The Third Minimal Randić Index Tree 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 \( G \). In this paper, we investigate some minimal Randić index properties and give the tree with the third minimal Randić index among the trees with \( n \) vertices and \( k \) 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, 3]). Among the numerous topological indices considered in chemical graph theory, only a few have been found noteworthy in practical application (see [4]). 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 [5, 6]) 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 \( G \). 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 (see [7]). There are many works to study the trees with extremal Randić index and the bounds in some graph sets (see [8]).

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In this paper, we are interested in the Randić indices for trees. First we provide a survey of some known results concerning our results. Let \( T \) be a tree of order \( n \). Yu (see [9]) gave a sharp upper bound of
\[
R(T) \leq \frac{n + 2\sqrt{2} - 3}{2}.
\]
In [10], trees with large general Randić index are 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 [11]). In order to illustrate some more results on the minimal Randić index, we need some notations as follows.

Let \( K_{1,k}(p_1, p_2, \ldots, p_s), (s \leq k) \) be a tree created from the star \( K_{1,k} \) of \( k+1 \) vertices by attaching paths of lengths \( p_1, p_2, \ldots, p_s \) to \( s \) pendant vertices of \( K_{1,k} \), respectively (see Fig. 1(a)). Let \( K_{n,k-s}^n \) be the tree created 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)). Denote
\[
S_{n, k-s}^n = \{ K_{1,k}(p_1, p_2, \ldots, p_s) : p_i > 0, \ \sum_{i=1}^{s} p_i = n - k - 1 \},
\]
\[
S_{n,k} = \bigcup_{s=1}^{k} S_{n,k-s}^n,
\]
\[
U_{n,k} = \{ K_{n,k-s}^n : s = 2, \ldots, \lfloor \frac{k}{2} \rfloor \},
\]
\[
T_{n,k} = \{ T : T \ \text{is a tree with} \ n \ \text{vertices and} \ k \ \text{pendant vertices} \}.
\]
Clearly, \( S_{n,k}, U_{n,k} \subseteq T_{n,k} \).

The trees with the minimum and the second minimum Randić index in \( T_{n,k} \) are characterized by Liu, Lu and Tian (see [12]) and Li et al. (see [8, 13]), respectively. A tree \( T \in T_{n,k} \) has the minimum Randić index if and only if \( T \in S_{1,k-1}^n \) 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 $T \in T_{n,k}$ has the second minimum Randić index if and only if $T \in S_{2,k-2}^n$ and its Randić index

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

Furthermore, we investigate some minimal Randić index properties, and characterize the tree $K_{2,k-2}^n$ with the third minimal Randić index and its Randić index

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

2. Notations and Lemmas

Let $G(V,E)$ be a graph with vertex set $V$ and edge set $E$. Suppose $x \in V(G)$, $S \subseteq V(G)$. Denote the neighborhood of $x$ by $N_G(x)$, $N_G(S) = \bigcup_{v \in S} N_G(v)$ 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 the 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 $V_1(T)$. A path $P = v_0v_1 \cdots v_s$ of $T$ is called a chain of $T$ if $s > 1$ and $d(v_1) = \cdots = d(v_{s-1}) = 2$. If $d(v_0) = 1$, $d(v_s) \geq 3$ or $d(v_s) = 1$ and $d(v_0) \geq 3$, then $P$ is called a pendant chain of $T$.

In order to compare the Randić index between trees, we need two functions with monotonous properties in the following lemma.

**Lemma 1.**

1. 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 $F(x,b)$ is a monotonously increasing function.

2. Let $G(x) = \frac{3}{\sqrt{x}} - \frac{1}{\sqrt{x-1}}$. If $x \geq 3$, then $G(x)$ is a monotonously decreasing function.

