

# Tree with minimal Laplacian spectral radius and diameter $n - 4$

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## Abstract

Let  $\mathcal{T}_{n,n-4}$  be the set of trees on  $n$  vertices with diameter  $n - 4$ . In this paper, we determine the unique tree which has the minimal Laplacian spectral radius among all trees in  $\mathcal{T}_{n,n-4}$ . The work is related with that of Yuan [The minimal spectral radius of graphs of order  $n$  with diameter  $n - 4$ , *Linear Algebra Appl.* 428(2008)2840-2851], which determined the graph with minimal spectral radius among all the graphs of order  $n$  with diameter  $n - 4$ . We can observe that the extremal tree on the Laplacian spectral radius is different from that on the spectral radius.

AMS Classification: 05C50

Keywords: Tree; Laplacian spectral radius; Diameter

## 1 Introduction

In this paper, we consider only connected simple graphs and, in particular, trees. Let  $G = (V(G), E(G))$  be a graph on vertex set  $V(G)$  and edge set  $E(G)$ . The degree of a vertex  $v$  in  $G$ , written by  $d_G(v)$ , is the number of edges incident with  $v$ . Let  $N_G(v)$  be the set of vertices which are adjacent to  $v$  in  $G$ . The distance between vertices  $u$  and  $v$  is denoted by  $d(u, v)$ , the

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\*Supported by the National Natural Science Foundation of China (No. 11201432) and the China Postdoctoral Science Foundation (No. 2011M501185 and 2012T50636). E-mail address: rfiu@zzu.edu.cn(R.Liu).

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‡Supported by the National Natural Science Foundation of China (No. 11271338).

diameter  $d$  of a connected graph  $G$  is the maximum distance between pairs of its vertices. Denote by  $L_G$  the line graph of graph  $G$ .

The adjacency matrix of a graph  $G$  is defined to be a  $(0, 1)$ -matrix  $A(G) = (a_{ij})$  of order  $n$ , where  $a_{ij} = 1$  if  $v_i$  is adjacent to  $v_j$ , and  $a_{ij} = 0$  otherwise. We call the largest eigenvalue of  $A(G)$  the spectral radius of the graph  $G$ , denoted by  $\rho(G)$ . The characteristic polynomial of graph  $G$  is just  $\det(xI - A(G))$ , denoted by  $\Phi(G)$ . The Laplacian matrix  $L(G) = D(G) - A(G)$  is the difference of the diagonal matrix of vertex degrees and the adjacency matrix. The largest eigenvalue of  $L(G)$  is usually called the Laplacian spectral radius of the graph  $G$ , denoted by  $\mu(G)$ .

In order to adjust the robustness of a network against the spread of viruses and the quality of the service running over the network, van Dam and Kooij [4] proposed the following problem: *which connected graph of order  $n$  with a given diameter  $d$  has minimal spectral radius?* In [4], the problem of cases with  $d \in \{1, 2, \lfloor \frac{n}{2} \rfloor, n-3, n-2, n-1\}$  are explicitly solved. Let  $P_{n_1, n_2, \dots, n_t, k}^{m_1, m_2, \dots, m_t}$  be the tree (of order  $n_1 + n_2 + \dots + n_t + k$ ) obtained from  $P_k$ , labeled as  $v_0 v_1 \dots v_{k-1}$ , by attaching pendant paths of order  $n_i + 1$  at vertices  $v_{m_i}$  for each  $i = 1, 2, \dots, t$ . van Dam and Kooij [4] proposed the following conjecture:

*For a fixed integer  $e$ , the tree  $P_{\lfloor \frac{e-1}{2} \rfloor, n-e-\lfloor \frac{e-1}{2} \rfloor}^{\lfloor \frac{e-1}{2} \rfloor, \lfloor \frac{e-1}{2} \rfloor, n-e+1}$  has the minimal spectral radius among the graphs of order  $n$  with diameter  $d = n - e$ , for  $n$  large enough.*

Yuan et al. [13] proved that the conjecture holds for  $e = 4$  (i.e.  $d = n - 4$ ), and pointed out for  $n \geq 11$ ,  $P_{1,2,n-3}^{1,n-6}$  has the minimal spectral radius. Furthermore, Cioabă et al. [3] proved that the conjecture also holds for  $e = 5$  (i.e.  $d = n - 5$ ) and  $n \geq 18$ , and for  $e \geq 6$  the conjecture does not hold. Belardo et al. [2] determined the trees with minimal spectral radius and diameter at most 4.

