Small Randić Index Ordering of Trees with k Pendant Vertices

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Abstract

The Randić index of an organic molecule whose molecular graph is G is the sum of the weights $(d(u)d(v))^{-\frac{1}{2}}$ of all edges uv of G, where $d(u)$ denotes the degree of the vertex u of the molecular graph G. Among all trees with n vertices and k pendant vertices, the extremal trees with the minimum, the second minimum and the third minimum Randić index were characterized by Hansen, Li and Wu et al., respectively. In this paper, we further investigate some small Randić index properties and give other elements of small Randić index ordering of trees with k pendant vertices.

1 Introduction

Mathematical descriptors of molecular structure, such as various topological indices, have been widely used in structure-property-activity studies (see [1, 2, 6]). The connectivity index or Randić index is one of the most useful molecular-graph-based structure-descriptors (see [3]). The Randić index of an organic molecule whose molecular graph is G is defined (see

[4, 5]) as

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

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. The graph invariant $R(G)$ was put forward by the chemist Milan Randić in 1975, aimed to be a measure of the branching of the carbon atom skeleton of organic molecules (see [5]). In Randić's study of alkanes, he noticed that there is a good correlation between $R(G)$ and several physicochemical properties of alkanes: boiling points, parameters in the Antoine equation for vapor pressure, surface areas, etc (see [5]). And he showed that if alkanes are ordered so that their $R(G)$-value decreases then the extent of their branching increases (see [5]). There are many publications to study the trees with extremal Randić index and the bounds in some graph sets (see [7]).

In this paper, we are interested in the small Randić index ordering of trees. First we provide a survey of some known results concerning our results. Let T be a tree of order n. Yu (see [8]) gave a sharp upper bound of

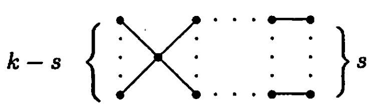
$$R(T) \leq \frac{n + 2\sqrt{2} - 3}{2}.$$

In[9], trees with large general Randić index were considered. For a tree T of order n with k pendant vertices, the sharp upper bound on Randić index in the case $3 \leq k \leq n-2, n \geq 3k-2$ was given by Zhang, Lu and Tian (see [10]). In order to illustrate some more results on the minimal Randić index, we need some notations as follows.

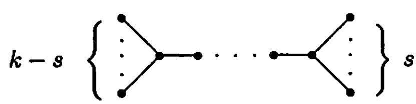
Let $K_{1,k}(p_1, p_2, \cdots, p_s)$, $(s \leq k)$ be a tree created from the star $K_{1,k}$ of $k+1$ vertices by attaching paths of lengths p_1, $p_2, \cdots, p_s$ to s pendant vertices of $K_{1,k}$, respectively(see Fig. 1(a)). And let $K^n_{s,k-s}$ be a tree constructed from a path of length $n-k-1$ by adding s pendant edges and $k-s$ pendant edges to two ends of the path, respectively (see Fig. 1(b)). Writing $\mathcal{F}_k^n$ for a tree set, and every tree in $\mathcal{F}_k^n$ is obtained from a path of length $n-k$ by adding $k-2$ pendant edges to one end of the path and adding a pendant edge to one 2-degree vertex of the path not adjacent to its ends, respectively (see Fig. 1(c)). Denote

$$\mathcal{S}_{s,k-s}^n = \{K_{1,k}(p_1, p_2, \cdots, p_s) : p_i > 0, \ \textstyle\sum_{i=1}^s p_i = n-k-1\},$$
$$\mathcal{S}_{n,k} = \textstyle\bigcup_{s=1}^k \mathcal{S}_{s,k-s}^n,$$
$$\mathcal{U}_{n,k} = \{K_{s,k-s}^n : s = 2, \ldots, \lfloor \tfrac{k}{2} \rfloor\},$$
$$\mathcal{T}_{n,k} = \{T : T \text{ is a tree with } n \text{ vertices and } k \text{ pendant vertices }\}.$$

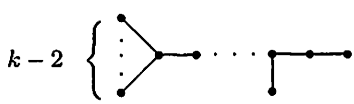
Clearly, $\mathcal{S}_{n,k}, \mathcal{U}_{n,k} \subseteq \mathcal{T}_{n,k}$.