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

$$F'_x(x,b) = \frac{1}{2\sqrt{x}} - \frac{b}{2\sqrt{x}^3} - \frac{1}{2\sqrt{x} + 1} + \frac{b}{2\sqrt{(x+1)^3}} = \frac{1}{2}\left(\frac{1}{\sqrt{x}} - \frac{1}{\sqrt{x+1}}\right) - \frac{b}{2}\left(\frac{1}{\sqrt{x}^3} - \frac{1}{\sqrt{(x+1)^3}}\right) > 0$$
when $x > 0$ and $b < 0$.

$$G'(x) = -\frac{3}{2\sqrt{x^3}} + \frac{1}{2\sqrt{(x-1)^3}}$$

$$= \frac{1}{2} \left( \frac{1}{\sqrt{(x-1)^3}} - \frac{1}{\sqrt{x^3}} \right)$$

$$< 0$$

when $x \geq 3$.

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

**Lemma 2.** Let $T \in T_{n,k}$. If $T$ has $s(\geq 2)$ pendant chains, then there exist $\overline{T} \in T_{n,k}$ with $s-1$ pendant chains such that $R(\overline{T}) < R(T)$.

**Proof.** Assume that $T$ has $s$ pendant chains, and $P = v_0v_1\cdots v_h$, $P' = v'_0v'_1\cdots v'_l$ ($h, l \geq 2$) are its two pendant chains with $d(v_0) = 1$ and $d(v_h), d(v'_l) \geq 3$. Let $\overline{T} = T - v_{h-1}v_{h-2} + v_0v'_0$. Then $\overline{T} \in T_{n,k}$ with $s-1$ pendant chains (see Fig.2).

It is not difficult to check that

$$R(T) - R(\overline{T}) = \left( \frac{1}{\sqrt{d(v_h)}} - \frac{1}{\sqrt{2}} \right) \left( \frac{1}{\sqrt{2}} - 1 \right)$$

$$> 0.$$ 

Therefore $R(\overline{T}) < R(T)$.

It is not difficult to check that $R(T_1) = R(T_2)$ for $T_1, T_2 \in S^n_{i,k-i}, i = 1, 2, \ldots, k$. The Randić index ordering of trees in $S_{n,k}$ is obtained immediately by Lemma 2.

**Corollary.** For any $T_1, T_2 \in S_{n,k}$, suppose $T_1 \in S^n_{i,k-i}$ and $T_2 \in S^n_{j,k-j}, i \leq j \leq k$. 

(1) If \( i = j \) then \( R(T_1) = R(T_2) \);
(2) if \( i < j \) the \( R(T_1) < R(T_2) \).

In order to characterize the tree with the third minimum Randić index, we first characterize two extremal properties of trees in \( T_{n,k} \setminus (S_{1,k-1}^n \cup S_{2,k-2}^n) \).

**Lemma 3.** Suppose \( T \in T_{n,k} \setminus (S_{1,k-1}^n \cup S_{2,k-2}^n) \), \( k \geq 4 \). If \( R(T) = \min \{ R(T) : T \in T_{n,k} \setminus (S_{1,k-1}^n \cup S_{2,k-2}^n) \} \), then \( T \notin S_{n,k} \).

**Proof.** By contradiction. Choose a tree \( T \in T_{n,k} \) such that \( R(T) = \min \{ R(T) : T \in T_{n,k} \setminus (S_{1,k-1}^n \cup S_{2,k-2}^n) \} \). If \( T \in S_{n,k} \), then \( T \in S_{3,k-3} \) by the choice of \( T \) and Corollary. It is easy to obtain that \( R(T) = \frac{1}{2} (n-k) + \frac{1}{\sqrt{k}} (k + \frac{3}{\sqrt{2}} - 3) + \frac{3}{\sqrt{2}} - 2 \). Clearly, \( K_{2,k-2}^n \in T_{n,k} \setminus (S_{1,k-1}^n \cup S_{2,k-2}^n) \), and we have

\[
R(T) - R(K_{2,k-2}^n) = \frac{1}{\sqrt{k}} (k + \frac{3}{\sqrt{2}} - 3) - \frac{1}{\sqrt{k-1}} (k + \frac{1}{\sqrt{2}} - 2) + \frac{3}{\sqrt{3}} - \frac{2}{\sqrt{6}} - \frac{1}{2} - \frac{1}{2} \]