Recent discoveries indicate that the Laplacian spectral radius of trees plays an important role in the theory of the photoelectron spectra of saturated hydrocarbons (see [5] and the references therein). Liu et al. [10] characterized the trees with minimal Laplacian spectral radii among the trees on order  $n$  and  $d \in \{1, 2, 3, 4, n-3, n-2, n-1\}$ .

**A problem arises naturally what is the tree whose Laplacian spectral radius is minimum among all trees of order  $n$  with diameter  $n - 4$ .**

Let  $\mathcal{T}_{n,n-4}$  be the set of trees on  $n$  vertices with diameter  $n - 4$ . In this paper, we determine the unique tree which has the minimal Laplacian spectral radius among all trees in  $\mathcal{T}_{n,n-4}$ .

## 2 Preliminaries

In this section, we introduce some lemmas which are useful in the presentations and proofs of our main results.

**Lemma 2.1** ([6, 14]) *Let  $v$  be a vertex of a tree  $T$  with at least two vertices. Let  $T_{k,l}$  ( $k \geq l \geq 1$ ) be the tree obtained from  $T$  by attaching two new paths  $P : vv_1v_2 \cdots v_k$  and  $Q : vu_1u_2 \cdots u_l$  of length  $k$  and  $l$ , respectively, at vertex  $v$ . Let  $T_{k+1,l-1} = T_{k,l} - u_{l-1}u_l + v_ku_l$ . Then  $\mu(T_{k+1,l-1}) < \mu(T_{k,l})$ .*

**Lemma 2.2** ([14]) *Suppose that  $uv$  is an edge on an internal path of tree  $T$ . Let  $T_{uv}$  be the tree obtained from  $T$  by the subdivision of the edge  $uv$  (i.e., by deleting the edge  $uv$ , adding a new vertex  $w$  and two new edges  $uw$  and  $wv$ .) Then  $\mu(T_{uv}) < \mu(T)$ .*

**Lemma 2.3** ([6]) *Let  $u, v$  be two distinct vertices of a tree  $T$ . Suppose  $v_1, v_2, \dots, v_s$  ( $1 \leq s \leq d_v$ ) are some vertices of  $N_T(v) \setminus N_T(u)$  and  $X = (x_1, x_2, \dots, x_n)^T$  is a unit eigenvector of tree  $T$ , where  $x_i$  corresponds to the vertex  $v_i$  ( $1 \leq i \leq n$ ). Let  $T^*$  be the tree obtained from  $T$  by deleting the edge  $vv_i$  and adding the edges  $uv_i$  ( $1 \leq i \leq s$ ). If  $|x_u| \geq |x_v|$ , then  $\mu(T) < \mu(T^*)$ .*

**Lemma 2.4** ([11]) *Let  $v$  be a vertex of a graph  $G$ , let  $\mathcal{C}(v)$  be the collection of circuits containing  $v$ , and let  $V(Z)$  denote the set of vertices in the circuit  $Z$ . Then the characteristic polynomial  $\Phi(G)$  satisfies*

$$\Phi(G) = x\Phi(G-v) - \sum_{w \in N_G(v)} \Phi(G-v-w) - 2 \sum_{Z \in \mathcal{C}(v)} \Phi(G-V(Z)).$$

**Lemma 2.5** ([11]) *Let  $e = vw$  be an edge of  $G$ , and let  $\mathcal{C}(e)$  be the set of all circuits containing  $e$ . Then the characteristic polynomial  $\Phi(G)$  satisfies*

$$\Phi(G) = \Phi(G-e) - \Phi(G-v-w) - 2 \sum_{Z \in \mathcal{C}(e)} \Phi(G-V(Z)).$$

Next, we denote  $\Phi(P_n)$  by  $P_n$  for short. By Lemma 2.4, the following result can be easily obtained.

**Corollary 2.6** *Let  $P_0 = 1$ , then we have*

- (i)  $P_{n+1} = xP_n - P_{n-1}$  ( $n \geq 1$ );
- (ii) For  $1 \leq s \leq t$ , then  $P_s P_t - P_{s-1} P_{t+1} = P_{t-s}$ .

