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Trees with Small Randić Connectivity Indices

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Abstract

Let T be a tree and $d(v)$ the degree of its vertex v. Then the connectivity index, or Randić index, of T is defined as $\chi(T) = \sum_{uv} \frac{1}{\sqrt{d(u)d(v)}}$, where the summation goes over all edges uv of T. In the existing literature, trees of order n with m pending vertices and with the smallest connectivity index were determined by Hansen et al, whereas the unique tree of order n with the smallest connectivity index was determined by Bollobás et al. In this paper, we determine all trees of order n with m pending vertices and with the second smallest connectivity index and all trees of order n with diameter r and with the smallest and the second smallest connectivity indices. The unique tree of order n with, respectively, the second, the third and the fourth smallest connectivity index is also determined.

1 Introduction

The connectivity index, or Randić index, χ is a topological index proposed by Randić in 1975. Randić himself demonstrated that the Randić index χ was well correlated with a variety of physico-chemical properties of alkanes, such as boiling point, surface area and solubility in water. Eventually, χ became one of the most popular molecular graph-based structure-descriptors, used in QSPR and QSAR studies. On its applications for predicting physico-chemical and pharmacologic properties of organic compounds two books (Kier and Hall, 1976, 1986) and scores of papers were published; details and further bibliography can be found in [1,2] and [5-14].

Let G be a graph with the vertex set $V(G)$ and the edge set $E(G)$. Then the connectivity index is defined as

$$\chi(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_G(u)d_G(v)}},$$

where $d_G(x)$, or simply $d(x)$, denotes the degree of a vertex x in G.

For a graph G and $u \in V(G)$, we denote by $N_G(u)$ the set of all neighbors of u in G and by $n(G)$ the number of vertices of G. We denote respectively by S_n and P_n the star and the path with n vertices. By $P_{n,m}$ we denote the graph obtained from S_{n+1} and P_m by identifying the center of S_{n+1} with a vertex of degree 1 of P_m. By $S_{n,m}$ we denote the graph obtained from S_{n+2} and S_{m+1} by identifying a vertex of degree 1 of S_{n+2} with the center of S_{m+1}. We denote by $D(G)$ the diameter of G, which is defined as $D(G) = \max\{d(u,v)|u,v \in V(G)\}$ where $d(u,v)$ denotes the distance between the vertices u and v in G. We denote by $\mathcal{T}(n,r)$ the set of all trees with n vertices such that $D(T) = r$. Undefined notations and terminology will conform to those in [3].

Bollobás and Erdős [4] in 1998 got the fundamental result that among all connected graphs G with n vertices the star S_n has the smallest connectivity index χ, that is $\chi(G) \geq \sqrt{n-1}$ for any such a graph G. Caporossi et al [5] in 1999 proved that $\chi(T) \leq \frac{n-3}{2} + \sqrt{2}$ for all trees T of order n and the equality holds if and only if $G \cong P_n$. Very recently, Hansen et al [10] obtained the following result.

Theorem 1.([10]) Let T be a tree of order $n \geq 3$ with m pending vertices. Then if $m < n-1$,

$$\chi(T) \geq \sqrt{m} + \left(\frac{1}{\sqrt{2}} - 1\right)\frac{1}{\sqrt{m}} + \frac{n-m-3}{2} + \frac{1}{\sqrt{2}},$$

and the equality holds if and only if T is the comet $T_{n,m}$, where $T_{n,m} \cong P_{m-1,n-m+1}$.

In this paper, we determine all trees of order n with m pending vertices and with the second smallest connectivity index and the unique tree of order n with, respectively, the second, the third and the fourth smallest connectivity index. Trees of order n with diameter r and with the smallest and the second smallest connectivity indices are also determined.

2 Lower Bounds for the Connectivity Index of Trees

In this section, we determine all trees with the second smallest connectivity index among all trees T of order n with m pending vertices. Let T be a tree with $n(T)$ vertices and u a vertex of T. Denote by $T + uv$ the tree obtained from T by adding a pendent edge uv. For convenience, we write $f(k) = \frac{1}{\sqrt{k+1}+\sqrt{k}}$ and $g(k) = \frac{1}{\sqrt{k(k+1)}(\sqrt{k+1}+\sqrt{k})}$.

