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ON THE MERRIFIELD–SIMMONS INDEX OF TREES[1]

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Abstract

The Merrifield–Simmons index $\sigma(G)$ of a (molecular) graph G is defined as the number of subsets of the vertex set, in which no two vertices are adjacent in G, i. e., the number of independent–vertex sets of G. Let $\mathcal{T}(n,k)$ be the set of trees with n vertices and with diameter k. The unique tree with the largest σ-value in $\mathcal{T}(n,k)$ is determined. We also determine all trees T of order n, for which $2^{n-2} \leq \sigma(T) \leq 2^{n-1}$.

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INTRODUCTION

A topological index is a map from the set of chemical compounds represented by molecular graphs to the set of real numbers. Many topological indices are closely correlated with some physico–chemical characteristics of the underlying compounds. The Merrifield–Simmons index σ [1–3] is one of the topological indices whose mathematical properties were studied in some detail [4–19] whereas its applicability for QSPR and QSAR was examined to a much lesser extent; in [2] it was shown that σ is correlated with the boiling points.

Given a molecular graph G, the Merrifield–Simmons index $\sigma = \sigma(G)$ is defined as the number of subsets of $V(G)$ in which no two vertices are adjacent i. e., in graph–theoretical terminology, the number of independent–vertex sets of G, including the empty set. For example, for the 4-membered cycle C_4 with vertex set $V(C_4) = \{v_1, v_2, v_3, v_4\}$, such that v_i and v_{i+1}, $i = 1, 2, 3$, as well as v_1 and v_4 are adjacent, the independent–vertex subsets are: $\emptyset$, $\{v_1\}$, $\{v_2\}$, $\{v_3\}$, $\{v_4\}$, $\{v_1, v_3\}$, $\{v_2, v_4\}$, and thus, $\sigma(C_4) = 7$. For the path P_n, $\sigma(P_n)$ is equal to the Fibonacci number[2] F_{n+1}. This is perhaps why some authors [6] called σ the "*Fibonacci number*" of the graph. For further details on σ see the book [2], the papers [4–19] and the references cited therein.

All graphs considered here are finite and simple. Undefined notation and terminology will conform to those in [20]. For a graph G with the set of vertices $V(G)$ and $u \in V(G)$, by $N_G(u)$ we denote the set of all neighbors of u in G. For $u, v \in V(G)$, $d(u, v)$ denotes the distance between u and v in G, which is the length of the shortest path between u and v. We denote by $d(G)$ the diameter of G, which is defined as $d(G) = \max\{d(u, v) \,|\, u, v \in V(G)\}$. By $G \cup H$ is denoted the disjoint union of two graphs G and H, and by $m\,H$ the disjoint union of m copies of H.

Let T be a tree with $n = n(T)$ vertices. By $\mathcal{T}(n)$ is denoted the set of all trees with n vertices and by $\mathcal{T}(n, k)$ the set of all trees with n vertices and diameter k.

In this paper we investigate the Merrifield–Simmons index of trees. We characterize the unique tree in $\mathcal{T}(n, k)$ with the largest σ-value, as well as the trees whose

[2] Recall that $F_n = F_{n-1} + F_{n-2}$ with initial conditions $F_0 = 1$ and $F_1 = 1$.

σ-values lie between 2^{n-2} and 2^{n-1}. From [17] we know that these results may have potential use in combinatorial chemistry.

The interval in which the σ-values of trees vary is determined by:

Lemma 1 [2, 6, 17]. Let $T \in \mathcal{T}(n)$. Then $F_{n+1} \leq \sigma(T) \leq 2^{n-1} + 1$. In addition, $\sigma(T) = F_{n+1}$ if and only if $T \cong P_n$ whereas $\sigma(T) = 2^{n-1} + 1$ if and only if $T \cong S_n$, where P_n and S_n are the n-vertex path and star, respectively.

The graphs shown in Fig. 1 are frequently used throughout this paper. Their construction and the parameters on which they depend are evident from Fig. 1 and will not be formally defined.

