Journal of Mathematical Chemistry, Vol. 41, No. 2, February 2007 (© 2006)
DOI: 10.1007/s10910-006-9066-0

Maximum Randić index on trees with k-pendant vertices

Lian-Zhu Zhang*
School of Mathematical Science, Xiamen University, Xiamen, Fujian 361005, China
E-mail: lz_zhang@126.com

Mei Lu
Department of Mathematical Sciences, Tsinghua University, Beijing 100084, China

Feng Tian
Institute of Systems Science, Academy of Mathematics and Systems Sciences, Chinese Academy of Sciences, Beijing 100080, China

Received 18 November 2005; revised 10 December 2005

The Randić index of an organic molecule whose molecular graph is G is the sum of the weights $(d(u)d(v))^{-1/2}$ of all edges uv of G, where $d(u)$ and $d(v)$ are the degrees of the vertices u and v in G. Let T be a tree with n vertices and k pendant vertices. In this paper, we give a sharp upper bound on Randić index of T.

KEY WORDS: Randić index, tree, pendant vertex

1. Introduction and notations

Mathematical descriptors of molecular structure, such as various topological indices, have been widely used in structure-property-activity studies (see [5, 6, 12]). Among the numerous topological indices considered in chemical graph theory, only a few have been found noteworthy in practical application (see [10]). One of these is the connectivity index or Randić index. The Randić index of an organic molecule whose molecular graph is G is defined (see [2,11]) as

$$R(G) = \sum_{u,v} (d(u)d(v))^{-1/2},$$

where $d(u)$ denotes the degree of the vertex u of the molecular graph G, the summation goes over all pairs of adjacent vertices of G. In Randić's study of alkanes: he showed that if alkanes are ordered so that their $R(G)$-value decrease then the extent of their branching should increase. (More details on the concept

*Corresponding author.

of branching and on ordering of alkanes with respect to other topological indices can be found in a recent study by Balaban et al. in [1]). In this paper, we are interested in the Randić index for trees. First we introduce some graph notations used in this paper and provide a survey of some known results.

We only consider trees here. For a vertex x of a tree T, we denote the neighborhood and the degree of x by $N_T(x)$ and $d_T(x)$, respectively. The maximum degree of T is denoted by $\Delta(T)$. We will use $T - xy$ to denote the graph that arises from T by deleting the edge $xy \in E(T)$. Let $P_s = v_0v_1 \cdots v_s$ be a path of T with $d(v_1) = \cdots = d(v_{s-1}) = 2$ (unless $s = 1$). If $d(v_0) = 1$ and $d(v_s) \geqslant 3$, then we call P_s a *pendant chain* of T and we also call that s the length of the pendant chain P_s.

Let T be a tree of order n. In [13], Yu gave a sharp upper bound of $R(T) \leqslant \dfrac{n + 2\sqrt{2} - 3}{2}$.

In [9,14], trees with small and large Randić index are considered. In [7], Liu et al. gave the sharp lower bound on Randić index of trees with n vertices and k pendant vertices, $3 \leqslant k \leqslant n - 2$. Other results about Randić index on Trees can be found in [3,4,8]. Here, we consider a tree T that has n vertices and k pendant vertices, and give sharp upper bound of $R(T)$.

Note that if $k = 2$, then T is a path, and hence $R(T) = \dfrac{n + 2\sqrt{2} - 3}{2}$. On the other hand, if $k = n - 1$, then T is a star, and hence $R(T) = \sqrt{(n-1)}$. Therefore in the following result, we always assume that $3 \leqslant k \leqslant n - 2$, and then $n \geqslant 5$.

Let $\mathcal{T}_{n,k} = \{T : T$ is a tree with n vertices and k pendant vertices, $3 \leqslant k \leqslant n - 2\}$. Denote

$$V_i(G) = \{v : v \in V(G), d_G(v) = i\}, n_i(G) = |V_i(G)|,$$

$E_2(G) = \{e : e = uv \in E(G), d(u) = d(v) = 2\}$ and $\mathcal{P}(T) = \{P : P$ is a pendant chain of the tree $T\}$.

