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The smallest Randić index for trees

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Abstract. The general Randić index $R_\alpha(G)$ is the sum of the weight $d(u)d(v)^\alpha$ over all edges uv of a graph G, where α is a real number and $d(u)$ is the degree of the vertex u of G. In this paper, for any real number $\alpha \neq 0$, the first three minimum general Randić indices among trees are determined, and the corresponding extremal trees are characterized.

Keywords. Extremal graph; tree; the general Randić index.

1. Introduction

In 1975, Randić [6] introduced the branching index as the sum of $d(u)d(v)^{-1/2}$ over all edges uv of a (molecular) graph $G = (V, E)$, i.e.

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

where $d(u)$ denotes the degree of $u \in V(G)$.

Randić noticed that there is a good correlation between the Randić index R and several physio-chemical properties of alkanes: boiling points, chromatographic retention times, enthalpies of formation, parameters in the Antoine equation for vapor pressure, surface areas, etc [6]. So finding the graphs having maximum and minimum Randić indices attracted the attention of many researchers. The Randić index has been extensively studied by both mathematicians and theoretical chemists (see [1, 6]).

Later in 1998, Bollobás and Erdös [2] generalized this index by replacing $-\frac{1}{2}$ with any real number α, which is called the general Randić index, i.e.

$$R_\alpha(G) == \sum_{uv \in E(G)} (d(u)d(v))^\alpha.$$

For a survey of results, we refer the reader to a book, which is written by Li and Gutman [5].

Let $d(u)$ and $N(u)$ denote the degree and neighborhood of vertex u, respectively. A vertex of degree i is also addressed as an *i-degree vertex*. A vertex of degree 1 is called a pendant vertex or a leaf. A connected graph without any cycle is a tree. The path P_n is a tree of order n with exactly two pendant vertices. The star of order n, denoted by S_n, is the tree with $n-1$ pendant vertices. The double star $S_{p,q}$ is the tree with one p-degree vertex, one q-degree vertex and $p+q-2$ pendant vertices. If $|p-q| \leq 1$, then the double star is said to be balanced. A comet is a tree composed of a star and a pendant path. For any number n and $2 \leq n_1 \leq n-1$, we denote by P_{n,n_1} the comet of order n with n_1 pendant vertices, i.e. a tree formed by a path P_{n-n_1} of which one end vertex coincides with a pendant vertex of a star S_{n_1+1} of order n_1+1. Let $L_{n,k,i}$ $(1 \leq k, i \leq n-i)$ denote the tree obtained from a path $v_1 v_2 \cdots v_{n-i}$ of length $n-i$ by attaching a suspended path of length i rooted at v_k. A quasi double star graph $QS_{n,p,q}$ is a tree obtained from connecting the centers of S_p and S_q by a path of length $n-p-q$ as shown in figure 1.

The question of finding the minimum general Randić index and the corresponding extremal graphs also attracted the attention of many researchers. Hu *et al.* [4] showed that among trees with $n \geq 5$ vertices, the path P_n for $\alpha > 0$ and the star S_n for $\alpha < 0$, respectively, has the minimum general Randić index. And in the same paper the trees of order $n \geq 6$ with second minimum and third minimum general Randić index for $0 < \alpha \leq -1$ are characterized. Chang and Liu [3] showed that among trees with $n \geq 7$ vertices, the comet $P_{n,3}$ has second minimum general Randić index for $\alpha > 0$.

In this paper, we discuss the first three minimum general Randić index for trees. We use a relatively simple way to prove results mentioned above, and determine trees with the third minimum general Randić index for $\alpha > 0$ (answering a question posed by Chang and Liu [3]). We proved that trees with second and third minimum general Randić index are double stars for $\alpha < -1$, and we show that the extremal trees with $n \geq 7$ vertices having second and third general Randić index are the balanced double star and $S_{p,q}$ with $|p-q| = 2$ or 3, respectively.

In the following, we distinguish α in two different intervals, $(0, +\infty)$ and $(-\infty, 0)$, to solve the problem.