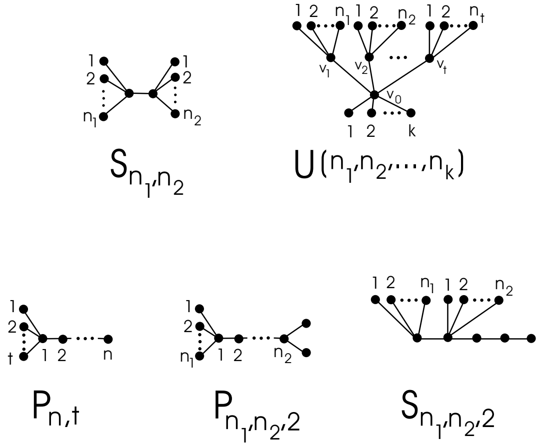

Figure 1. Trees considered in this work, the parameters on which they depend, and the labelling of their vertices.

PRELIMINARIES

Lemma 2 [2, 17]. Let G be a graph with k components $G_1, G_2, \ldots, G_k$. Then

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

Lemma 3 [2, 17]. For $v \in V(G)$,

$$\sigma(G) = \sigma(G - v) + \sigma(G - v - N_G(v)) \ .$$

From Lemmas 2 and 3, we can easily get the following:

Lemma 4. For two positive integers n_1 and n_2,

$$\sigma(S_{n_1,n_2}) = 2^{n_1+n_2} + 2^{n_1} + 2^{n_2} \ .$$

Lemma 5. Suppose that $n_1 \geq n_2 \geq \cdots \geq n_t \geq 0$ and $m = \sum_{i=1}^{t} n_i$. Then

$$\sigma(U_k(n_1, n_2, \ldots, n_t)) = 2^k \prod_{i=1}^{t} (2^{n_i} + 1) + 2^m \tag{1}$$

$$\sigma(U_k(n_1, n_2, \ldots, n_i{+}1, \ldots, n_j{-}1, \ldots, n_t)) > \sigma(U_k(n_1, n_2, \ldots, n_i, \ldots, n_j, \ldots, n_t)) \tag{2}$$

and if $2^{k-1}\,3^{t-1} > 2^m$, then

$$\sigma(U_k(m-t+1, \overbrace{1, \ldots, 1}^{t-1})) > \sigma(U_{k-1}((m-t+2, \overbrace{1, \ldots, 1}^{t-1})) \tag{3}$$

otherwise,

$$\sigma(U_k(m-t+1, \overbrace{1, \ldots, 1}^{t-1})) \leq \sigma(U_{k-1}((m-t+2, \overbrace{1, \ldots, 1}^{t-1})) \ . \tag{4}$$

Proof. Eq. (1): From Lemmas 2 and 3 we have

$$\sigma(U_k(n_1, n_2, \ldots, n_t)) = 2^k \prod_{i=1}^{t} \sigma(S_{n_i+1}) + 2^m = 2^k \prod_{i=1}^{t} (2^{n_i} + 1) + 2^m \ .$$

Eq. (2): Since $n_i \geq n_j$, we have $(2^{n_i+1}+1)(2^{n_j-1}+1) > (2^{n_i}+1)(2^{n_j}+1)$. Then, from (1) we get (2).

Eqs. (3) and (4): From (1) we have that

$$\sigma(U_k(m-t+1, \overbrace{1, \ldots, 1}^{t-1})) = 2^k\,(2^{m-t+1}+1)\,3^{t-1} + 2^m$$

and

$$\sigma(U_{k-1}(m-t+2, \overbrace{1, \ldots, 1}^{t-1})) = 2^{k-1}\,(2^{m-t+2}+1)\,3^{t-1} + 2^{m+1} \ .$$

Thus,

$$\sigma(U_k(m-t+1, \overbrace{1, \ldots, 1}^{t-1})) - \sigma(U_{k-1}(m-t+2, \overbrace{1, \ldots, 1}^{t-1})) = 2^{k-1}3^{t-1} - 2^m.$$

Obviously, (3) and (4) hold. $\square$

In a similar manner as Lemma 5, we prove:

Lemma 6. For all $n_1 \geq 2$ and $n_2 \geq 2$,

$$\sigma(P_{n_1,n_2}) = 2^{n_2} F_{n_1} + F_{n_1-1} \tag{5}$$

$$\sigma(P_{n_1,n_2}) > \sigma(P_{n_1+1,n_2-1}) . \tag{6}$$

Lemma 7. If $n \geq 7$, then

$$\sigma(P_{4,n-6,2}) = 2^{n-3} + 2^{n-4} + 2^{n-5} + 9 .$$

If $n_1 \geq 1$, $n_2 \geq 1$, and $n_1 + n_2 = n - 5$, then

$$\sigma(S_{n_1,n_2,2}) = 2^{n-3} + 2^{n-5} + 2^{n_2+2} + 2^{n_2} + 2^{n_1+1} + 2^{n_1}$$

and

$$\sigma(S_{n_1,n_2,2}) \leq \sigma(S_{1,n-6,2}) = 2^{n-3} + 2^{n-4} + 2^{n-5} + 2^{n-6} + 6$$

for all $n_1 \geq 1$ and $n_2 \geq 1$.

THE MAIN RESULTS

Lemma 8. If $T \in \mathcal{T}(n, n-1)$, then $\sigma(T) \leq 4\,F_{n-2} + F_{n-3}$. Equality holds if and only if $T \cong P_{n-2,2}$.

Proof. Since $T \in \mathcal{T}(n, n-1)$, we have $d(T) = n-1$. Then, T must be a tree obtained from P_2 and P_{n-1} by identifying one vertex in P_2 with one vertex of P_{n-1} of degree 2. Assume that $P_{n-1} = u_1, u_2, \ldots, u_{n-1}$ and that T is the tree obtained from P_{n-1} by adding a pendent edge at the vertex u_k, where $2 \leq k \leq n-2$. From Lemmas 1, 2, and 3, we have

$$\sigma(T) = \sigma(P_{n-1}) + \sigma(P_{k-1})\sigma(P_{n-k-1}) = F_n + F_k\,F_{n-k} .$$

Based on a result from [6], if $2 \leq k \leq n-2$, then $F_k\,F_{n-k} \leq F_2\,F_{n-2}$ and the equality holds if and only if $k = 2$. This completes the proof. □

Theorem 1. If $T \in \mathcal{T}(n, k)$, then $\sigma(T) \leq 2^{n-k+1}\,F_{k-1} + F_{k-2}$. Equality holds if and only if $T \cong P_{k,n-k}$.

Proof. Since $T \in \mathcal{T}(n,k)$, we have that $d(T) = k$ and $n \geq k+1$. We prove the theorem by double induction on k and n.

From Lemmas 1 and 4 follows that the theorem is true for $k = 2, 3$ and $n(T) \geq 4$.

Suppose that the theorem holds for all $d(T) \leq k-1$ and $k \geq 4$ and $n(T) \geq d(T)+2$.

Now for a tree T with $d(T) = k$, from Lemma 8 the theorem is true for $d(T) = k$ and $n(T) = k+2$. We assume that the theorem holds for $d(T) = k$ and $n(T) \leq n-1$. When $d(T) = k$ and $n(T) = n$, we distinguish the following two cases:

Case 1. There is at least one path $u_1, u_2, u_3, \ldots, u_k, u_{k+1}$ in T, such that $d_{u_2} = 2$ or $d_{u_k} = 2$. Without loss of generality, assume that $d_{u_2} = 2$. From Lemma 3 we have

$$\sigma(T) = \sigma(T - u_1) + \sigma(T - \{u_1, u_2\})$$

and

$$\sigma(P_{k,n-k}) = \sigma(P_{k-1,n-k}) + \sigma(P_{k-2,n-k}) \ .$$

Now, $T - u_1$ and $T - \{u_1, u_2\}$ are trees with $n-1$ and $n-2$ vertices, respectively. In addition, $k-1 \leq d(T-u_1) \leq k$ and $k-2 \leq d(T - \{u_1,u_2\}) \leq k$.