(a) $K_{1,k}(p_1, p_2, \cdots, p_s) \in \mathcal{S}_{s,k-s}^n$



(b) $K_{s,k-s}^n \in \mathcal{U}_{n,k}$



(c) $T \in \mathcal{F}_k^n$

Fig. 1

The trees with the minimum and the second minimum Randić index in $\mathcal{T}_{n,k}$ were given by Hansen et al. (see[11]) and Li et al. (see [7, 12]), respectively. A tree $T \in \mathcal{T}_{n,k}$ has the minimum Randić index if and only if $T \in \mathcal{S}^n_{1,k-1}$ and its Randić index

$$R(T) = \frac{1}{2}(n-k) + \frac{1}{\sqrt{k}}(k + \frac{1}{\sqrt{2}} - 1) + \frac{1}{\sqrt{2}} - 1.$$

And a tree $T \in \mathcal{T}_{n,k}$ has the second minimum Randić index if and only if $T \in \mathcal{S}^n_{2,k-2}$ and its Randić index

$$R(T) = \frac{1}{2}(n-k) + \frac{1}{\sqrt{k}}(k + \sqrt{2} - 2) + \sqrt{2} - \frac{3}{2}.$$

The tree with the third minimum Randić index in $\mathcal{T}_{n,k}$ was determined by Wu and Zhang (see [13]). And a tree $T \in \mathcal{T}_{n,k}$ has the third minimum Randić index if and only if $T \cong K^n_{2,k-2}$ and its Randić index

$$R(T) = \frac{1}{2}(n-k) + \frac{1}{\sqrt{k-1}}(k + \frac{1}{\sqrt{2}} - 2) + \frac{2}{\sqrt{3}} + \frac{1}{\sqrt{6}} - \frac{3}{2}.$$

In this paper, we are interested in the ordering of trees with respect to Randić index. Furthermore, we investigate some small Randić index properties and give other elements of small Randić index ordering of trees with k pendant vertices.

2 Notations and Lemmas

Let $G(V, E)$ be a graph with vertex set V and edge set E. Suppose that $x \in V(G)$, $S \subseteq V(G)$. Writing $N_G(x)$ for the neighborhood of x, denote $N_G(S) = \bigcup_{v \in S} N_G(v)$ and $V_i(G) = \{v : v \in V(G), d(v) = | N_G(v) | = i\}$. The maximum degree of G is denoted by $\Delta(G)$. Let T be a tree. For $x, y \in V(T)$, we use $T - x$ or $T - xy$ to denote a graph which arises from the tree T by deleting the vertex $x \in V(T)$ or the edge $xy \in E(T)$. Similarly, $T + xy$ is a graph that arises from T by adding an edge $xy \notin E(T)$. A vertex $x \in V(T)$ is called a pendant vertex if $x \in V_1(T)$. An edge in $E(T)$ is called a pendant edge if one end of the edge is in $V_1(T)$. Let $P = v_0v_1\cdots v_s$ be a path in T with $d(v_1) = \cdots = d(v_{s-1}) = 2$ (unless $s = 1$). If $d(v_0) = 1$, $d(v_s) \geq 3$ or $d(v_s) = 1$, $d(v_0) \geq 3$, then we call P a *pendant chain* of T; if $d(v_0)$, $d(v_s) \geq 3$, then P is called a *non-pendant chain* of T. Set

$$\mathcal{P}(T) = \{P : P \text{ is a pendant chain of length at least 2 in } T\},$$

$$\widetilde{\mathcal{P}}(T) = \{P : P \text{ is a non-pendant chain in } T\}.$$

We first show the following lemma.

Lemma 1.

(i) Let $F(x,b) = f(x,b) - f(x+1,b)$, where $f(x,b) = \sqrt{x} + \frac{b}{\sqrt{x}}$. If $x > 0$ and $b < 0$, then the function $F(x,b)$ is monotonously increasing in x.

(ii) Let $G(x,c) = \frac{c}{\sqrt{x}} - \frac{1}{\sqrt{x-1}}$. If $x \geq 3$ and $c \geq 3$, then the function $G(x,c)$ is monotonously decreasing in x.

(iii) Let $H(x) = \sqrt{x-1} - \sqrt{x}$. If $x \geq 3$, then the function $H(x)$ is monotonously increasing in x.

Proof. By derivation to functions $F(x,b)$, $G(x,c)$ and $H(x)$ in x, we obtain

$$\begin{aligned} F'_x(x,b) &= \frac{1}{2\sqrt{x}} - \frac{b}{2\sqrt{x^3}} - \frac{1}{2\sqrt{x+1}} + \frac{b}{2\sqrt{(x+1)^3}} \\ &= \frac{1}{2}(\frac{1}{\sqrt{x}} - \frac{1}{\sqrt{x+1}}) - \frac{b}{2}(\frac{1}{\sqrt{x^3}} - \frac{1}{\sqrt{(x+1)^3}}) \\ &> 0 \end{aligned}$$

when $x > 0$ and $b < 0$.

$$\begin{aligned} G'_x(x,c) &= -\frac{c}{2\sqrt{x^3}} + \frac{1}{2\sqrt{(x-1)^3}} \\ &= \frac{1}{2}\left(\frac{1}{\sqrt{(x-1)^3}} - \frac{1}{\sqrt{\frac{x^3}{c^2}}}\right) \\ &< 0 \end{aligned}$$

when $x \geq 3$ and $c \geq 3$.

$$\begin{aligned} H'(x) &= \frac{1}{2\sqrt{x-1}} - \frac{1}{2\sqrt{x}} \\ &= \frac{1}{2}\left(\frac{1}{\sqrt{x-1}} - \frac{1}{\sqrt{x}}\right) \\ &> 0 \end{aligned}$$

when $x \geq 3$.