2. The case for $\alpha > 0$

Lemma 2.1. *Let T_1 be a tree of order $n \geq 7$ which is not a star, $\alpha > 0$. Assume that $P = v_1 v_2 \cdots v_t$ is a longest path in T_1 with $d = d(v_2) > 2$, and $u_1, u_2, \ldots, u_{d-2}$ are neighbours of v_2 other than v_1, v_3. T_2 is formed by deleting the edges $v_2u_1, v_2u_2, \ldots, v_2u_{d-2}$ and adding the edges $v_1u_1, v_1u_2, \ldots, v_1u_{d-2}$, as shown in figure 2. Then $R_\alpha(T_1) > R_\alpha(T_2)$.*

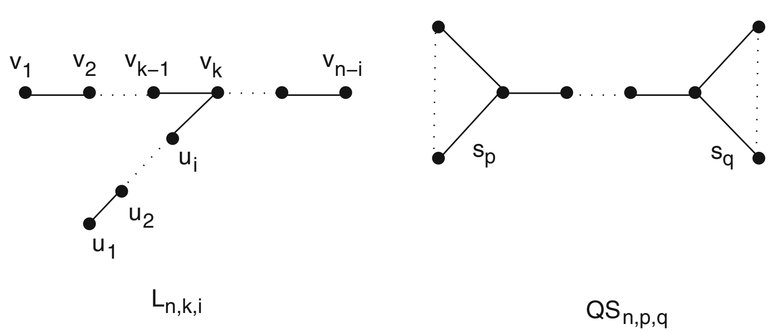

Figure 1. $L_{n,k,i}$ and $QS_{n,p,q}$.

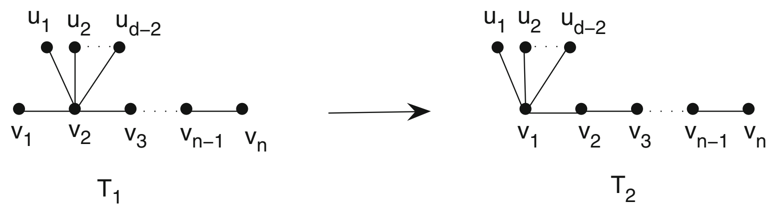

Figure 2. Transform T_1 to T_2.

Proof. Since T_1 is not a star and P is a longest path, $d(u_1) = d(u_2) = \cdots = d(u_{d-2}) = 1$ and $d(v_3) > 1$.

$$\begin{aligned} R_\alpha(T_1) - R_\alpha(T_2) &= d(v_3)^\alpha(d^\alpha - 2^\alpha) - 2^\alpha(d-1)^\alpha + (d-1)d^\alpha \\ &\quad - (d-2)(d-1)^\alpha \geq 2^\alpha(d^\alpha - 2^\alpha) + (d-1)d^\alpha \\ &\quad - 2^\alpha(d-1)^\alpha - (d-2)d^\alpha \\ &= 2^\alpha(d^\alpha - (d-1)^\alpha) + d^\alpha - 4^\alpha. \end{aligned}$$

If $d \geq 4$,

$$R_\alpha(T_1) - R_\alpha(T_2) > 0,$$

If $d = 3$,

$$\begin{aligned} &R_\alpha(T_1) - R_\alpha(T_2) > 2^\alpha(3^\alpha - (d-1)^\alpha) + 3^\alpha - 4^\alpha. \\ &\quad = 6^\alpha + 3^\alpha - 2 * 4^\alpha > 2 * \sqrt{18^\alpha} - 2 * \sqrt{16^\alpha} > 0. \end{aligned}$$

□

COROLLARY 2.1

The general Randić index of a comet P_{n,n_1} is monotonously decreasing in n_1 for $\alpha > 0$.

Lemma 2.2. *Let T_1 be a tree of order $n \geq 7$, $\alpha > 0$. Assume that $P = v_1v_2 \cdots v_t$ is the longest path in T_1 with $d(v_2) = d(v_{t-1}) = 2$, and $d = d(v_k) > 2$ for some $3 \leq k \leq t-2$. $u_1, u_2, \ldots, u_{d-2}$ are neighbors of v_k other than v_{k-1}, v_{k+1}. T_2 is formed by deleting the edge v_ku_1 and adding a new edge v_1u_1, as shown in figure 3. Then $R_\alpha(T_1) > R_\alpha(T_2)$.*

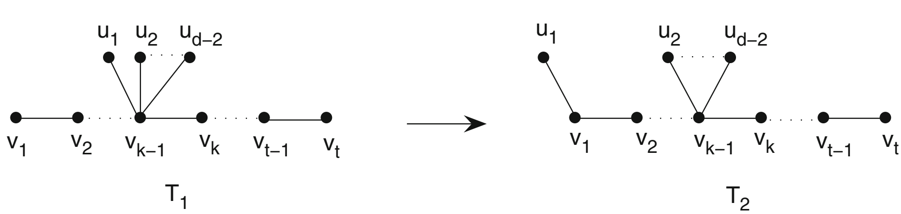

Figure 3. Transform T_1 to T_2.