For $T - u_1$, by the induction hypothesis we have that $\sigma(P_{k-1,n-k}) \geq (T - u_1)$ if $d(T-u_1) = k-1$ and $\sigma(P_{k,n-k-1}) \geq (T-u_1)$ if $d(T-u_1) = k$. Thus, from Lemma 6 we have that $\sigma(P_{k-1,n-k}) > \sigma(P_{k,n-k-1})$. It is not difficult to show that $\sigma(P_{k-1,n-k}) \geq (T - u_1)$ and that equality holds if and only if $T - u_1 \cong P_{k-1,n-k}$.

Similarly, for $T - \{u_1,u_2\}$ we have $\sigma(P_{k-2,n-k}) \geq \sigma(T - \{u_1,u_2\})$, and the equality holds if and only if $T \cong P_{k-2,n-k}$. Hence, $\sigma(T) \leq \sigma(P_{k,n-k})$ and the equality holds if only if $T \cong P_{k,n-k}$.

Case 2. $d_{u_2} \geq 3$ and $d_{u_k} \geq 3$ for each path $u_1, u_2, u_3, \ldots, u_k, u_{k+1}$ in T. Suppose that $d_{u_2} = r+1 \geq 3$. From Lemma 3 we have

$$\sigma(T) = \sigma(T - u_1) + \sigma(T - \{u_1, u_2\})$$

and

$$\sigma(P_{k,n-k}) = \sigma(P_{k,n-k-1}) + 2^{n-k-1} F_k \ .$$

Now, $T - u_1$ is an $(n-1)$-vertex tree of diameter k. Then, by the induction hypothesis, $\sigma(P_{k,n-k-1}) \geq \sigma(T - u_1)$ and the equality holds if and only if $P_{k,n-k-1} \cong T - u_1$. On the other hand, there is a tree H such that $T - \{u_1, u_2\} = (r-1)\,K_1 \cup H$.[3] Then from Lemma 2,

$$\sigma(T - \{u_1, u_2\}) = 2^{r-1}\,\sigma(H)\ .$$

Note that $n(H) = n - r - 1 < n$ and $k - 2 \leq d(H) \leq k$. Hence, by the induction hypothesis and Lemma 6, we have $\sigma(P_{k-2,n-k-r+1}) \geq \sigma(H)$ and $n - k - r + 1 \geq 1$. Thus, $n - k \geq r$ and we have

$$\sigma(T - \{u_1, u_2\}) \leq 2^{r-1}\,\sigma(P_{k-2,n-r-k+1}) = 2^{n-k}\,F_{k-2} + 2^{r-1}\,F_{k-3}\ .$$

Since $2^{n-k-1}\,F_k = 2^{n-k}\,F_{k-2} + 2^{n-k-1}\,F_{k-3}$ and $n - k \geq r$, we have $2^{n-k-1}\,F_{k+1} \geq \sigma(T - \{u_1, u_2\})$ and the equality holds if and only if $n - k = r$. So, we have

$$\sigma(P_{k,n-k}) \geq \sigma(T)$$

and the equality holds if and only if $P_{k,n-k-1} \cong T - u_1$ and $n - k = r$, that is, $T \cong P_{k,n-k}$. By this the proof of Theorem 1 is completed. □

Lemma 9. Let T be an n-vertex tree and $d(T) = 4$. Then for $n \geq 10$, $\sigma(T) \geq 2^{n-2}$ if and only if $T \in \{U_1(n-5,1)\,,\, U_{n-5}(1,1)\,,\, U_0(n_1,n_2)\,|\, n_1 + n_2 = n-3\}$.