Lemma 1. Let T a tree with a vertex u such that $d_T(u) = k$. Suppose that $N_T(u) = \{1, 2, 3, \cdots, k\}$ and $v \in V(T)$. Then

$$\chi(T + uv) = \chi(T) + f(k) + g(k)\left(k - \sum_{i \in N_T(u)} \frac{1}{\sqrt{d_T(i)}}\right).$$

Proof. Suppose that $Q = \{ui | i \in N_T(u)\}$ and $\Omega = \sum_{xy \in E(T)-Q} \frac{1}{\sqrt{d_T(x)d_T(y)}}$. Then we have

$$\begin{aligned}\chi(T) &= \sum_{xy \in E(T)} \frac{1}{\sqrt{d_T(x)d_T(y)}} \\ &= \Omega + \sum_{i \in N_T(u)} \frac{1}{\sqrt{kd_T(i)}}\end{aligned}$$

and

$$\begin{aligned}\chi(T + uv) &= \sum_{xy \in E(T+uv)} \frac{1}{\sqrt{d_{T+uv}(x)d_{T+uv}(y)}} \\ &= \Omega + \sum_{i \in N_T(u)} \frac{1}{\sqrt{(k+1)d_T(i)}} + \frac{1}{\sqrt{k+1}}.\end{aligned}$$

So, we get that

$$\begin{aligned}\chi(T + uv) - \chi(T) &= \frac{1}{\sqrt{k+1}} - \frac{1}{\sqrt{k(k+1)}(\sqrt{k+1}+\sqrt{k})}\left(\sum_{i \in N_T(u)} \frac{1}{\sqrt{d_T(i)}}\right) \\ &= f(k) + g(k)\left(k - \sum_{i \in N_T(u)} \frac{1}{\sqrt{d_T(i)}}\right).\end{aligned}$$

Clearly, the lemma holds. □

Let v be a vertex of T. One can see that there is a vertex $w \in N_T(v)$ such that $d_T(w) \geq 2$ except if v is the center of a star. So, we have

$$k - \sum_{i \in N_T(v)} \frac{1}{\sqrt{d_T(i)}} \geq 1 - \frac{1}{\sqrt{2}} \quad (1)$$

if $T + uv$ is not a star.

Denote by Q_{n_1,n_2} and P_{n_1,n_2,n_3} the two graphs shown in Figure 1, where G is a connected graph.

Figure 1. Graphs Q_{n_1,n_2} and P_{n_1,n_2,n_3}

Theorem 2. Let $n_1 \geq n_2 + 2 \geq 2$ and $d(v_2) \geq d(u_2)$. Then

$$\chi(Q_{n_1,n_2}) < \chi(Q_{n_1-1,n_2+1}).$$

Proof. By Lemma 1 it follows that

$$\chi(Q_{n_1,n_2}) = \chi(Q_{n_1-1,n_2}) + f(n_1) + g(n_1)\left(1 - \frac{1}{\sqrt{d(u_2)}}\right)$$

and

$$\chi(Q_{n_1-1,n_2+1}) = \chi(Q_{n_1-1,n_2}) + f(n_2+1) + g(n_2+1)\left(1 - \frac{1}{\sqrt{d(v_2)}}\right).$$

Since $n_1 \geq n_2 + 2$ and $d(v_2) \geq d(u_2)$, the theorem holds. □

It is not hard to see that the proof of Theorem 2 is valid for the graph P_{n_1,n_2,n_3}, where $n_1 \geq n_3 + 2 \geq 2$ and $n_2 \geq 2$. So, we have the following lemma.

Lemma 2. Let $n_1 \geq n_3 + 2 \geq 2$ and $n_2 \geq 2$. Then

$$\chi(P_{n_1,n_2,n_3}) < \chi(P_{n_1-1,n_2,n_3+1}). \qquad \square$$

Lemma 3. Let $n_1 \geq n_2 \geq 2$ and G be a tree. If Q_{n_1,n_2} has n vertices and m pending vertices, then $\chi(Q_{n_1,n_2}) \geq \chi(P_{m-2,n-m,2})$.