Therefore the functions $F(x,b) = f(x,b) - f(x+1,b)$, $G(x,c)$ and $H(x)$ are monotonously increasing, monotonously decreasing and monotonously increasing respectively in x. ■

Lemma 2 [13]. For any $T_1, T_2 \in \mathcal{S}_{n,k}$, suppose that $T_1 \in \mathcal{S}^n_{i,k-i}$ and $T_2 \in \mathcal{S}^n_{j,k-j}$, $i \leq j \leq k$.

(i) If $i = j$ then $R(T_1) = R(T_2)$;

(ii) If $i < j$ then $R(T_1) < R(T_2)$.

In order to characterize the trees with the fourth minimum Randić index, we first characterize a extremal property of trees in $\mathcal{T}_{n,k} \setminus (\mathcal{S}^n_{1,k-1} \cup \mathcal{S}^n_{2,k-2} \cup \{K^n_{2,k-2}\})$.

Lemma 3. Let $T \in \mathcal{T}_{n,k} \setminus (\mathcal{S}^n_{1,k-1} \cup \mathcal{S}^n_{2,k-2} \cup \{K^n_{2,k-2}\})$, $4 \leq k \leq n-4$. If $R(T) = min\{R(T) : T \in \mathcal{T}_{n,k} \setminus (\mathcal{S}^n_{1,k-1} \cup \mathcal{S}^n_{2,k-2} \cup \{K^n_{2,k-2}\})\}$, then $\widetilde{\mathcal{P}}(T) \neq \emptyset$.

Proof. By contradiction. Choose a tree $T \in \mathcal{T}_{n,k}$ such that $R(T) = min\{R(T) : T \in \mathcal{T}_{n,k} \setminus (\mathcal{S}^n_{1,k-1} \cup \mathcal{S}^n_{2,k-2} \cup \{K^n_{2,k-2}\})\}$. If $\widetilde{\mathcal{P}}(T) = \emptyset$, then $T \in \mathcal{S}^n_{3,k-3}$ by the choice of T and Lemma 2. And it is easy to obtain that $R(T) = \frac{1}{2}(n-k) + \frac{1}{\sqrt{k}}\left(k + \frac{3}{\sqrt{2}} - 3\right) + \frac{3}{\sqrt{2}} - 2$. Clearly, for any $T_0 \in \mathcal{F}^n_k$, we can get $R(T_0) = \frac{1}{2}(n-k) + \frac{1}{\sqrt{k-1}}\left(k + \frac{1}{\sqrt{2}} - 2\right) + \frac{2}{\sqrt{6}} + \frac{1}{\sqrt{3}} + \frac{1}{\sqrt{2}} - 2$ and $T_0 \in \mathcal{F}^n_k \subset \mathcal{T}_{n,k} \setminus (\mathcal{S}^n_{1,k-1} \cup \mathcal{S}^n_{2,k-2} \cup \{K^n_{2,k-2}\})$. Considering the value

$R(T) - R(T_0)$, we have

$$\begin{aligned} R(T) - R(T_0) &= \left(\sqrt{k} - \sqrt{k-1}\right) + \left(\frac{1}{\sqrt{2}} - 1\right)\left(\frac{3}{\sqrt{k}} - \frac{1}{\sqrt{k-1}}\right) \\ &\quad + \sqrt{2} - \frac{2}{\sqrt{6}} - \frac{1}{\sqrt{3}} \\ &> \left(\frac{1}{\sqrt{2}} - 1\right)\left(\frac{3}{\sqrt{k}} - \frac{1}{\sqrt{k-1}}\right) + \sqrt{2} - \frac{2}{\sqrt{6}} - \frac{1}{\sqrt{3}}. \end{aligned}$$

When $4 \le k \le 829$, by means of mathematical programming, one easily calculates that $R(T) - R(T_0) > 0.0024$.