Proof. Since T is a tree with $d(T) = 4$ and $n(T) = n$, there are integers $n_i \geq 1$, $i = 1, 2, \ldots, t$, $k \geq 0$ and $t \geq 2$, such that $T \cong U_k(n_1, n_2, \ldots, n_t)$. Let $m = \sum_{i=1}^{t} n_i$. Since $t \geq 2$, from Lemma 5 we have

$$\sigma(U_k(m - t + 1, \overbrace{1, \ldots, 1}^{t-1})) \geq \sigma(U_k(n_1, n_2, \ldots, n_t)) \tag{7}$$

for $n_1 \geq n_2 \geq \cdots \geq n_t \geq 1$ and

$$\sigma(U_{k+s}(m - t + s, \overbrace{1, \ldots, 1}^{t-s})) > \sigma(U_{k+l}(m - t + l, \overbrace{1, \ldots, 1}^{t-l})) \tag{8}$$

[3] If this would not be the case, then it would be $T - \{u_1, u_2\} = r_1\,K_1 \bigcup_{i=1}^{t} H_i$, such that H_i is a tree with $n(H_i) \geq 2$ and $t \geq 2$, where $r_1 + t = r$. Since $d(T) = k$, there would have to be a tree, say H_1, such that $d(H_1) = k - 2$ and $d(H_i) \geq 1$ for $i \geq 2$. Thus we would have $d(T) \geq k + 1$, which would contradict to the fact $d(T) = k$.

for $s > l \geq 1$. So, from (7) and (8) we have

$$\max\{\sigma(U_{k-1}(m-2,1,1)) \,|\, k+m = n-4\} \geq \sigma(U_k(n_1, n_2, \ldots, n_t)) \tag{9}$$

for all $t \geq 3$ and $n_1 \geq n_2 \geq \cdots \geq n_t \geq 1$.

From (3) it follows that

$$\begin{aligned} & \max\{\sigma(U_{k-1}(m-2,1,1)) \,|\, k+m = n-4\} \\ = & \max\{\sigma(U_0(n-6,1,1)), \sigma(U_{n-7}(1,1,1))\} \\ = & 2^{n-3} + 2^{n-4} + 2^{n-6} + 9 \ . \end{aligned} \tag{10}$$

For $t = 2$,

$$\sigma(U_k(m-1,1)) > \sigma(U_k(m-2,2)) > \sigma(U_k(m-3,3) > \sigma(U_k(m-s,s)) \tag{11}$$

where $k + m = n - 4$ and $s \geq 4$. From Lemma 5 and the inequality (11) we infer the following:]

For $k = 0$ and $n_1 + n_2 = n - 3$,

$$\sigma(U_0(n_1, n_2)) = 2^{n-2} + 2^{n_1} + 2^{n_2} + 1 \ . \tag{12}$$

For $k = 1$ and $s \geq 1$,

$$\sigma(U_1(n-5,1)) > \sigma(U_1(n-6,2)) > \sigma(U_1(n-6-s, s+2)) \ . \tag{13}$$

For $k = 2$ and $s \geq 1$,

$$\sigma(U_2(n-6,1)) > \sigma(U_2(n-6-s, s+1)) \ . \tag{14}$$

For $k = n - 5$ and $s \geq 1$,

$$\sigma(U_{n-5}(1,1)) > \sigma(U_{n-6}(2,1)) > \sigma(U_{n-6-s}(1, 2+s)) \ . \tag{15}$$

For $k \geq 3$, $s_1 \geq 2$, and $s_2 \geq 1$,

$$\max\{\sigma(U_2(n-6,1)), \sigma(U_{n-6}(2,1))\} \geq \sigma(U_k(s_1, s_2)) \ . \tag{16}$$

In addition, by direct calculation we obtain:

$$\sigma(U_0(n_1,n_2)) = 2^{n-2} + 2^{n_1} + 2^{n_2} + 1 \quad (17)$$

$$\sigma(U_1(n-5,1)) = 2^{n-2} + 6 \quad (18)$$

$$\sigma(U_1(n-6,2)) = 2^{n-3} + 2^{n-4} + 2^{n-5} + 10 \quad (19)$$

$$\sigma(U_2(n-6,1)) = 2^{n-3} + 2^{n-4} + 2^{n-5} + 12 \quad (20)$$

$$\sigma(U_{n-5}(1,1)) = 2^{n-2} + 2^{n-5} + 4 \quad (21)$$

$$\sigma(U_{n-6}(1,2)) = 2^{n-3} + 2^{n-4} + 2^{n-5} + 2^{n-6} + 8 \quad (22)$$

Note that if $n \geq 10$, then $2^{n-5} > 12$ and $2^{n-6} > 8$. Therefore, from the inequalities (9)–(16) and Eqs. (17)–(22), we conclude that if $d(T) = 4$, then $\sigma(T) \geq 2^{n-2}$ if and only if $T \in \{U_1(n-5,1)\,,\, U_{n-5}(1,1)\,,\, U_0(n_1,n_2)\,|\, n_1+n_2 = n-3\}$. $\Box$

Lemma 10. Let T be an n-vertex tree with $d(T) = k$. If there exists a path $u_1, u_2, \ldots, u_{k+1}$ such that $d_{u_2} \geq 3$ and $d_{u_k} \geq 3$, then $\sigma(T) \leq \sigma(P_{k-1,n_1,2})$, where $n_1 = n-k-1$.

Proof follows by induction on $n(T)$. From the condition of the lemma, we know that $n(T) \geq k+3$ and the equality holds if and only if $T \cong P_{k-1,2,2}$. So, the lemma is true for $n(T) = k+3$.

Suppose that $n(T) \geq k+4$ and that the lemma holds for all trees with $n(T) < n$. Let $u_1, u_2, \ldots, u_{k+1}$ be a path, such that $d_{u_2} \geq 3$ and $d_{u_k} \geq 3$. We distinguish the following two cases:

Case 1. $d_{u_2} = 3$ or $d_{u_k} = 3$. Suppose that $d_{u_2} = 3$. From Lemma 2 we have

$$\sigma(T) = \sigma(T-u_1) + \sigma(T - \{u_1,u_2\})$$

and

$$\sigma(P_{k-1,n_1,2}) = \sigma(P_{k,n-k-1}) + 2\,\sigma(P_{k-2,n-k-1})\ .$$

Note that $n(T-u_1) = n-1$, $d(T-u_1) = k$, $T - \{u_1,u_2\} = K_1 \cup H$, and $k-2 \leq d(H) \leq k$, where H is a tree. From Theorem 1, $\sigma(T-u_1) \leq \sigma(P_{k,n-k-1})$ and

$\sigma(T-\{u_1,u_2\}) \le 2\,\sigma(P_{k-2,n-k-1})$, and each equality holds if and only if $T \cong P_{k-1,n_1,2}$. In view of this, the lemma holds.

Case 2. $d_{u_2} \ge 4$ and $d_{u_k} \ge 4$. Let $d_{u_2} = r \ge 4$. From Lemma 2 we have

$$\sigma(T) = \sigma(T-u_1) + \sigma(T-\{u_1,u_2\})$$

and

$$\sigma(P_{k-1,n_1,2}) = \sigma(P_{k-1,n_1-1,2}) + 2^{n_1-1}\,\sigma(P_{k-2,2})\ .$$

Since $T-u_1$ has a path $u_1,u_2,\ldots,u_{k+1}$ such that $d_{u_2} = r-1 \ge 3$ and $d_{u_k} \ge 4$, by the induction hypothesis, $\sigma(P_{k-1,n_1-1,2}) \ge \sigma(T-u_1)$ and the equality holds if and only if $P_{k,n-k-1} \cong T-u_1$. For $T-\{u_1,u_2\}$, by $d(T)=k$ we know that there is a tree H such that $T-\{u_1,u_2\} = (r-2)\,K_1 \cup H$ and $k-2 \le d(H) \le k$. Since $n(H) = n-r$, from Theorem 1 we have