Since \( F(k-1, \frac{1}{\sqrt{2}} - 1) \) is a monotonously increasing in \( k \) by Lemma 1(1). Moreover, \( \frac{2}{\sqrt{k}} (\frac{1}{\sqrt{2}} - 1) \) is monotonously increasing in \( k \). Thus

\[
R(T) - R(K_{2,k-2}^n) \geq \begin{cases}
\frac{2}{\sqrt{3}} (\frac{1}{\sqrt{2}} - 1) - F(4, \frac{1}{\sqrt{2}} - 1) + \frac{3}{\sqrt{2}} - \frac{2}{\sqrt{3}} - \frac{1}{\sqrt{6}} - \frac{1}{2}, & \text{if } 4 \leq k \leq 5 \\
\frac{2}{\sqrt{6}} (\frac{1}{\sqrt{2}} - 1) - F(7, \frac{1}{\sqrt{2}} - 1) + \frac{3}{\sqrt{2}} - \frac{2}{\sqrt{3}} - \frac{1}{\sqrt{6}} - \frac{1}{2}, & \text{if } 6 \leq k \leq 8 \\
\frac{2}{\sqrt{15}} (\frac{1}{\sqrt{2}} - 1) - F(28, \frac{1}{\sqrt{2}} - 1) + \frac{3}{\sqrt{2}} - \frac{2}{\sqrt{3}} - \frac{1}{\sqrt{6}} - \frac{1}{2}, & \text{if } 9 \leq k \leq 14 \\
\frac{2}{\sqrt{30}} (\frac{1}{\sqrt{2}} - 1) - F(99, \frac{1}{\sqrt{2}} - 1) + \frac{3}{\sqrt{2}} - \frac{2}{\sqrt{3}} - \frac{1}{\sqrt{6}} - \frac{1}{2}, & \text{if } 15 \leq k \leq 29 \\
\end{cases}
\]

\( > 0 \) for \( k \leq 100 \).
For $k > 100$, we have

$$R(T) = R(K_{2,k-2}^n)$$

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

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

$$> (\frac{1}{\sqrt{2}} - 1)G(k) + 3\frac{3}{\sqrt{2}} - \frac{2}{\sqrt{3}} - \frac{1}{\sqrt{6}} - \frac{1}{2}$$

$$\geq (\frac{1}{\sqrt{2}} - 1)G(101) + \frac{3}{\sqrt{2}} - \frac{2}{\sqrt{3}} - \frac{1}{\sqrt{6}} - \frac{1}{2}$$

$$> 0$$

By Lemma 1(2), $G(k)$ is monotonous decreasing in $k$. This contradicts to $R(T) = \min\{R(T) : T \in T_{n,k} \setminus (S_{1,k-1}^n \cup S_{2,k-2}^n)\}$. Consequently, $T \notin S_{n,k}$.

**Lemma 4.** Suppose $T \in T_{n,k} \setminus (S_{1,k-1}^n \cup S_{2,k-2}^n)$, $k \geq 4$. If $R(T) = \min\{R(T) : T \in T_{n,k} \setminus (S_{1,k-1}^n \cup S_{2,k-2}^n)\}$, then $T$ contains no any pendant chains.

**Proof.** By contradiction. Assume that $T \in T_{n,k} \setminus (S_{1,k-1}^n \cup S_{2,k-2}^n)$ with $R(T) = \min\{R(T) : T \in T_{n,k} \setminus (S_{1,k-1}^n \cup S_{2,k-2}^n)\}$ and $T$ has a pendant chain $P = v_0v_1\cdots v_s$ with $d(v_0) = 1$. There are at least two vertices of degrees greater than 2 in the tree $T$ by Lemma 3. Therefore there exists an edge or a chain $P' = v_0v'_1\cdots v'_l$ ($l \geq 1$) with $d(v'_0), d(v'_l) \geq 3$. Let $T'$ be obtained from $T - \{v_0, v_1, \ldots, v_{s-2}\}$ by using the path $P'' = v'_0v'_1\cdots v'_{l+s-1}$ of length $l+s-1$ instead of the path $P' = v'_0v'_1\cdots v'_l$ (see Fig. 3). Then $T' \in T_{n,k} \setminus (S_{1,k-1}^n \cup S_{2,k-2}^n)$.