Proof.

$$\begin{aligned}
R_\alpha(T_1) - R_\alpha(T_2) &\geq (d * d(u_1))^\alpha + (d * d(v_{k-1}))^\alpha \\
&\quad + 2^\alpha - (2 * d(u_1)^\alpha + (d(v_{k-1})(d-1))^\alpha - 4^\alpha) \\
&= d(u_1)^\alpha (d^\alpha - 2^\alpha) + d(v_{k-1})^\alpha (d^\alpha - (d-1)^\alpha) \\
&\quad + 2^\alpha - 4^\alpha \\
&\geq d^\alpha - 2^\alpha + 2^\alpha (d^\alpha - (d-1)^\alpha) + 2^\alpha - 4^\alpha \\
&= d^\alpha - 4^\alpha + 2^\alpha (d^\alpha - (d-1)^\alpha).
\end{aligned}$$

If $d \geq 4$,

$$R_\alpha(T_1) - R_\alpha(T_2) > 0.$$

If $d = 3$,

$$R_\alpha(T_1) - R_\alpha(T_2) = 6^\alpha + 3^\alpha - 2 * 4^\alpha > 2 * \sqrt{18^\alpha} - 2 * \sqrt{16^\alpha} > 0.$$

□

Theorem 2.1. *Let $\alpha > 0$, among trees with $n \geq 7$ vertices.*

(1) *The path P_n has minimum general Randić index*;
(2) *The comet $P_{n,3}$ has second minimum general Randić index*;
(3) *Let μ be approximately equal to 3.6475, if $\alpha > \mu$, $L_{n,k,1}$ $(k = 3, 4, \ldots, n-3)$ has third general Randić index. If $\alpha < \mu$, the quasi double star $QS_{3,3}$ has third general Randić index.*

Proof.

(1) Assume that $P = v_1 v_2 \cdots v_t$ is a longest path in T. If $d(v_i) > 2$ for some $i = 2, 3, \ldots, n-1$, by Lemmas 2.1 and 2.2, we can delete some edges and add them to the end vertices to get a new tree with the general Randić index smaller than that of T. Therefore, tree with minimum general Randić index should contain no vertex with degree bigger than 2. Hence the path P_n has minimum general Randić index.

(2) Let T' be a tree with second minimum general Randić index. We assert that T_1 contains no vertex with degree bigger than 3 or two 3-degree vertices. Assume the contrary, if $d(v_i) \geq 4$ or $d(v_j) = d(v_k) = 3$ for some $1 \leq i, j, k \leq n$, then we can delete one edge adjacent to v_i or v_j and add it to a pendant vertex to get a new tree T'. By Lemmas 2.1 and 2.2, $R_\alpha(T'') > R_\alpha(T')$. Obviously, T'' is not a path, a contradiction. Hence, T' contains exactly one 3-degree vertex. Note that $R_\alpha(L_{n,3,1}) = R_\alpha(L_{n,4,1}) = \cdots = R_\alpha(L_{n,n-2,1})$ and $R_\alpha(L_{n,k,l})$ are the same for $3 \leq k \leq n-2$ and $2 \leq l \leq k$. Thus it suffices to compare the general Randić index of the following trees, which are shown in figure 4:

$$\begin{aligned}
R_\alpha(H_2) - R_\alpha(H_1) &= 2 * 6^\alpha + 3^\alpha + 2 * 2^\alpha - 2 * 3^\alpha - 2^\alpha - 6^\alpha - 4^\alpha \\
&= 6^\alpha + 2^\alpha - 3^\alpha - 4^\alpha \\
&= 3^\alpha * 2^\alpha + 2^\alpha - 3^\alpha - 2^\alpha * 2^\alpha \\
&= (3^\alpha - 2^\alpha)(2^\alpha - 1) > 0,
\end{aligned}$$