$$\sigma(H) \le \sigma(P_{k-2,n-k-r+2}) = 2^{n-k-r+2}\,F_{k-2} + F_{k-3}$$

where $n-k-r+2 \ge 0$. Consequently,

$$\sigma(T-\{u_1,u_2\}) \le 2^{n-k}\,F_{k-2} + 2^{r-2}\,F_{k-3}\ .$$

Note that

$$2^{n_1-1}\,\sigma(P_{k-2,2}) = 2^{n-k}\,F_{k-2} + 2^{n-k-2}\,F_{k-3}\ .$$

Since $n-k-2 \ge r$, we have

$$\sigma(T-\{u_1,u_2\}) < 2^{n_1-1}\,\sigma(P_{k-2,2})$$

which completes the proof. $\square$

Lemma 11. If $T \in \mathcal{T}(n,5) \setminus \{P_{5,n-5}\}$, then $\sigma(T) \le 2^{n-3} + 2^{n-4} + 2^{n-5} + 2^{n-6} + 6$, and the equality holds if and only if $T \cong S_{1,n-5,2}$.

Proof. Since $T \in \mathcal{T}(n,5) \setminus \{P_{5,n-5}\}$, we only need to consider the following cases:

Case 1. There is a path u_1,u_2,u_3,u_4,u_5,u_6, such that $d_{u_2} \ge 3$ and $d_{u_5} \ge 3$. Then, from Lemmas 7 and 10,

$$\sigma(T) \le \sigma(P_{4,n-6,2}) = 2^{n-3} + 2^{n-4} + 2^{n-5} + 9\ .$$

Case 2. For each path $u_1, u_2, u_3, u_4, u_5, u_6$, we have, $d_{u_2} = 2$ or $d_{u_5} = 2$. Without loss of generality, assume, that $d_{u_2} = 2$. Then, from Lemma 3,

$$\sigma(T) = \sigma(T - u_1) + \sigma(T - \{u_1, u_2\})$$

and

$$\sigma(S_{1,n-5,2}) = \sigma(P_{4,n-5}) + \sigma(P_{4,n-6}) \ .$$

Note that $4 \leq d(T - u_1) \leq 5$ and $3 \leq d(T - \{u_1, u_2\}) \leq 5$. From Lemma 8 and Theorem 1, one concludes that if $d(T - \{u_1, u_2\}) \geq 4$, then $\sigma(T - u_1) \leq \sigma(P_{4,n-5})$ and $\sigma(T - \{u_1, u_2\}) \leq \sigma(P_{4,n-6})$. Therefore, $\sigma(T) \leq \sigma(S_{1,n-5,2})$ and the equality holds if and only if $T \cong S_{1,n-5,2}$. On the other hand, if $d(T - \{u_1, u_2\}) = 3$, then we have $d(T - u_1) = 4$. Then $T \cong S_{n_1,n_2,2}$, where $n_1 + n_2 = n - 6$. From Lemma 7, $\sigma(T) \leq \sigma(S_{1,n-5,2})$ and the equality holds if and only if $T \cong S_{1,n-5,2}$.

This completes the proof. □

Before stating Theorem 2 we first list a few results that can be obtained by direct calculation. These cover the case of trees with fewer than 10 vertices.

For any n, from Lemma 1 and Theorem 1 follows that there exists a unique tree such that $2^{n-1} \leq \sigma(T) \leq 2^n$, which is the star S_n.

For $1 \leq n \leq 7$ and $T \in \mathcal{T}(n) \setminus \{S_n\}$, $2^{n-2} \leq \sigma(T) < 2^{n-1}$.

For $n = 8$, if $T \in \{A_8, U_1(2,2), U_2(2,1), P_{4,2,2}, S_{1,2,2}, U_1(3,1), U_3(1,1), S(n_1, n_2), U_0(s_1, s_2) \mid n_1 + n_2 = 6, s_1 + s_2 = 5\}$ then $2^6 \leq \sigma(T) < 2^7$. Otherwise, $2^5 \leq \sigma(T) < 2^6$. In the above expression A_8 stands for the tree obtained from a path $u_1, u_2, u_3, u_4, u_5, u_6$ by adding a pendant edge at each of the vertices u_2 and u_4.

For $n = 9$, if $T \in \{U_3(2,1), P_{5,4}, U_1(4,1), U_4(1,1), U_0(s_1, s_2), S_{n_1,n_2} \mid n_1 + n_2 = 7, s_1 + s_2 = 6\}$ then $2^7 \leq \sigma(T) < 2^8$. Otherwise, $2^6 \leq \sigma(T) < 2^7$.