When $k \ge 830$, by Lemma 1(ii), function $G(k, 3)$ is monotonously decreasing in k. Thus

$$\begin{aligned} R(T) - R(T_0) &> \left(\frac{1}{\sqrt{2}} - 1\right)\left(\frac{3}{\sqrt{k}} - \frac{1}{\sqrt{k-1}}\right) + \sqrt{2} - \frac{2}{\sqrt{6}} - \frac{1}{\sqrt{3}} \\ &\ge \left(\frac{1}{\sqrt{2}} - 1\right) G(830, 3) + \sqrt{2} - \frac{2}{\sqrt{6}} - \frac{1}{\sqrt{3}}. \\ &> 0 \end{aligned}$$

Thus $R(T) > R(T_0)$, a contradiction. Therefore $\widetilde{\mathcal{P}}\ (T) \neq \emptyset$. ∎

Lemma 4 [13]. Let $T \in \mathcal{T}_{n,k}$. If $|\mathcal{P}(T)| = s$ $(s \ge 2)$, then there exists $\overline{T} \in \mathcal{T}_{n,k}$ with $|\mathcal{P}(\overline{T})| = s - 1$ such that $R(\overline{T}) < R(T)$.

3 Trees with Small Randić Index

Clearly, to determine a tree with the fourth minimum Randić index in $\mathcal{T}_{n,k}$ is equivalent to determine a tree with the minimum Randić index in $\mathcal{T}_{n,k} \setminus (\mathcal{S}^n_{1,k-1} \cup \mathcal{S}^n_{2,k-2} \cup \{K^n_{2,k-2}\})$. Note that $\mathcal{T}_{n,2} = \{P_n\}$, $\mathcal{T}_{n,n-1} = \{K_{1,n-1}\}$, $\mathcal{T}_{n,n-2} = \mathcal{U}_{n,n-2}$, and $\mathcal{T}_{n,3} = \mathcal{S}^n_{1,2} \cup \mathcal{S}^n_{2,1} \cup \mathcal{S}^n_{3,0}$. Therefore we just need to show the cases $4 \le k \le n-3$ and $n \ge 7$.

Theorem 1. Suppose that $T \in \mathcal{T}_{n,k} \setminus (\mathcal{S}^n_{1,k-1} \cup \mathcal{S}^n_{2,k-2} \cup \{K^n_{2,k-2}\})$ $(4 \leq k \leq n-3,\ n \geq 7)$ with the minimum Randić index. Let F_0^m, $7 \leq m \leq 10$ and $F_0^n, n \geq 11$ be the trees shown in Fig. 2.

(i) If $k = 4$ and $n = 7$, then $T \cong F_0^7$ and $R(T) = \sqrt{3} + \frac{1}{3} + \frac{1}{\sqrt{6}} + \frac{1}{\sqrt{2}}$;

(ii) If $k = 5$ and $n = 8$, then $T \cong F_0^8$ and $R(T) = \frac{3}{2} + \frac{3+\sqrt{2}+\sqrt{6}}{\sqrt{12}}$;

(iii) If $k = 6$ and $n = 9$, then $T \cong F_0^9$ and $R(T) = 3 + \frac{1}{\sqrt{2}}$;

(iv) If $k = 7$ and $n = 10$, then $T \cong F_0^{10}$ and $R(T) = \frac{3}{2} + \frac{4}{\sqrt{5}} + \frac{1}{\sqrt{8}} + \frac{1}{\sqrt{10}}$;

(v) If $4 \leq k \leq n-4$, $n \geq 8$, then $T \in \mathcal{F}_k^n$ and

$$R(T) = \frac{1}{2}(n-k) + \frac{1}{\sqrt{k-1}}\left(k + \frac{1}{\sqrt{2}} - 2\right) + \frac{2}{\sqrt{6}} + \frac{1}{\sqrt{3}} + \frac{1}{\sqrt{2}} - 2;$$

(vi) If $k = n-3$, $n \geq 11$, then $T \cong F_0^n$ and

$$R(T) = \frac{1}{\sqrt{n-4}}(n + \frac{1}{\sqrt{3}} - 5) + \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{3}} + \frac{1}{\sqrt{6}}.$$

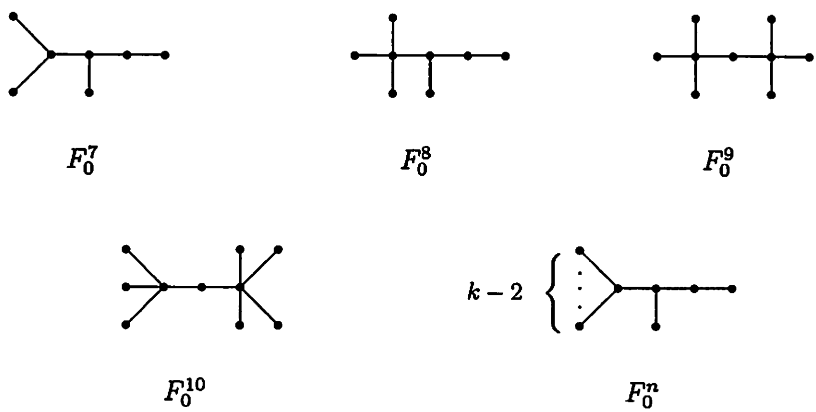


Fig. 2

Proof. In [14], it is obtained that all different trees in $\mathcal{T}_{n,k}$ with $(n,k) = (7,4)$, $(8,5)$, $(9,6)$, and $(10,7)$ up to isomorphism. And there are