**Lemma 2.7** ([9]) *Let  $G$  and  $H$  be two simple connected graphs. If  $\Phi(H) > \Phi(G)$  for  $x \geq \rho(G)$ , then  $\rho(G) > \rho(H)$ .*

**Lemma 2.8** ([7]) Let  $G$  be a connected bipartite graph, and  $G_1$  be a proper subgraph of graph  $G$ , then  $\mu(G_1) < \mu(G)$ .

**Lemma 2.9** ([12]) Let  $G$  be a connected graph, then  $\mu(G) \leq 2 + \rho(L_G)$ . The equality holds if and only if  $G$  is bipartite.

**Lemma 2.10** Let  $G$  be a connected graph,  $\Delta$  be its maximum degree,  $d_i$  be the degree of vertex  $v_i$ . Then

(i) ([8])  $\mu(G) \geq \Delta + 1$ , the equality holds if and only if  $\Delta = n - 1$ .

(ii) ([1])  $\mu(G) \leq \max\{d_i + d_j | v_i v_j \in E(G)\}$ , the equality holds if and only if  $G$  is either a regular bipartite graph or a semiregular bipartite graph.

### 3 Tree with minimal Laplacian spectral radius

For  $T \in \mathcal{T}_{n,n-4}$ ,  $T$  must be obtained from  $P_{n-3} : v_0 \cdots v_i \cdots v_j \cdots v_k \cdots v_{n-4}$  by attaching other three vertices to  $v_i, v_j$  and  $v_k$  as the following seven forms, where  $1 \leq i, j, k \leq n - 5$ . Let  $\mathcal{T}_i$  denote the set of each kind of trees, clearly,  $\mathcal{T}_{n,n-4} = \bigcup_{i=1}^7 \mathcal{T}_i$  (See Fig.1).

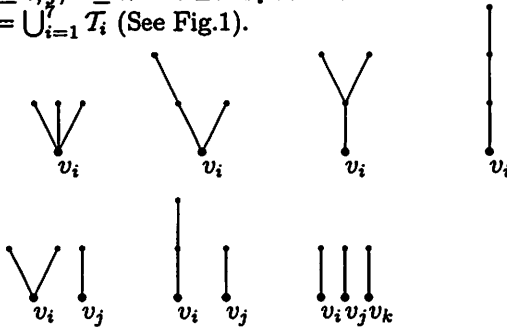


Fig.1. Seven kinds of trees in  $\mathcal{T}_{n,n-4}$ .

Let  $T_i^*$  be a tree in  $\mathcal{T}_i$ , where  $1 \leq i \leq 7$  (see Fig.2).

**Lemma 3.1** For any  $T \in \mathcal{T}_i$ , we have  $\mu(T) \geq \mu(T_i^*)$ , with the equality if and only if  $T \cong T_i^*$ , where  $1 \leq i \leq 6$ .

**Proof.** According to Lemma 2.1, for  $1 \leq i \leq 4$ , we have  $\mu(T) \geq \mu(T_i^*)$ , with the equality if and only if  $T \cong T_i^*$ .

By Lemmas 2.2 and 2.8, for  $5 \leq i \leq 6$ , we have  $\mu(T) \geq \mu(T_i^*)$ , with the equality if and only if  $T \cong T_i^*$ .  $\square$

**Lemma 3.2** For any  $T \in \mathcal{T}_7$ , we have  $\mu(T) \geq \mu(T_7^*)$ , with the equality if and only if  $T \cong T_7^*$ .

**Proof.** For any  $T \in \mathcal{T}_7$ , by Lemmas 2.2 and 2.8, we have  $\mu(T) \geq \mu(P_{1,1,1,n-3}^{1,j,n-5})$ , where  $2 \leq j \leq n-6$ .

Next we consider tree  $P_{1,1,1,n-3}^{1,j,n-5}$ , it suffices to prove that  $\mu(P_{1,1,1,n-3}^{1,j,n-5}) \geq \mu(T_7^*)$ . Note that line graph  $L_{P_{1,1,1,n-3}^{1,j,n-5}} \cong G_{l_1, l_2}$  (see Fig.3), by Lemma 2.9, we consider its line graph  $G_{l_1, l_2}$ . Without loss of generality, suppose that  $l_2 \geq l_1$ . Let  $G_{l_1, l_2}$  be the graph which has the minimal spectral radius. We can claim that  $l_2 \leq l_1 + 1$ , that is to say,  $T_7^*$  has the minimal Laplacian spectral radius in  $\mathcal{T}_7$ .