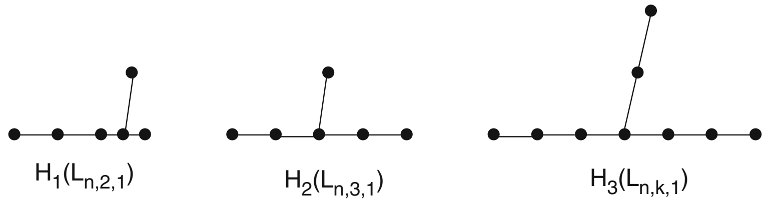

Figure 4. Trees possible with second minimum general Randić index.

$$\begin{aligned} R_\alpha(H_3) - R_\alpha(H_2) &= 3*6^\alpha + 3*2^\alpha - 2*6^\alpha - 3^\alpha - 4^\alpha - 2*2^\alpha \\ &= 6^\alpha + 2^\alpha - 3^\alpha - 4^\alpha \\ &= 3^\alpha * 2^\alpha + 2^\alpha - 3^\alpha - 2^\alpha * 2^\alpha \\ &= (3^\alpha - 2^\alpha)(2^\alpha - 1) > 0. \end{aligned}$$

Hence H_1 (the comet $P_{n,3}$) has the second general Randić index.
(3) Let $\bar{T}$ be a tree with third minimum general Randić index. By Lemmas 2.1 and 2.2, we assert that $\bar{T}$ contains no vertex with degree bigger than 4, or two 4-degree vertices, or one 4-degree vertex and one 3-degree vertex. Hence $\bar{T}$ must be one of the following, which are shown in figure 5:

If $d(u_1) > 1$ or $d(u_2) > 1$, by Lemma 2.2, $R_\alpha(T_2) > R_\alpha(T_5)$. If $d(u_1) = d(u_2) = 1$, by Lemma 2.2, $R_\alpha(T_2) > R_\alpha(T_3)$. By the proof of (2), $R_\alpha(T_5) > R_\alpha(T_3)$. For T_6, if $d(v_1) > 1$ or $d(v_2) > 1$, by Lemma 2.2, $R_\alpha(T_6) > R_\alpha(T_5)$. So if $d(v_1) = d(v_2) = 1$, by Lemma 2.2, $R_\alpha(T_6) > R_\alpha(T_3)$. Therefore, $\bar{T}$ must be one of T_1, T_3, T_4.

$$\begin{aligned} R_\alpha(T_1) - R_\alpha(T_3) &= 3*4^\alpha + 8^\alpha + 2^\alpha - 2*6^\alpha - 3^\alpha - 2*2^\alpha \\ &= 8^\alpha + 3*4^\alpha - 2*6^\alpha - 3^\alpha - 2^\alpha. \end{aligned}$$

Let

$$\begin{aligned} f(x) &= 8^x + 3*4^x - 2*6^x - 3^x - 2^x, \quad x \geq 0, \\ f(0) &= 0, \\ f'(x) &= 3*8^x \ln 2 + 6*4^x \ln 2 - 2*6^x \ln 6 - 3^x \ln 3 - 2^x \ln 2 \end{aligned}$$

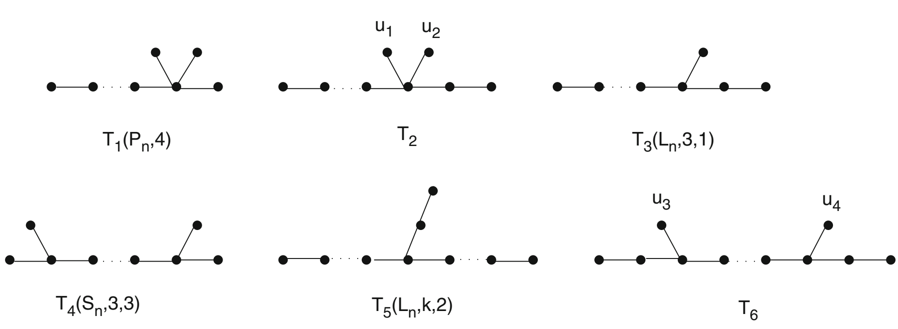

Figure 5. Trees possible with third minimum general Randić index.