Proof. By induction on m. Clearly, $m \geq 4$. When $m = 4$, $Q_{n_1,n_2} \cong P_{2,n-4,2}$. So, the lemma is true for $m = 4$ and all $n \geq m + 2$.

Suppose that $m \geq 5$ and the lemma holds for every Q_{s_1,s_2} of order n with $m - 1$ pending vertices, where $s_1 \geq s_2 \geq 2$ and $s_1 + s_2 = n_1 + n_2$. We distinguish the following cases:

Case 1. $n_1 = 2$ or $n_2 = 2$.

Let $n_2 = 2$ and $T' = Q_{n_1,1}$. By Lemma 1, we have

$$\chi(Q_{n_1,n_2}) = \chi(T') + f(2) + g(2)\left(1 - \frac{1}{\sqrt{d_{T'}(v_2)}}\right)$$

and

$$\chi(P_{m-2,n-m,2}) = \chi(P_{m-2,n-m+1}) + f(2) + g(2)\left(1 - \frac{1}{\sqrt{2}}\right).$$

Note that T' has $n-1$ vertices and $m-1$ pending vertices. From Theorem 1 we have that $\chi(T') \geq \chi(P_{m-2,n-m+1})$ and the equality holds if and only if $T' \cong P_{m-2,n-m+1}$. So, we have that $\chi(Q_{n_1,n_2}) \geq \chi(P_{m-2,n-m,2})$ and the equality holds if and only if $Q_{n_1,n_2} \cong P_{m-2,n-m,2}$.

Case 2. $n_1 \geq 3$ and $n_2 \geq 3$.

Let $T' = Q_{n_1-1,n_2}$. By Lemma 1, we have

$$\chi(Q_{n_1,n_2}) = \chi(T') + f(n_1) + g(n_1)\left(1 - \frac{1}{\sqrt{d_{T'}(u_2)}}\right) \tag{2}$$

and

$$\chi(P_{m-2,n-m,2}) = \chi(P_{m-3,n-m,2}) + f(m-2) + g(m-2)\left(1 - \frac{1}{\sqrt{2}}\right). \tag{3}$$

Since $T' \cong Q_{n_1-1,n_2}$ and T' has $m-1$ pending vertices, by the induction hypothesis, $\chi(P_{m-3,n-m,2}) \leq \chi(T')$. Note that $n_1 \leq m-3$ and Q_{n_1,n_2} is not a star. Thus from (1), (2) and (3) we have

$$\chi(Q_{n_1,n_2}) > \chi(P_{m-2,n-m,2}).$$

This completes the proof. □

Let $v_1v_2v_3\cdots v_k$ be a path P_k and $T_{k,v_i,m}$ be a graph shown in Figure 2, where $k \geq 5$ and $m \geq 1$.

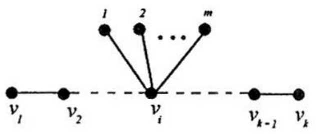

Figure 2. Graph $T_{k,v_i,m}$

Lemma 4. Let $r \geq 4$ and $n \geq r+3$. Then

$$\chi(P_{n-r-1,r-1,2}) > \chi(T_{r+1,v_3,n-r-1}).$$

Proof. By the definition of χ, we have

$$\chi(P_{n-r-1,r-1,2}) = \frac{n-r-1}{\sqrt{n-r}} + \frac{1}{\sqrt{2(n-r)}} + \frac{r-4}{2} + \frac{2}{\sqrt{3}} + \frac{1}{\sqrt{6}}$$

and

$$\chi(T_{r+1,v_3,n-r-1}) = \frac{n-r-1}{\sqrt{n-r+1}} + \frac{\sqrt{2}}{\sqrt{n-r+1}} + \frac{r-4}{2} + \sqrt{2}.$$