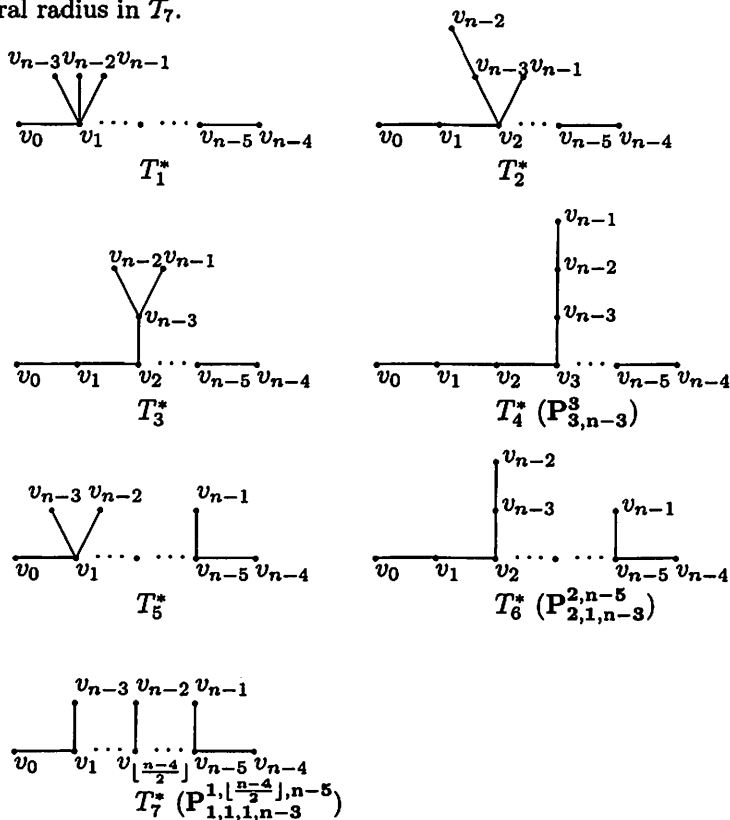


Fig.2. Trees  $T_1^*, T_2^*, \dots, T_7^*$ .

In the following, we prove by contradiction. Suppose  $l_2 \geq l_1 + 2$ . Note that  $G_{l_1, l_2}$  is the graph which has the minimal spectral radius, it suffices to prove that  $\rho(G_{l_1, l_2}) > \rho(G_{l_1+1, l_2-1})$ .

According to Lemma 2.5, we have

$$\begin{aligned} \Phi(G_{l_1, l_2}) &= \Phi(G_{l_1, l_2} - uv) - \Phi(G_{l_1, l_2} - u - v) - 2\Phi(G_{l_1, l_2} - u - v - w) \\ &= \Phi(G_{l_1, l_2} - uv) - (x + 2)\Phi(G_{l_1})\Phi(G_{l_2}), \end{aligned}$$

$$\begin{aligned}
\Phi(G_{l_1+1, l_2-1}) &= \Phi(G_{l_1+1, l_2-1} - uv) - \Phi(G_{l_1+1, l_2-1} - u - v) \\
&\quad - 2\Phi(G_{l_1+1, l_2-1} - u - v - w) \\
&= \Phi(G_{l_1+1, l_2-1} - uv) - (x+2)\Phi(G_{l_1+1})\Phi(G_{l_2-1}).
\end{aligned}$$

Note that

$$\begin{aligned}
\Phi(G_l) &= \Phi(G_l - v_1 v_{l+1}) - \Phi(G_l - v_1 - v_{l+1}) \\
&\quad - 2\Phi(G_l - v_1 - v_{l+1} - v_{l+2}) \\
&= P_{l+2} - (x+2)P_{l-1},
\end{aligned}$$

hence

$$\begin{aligned}
&\Phi(G_{l_1, l_2}) - \Phi(G_{l_1+1, l_2-1}) \\
&= (x+2)(\Phi(G_{l_1+1})\Phi(G_{l_2-1}) - \Phi(G_{l_1})\Phi(G_{l_2})) \\
&= (x+2) \cdot (*),
\end{aligned}$$

where

$$\begin{aligned}
(*) &= P_{l_1+3}P_{l_2+1} - (x+2)P_{l_1+3}P_{l_2-2} \\
&\quad - (x+2)P_{l_1}P_{l_2+1} + (x+2)^2P_{l_1}P_{l_2-2} \\
&\quad - P_{l_1+2}P_{l_2+2} + (x+2)P_{l_1+2}P_{l_2-1} \\
&\quad + (x+2)P_{l_1-1}P_{l_2+2} - (x+2)^2P_{l_1-1}P_{l_2-1}.
\end{aligned}$$

Let  $k = l_2 - l_1$ , clearly  $k \geq 2$ .

