbf{t}}(n,2)$ of the form $T = S(\underbrace{1,\ldots,1}_{p};\mathbf{t};\underbrace{1,\ldots,1}_{q})$. We may assume that $p \leq q$. Now, a repeated application of Lemma 2.4 gives that $\sigma(T) < \sigma(S(1,1;\mathbf{t};\underbrace{1,\ldots,1}_{n-\mathbf{t}-2}))$. □

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

$$\sigma(T) > \sigma\left(S(2,2;\mathbf{t};2,n-\mathbf{t}-6)\right).$$

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 $\mathbf{t} \geq 3$ and trees in $\Omega^{\mathbf{t}}(n,2)$ of the form $T = S(w,x;\mathbf{t};y,z)$.

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

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