Let $x = n-r$. Obviously, x is an integer and $x \geq 3$. So, we get that

$$\chi(P_{n-r-1,r-1,2}) - \chi(T_{r+1,v_3,n-r-1}) = \phi(x), \tag{4}$$

where $\phi(x) = (\sqrt{2}-1)\left(\frac{\sqrt{2}}{\sqrt{x+1}} - \frac{1}{\sqrt{2x}}\right) + \frac{2\sqrt{2}+1-\sqrt{12}}{\sqrt{6}} - \frac{1}{\sqrt{x+1}+\sqrt{x}}$. By calculation, one can check that $\phi(x) > 0$ for each $x \in \{3,4,5,6,7,8,9,10\}$ and $\phi(x) > \frac{2\sqrt{2}+1-\sqrt{12}}{\sqrt{6}} - \frac{1}{\sqrt{11}+\sqrt{12}} > 0$ for $x \geq 11$. Thus by formula (4) the lemma is true.

Lemma 5. If $T \in \mathcal{T}(n,4) - \{P_{n-4,4}\}$, then $\chi(T) \geq \frac{n-5}{\sqrt{n-3}} + \frac{\sqrt{2}}{\sqrt{n-3}} + \sqrt{2}$ and the equality holds if and only if $T \cong T_{5,v_3,n-5}$.

Proof. Clearly, $T \in \mathcal{T}(n,4) - \{P_{n-5,5}\}$ if and only if T has $n-3$ pending vertices. So, we have the following cases:

Case 1. There is a path $u_1u_2u_3u_4u_5$ in T such that $d(u_2) \geq 3$ and $d(u_4) \geq 3$. By Lemmas 3 and 4,

$$\chi(T) \geq \chi(P_{n-5,3,2}) > \chi(T_{5,v_3,n-5}).$$

Case 2. For each path $u_1u_2u_3u_4u_5$ in T, we must have $d(u_2) = 2$ or $d(u_r) = 2$. Recalling that $D(T) = 4$, one can see that T must be the graph $U_k(n_1,t)$ shown in Figure 2, where $k \geq 0$, $n_1 \geq 1$, $t \geq 2$ and $n_1 + 2t + k = n$.

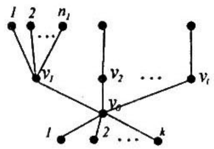

Figure 3. Graph $U_k(n_1,t)$

By Lemma 1,

$$\chi(T_{5,v_3,n-5}) = \chi(T_{5,v_3,n-6}) + f(n-4) + g(n-4)(2-\sqrt{2}). \tag{5}$$

Subcase 2.1. $k \geq 1$ in $U_k(n_1,t)$.

By Lemma 1, we have

$$\chi(U_k(n_1,t)) \geq \chi(U_{k-1}(n_1,t)) + f(k+t-1) + g(k+t-1)(2-\sqrt{2}) \tag{6}$$

and the equality holds if and only if $n_1 = 1$ and $t = 2$, that is, $U_k(n_1,t) \cong T_{5,v_3,n-5}$. Since $k+t-1 \leq n-4$, by (5) and (6) we have

$$\chi(U_k(n_1,t)) \geq \chi(T_{5,v_3,n-5})$$

and the equality holds if and only if $U_k(n_1,t) \cong T_{5,v_3,n-5}$.

Subcase 2.2. $k = 0$ and $t \geq 3$ in $U_k(n_1,t)$.

By Lemma 1, we have that

$$\chi(U_0(n_1,t)) = \chi(U_1(n_1,t-1)) + f(1) + g(1)(1 - \frac{1}{\sqrt{t}})$$

and

$$\chi(U_1(n_1+1,t-1)) = \chi(U_1(n_1,t-1)) + f(n_1+1) + g(n_1+1)(1 - \frac{1}{\sqrt{t}}).$$

Clearly, $n_1 + 1 > 1$. So, $\chi(U_0(n_1,t)) > \chi(U_1(n_1+1,t-1))$. From Subcase 2.1, we have

$$\chi(U_0(n_1,t)) > \chi(U_1(n_1+1,t-1)) \geq \chi(T_{5,v_3,n-5}).$$

Subcase 2.3. $k = 0$ and $t = 2$ in $U_k(n_1,t)$.

So, $U_0(n_1,2) \cong P_{5,n-5}$, which contradicts to the condition of the lemma.