We call T a $(k, 3)$-regular tree if T is a tree with k-pendent vertices and for any vertex v in $V(T)\backslash V_1(T)$, $d_T(v) = 3$ (see figure 1). It is easy to see that $|V(T)| = 2k - 2$.

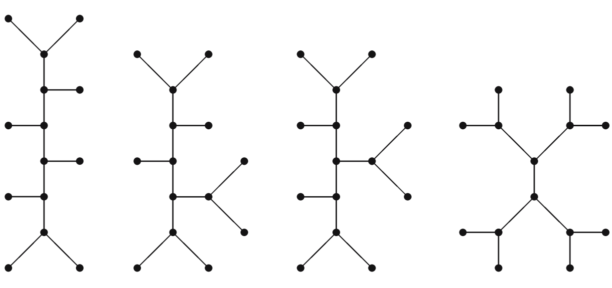


Figure 1. (8, 3)-regular trees.

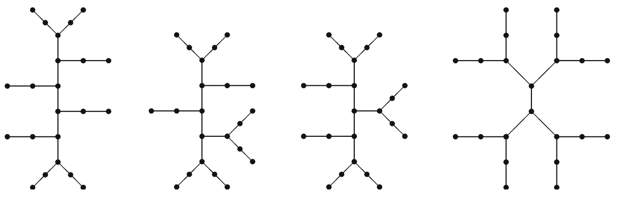


Figure 2. Trees in $\mathcal{T}^*_{22,8}$.

Let $\mathcal{T}^*_{n,k} = \{T : T$ is obtained from a $(k, 3)$-regular tree by adding at least one new vertex on each pendant edge, and total number of new vertices is $n - 2k + 2\}$ (see figure 2).

2. Definitions

Now we define three kinds of operations of $T \in \mathcal{T}_{n,k}$.

(i) If $e = uv$ is an edge of T and T' is obtained from T by contracting uv, i.e., identifying vertices u and v in $T - uv$, we say that T' is obtained from T by operation I and denote T'=T_{uv}. Clearly, $|V(T_{uv})| = |V(T)| - 1$, and $|E(T_{uv})| = |E(T)| - 1$.

(ii) Let $N_T(v) = V' \cup V''$ such that $V' \cap V'' = \emptyset$, $|V'| = s_1 \geqslant 1$ and $|V''| = s_2 \geqslant 1$, where $v \in V(T)$. If T' is obtained from T by using tow new vertices v' and v'' instead of the vertex v, connecting v' and v'', and connecting v' to each vertex in V' and v'' to each vertex in V'', we say that T' is obtained from T by operation II and denote $T' = T_{v\to(s_1,s_2)}$. Thus $|V(T_{v\to(s_1,s_2)})| = |V(T)| + 1$, and $|E(T_{v\to(s_1,s_2)})| = |E(T)| + 1$.

(iii) If $v \in V(T)$ with $d(v) = s > 3$ and T'' is obtained form T by a $(s, 3)$-regular tree T' instead of the vertex v such that each vertex in $N_T(v)$ and each pendant of T' is identified one by one, we say that T'' is obtained from T by operation III and denote $T'' = T_{v\to(3-\text{reg})}$. Thus $|V(T_{v\to(3-\text{reg})})| = |V(T)| + s - 3$, and $|E(T_{v\to(3-\text{reg})})| = |E(T)| + s - 3$.

Let T be a Tree. Then $T_{uv}, T_{v\to(3-\text{reg})}, T_{v\to(2,4)}$ are illustrated in figure 3.