For  $k \geq 5$ , by Corollary 2.6, we have

$$\begin{aligned}
(*) &= P_{k-2} - (x+2)P_{k-5} - (x+2)P_{k+1} + (x+2)^2P_{k-2} \\
&= (x^2 + 4x + 5)P_{k-2} - (x+2)P_{k-5} - (x+2)P_{k+1} \\
&= -(x-1)(x+1)^3(x^2-5)P_{k-4} + x(x+1)^2(x^2-5)P_{k-5} \\
&= (x+1)^2(x^2-5)(xP_{k-5} - (x^2-1)P_{k-4}) \\
&= (x+1)^2(x^2-5)(-x(P_{k-4} - P_{k-5}) + P_{k-4}) \\
&= -(x+1)^2(x^2-5)P_{k-2}.
\end{aligned}$$

$$\Phi(G_{l_1, l_2}) - \Phi(G_{l_1+1, l_2-1}) = -(x+2)(x+1)^2(x^2-5)P_{k-2}.$$

For  $k = 4$ , let  $l_1 = l$ ,  $l_2 = l + 4$ , then

$$\begin{aligned}
(*) &= P_2 - (x+2)P_5 + (x+2)^2P_2 - (x+2)(P_{l+3}P_{l+2} - P_{l+2}P_{l+3}) \\
&= -(x-1)(x^2-5)(x+1)^3,
\end{aligned}$$

$$\Phi(G_{l_1, l_2}) - \Phi(G_{l_1+1, l_2-1}) = -(x+2)(x-1)(x^2-5)(x+1)^3.$$

Similarly, for  $k = 3$  and  $k = 2$ , we have

$$\Phi(G_{l_1, l_2}) - \Phi(G_{l_1+1, l_2-1}) = -(x+2)(x-1)(x^2-5)(x+1)^2.$$

$$\Phi(G_{l_1, l_2}) - \Phi(G_{l_1+1, l_2-1}) = -(x+2)(x^2-5)(x+1)^2.$$

Note that  $\triangleleft$  is a proper subgraph of  $G_{l_1, l_2}$  for any  $l_1 \geq 0$ . And by Lemma 2.4, we can get that  $\Phi(\triangleleft) = x(x^2+x-1)(x^2-x-3)$ , then  $\rho(\triangleleft) = \frac{1+\sqrt{13}}{2} > \sqrt{5}$ . So  $\rho(G_{l_1, l_2}) > \rho(\triangleleft) > \sqrt{5}$ . Then for any  $x \geq \rho(G_{l_1, l_2}) > \sqrt{5}$ , we have  $\Phi(G_{l_1, l_2}) - \Phi(G_{l_1+1, l_2-1}) < 0$ . By Lemma 2.7,  $\rho(G_{l_1, l_2}) > \rho(G_{l_1+1, l_2-1})$ . This completes the proof of Lemma 3.2.  $\square$

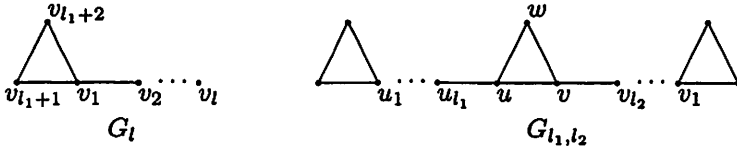


Fig.3.  $G_l$  and  $G_{l_1, l_2}$ .

**Theorem 3.3** For  $T \in T_{n, n-4}$  ( $n \geq 11$ ), then  $\mu(T) \geq \min\{\mu(T_7^*), \mu(T_6^*)\}$ , with the equality if and only if  $T \cong T_7^*$  or  $T \cong T_6^*$ .