4 trees, 6 trees, 9 trees and 12 trees for $(n,k) = (7,4)$, $(8,5)$, $(9,6)$ and $(10,7)$ respectively. An examination by direct calculation, we can prove and obtain (i) to (iv). Next we prove (v) and (vi).

(v) For convenience, denote

$$\phi(n,k) = \frac{1}{2}(n-k) + \frac{1}{\sqrt{k-1}}\left(k + \frac{1}{\sqrt{2}} - 2\right) + \frac{2}{\sqrt{6}} + \frac{1}{\sqrt{3}} + \frac{1}{\sqrt{2}} - 2.$$

It is easy to obtain that

$$\phi(n-1,k-1) - \phi(n,k) = F(k-2, \frac{1}{\sqrt{2}} - 1)$$

and for every tree $T \in \mathcal{F}_k^n$

$$R(T) = \frac{1}{2}(n-k) + \frac{1}{\sqrt{k-1}}(k + \frac{1}{\sqrt{2}} - 2) + \frac{2}{\sqrt{6}} + \frac{1}{\sqrt{3}} + \frac{1}{\sqrt{2}} - 2.$$

Choose a tree $T \in \mathcal{T}_{n,k} \backslash (\mathcal{S}_{1,k-1}^n \cup \mathcal{S}_{2,k-2}^n \cup \{K_{2,k-2}^n\})$ such that $R(T) = min\{R(T) : T \in \mathcal{T}_{n,k} \setminus (\mathcal{S}_{1,k-1}^n \cup \mathcal{S}_{2,k-2}^n \cup \{K_{2,k-2}^n\})\}$. By Lemma 3 and Lemma 4, $\widetilde{\mathcal{P}}(T) \neq \emptyset$ and $|\mathcal{P}(T)| \leq 1$.

We now prove the conclusion by induction on k. When $k = 4$, we have $\Delta(T) = 3$. Otherwise $T \in \mathcal{S}_{n,4}$ and $\widetilde{\mathcal{P}}(T) = \emptyset$, a contradiction. Thus, $|V_3(T)| = 2$ and $|\widetilde{\mathcal{P}}(T)| = 1$. By the choice of T, we have $|\mathcal{P}(T)| = 1$. And it is easy to check that the length of this non-pendant chain is at least 2. Therefore $T \in \mathcal{F}_4^n$.

Assume that $k \geq 5$ and the result holds for $k-1$. Next, choose a vertex $u \in N_T(V_1)$ such that $d(u)$ is the maximum and $3 \leq d(u) \leq k-1$. Let $d(u) = t$, $N_T(u) \cap V_1(T) = \{v_1, \cdots, v_r\}$ $(r \geq 1)$, $N_T(u) \backslash V_1(T) = \{x_1, \cdots, x_{t-r}\}$ and $d(x_j) = d_j$ $(1 \leq j \leq t-r)$, then $t - r \geq 1$ $(T \ncong K_{1,n-1})$, $d_j \geq 2$ $(1 \leq j \leq t-r)$. If possible, choosing the vertex u satisfying $r > \frac{d(u)}{2}$. In particular, $T \ncong K_{3,3}^n$ when $k = 6$. Otherwise, choose $T_0 \in \mathcal{F}_6^n \subset \mathcal{T}_{n,k} \setminus (\mathcal{S}_{1.5}^n \cup \mathcal{S}_{2,4}^n \cup \{K_{2,4}^n\})$, by direct calculation,

$R(T)-R(T_0)>0.001$, a contradiction. Set $\overline{T}=T-v_1$. Thus $\overline{T}=T-v_1\in \mathcal{T}_{n-1,k-1}\setminus(\mathcal{S}^{n-1}_{1,k-2}\cup\mathcal{S}^{n-1}_{2,k-3}\cup\{K^{n-1}_{2,k-3}\})$ and $R(\overline{T})\geq\phi(n-1,k-1)$ by the hypothesis of induction. Therefore