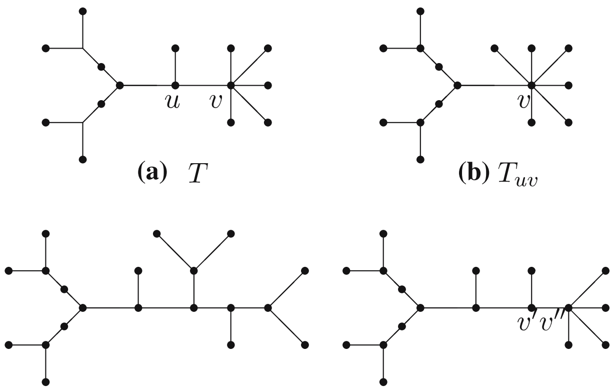
3. Useful formulas

In this section, we will give some useful formulas. Let $T \in \mathcal{T}_{n,k}$. Then

$$k = n_3(T) + 2n_4(T) + \cdots + (\Delta - 2)n_\Delta(T) + 2. \tag{1}$$

If T is a tree and $e = uv \in E_2(T)$, then

$$R(T) - R(T_{uv}) = \tfrac{1}{2}. \tag{2}$$



(a) T (b) T_{uv}

(c) $T_{v\to(3-reg)}$ (d) $T_{v\to(2,4)}$

Figure 3. Three kinds of operations.

Denote $R_T(v)=\sum_{w\in N_T(v)}\frac{1}{\sqrt{d_T(w)}}$. If $v\in V(T)$ with $d(v)=s>3$, then

$$R(T)-R(T_{v\to(s_1,s_2)})=-\frac{1}{\sqrt{(s_1+1)(s_2+1)}}+\left(\frac{1}{\sqrt{d_T(v)}}-\frac{1}{\sqrt{s_1+1}}\right)R_{T_{v\to(s_1,s_2)}}(v') \\ +\left(\frac{1}{\sqrt{d_T(v)}}-\frac{1}{\sqrt{s_2+1}}\right)R_{T_{v\to(s_1,s_2)}}(v''). \quad (3)$$

Particularly, if $s_1=s_2$, then

$$R(T)-R(T_{v\to(s_1,s_1)})=-\frac{1}{s_1+1}+\left(\frac{1}{\sqrt{d_T(v)}}-\frac{1}{\sqrt{s_1+1}}\right)R_T(v). \quad (4)$$

If $v\in V(T)$ with $d(v)=s>3$, then

$$R(T)-R(T_{v\to(3-\mathrm{reg})})=-\frac{s-3}{3}+\left(\frac{1}{\sqrt{d_T(v)}}-\frac{1}{\sqrt{3}}\right)R_T(v). \quad (5)$$

4. Lemmas

We will give some lemmas in this section which will be used in the proofs of our main results.

Lemma 1. Suppose $T\in\mathcal{T}_{n,k}$, $v\in V(T)$ with $d(v)=2$ and the degrees of the vertices adjacent to v are at least 2. Then there is a tree $\overline{T}\in\mathcal{T}_{n,k}$ such that $R(T)\leqslant R(\overline{T})$.

Proof. Suppose $N_T(v)=\{u,w\}$, where $v\in V(T)$ with $d_T(v)=2$ and $d_T(u)\geqslant 2$, $d_T(w)\geqslant 2$. Let x be a pendant vertex of T and y its neighbor. Let $\overline{T}$ be obtained from T_{uv} by adding an edge to the vertex x. Then $\overline{T} \in \mathcal{T}_{n,k}$. Note that $d_T(u), d_T(w), d_T(y) \geqslant 2$, we have

$$\begin{aligned} R(T) - R(\overline{T}) &= \frac{1}{\sqrt{2d_T(u)}} + \frac{1}{\sqrt{2d_T(w)}} + \frac{1}{\sqrt{d_T(y)}} \\ &\quad - \frac{1}{\sqrt{d_T(u)d_T(w)}} - \frac{1}{\sqrt{2d_T(y)}} - \frac{1}{\sqrt{2}} \\ &= \left(\frac{1}{\sqrt{d_T(u)}} - \frac{1}{\sqrt{2}}\right)\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{d_T(w)}}\right) \\ &\quad + \left(\frac{1}{\sqrt{2}} - 1\right)\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{d_T(y)}}\right) \\ &\leqslant 0. \end{aligned}$$