$$
\begin{aligned}
&> 3*8^x \ln 2 + 6*4^x \ln 2 - 2*6^x \ln 6 - 3^x \ln 6 = g(x),\\
g(0) &= 3*\ln 2 + 6*\ln 2 - 2*\ln 6 - \ln 6 = \ln(2^9) - \ln(6^3) > 0.
\end{aligned}
$$

Since $(\ln 6)^2 < 7(\ln 2)^2$ and $\ln 6 * \ln 3 < 6*(\ln 2)^2$, then

$$
\begin{aligned}
g'(x) &= 9*8^x(\ln 2)^2 + 12*4^x(\ln 2)^2 - \ln 6(2*6^x \ln 6 - 3^x \ln 3)\\
&> (9*8^x + 12*4^x - 14*6^x - 6*3^x \ln 3)(\ln 2)^2\\
&> (9*8^x + 6*4^x - 14*6^x)(\ln 2)^2.
\end{aligned}
$$

Let $h(x) = 9*8^x + 6*4^x - 14*6^x$, $h(0) > 0$.

$$
\begin{aligned}
h'(x) &= 27*8^x*\ln 2 + 12*4^x \ln 2 - 14*6^x*\ln 6,\\
h''(x) &> 81*8^x*(\ln 2)^2 + 24*4^x*(\ln 2)^2 - 14*6^x*(\ln 6)^2,\\
h''(0) &= 81*(\ln 2)^2 + 24*(\ln 2)^2 - 14*(\ln 6)^2\\
&> 105*(\ln 2)^2 - 98(\ln 2)^2 > 0,\\
h'''(x) &> 243*8^x*(\ln 2)^3 - 14*6^x*(\ln 6)^3\\
&> (243*(\ln 2)^3 - 14*(\ln 6)^3)*8^x > 0.
\end{aligned}
$$

Therefore, $h(x) > 0$ for $x > 0$. Thus $f(x) > 0$ for $x > 0$. Hence $R_\alpha(T_1) > R_\alpha(T_3)$.

$$
\begin{aligned}
R_\alpha(T_4) - R_\alpha(T_3) &= 4*3^\alpha + 2*6^\alpha - (2*6^\alpha + 3^\alpha + 2*2^\alpha + 4^\alpha)\\
&= 3*3^\alpha - 4^\alpha - 2*2^\alpha
\end{aligned}
$$

It is easy to calculate that for μ approximately equal to 3.6457, if $\alpha > \mu$, $R_\alpha(T_4) > R_\alpha(T_3)$; otherwise, $R_\alpha(T_3) > R_\alpha(T_4)$. Therefore, if $\alpha > \mu$, $L_{n,k,1}$ $(k = 3, 4, \ldots, n-3)$ has third general Randić index. If $\alpha < \mu$, the quasi double star $QS_{3,3}$ has third general Randić index. □

3. The case for $\alpha < 0$

The following lemma is due to Wu and Zhang [7].

Lemma 3.1. *Suppose the star S_n, $n \geq 1$, is disjoint from a graph G with v as its center. For a vertex $u \in V(G)$, let $G_1 = G \cup S_n$, and G_2 be the graph obtained from G by attaching a star S_{n+1} to the vertex u with u as its center as shown in figure 6. If u is not an isolates vertex, then $R_\alpha(G_1) > R_\alpha(G_2)$ for $\alpha < 0$.*

Lemma 3.2. *The general Randić index of a double star $S_{p,q}$ $(p \leq q)$, i.e. $R_\alpha(S_{p,q}) = (p-1)p^\alpha + (q-1)q^\alpha + (pq)^\alpha$, is monotonously increasing for $-1 \leq \alpha < 0$ in p.*

Lemma 3.3. *The general Randić index of a double star $S_{p,q}(p \leq q)$, i.e. $R_\alpha(S_{p,q}) = (p-1)p^\alpha + (q-1)q^\alpha + (pq)^\alpha$, is monotonically decreasing for $\alpha < -2$ in p.*

Proof. Let $f(x) = x(x+1)^\alpha$. We may assume that $q > p+1$.