![Fig. 3](image-url)
When \( l = 1 \),
\[
R(T) - R(T) = \frac{1}{\sqrt{d(v_0')}} + \frac{1}{\sqrt{d(v_s')}} + \frac{1}{\sqrt{d(v')}} - \frac{1}{\sqrt{d(v_0')}} - \frac{1}{\sqrt{d(v')}} - \frac{1}{\sqrt{d(v_s')}}
\]
\[
= (1 - \frac{1}{\sqrt{2}})(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{d(v_s')}}) + (\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{d(v')}})(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{d(v)')})
\]
\[
> 0.
\]
And when \( l \geq 2 \),
\[
R(T) - R(T) = \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2d(v_s)}} - \frac{1}{\sqrt{4}} - \frac{1}{\sqrt{d(v_s)}}
\]
\[
= (1 - \frac{1}{\sqrt{2}})(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{d(v_s)}})
\]
\[
> 0.
\]
This is a contradiction to \( R(T) = \min\{R(T) : T \in \mathcal{T}_{n,k} \}\).

**Lemma 5 [8,13].** Suppose \( K_{s,k-s}^n \), \( K_{t,k-t}^n \in U_{n,k} \). If \( s < t < k - t \), then \( R(K_{s,k-s}^n) < R(K_{t,k-t}^n) \).

3. Extremal Property of \( K_{2,k-2}^n \)

Clearly, to determine that \( K_{2,k-2}^n \) has the property of the third minimum Randić index in \( \mathcal{T}_{n,k} \) (\( 3 \leq k \leq n - 3 \)) is equivalent to determine it has the minimum Randić index in \( \mathcal{T}_{n,k} \) \( (S_{1,k-1}^n \cup S_{2,k-2}^n) \). Suppose \( T \in \mathcal{T}_{n,k} \). Note that if \( k = 2 \), then \( T \) is a path, and hence \( R(T) = \frac{n+2\sqrt{2}}{2} \); if \( k = n-1 \), then \( T \) is a star, and hence \( R(T) = \sqrt{n-1} \). Moreover, \( T \in S_{1,2}^n \) in the case \( k = 3 \) and \( n = 5 \); \( T \in S_{1,2}^n \cup S_{2,1}^n \) in the case \( k = 3 \) and \( n = 6 \); \( R(T) = \frac{1+4\sqrt{3}}{9} \) or \( T \in S_{1,3}^n \) in the case \( k = 3 \) and \( n = 6 \). If \( k = 3 \) and \( n \geq 7 \), then we have \( T_{n,3} = S_{1,2}^n \cup S_{2,1}^n \cup S_{3,0}^n \). Thus, for any \( T_i \in S_{1,k-2}^n \) (\( 1 \leq i \leq 3 \)), we get \( R(T_1) < R(T_2) < R(T_3) \) by Corollary. If \( k = n-2 \) and \( n \geq 7 \), then we have \( T_{n,n-2} = U_{n,n-2} \). Thus \( R(K_{2,n-4}^n) < R(K_{3,n-5}^n) < \cdots < R(K_{[n-2],[n-2]}^n) \) by Lemma 5. Therefore we just need to show the final case \( 4 \leq k \leq n - 3 \) and \( n \geq 7 \).

**Theorem.** Suppose \( T \in \mathcal{T}_{n,k} \), \( 4 \leq k \leq n - 3 \), \( n \geq 7 \). If \( R(T) \) is the third minimal Randić index in \( \mathcal{T}_{n,k} \), then \( T \cong K_{2,k-2}^n \) and
\[
R(T) = \frac{1}{2}(n - k) + \frac{1}{\sqrt{k-1}}(k + \frac{1}{\sqrt{2}} - 2) + \frac{2}{\sqrt{3}} + \frac{1}{\sqrt{6}} - \frac{3}{2}.
\]
Proof. For convenience, denote
\[ \phi(n,k) = \frac{1}{2}(n-k) + \frac{1}{\sqrt{k-1}}(k + \frac{1}{\sqrt{2}} - 2) + \frac{2}{\sqrt{3}} + \frac{1}{\sqrt{6}} - \frac{3}{2}. \]