Therefore $R(T) \leqslant R(\overline{T})$. □

Lemma 2. Suppose $T \in \mathcal{T}_{n,k}$. If $n \geqslant 3k - 2$ and $E_2(T) \subseteq E(\mathcal{P}(T))$, then

$$|E_2(T)| \geqslant n_4(T) + 2n_5(T) + \cdots + (\Delta - 3)n_\Delta(T). \tag{6}$$

Proof. Note that $|E(T) - E(\mathcal{P}(T))| = (n_3 + n_4 + \cdots + n_\Delta - 1)$. By $E_2(T) \subseteq E(\mathcal{P}(T))$, each pendant chain has at most two edge which are not in $E_2(T)$. So,

$$|E_2(T)| \geqslant (n(T) - 1) - 2n_1(T) - (n_3(T) + n_4(T) + \cdots + n_\Delta(T) - 1).$$

By formula (1) and noting $3n_1 - 2 = 3k - 2 \leqslant n = n_1 + \cdots + n_\Delta$, (6) holds. □

Lemma 3. Suppose $T \in \mathcal{T}_{n,k}$, $v \in V(T)$ with $d_T(v) = s > 3$, $N_T(v) = \{u_1, u_2, \ldots, u_s\}$ and $d_T(u_1) \leqslant d_T(u_2) \leqslant \cdots \leqslant d_T(u_s)$. If $|E_2(T)| \geqslant s - 3$, then there is a tree $\overline{T} \in \mathcal{T}_{n,k}$ such that the following statements are hold.

(i) If $d_T(u_{s-1}) \leqslant 3$ and $d_T(v) \geqslant 6$, then $R(T) < R(\overline{T})$.

(ii) If $d_T(u_{s-1}) \leqslant 4$ and $d_T(v) \geqslant 10$, then $R(T) < R(\overline{T})$.

(iii) If $d_T(u_{s-1}) \leqslant 5$ and $d_T(v) \geqslant 16$, then $R(T) < R(\overline{T})$.

Proof. Let T' be obtained from T by contracting $s - 3$ edges in $E_2(T)$ and $\overline{T} = T'_{v \to (3-\text{reg})}$. Then $\overline{T} \in \mathcal{T}_{n,k}$. Denote $d_T(u_{s-1}) = r$. By formulas (2) and (5), we have

$$\begin{aligned} R(T) - R(\overline{T}) &= \frac{s-3}{6} + \left(\frac{1}{\sqrt{s}} - \frac{1}{\sqrt{3}}\right) R_T(v) \\ &< \frac{s-3}{6} + \left(\frac{1}{\sqrt{s}} - \frac{1}{\sqrt{3}}\right) \frac{s-1}{\sqrt{r}}. \end{aligned}$$

Let

$$f(r,s) = \frac{s-3}{6} + \left(\frac{1}{\sqrt{s}} - \frac{1}{\sqrt{3}}\right)\frac{s-1}{\sqrt{r}}.$$

We consider some partial derivatives. Since

$$\frac{\partial f(r,s)}{\partial r} = -\left(\frac{1}{\sqrt{s}} - \frac{1}{\sqrt{3}}\right)\frac{s-1}{2r\sqrt{r}} > 0,$$

we have $f(r,s)$ is monotonously increasing in r. On the other hand,

$$\frac{\partial f(r,s)}{\partial s} = \frac{1}{6} - \frac{1}{\sqrt{3r}} + \frac{1}{2\sqrt{r}}\left(\frac{1}{\sqrt{s^3}} + \frac{1}{\sqrt{s}}\right)$$

and

$$\frac{\partial^2 f(r,s)}{\partial s^2} = -\frac{1}{4\sqrt{r}}\left(\frac{3}{\sqrt{s^5}} + \frac{1}{\sqrt{s^3}}\right) < 0.$$

Thus $\dfrac{\partial f(r,s)}{\partial s}$ is monotonously decreasing in s.