By calculation, we have

$$\chi(T_{5,v_3,n-5}) = \frac{n-5}{\sqrt{n-3}} + \frac{\sqrt{2}}{\sqrt{n-3}} + \sqrt{2}.$$

This completes the proof. □

Let T be a tree of order $n \geq 3$ with m pending vertices. Obviously, $m \leq n-1$ and the equality holds if and only if $T = S_n$. When $m = n-2$, one can see that $T \in \{S_{n_1,n_2} | n_1 + n_2 = n-2, n_1 \geq n_2\}$. By Lemma 2, for all $t \geq 5$ we have

$$\chi(S_{n-3,1}) > \chi(S_{n-4,2}) > \chi(S_{n-t,t-2}).$$

So, $S_{n-4,2}$ has the second smallest connectivity index among all trees of order n with $n-2$ pending vertices. For $m < n-2$, we have

Theorem 3. Let T be a tree of order $n \geq 3$ with m pending vertices. If $m < n-2$ and $T \ncong P_{m-1,n-m+1}$, then

$$\chi(T) \geq \sqrt{m} + \left(\sqrt{2}-2\right)\frac{1}{\sqrt{m}} + \frac{n-m-3}{2} + \sqrt{2}$$

and the equality holds if and only if $T \in \{T_{n-m+2,v_i,m-2} | 3 \leq i \leq n-m\}$.

Proof. Let T be a tree of order $n \geq 3$ with m pending vertices. By the condition of the theorem, $m \geq 3$ and $n \geq m+3$. By calculation, it is not difficult to obtain that for $3 \leq i \leq r-1$,

$$\chi(T_{n-m+2,v_3,m-2}) = \chi(T_{n-m+2,v_i,m-2}) = \sqrt{m} + \left(\sqrt{2}-2\right)\frac{1}{\sqrt{m}} + \frac{n-m-3}{2} + \sqrt{2}.$$

So, we need only to prove that $\chi(T) \geq \chi(T_{n-m+2,v_3,m-2})$. We prove it by induction on n.

For any $m \geq 3$, one can see that $n = m+3$ if and only if $D(T) = 4$. By Lemma 5, the theorem holds for $n = m+3$ with $m \geq 3$.

Suppose that $n \geq m+4$ and that the theorem is true for all trees T of order $n-1$ with m pending vertices. Then for a tree T of order n with m pending vertices, we consider the following cases:

Case 1. T is a tree of form Q_{n_1,n_2} such that $n_1 \geq n_2 \geq 2$. Then, from Lemmas 3 and 4, it follows that

$$\chi(T) \geq \chi(P_{m-2,n-m,2}) > \chi(T_{n-m+2,v_3,m-2}).$$

Case 2. There is a path $u_1u_2u_3$ in T such that $d(u_1) = 1$, $d(u_2) = 2$ and $d(u_3) \geq 2$. Let $T' = T - u_1$. Then, by Lemma 1 we have that

$$\chi(T) \geq \chi(T') + f(1) + g(1)(1 - \frac{1}{\sqrt{d_{T'}(u_3)}}) \tag{7}$$

and

$$\chi(T_{n-m+2,v_3,m-2}) = \chi(T_{n-m+1,v_3,m-2}) + f(1) + g(1)(1 - \frac{1}{\sqrt{2}}). \tag{8}$$

Clearly, T' has $n-1$ vertices and m pending vertices. Since $T \ncong P_{m-1,n-m+1}$, we have $T \cong T_{n-m+2,v_3,m-2}$ if $T' \cong P_{m-1,n-m}$. For $T' \ncong P_{m-1,n-m}$, by the induction hypothesis we have $\chi(T') \geq \chi(T_{n-m+1,v_3,m-2})$. So, from (7) and (8),

$$\chi(T) \geq \chi(T_{n-m+2,v_3,m-2})$$

and the equality holds if and only if $T' \in \{T_{n-m+1,v_i,m-2} | 3 \leq i \leq n-m-1\}$ and $d_{T'}(u_3) = 2$. Furthermore, the equality holds if and only if $d_T(u_3) = 2$ and $T \in \{T_{n-m+2,v_i,m-2} | 3 \leq i \leq n-m\}$.