Theorem 2. If $T \in \mathcal{T}(n)$ and $n \geq 10$, then $2^{n-2} \leq \sigma(T) \leq 2^{n-1}$ if and only if $T \in \{P_{5,n-5}\,,\, U_1(n-5,1)\,,\, U_{n-5}(1,1)\,,\, U_0(s_1,s_2)\,,\, S_{n_1,n_2}\,|\, n_1+n_2=n-2\,,\, n_1 \geq n_2 \geq 1\,,\, s_1+s_2=n-3\,,\, s_1 \geq s_2 \geq 1\}$. In addition,

$$\begin{aligned}
\sigma(P_{5,n-5}) &= 2^{n-2}+5 \\
\sigma(U_1(n-5,1)) &= 2^{n-2}+6 \\
\sigma(U_{n-5}(1,1)) &= 2^{n-2}+2^{n-5}+4 \\
\sigma(U_0(s_1,s_2)) &= 2^{n-2}+2^{s_1}+2^{s_2}+1 \\
\sigma(S_{n_1,n_2}) &= 2^{n-2}+2^{n_1}+2^{n_2}\,.
\end{aligned}$$

Proof. Let T be a tree with $n(T) \geq 10$. Then $d(T) \geq 2$. For $d(T) = 2$, we have $T \cong S_n$ and $\sigma(S_n) > 2^{n-1}$.

For any tree T with $d(T) = 3$, from (5) and Lemma 1 we have $2^{n-2} \leq \sigma(T) \leq 2^{n-1}$.

For any tree T with $d(T) = 4$ and $n \geq 10$, from Lemma 9 we know that $2^{n-2} \leq \sigma(T) \leq 2^{n-1}$ if and only if $T \in \{U_1(n-5,1)\,,\, U_{n-5}(1,1)\,,\, U_0(s_1,s_2)\,|\, s_1+s_2=n-3\}$.

For any tree T with $d(T) = 5$, $\sigma(P_{5,n-5}) = 2^{n-2}+5$. From Theorem 1 and Lemmas 6 and 11 we know that $2^{n-2} \leq \sigma(T) \leq 2^{n-1}$ if and only if $T \cong P_{5,n-5}$.

For any tree T with $d(T) \geq 6$, from Theorem 1 and Lemma 6 we know that $\sigma(T) \leq \sigma(P_{6,n-6}) = 2^{n-3}+2^{n-4}+2^{n-6}+8$ and that equality holds if and only if $T \cong P_{6,n-6}$.

Theorem 2 follows from the above arguments, Lemma 4, and Eqs. (17)–(22). □

CONCLUDING REMARKS

Lemma 1 and Theorem 2 imply that there is a single n-vertex tree for which $2^{n-1}+1 \leq \sigma(T) \leq 2^n$. For $n \geq 10$ the number of n-vertex trees with with the property $2^{n-2}+1 \leq \sigma(T) \leq 2^{n-1}$ is exactly n. Above Theorem 2 all trees with fewer than 10 vertices were listed, for which $2^{n-t}+1 \leq \sigma(T) \leq 2^{n-t+1}$ for any possible integer t. We denote by $\mathcal{T}(2^t)$ the set of n-vertex trees T, such that $2^{n-t}+1 \leq \sigma(T) \leq 2^{n-t+1}$, and denote $|\mathcal{T}(2^t)|$ by $f(t)$.

Note that $\sigma(P_n) \geq 2^{\lfloor (n+2)/2 \rfloor}$. Therefore, $\lfloor (n+2)/2 \rfloor \leq t \leq n$. We have shown that $f(1) = 1$ and $f(2) = n$ if $n \geq 10$. An interesting problem would be to determine

$f(t)$ and $\mathcal{T}(2^t)$ for any $t \in [\lfloor (n+2)/2 \rfloor, n]$, and for any n, or to find good upper and lower bounds for $f(t)$.

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