(i) Since $f(r,s)$ is monotonously increasing in r and $r \leqslant 3$, we have that

$$R(T) - R(\overline{T}) < f(3,s).$$

By $\dfrac{\partial f(r,s)}{\partial s}$ being monotonously decreasing in s, $s \geqslant 7$, and $\dfrac{\partial f(3,s)}{\partial s}|_{s=7} < 0$, we have

$$R(T) - R(\overline{T}) < f(3,s) < f(3,7) < 0.$$

Now, we consider the case $r \leqslant 3$ and $s = 6$. Let T'' be obtained from T by contracting an edge in E_2 and $\overline{T} = T''_{v\to(3,3)}$. Then $\overline{T} \in \mathcal{T}_{n,k}$. By formula (2) and (4),

$$\begin{aligned} R(T) - R(\overline{T}) &= \frac{1}{2} - \frac{1}{4} + \left(\frac{1}{\sqrt{6}} - \frac{1}{\sqrt{4}}\right) R_T(v) \\ &< \frac{1}{4} + \left(\frac{1}{\sqrt{6}} - \frac{1}{2}\right)\frac{5}{\sqrt{3}} \\ &< 0. \end{aligned}$$

Thus, (i) holds.

(ii) Since $f(r,s)$ is monotonously increasing in r and $r \leqslant 4$, we have that

$$R(T) - R(\overline{T}) < f(4,s).$$

By $\frac{\partial f(r,s)}{\partial s}$ being monotonously decreasing in s, $s \geqslant 10$, and $\frac{\partial f(4,s)}{\partial s}|_{s=10} < 0$, we have

$$R(T) - R(\overline{T}) < f(4,s) < f(4,10) < 0.$$

Thus (ii) holds.

(iii) By the same argument as (ii), we easily have (iii) holds. □

Lemma 4. Suppose $T \in \mathcal{T}_{n,k}$, $v \in V(T)$ with $d_T(v) = s > 3$, $N(v) = \{u_1, u_2, \ldots, u_s\}$ and $d_T(u_1) \leqslant d_T(u_2) \leqslant \cdots \leqslant d_T(u_s)$. If $d_T(u_{s-1}) \leqslant 3$ and $|E_2(T)| \geqslant s-3$, then there is a tree $\overline{T} \in \mathcal{T}_{n,k}$ such that the following statements are hold.

(i) If $s = 4$ and $d_T(u_4) \leqslant 5$ then $R(T) < R(\overline{T})$.

(ii) If $s = 5$ and $d_T(u_5) \leqslant 15$ then $R(T) < R(\overline{T})$.

Proof. Let the tree T' be obtained from T by contracting $s-3$ edges in E_2 and $\overline{T} = T'_{v\to(3-\mathrm{reg})}$. Then $\overline{T} \in \mathcal{T}_{n,k}$. By formula (4), we have

$$\begin{aligned} R(T) - R(\overline{T}) &= \frac{s-3}{6} + \left(\frac{1}{\sqrt{s}} - \frac{1}{\sqrt{3}}\right) R_T(v) \\ &\leqslant \frac{s-3}{6} + \left(\frac{1}{\sqrt{s}} - \frac{1}{\sqrt{3}}\right)\left(\frac{s-1}{\sqrt{3}} + \frac{1}{\sqrt{d_T(u_s)}}\right) \\ &< 0. \end{aligned}$$

The last inequality holds when $s = 4, d_T(u_4) \leqslant 5$ or $s = 5, d_T(u_5) \leqslant 15$.