**Proof.** By Lemmas 3.1 and 3.2, it is known that for any  $T \in T_{n, n-4}$ ,  $\mu(T) \geq \min\{\mu(T_i^*) | 1 \leq i \leq 7\}$ . By Lemma 2.3,  $\mu(T_1^*) > \mu(T_5^*)$ . For  $n \geq 9$ , by Lemma 2.10,  $\mu(T_6^*) \leq \max\{d_i + d_j | v_i v_j \in E(G)\} = 5$  and  $\mu(T_5^*) > \Delta + 1 = 5$ , then  $\mu(T_5^*) > \mu(T_6^*)$ .

Consider the tree  $T_3^*$ , let  $X = (x_0, x_1, \dots, x_{n-1})^T$  be a unit eigenvector of  $T_3^*$ , where  $x_{v_2}$  and  $x_{v_{n-3}}$  correspond to  $v_2$  and  $v_{n-3}$ , respectively. If  $|x_{v_2}| \geq |x_{v_{n-3}}|$ , note that  $T_2^* = T_3^* - v_{n-3}v_{n-1} + v_2v_{n-1}$  and Lemma 2.3, then  $\mu(T_2^*) > \mu(T_3^*)$ . Otherwise  $|x_{v_2}| < |x_{v_{n-3}}|$ . Let  $T_0 = T_3^* - v_1v_2 + v_1v_{n-3}$ , then by Lemma 2.3,  $\mu(T_0) > \mu(T_3^*)$ . Consider the vertex  $v_{n-3}$ , according to Lemma 2.1,  $\mu(T_2^*) > \mu(T_0)$ . Hence,  $\mu(T_2^*) > \mu(T_3^*)$ . In tree  $T_3^*$ , we can view path:  $v_{n-2}v_{n-3}v_2 \dots v_{n-5}v_{n-4}$  as the diameter path, then by Lemmas 2.2 and 2.8, we can easily obtain that  $\mu(T_3^*) > \mu(T_6^*)$ .

For trees  $T_4^*$  and  $T_6^*$ , when  $n = 10$ , using Matlab to compute their Laplacian characteristic polynomial, we have  $\mu(P_{3,7}^3) = \mu(P_{2,1,7}^{2,5})$ . For  $n \geq 11$ , by Lemmas 2.2 and 2.8,  $\mu(T_4^*) \geq \mu(P_{3,7}^3) = \mu(P_{2,1,7}^{2,5}) > \mu(T_6^*)$ .

Hence for any  $n \geq 11$ , we have  $\mu(T) \geq \min\{\mu(T_7^*), \mu(T_6^*)\}$ , with the equality if and only if  $T \cong T_7^*$  or  $T \cong T_6^*$ .  $\square$

**Theorem 3.4** For  $n \geq 13$ , tree  $T_7^*(P_{1,1, \lfloor \frac{n-4}{3} \rfloor, n-5}^{1, \lfloor \frac{n-4}{3} \rfloor, n-5})$  has the minimal Laplacian spectral radius in  $T_{n, n-4}$ .

**Proof.** By Theorem 3.3, it suffices to prove that for  $n \geq 13$ ,  $\mu(T_6^*) > \mu(T_7^*)$ . Using Matlab, we have  $\mu(P_{1,1,1,1,10}^{1,4,8}) \approx 4.4397$  and  $\mu(P_{2,11}^2) \approx 4.4463$ . Note that  $P_{2,11}^2$  is a subgraph of  $P_{2,n-2}^2$  for  $n \geq 13$ , by Lemma 2.8, we have  $\mu(P_{2,n-2}^2) \geq \mu(P_{2,11}^2)$ . By Lemma 2.2,  $\mu(P_{1,1,1,1,10}^{1,4,8}) \geq \mu(P_{1,1,1,n-3}^{1, \lfloor \frac{n-4}{2} \rfloor, n-5})$ . According to Lemma 2.1,  $\mu(T_6^*) = \mu(P_{2,1,n-3}^{2,n-5}) > \mu(P_{2,n-2}^2)$ , then  $\mu(T_6^*) > \mu(P_{2,n-2}^2) \geq \mu(P_{2,11}^2) > \mu(P_{1,1,1,1,10}^{1,4,8}) \geq \mu(P_{1,1,1,n-3}^{1, \lfloor \frac{n-4}{2} \rfloor, n-5}) = \mu(T_7^*)$ .  $\square$

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