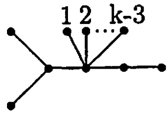
$$
\begin{aligned}
R(T) &= R(\overline{T})+\frac{r}{\sqrt{t}}-\frac{r-1}{\sqrt{t-1}}+\sum_{i=1}^{t-r}\frac{1}{\sqrt{d_i}}\left(\frac{1}{\sqrt{t}}-\frac{1}{\sqrt{t-1}}\right)\\
&\geq R(\overline{T})+\frac{r}{\sqrt{t}}-\frac{r-1}{\sqrt{t-1}}+\frac{1}{\sqrt{2}}(t-r)\left(\frac{1}{\sqrt{t}}-\frac{1}{\sqrt{t-1}}\right)\\
&\geq \phi(n-1,k-1)+\frac{r}{\sqrt{t}}-\frac{r-1}{\sqrt{t-1}}+\frac{1}{\sqrt{2}}(t-r)\left(\frac{1}{\sqrt{t}}-\frac{1}{\sqrt{t-1}}\right)\\
&= \phi(n,k)+F(k-2,\frac{1}{\sqrt{2}}-1)-F(t-1,\frac{1}{\sqrt{2}}-1)\\
&\quad+\left(\frac{1}{\sqrt{2}}-1\right)(t-r-1)\left(\frac{1}{\sqrt{t}}-\frac{1}{\sqrt{t-1}}\right)\\
&\geq \phi(n,k)+F(k-2,\frac{1}{\sqrt{2}}-1)-F(t-1,\frac{1}{\sqrt{2}}-1)\\
&\geq \phi(n,k),
\end{aligned}
$$

since $k-1\geq t$ and $F(x,\frac{1}{\sqrt{2}}-1)$ is monotonously increasing in x according to Lemma 1(i). $R(T)=\phi(n,k)$ if and only if all inequalities in the above argument are equalities. Thus we have $R(\overline{T})=\phi(n-1,k-1)$, $k-1=t$, $t-r=1$ and $d_1=2$. By the induction hypothesis, $\overline{T}\in\mathcal{F}^{n-1}_{k-1}$, $|\mathcal{P}(\overline{T})|=|\widetilde{\mathcal{P}}(\overline{T})|=1$ and the length of this non-pendant chain is at least 2. Therefore $T\in\mathcal{F}^n_k$ and the proof of Theorem 1(v) is completed.

(vi) $k=n-3$. For $T\in\mathcal{T}_{n,n-3}\setminus(\mathcal{S}^n_{1,n-4}\cup\mathcal{S}^n_{2,n-5}\cup\{K^n_{2,n-5}\})$, let $u\in N_T(V_1)$ with $d(u)=max\{d(v):v\in N_T(V_1)\}$. Since $n\geq 11$, $d(u)\leq k-1$. If $d(u)=k-1$, then there are only two trees up to isomorphism, i.e., $F^n_0,F^n_1\in\mathcal{T}_{n,n-3}\setminus(\mathcal{S}^n_{1,n-4}\cup\mathcal{S}^n_{2,n-5}\cup\{K^n_{2,n-5}\})$ (see Fig. 2, Fig. 3). By direct calculation,

$$R(F^n_0)=\frac{1}{\sqrt{n-4}}(n+\frac{1}{\sqrt{3}}-5)+\frac{1}{\sqrt{2}}+\frac{1}{\sqrt{3}}+\frac{1}{\sqrt{6}}$$

and $R(F^n_1)>R(F^n_0)$.



F_1^n

Fig. 3

If $d(u) \leq k-2$, then $T \in \mathcal{T}_{n,n-3} \setminus (\mathcal{S}_{1,n-4}^n \cup \mathcal{S}_{2,n-5}^n \cup \{K_{2,n-5}^n\} \cup \{F_0^n, F_1^n\})$ and $R(T) \geq \frac{1}{\sqrt{n-5}}(n+\frac{1}{\sqrt{2}}-6)+\frac{1}{\sqrt{8}}+\frac{3}{2}$, equality holds if and only if $T \cong K_{3,n-6}^n$. As an analogue to $\mathcal{F}_k^n$ $(4 \leq k \leq n-4)$, we can obtain $R(K_{3,n-6}^n) = \frac{1}{\sqrt{n-5}}(n+\frac{1}{\sqrt{2}}-6)+\frac{1}{\sqrt{8}}+\frac{3}{2}$, and similar to the above proof of Theorem 1(v), we can prove the result. Next, considering the value $R(K_{3,n-6}^n) - R(F_0^n)$.