This completes the proof. □

In the following, using Theorems 1 and 3 we find the smallest value of the connectivity index of trees in $\mathcal{T}(n,r)$ and determine the corresponding trees. Let $T \in \mathcal{T}(n,r)$ and $r \geq 3$. Then, there is a path $u_1u_2\cdots u_{r+1}$ in T such that $d(u_1) = d(u_{r+1}) = 1$ and $d(u_i) \geq 2$ for all $2 \leq i \leq r$. So, T has at most $n-r+1$ pending vertices. By Theorem 1, it is not difficult to see that $\chi(T) \geq \chi(P_{m-1,n-m+1})$ if T has m pending vertices. By Lemma 2, for $m \geq 3$ we have

$$\chi(P_{m-2,n-m+1,1}) > \chi(P_{m-1,n-m+1,0}),$$

that is,

$$\chi(P_{m-2,n-m+2}) > \chi(P_{m-1,n-m+1}). \tag{9}$$

Thus, we have $\chi(T) \geq \chi(P_{n-r,r})$ and the equality holds if and only if $T \cong P_{n-r,r}$.

For $r = 3$, we have that $S_{n-4,2}$ is the unique tree with the second smallest connectivity index among all trees of order n with diameter 3. For $r \geq 4$, by (9) and Theorems 1 and 3 we have that if $T \ncong P_{n-r,r}$, then $\chi(T) \geq \chi(T_{r+1,v_3,n-r-1})$ when T has $n-r+1$ pending vertices and $\chi(T) \geq \chi(P_{n-r-1,r+1})$ when T has no more than $n-r$ pending vertices. By calculation, we have

$$\chi(T_{r+1,v_3,n-r-1}) = \frac{n-r-1}{\sqrt{n-r+1}} + \frac{\sqrt{2}}{\sqrt{n-r+1}} + \frac{r-4}{2} + \sqrt{2}. \tag{10}$$

and

$$\chi(P_{n-r-1,r+1}) = \frac{n-r-1}{\sqrt{n-r}} + \frac{1}{\sqrt{2(n-r)}} + \frac{r-2}{2} + \frac{1}{\sqrt{2}}. \tag{11}$$

From (10) and (11), we have

$$\chi(P_{n-r-1,r+1}) - \chi(T_{r+1,v_3,n-r-1}) = \psi(x),$$

where $\psi(x) = \frac{x-1}{\sqrt{x}} - \frac{x-1}{\sqrt{x+1}} + \frac{1}{\sqrt{2x}} - \frac{\sqrt{2}}{\sqrt{x+1}} + 1 - \frac{1}{\sqrt{2}}$ and $x = n-r \geq 2$. It is easy to check that $\psi(x) > 0$ for $x = 2,3,4$. For $x \geq 5$, we have

$$\psi(x) > 1 - \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2(x+1)}} - \frac{\sqrt{2}}{\sqrt{x+1}} \geq 1 - \frac{1}{\sqrt{2}} - \frac{1}{\sqrt{12}} > 0.$$

So, from the above arguments and Theorems 1 and 3, we have

Theorem 4. (i) For $T \in \mathcal{T}(n,r)$ and $r \geq 3$, we have

$$\chi(T) \geq \frac{n-r}{\sqrt{n-r+1}} + \frac{1}{\sqrt{2(n-r+1)}} + \frac{r-3}{2} + \frac{1}{\sqrt{2}},$$

and the equality holds if and only if $T \cong P_{n-r,r}$.

(ii) For $r \geq 4$ and $T \in \mathcal{T}(n,r) - \{P_{n-r,r}\}$, we have

$$\chi(T) \geq \frac{n-r-1}{\sqrt{n-r+1}} + \frac{\sqrt{2}}{\sqrt{n-r+1}} + \frac{r-4}{2} + \sqrt{2},$$

and the equality holds if and only if $T \in \{T_{r+1,v_i,n-r-1} | 3 \leq i \leq r-1\}$. □

3 Trees with Small Connectivity Indices

In this section, we determine the unique tree of order n with, respectively, the second, the third and the fourth smallest connectivity index.