Therefore the statements (i) and (ii) are proved. □

Lemma 5. Let $T \in \mathcal{T}_{n,k}$ with $E_2(T) \neq \emptyset$, and $e = uv$ a pendant edge with $d_T(u) = r \geqslant 3$ and $d_T(v) = 1$. If $\overline{T} \in \mathcal{T}_{n,k}$ is obtained from T by contracting an edge in $E_2(T)$ and adding an edge to the pendant vertex v, then $R(\overline{T}) > R(T)$.

Proof. Obviously, $uv \notin E_2(T)$. It is not difficult to check that

$$\begin{aligned} R(T) - R(\overline{T}) &= \frac{1}{2} + \frac{1}{\sqrt{r}} - \frac{1}{\sqrt{2}} - \frac{1}{\sqrt{2r}} \\ &= \left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{r}}\right)\left(\frac{1}{\sqrt{2}} - 1\right) \\ &< 0. \end{aligned}$$

The last inequality holds by $d_T(u) \geqslant 3$. Therefore $R(\overline{T}) > R(T)$. □

5. Main results

Denote $R_{\max}(\mathcal{T}_{n,k}) = \max\{R(T) : T \in \mathcal{T}_{n,k}\}$. Then we have the following main result.

Theorem 1. For any $T \in \mathcal{T}_{n,k}$ with $n \geqslant 3k-2$ and $k \geqslant 3$,

$$R(T) \leqslant \frac{n}{2} + \frac{(3\sqrt{2}+\sqrt{6}-7)k}{6}.$$

Moreover, the equality holds if and only if $T \in \mathcal{T}^*_{n,k}$.

Proof. It is easy to see that if $T \in \mathcal{T}^*_{n,k}$, then

$$R(T) = \frac{n}{2} + \frac{(3\sqrt{2}+\sqrt{6}-7)k}{6}.$$

Hence we just need to show that if $T \in \mathcal{T}_{n,k}$ $(n \geqslant 3k-2, k \geqslant 3)$, and $R(T) = R_{\max}(\mathcal{T}_{n,k})$, then $T \in \mathcal{T}^*_{n,k}$.

By contradiction. Suppose $T \in \mathcal{T}_{n,k}$ and $R(T) = R_{\max}(\mathcal{T}_{n,k})$. By the proof of lemma 1, we can assume, without lost of generality, that all vertices of T with degree 2 are on pendant chains. Thus $E_2(T) \subseteq E(\mathcal{P}(T))$. Since $k \geqslant 3$, $\Delta(T) \geqslant 3$.

We first show that $\Delta(T) = 3$. Assume that $\Delta(T) \geqslant 4$. By lemma 2, we have that

$$|E_2(T)| \geqslant n_4(T) + 2n_5(T) + \cdots + (\Delta-3)n_\Delta(T) \geqslant \Delta - 3 \geqslant 1.$$

Let $u_0 \in V(T)$ with $d(u_0) = \Delta \geqslant 4$. Denote

$$\mathcal{Q} = \{P \mid P = u_0 \cdots u_t \text{ with } d(u_t) \geqslant 4\}.$$

Choose $P = u_0u_1\cdots u_t$ in $\mathcal{Q}$ such that the length of P as large as possible. By lemmas 3(i), 4, and $R(T) = R_{\max}(\mathcal{T}_{n,k})$, we have that $t \geqslant 1$.

Denote $\widetilde{N_T}(u_{t-1}) = N_T(u_{t-1}) \backslash \{u_{t-2}\}$ if $t \geqslant 2$, otherwise $\widetilde{N_T}(u_{t-1}) = N_T(u_{t-1})$. Clearly, $u_t \in \widetilde{N_T}(u_{t-1})$.