$$\begin{aligned}
R(K_{3,n-6}^n) &- R(F_0^n) \\
&= \frac{1}{\sqrt{n-5}}(n+\frac{1}{\sqrt{2}}-6)+\frac{1}{\sqrt{8}}+\frac{3}{2}-\frac{1}{\sqrt{n-4}}(n+\frac{1}{\sqrt{3}}-5) \\
&\quad -\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}-\frac{1}{\sqrt{6}} \\
&= \sqrt{n-5}-\sqrt{n-4}+\frac{1}{\sqrt{n-5}}(\frac{1}{\sqrt{2}}-1)-\frac{1}{\sqrt{n-4}}(\frac{1}{\sqrt{3}}-1) \\
&\quad +\frac{3}{2}-\frac{1}{\sqrt{3}}-\frac{1}{\sqrt{6}}-\frac{1}{\sqrt{8}} \\
&> \sqrt{n-5}-\sqrt{n-4}+\frac{1}{\sqrt{n-5}}(\frac{1}{\sqrt{2}}-1) \\
&\quad +\frac{3}{2}-\frac{1}{\sqrt{3}}-\frac{1}{\sqrt{6}}-\frac{1}{\sqrt{8}}.
\end{aligned}$$

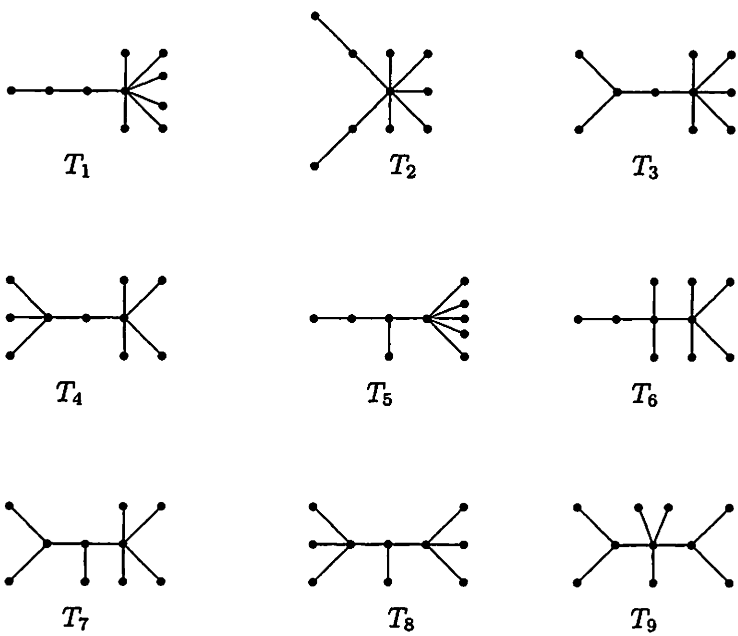
Since $H(n-4)$ is monotonously increasing in n by Lemma 1(iii). Clearly, $\frac{1}{\sqrt{n-5}}(\frac{1}{\sqrt{2}}-1)$ and $\frac{1}{\sqrt{n-4}}(\frac{1}{\sqrt{2}}-1)$ are monotonously increasing in n. Thus,

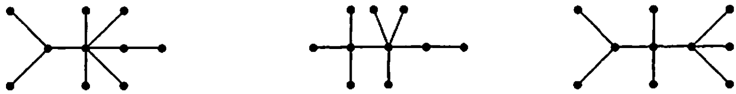
$$R(K_{3,n-6}^n)-R(F_0^n) \geq \begin{cases} H(7)+\frac{1}{\sqrt{6}}(\frac{1}{\sqrt{2}}-1)-\frac{1}{\sqrt{7}}(\frac{1}{\sqrt{3}}-1) & \\ +\frac{3}{2}-\frac{1}{\sqrt{3}}-\frac{1}{\sqrt{6}}-\frac{1}{\sqrt{8}}, & \text{if } n=11; \\ H(8)+\frac{1}{\sqrt{7}}(\frac{1}{\sqrt{2}}-1)-\frac{1}{\sqrt{10}}(\frac{1}{\sqrt{3}}-1) & \\ +\frac{3}{2}-\frac{1}{\sqrt{3}}-\frac{1}{\sqrt{6}}-\frac{1}{\sqrt{8}}, & \text{if } 12 \leq n \leq 14 \\ H(11)+\frac{1}{\sqrt{10}}(\frac{1}{\sqrt{2}}-1)-\frac{1}{\sqrt{24}}(\frac{1}{\sqrt{3}}-1) & \\ +\frac{3}{2}-\frac{1}{\sqrt{3}}-\frac{1}{\sqrt{6}}-\frac{1}{\sqrt{8}}, & \text{if } 15 \leq n \leq 28 \\ H(25)+\frac{1}{\sqrt{24}}(\frac{1}{\sqrt{2}}-1) & \\ +\frac{3}{2}-\frac{1}{\sqrt{3}}-\frac{1}{\sqrt{6}}-\frac{1}{\sqrt{8}}, & \text{if } n \geq 29; \end{cases}$$

$$> 0 \text{ for } n \geq 11.$$

Hence the proof of Theorem 1(vi) is completed. ■

And it is of particular interest to determine the ordering of trees with respect to Randić index. An examination of all 12 trees of order 10 with $k = 7$ pendant vertices up to isomorphism (see [14]), obtaining that the tree T_5 with the fifth minimum Randić index in $\mathcal{T}_{10,7}$ (see Fig. 4).