Let T be a tree of order n. Then, for smaller n we have the following: for $n = 1, 2, 3$, we have $T \cong S_n$; for $n \geq 4$, we can easily check that

(a) for $n = 4$, $\chi(P_3) > \chi(S_3)$;

(b) for $n = 5$, $\chi(P_5) > \chi(S_{2,1}) > \chi(S_4)$;

(c) for $n = 6, 7$, $\chi(T) > \chi(P_{n-4,4}) > \chi(S_{n-4,2}) > \chi(S_{n-3,1}) > \chi(S_n)$ if $T \notin \{P_{n-4,4}, S_{n-4,2}, S_{n-3,1}, S_n\}$.

Now we consider the case $n \geq 8$. By Lemma 2, we have

$$\chi(S_{n_1,n_2}) > \chi(S_{n_1+1,n_2-1}) \quad for \quad n_1 \geq n_2 \geq 2. \tag{12}$$

By (9) and Theorem 4, we have

$$\chi(T) > \chi(P_{n-4,4}) \quad if \quad T \in \mathcal{T}(n,r) - P_{n-4,4} \quad and \quad r \geq 4. \tag{13}$$

By calculation, we obtain the following:

(i) $\chi(S_{n-3,1}) = \frac{n-3}{\sqrt{n-2}} + \frac{1}{\sqrt{2(n-2)}} + \frac{1}{\sqrt{2}}$,

(ii) $\chi(S_{n-4,2}) = \frac{n-4}{\sqrt{n-3}} + \frac{1}{\sqrt{3(n-3)}} + \frac{2}{\sqrt{3}}$,

(iii) $\chi(S_{n-5,3}) = \frac{n-5}{\sqrt{n-4}} + \frac{1}{2\sqrt{n-4}} + \frac{3}{2}$,

(iv) $\chi(P_{n-4,4}) = \frac{n-4}{\sqrt{n-3}} + \frac{1}{\sqrt{2(n-3)}} + \frac{1+\sqrt{2}}{2}$.

From (i) to (iv), it is not difficult to obtain that $\chi(S_{n-5,3}) > \chi(S_{n-4,2}) > \chi(S_{n-3,1})$ and $\chi(P_{n-4,4}) > \chi(S_{n-4,2}) > \chi(S_{n-3,1})$ for $n \geq 8$. On the other hand, we have

$$\chi(S_{n-5,3}) - \chi(P_{n-4,4}) = z(x), \tag{14}$$

where $z(x) = 1 - \frac{\sqrt{2}}{2} - \frac{1}{2\sqrt{x}} - \frac{1}{\sqrt{2(x+1)}} + \frac{x}{\sqrt{x}} - \frac{x}{\sqrt{x+1}}$ and $x = n - 4 \geq 4$. By calculation, one obtains that $z(x) < 0$ for $n = 8, 9$ and $z(x) > 0$ for $10 \leq n \leq 20$. For $n \geq 21$, it follows that

$$z(x) > 1 - \frac{\sqrt{2}}{2} - \frac{1}{2\sqrt{17}} - \frac{1}{\sqrt{36}} > 0.$$

So, by (14) we have that $\chi(S_{n-5,3}) < \chi(P_{n-4,4})$ for $n = 8, 9$ and $\chi(S_{n-5,3}) > \chi(P_{n-4,4})$ for $n \geq 10$. Thus, by (c), (12) and (13), we have the following theorem.

Theorem 5. Let T be a tree of order n and let $T \notin \{S_{n-4,2}, S_{n-3,1}, S_n\}$. Then,

(i) $\chi(T) \geq \chi(S_{n-5,3}) > \chi(S_{n-4,2}) > \chi(S_{n-3,1}) > \chi(S_n)$ for $n = 8, 9$ and the equality holds if and only if $T \cong S_{n-5,3}$.

(ii) $\chi(T) \geq \chi(P_{n-4,4}) > \chi(S_{n-4,2}) > \chi(S_{n-3,1}) > \chi(S_n)$ for $n = 6, 7$ or $n \geq 10$ and the equality holds if and only if $T \cong P_{n-4,4}$. □

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