Claim 1. *For any $x \in \widetilde{N_T}(u_{t-1})$, $d_T(x) \leqslant 4$ and $|\{x \mid x \in \widetilde{N_T}(u_{t-1})$ and $d(x) = 4\}| \geqslant 1$.*

Proof of claim 1. For any $x \in \widetilde{N_T}(u_{t-1})$, denote $N_T(x) = \{v_1, v_2, \ldots, v_s\}$ and $d_T(v_1) \leqslant d_T(v_2) \leqslant \cdots \leqslant d_T(v_s)$. By the choice of P, we have $d_T(v_{s-1}) \leqslant 3$ and $v_s = u_{t-1}$. From lemma 3(i), we obtain $d_T(x) \leqslant 5$. By lemma 3(iii), we obtain $d_T(u_{t-1}) \leqslant 15$. Finally, by lemma 4(ii), $d_T(x) \neq 5$. Therefore $d_T(x) \leqslant 4$. Since $d(u_t) \geqslant 4$ and $u_t \in \widetilde{N_T}(u_{t-1})$, we have $d(u_t) = 4$. Thus $|\{x \mid x \in \widetilde{N_T}(u_{t-1})$ and $d(x) = 4\}| \geqslant 1$.

Claim 2. $d_T(u_{t-1}) = 6$.

Proof of claim 2. By claim 1, for any $x \in \widetilde{N_T}(u_{t-1}), d_T(x) \leqslant 4$. By lemma 3(ii) and $R(T) = R_{\max}(\mathcal{T}_{n,k})$, we have $d(u_{t-1}) \leqslant 9$, and then by lemma 4(i) and claim 1, $d_T(u_{t-1}) \geqslant 6$. Hence $6 \leqslant d_T(u_{t-1}) \leqslant 9$. Denote $d_T(u_{t-1}) = r$ and $N_T(u_{t-1}) = \{w_1, w_2, \ldots, w_r\}$. Let T' be obtained by contracting one edge in $E_2(T)$ and $\overline{T} = T'_{u_{t-1}\to(3,r-3)}$. Then $\overline{T} \in \mathcal{T}_{n,k}$. By formulas (2) and (3),

$$\begin{aligned}
&R(T) - R(\overline{T})\\
&\quad = \frac{1}{2} - \frac{1}{\sqrt{4(r-2)}} + \left(\frac{1}{\sqrt{r}} - \frac{1}{\sqrt{4}}\right)\left(\frac{1}{\sqrt{d_T(w_1)}} + \frac{1}{\sqrt{d_T(w_2)}} + \frac{1}{\sqrt{d_T(w_3)}}\right)\\
&\qquad + \left(\frac{1}{\sqrt{r}} - \frac{1}{\sqrt{r-2}}\right)\left(\frac{1}{\sqrt{d_T(w_4)}} + \frac{1}{\sqrt{d_T(w_5)}} + \cdots + \frac{1}{\sqrt{d_T(w_r)}}\right)\\
&\quad < \frac{1}{2} - \frac{1}{\sqrt{4(r-2)}} + \left(\frac{1}{\sqrt{r}} - \frac{1}{\sqrt{4}}\right)\frac{3}{\sqrt{4}}\\
&\qquad + \left(\frac{1}{\sqrt{r}} - \frac{1}{\sqrt{r-2}}\right)\frac{r-4}{\sqrt{4}}.
\end{aligned}$$

By an elementary calculation, we have

$$R(T) - R(\overline{T}) < \begin{cases} -0.01, & \text{if} \quad r = 7,\\ -0.03, & \text{if} \quad r = 8,\\ -0.05, & \text{if} \quad r = 9.\end{cases}$$

So $R(T) < R(\overline{T})$ when $7 \leqslant d_T(u_{t-1}) \leqslant 9$, a contradiction. Therefore, $d_T(u_{t-1}) = 6$.