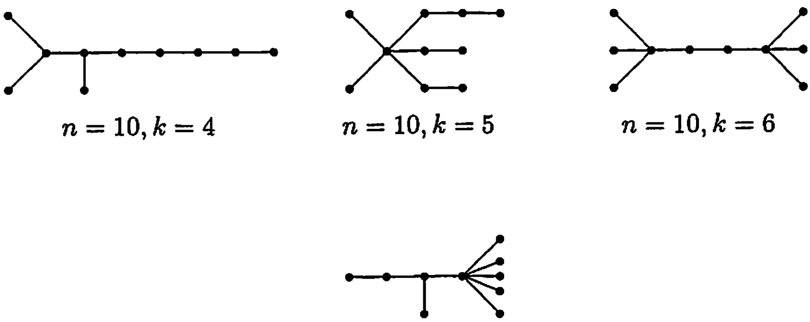




T_{10} T_{11} T_{12}

Fig. 4

Similarly, an examination of all trees of order 10 with $k = 4, 5, 6$ pendant vertices up to isomorphism (see [14]), finding that the structural properties of these trees with the fifth minimum Randić index differ significantly (see Fig. 5).



$n = 10, k = 4$ $n = 10, k = 5$ $n = 10, k = 6$

$n = 10, k = 7$

Fig. 5

This implies it is a non-trivial task to characterize other elements of this ordering. Particularly, in the case when $k = n-3$ and $n \geq 11$, searching for graphically feasible combinations of n_1, n_2 and n_3 pendant vertices adjacent to only three non-pendant vertices of a tree T, respectively, where $n_1 + n_2 + n_3 = k$, there is the same story about the structural properties of trees with the sixth minimum Randić index. In view of this, for $k = n - 3$ and $n \geq 11$, we determine the fifth minimum Randić index.

Theorem 2. Let $T \in \mathcal{T}_{n,k}$. If $k = n-3$, $n \geq 11$ and $R(T)$ is the fifth minimum Randić index, then $T \cong K^n_{3,n-6}$ and

$$R(T) = \frac{1}{\sqrt{n-5}}(n + \frac{1}{\sqrt{2}} - 6) + \frac{1}{\sqrt{8}} + \frac{3}{2}.$$

Proof. Similar to the above proof of Lemma 3, we can verify $R(F^n_1) - R(K^n_{3,n-6}) > 0$, where F^n_1 is the graph shown in Fig. 3, that is,

$$\begin{aligned} R(F^n_1) \quad - & \quad R(K^n_{3,n-6}) \\ = & \quad \frac{1}{\sqrt{n-4}}(n + \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{3}} - 6) + \frac{1}{\sqrt{2}} + \frac{2}{\sqrt{3}} \\ & -\frac{1}{\sqrt{n-5}}(n + \frac{1}{\sqrt{2}} - 6) - \frac{1}{\sqrt{8}} - \frac{3}{2} \\ = & \quad \sqrt{n-4} - \sqrt{n-5} + (\frac{1}{\sqrt{n-4}} - \frac{1}{\sqrt{n-5}})(\frac{1}{\sqrt{2}} - 1) \\ & + \frac{1}{\sqrt{n-4}}(\frac{1}{\sqrt{3}} - 1) + \frac{1}{\sqrt{8}} + \frac{2}{\sqrt{3}} - \frac{3}{2} \\ > & \quad \frac{1}{\sqrt{n-4}}(\frac{1}{\sqrt{3}} - 1) + \frac{1}{\sqrt{8}} + \frac{2}{\sqrt{3}} - \frac{3}{2}. \end{aligned}$$

For $11 \leq n \leq 2630$, by means of mathematical programming, one easily calculates that $R(F^n_1) - R(K^n_{3,n-6}) > 0.009$, and for $n > 2630$, we also have $R(F^n_1) - R(K^n_{3,n-6}) > 0$. By the proof of Theorem 1(vi), we have $T \in \mathcal{T}_{n,n-3} \backslash (S^n_{1,n-4} \cup S^n_{2,n-5} \cup \{K^n_{2,n-5}\} \cup \{F^n_0, F^n_1\})$ and $R(T) \geq \frac{1}{\sqrt{n-5}}(n + \frac{1}{\sqrt{2}} - 6) + \frac{1}{\sqrt{8}} + \frac{3}{2}$, equality holds if and only if $T \cong K^n_{3,n-6}$. Hence it is immediate that $R(K^n_{3,n-6})$ has the property of the fifth minimum Randić index when $k = n-3$ by Theorem 1(vi). ■

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