It is easy to obtained that
\[ \phi(n-1,k-1) - \phi(n,k) = F(k-2, \frac{1}{\sqrt{2}} - 1) \]
and
\[ R(K_{2,k-2}^n) = \frac{1}{2}(n-k) + \frac{1}{\sqrt{k-1}}(k + \frac{1}{\sqrt{2}} - 2) + \frac{2}{\sqrt{3}} + \frac{1}{\sqrt{6}} - \frac{3}{2} = \phi(n,k). \]

Choose a tree \( T \in T_{n,k} \setminus (S^{n}_{1,k-1} \cup S^{n}_{2,k-2}) \) such that \( R(T) = \min\{R(T) : T \in T_{n,k} \setminus (S^{n}_{1,k-1} \cup S^{n}_{2,k-2})\} \). By Lemma 3 and Lemma 4, \( T \not\in S_{n,k} \) and the tree \( T \) contains no pendant chain.

We now prove the conclusion by induction on \( k \). When \( k = 4 \), we have \( \Delta(T) = 3 \). Otherwise \( T \in S_{n,4} \), a contradiction. Furthermore, \( |V_3(T)| = 2 \) and \( V_3(T) \subseteq N_T(V_1) \). Thus \( T \cong K_{2,2}^n \).

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 \( N_T(u) \cap V_1(T) = \{v_1, \ldots, v_r\} (r \geq 1) \), \( N_T(u) \setminus V_1(T) = \{x_1, \ldots, x_{t-r}\} \), and \( d(x_j) = d_j \) (\( 1 \leq j \leq t-r \)). Then \( t-r \geq 1 \) (\( T \not\cong K_{1,n-1} \)) and \( d_j \geq 2 \) (\( 1 \leq j \leq t-r \)). Let \( \overline{T} = T - v_1 \). Thus \( \overline{T} = T - v_1 \in T_{n-1,k-1} \setminus (S^{n-1}_{1,k-2} \cup S^{n-1}_{2,k-3}) \) and \( R(T) = \phi(n-1,k-1) \) by the hypothesis of induction. Therefore

\[
R(T) = R(\overline{T}) + \frac{r}{\sqrt{t}} - \frac{r-1}{\sqrt{t-1}} + \sum_{i=1}^{l-r} \frac{1}{\sqrt{d_i}} (\frac{1}{\sqrt{t}} - \frac{1}{\sqrt{t-1}}) \\
\geq R(\overline{T}) + \frac{r}{\sqrt{t}} - \frac{r-1}{\sqrt{t-1}} + \frac{1}{\sqrt{2}}(t-r)(\frac{1}{\sqrt{t}} - \frac{1}{\sqrt{t-1}}) \\
\geq \phi(n-1,k-1) + \frac{r}{\sqrt{t}} - \frac{r-1}{\sqrt{t-1}} + \frac{1}{\sqrt{2}}(t-r)(\frac{1}{\sqrt{t}} - \frac{1}{\sqrt{t-1}}) \\
= \phi(n,k) + F(k-2, \frac{1}{\sqrt{2}} - 1) - F(t-1, \frac{1}{\sqrt{2}} - 1) + (\frac{1}{\sqrt{2}} - 1)(t-r-1)(\frac{1}{\sqrt{t}} - \frac{1}{\sqrt{t-1}}) \\
\geq \phi(n,k) + F(k-2, \frac{1}{\sqrt{2}} - 1) - F(t-1, \frac{1}{\sqrt{2}} - 1) \\
\geq \phi(n,k),
\]
since \( k-1 \geq t \) and \( F(x, \frac{1}{\sqrt{2}} - 1) \) is monotonously increasing according to Lemma 1(1). \( R(T) = \phi(n,k) \) if and only if all inequalities above must be equalities. Thus we have \( R(\overline{T}) = \phi(n-
1, k − 1), k − 1 = t, t − r = 1 and d₀ = 2. By the induction hypothesis, T ≅ Kⁿ−₁₂, k−³. Therefore $T ≅ K_{2,k−2}$ and the proof is completed.

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