Suppose $d_T(w_1) \leqslant \cdots \leqslant d_T(w_6)$. By claim 1 and the choice of P, we have that $d(w_i) \leqslant 4$ $(1 \leqslant i \leqslant 5)$ and for any $y \in N_T(w_i)(1 \leqslant i \leqslant 5), d_T(y) \leqslant 3$. By claim 1, we can assume that $d_T(w_{p+1}) = \cdots = d_T(w_5) = 4$, where $0 \leqslant p \leqslant 4$. Then $d_T(w_1) \leqslant \cdots \leqslant d_T(w_p) \leqslant 3$ if $p \geqslant 1$ and $n_4(T) \geqslant 5 - p$. By lemma 2, we have that $|E_2(T)| \geqslant n_4 + 3n_6 \geqslant 8 - p$.

Let T_1 be obtained from T by contracting an edge in $E_2(T)$ and splitting the vertex u_1 in to (3, 3). Then $T_1 \in \mathcal{T}_{n,k}$ and $|E_2(T_1)| \geqslant 7 - p$. By (2) and (4),

$$\begin{aligned}
R(T) - R(T_1) &= \frac{1}{2} - \frac{1}{4} + \left(\frac{1}{\sqrt{6}} - \frac{1}{\sqrt{4}}\right)R_T(v)\\
&< \frac{1}{4} + \left(\frac{1}{\sqrt{6}} - \frac{1}{2}\right)\left(\frac{p}{\sqrt{3}} + \frac{5-p}{\sqrt{4}}\right).
\end{aligned}$$

Now let $\overline{T}$ be obtained from T_1 by contracting $5 - p$ edges in $E_2(T_1)$ and splitting the vertices $w_{p+1}, \ldots, w_5$ into (2,2), respectively. Then $\overline{T}$ is in $\mathcal{T}_{n,k}$.

Combining (2) and (4), we have that

$$\begin{aligned}
R(T_1) - R(\overline{T}) &= \frac{5-p}{6} + \left(\frac{1}{\sqrt{4}} - \frac{1}{\sqrt{3}}\right)\left(R_{T_1}(w_{p+1}) + R_{T_1}(w_{p+2}) + \cdots + R_{T_1}(w_5)\right) \\
&\leqslant \frac{5-p}{6} + \left(\frac{1}{\sqrt{4}} - \frac{1}{\sqrt{3}}\right)\left(\frac{3(5-p)}{\sqrt{3}} + \frac{5-p}{\sqrt{4}}\right).
\end{aligned}$$

Note that $0 \leqslant p \leqslant 4$, we have that

$$\begin{aligned}
R(T) - R(\overline{T}) &= (R(T) - R(T_1)) + \left(R(T_1) - R(\overline{T})\right) \\
&< \frac{1}{4} + \left(\frac{1}{\sqrt{6}} - \frac{1}{2}\right)\left(\frac{p}{\sqrt{3}} + \frac{5-p}{\sqrt{4}}\right) \\
&\quad + \frac{5-p}{6} + \left(\frac{1}{\sqrt{4}} - \frac{1}{\sqrt{3}}\right)\left(\frac{3(5-p)}{\sqrt{3}} + \frac{5-p}{\sqrt{4}}\right) \\
&= \frac{5\sqrt{6} + 20\sqrt{3} - 47}{12} + \frac{(10 + 2\sqrt{2} - 6\sqrt{3} - \sqrt{6})p}{12} \\
&< -0.009 - 0.0012p \\
&< 0,
\end{aligned}$$

a contradiction. Thus we have $\Delta = 3$.

Now, we will show that $n_2(T) \geqslant k$. By (1), we have $n_3(T) = k - 2$. On the other hand, we have $n_1(T) + 2n_2(T) + 3n_3(T) = 2(n-1)$. Noting that $n_1(t) = k$ and $n \geqslant 3k - 2$, we easily have $n_2(T) \geqslant k$. By lemma 5, we have that the length of each pendant chains of T are at least tow. Thus $T \in \mathcal{T}^*_{n,k}$ and the proof of theorem 1 is complete. □

Acknowledgments

Lian-zhu Zhang partially supported by NSFC(NO.10571105). Mei Lu partially supported by NSFC(NO.10571105). Feng Tian partially supported by NSFC(No. 10431020).

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