$$
\begin{aligned}
R_\alpha(S_{p,q}) - R_\alpha(S_{p+1,q-1}) &= (p-1)p^\alpha + (q-1)q^\alpha + (pq)^\alpha\\
&\quad - (p(p+1)^\alpha + (q-2)(q-1)^\alpha
\end{aligned}
$$

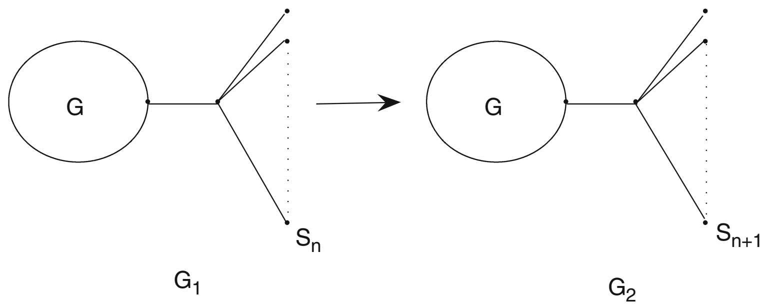

Figure 6. Transform G_1 to G_2.

$$
\begin{aligned}
&\quad + (p+1)^{\alpha}(q-1)^{\alpha})\\
&\geq ((q-1)q^{\alpha} - (q-2)(q-1)^{\alpha})\\
&\quad - (p(p+1)^{\alpha} - (p-1)p^{\alpha})\\
&= f'(\xi_1) - f'(\xi_2) p \leq \xi_2 \leq p+1 \leq q-1\\
&\leq \xi_1 \leq q)\\
&= f''(\xi_3)(\xi_1 - \xi_2)(\xi_2 \leq \xi_3 \leq \xi_1)\\
&= \alpha(\xi_3+1)^{\alpha-1}\left(2 + (\alpha-1)\frac{\xi_3}{\xi_3+1}\right).
\end{aligned}
$$

Since $2 \leq p \leq \xi_2 \leq \xi_3$ and $\alpha < -2$, $R_{\alpha}(S_{p,q}) > R_{\alpha}(S_{p+1,q-1})$, as asserted. □

Theorem 3.1. *Among trees with n vertices, $n \geq 7$, $\alpha < 0$, we have the following*:

(1) *The star S_n has minimum general Randić index*;
(2) *One double star has second general Randić index*; $S_{2,n-2}$ *has second general Randić index for* $-1 \leq \alpha < 0$; *the balanced double star has second minimum general Randić index for* $\alpha \leq -2$;
(3) $S_{3,n-3}$ *has third general Randić index for* $-1 \leq \alpha < 0$; $S_{\lfloor \frac{n}{2} \rfloor -1, \lceil \frac{n}{2} \rceil +1}$ *has third general Randić index for* $\alpha \leq -2$.

Proof.

(1) Assume that T_1 has minimum general Randić index and T_1 contains a path of length longer than 2. Let $P = v_1 v_2 \cdots v_t$ is a longest path in T with $t > 2$, $N(v_2)$ denotes the neighbour of v_2. Then $\{v_2\} \cup N(v_2) \setminus \{v_3\}$ induces a star S_d where $d = d(v_2)$. By contracting the edge $v_2 v_3$ and adding a new pendant vertex u as a neighbor of v_2, we get a new tree T'. By Lemma 3.1, $R_{\alpha}(T) > R_{\alpha}(T')$. Thus trees with minimum general Randić index contains no path of length longer than 2. Therefore, the star S_n has a minimum general Randić index.
(2) Let T_2 be a tree with second minimum general Randić index. We assert that T_2 contains no path with length longer than 3. Assuming the contrary, let $P = v_1 v_2 \cdots v_t$ be a longest path in T_2 with $t > 3$. Then we can contract the edge $v_2 v_3$ and add a new pendant vertex u as a neighbour of v_2 to get a new tree T_3. By Lemma 3.1, $R_{\alpha}(T_3) > R_{\alpha}(T_2)$. Obviously, $T_2 \ncong S_n$, a contradiction.

Hence T_1 contains no path with length longer than 3, hence T_1 must be a double star. For $-1 \leq \alpha < 0$, by Lemma 3.2, $S_{2,n-2}$ has second general Randić index. For $\alpha \leq -2$, by Lemma 3.3, the balanced double star has second minimum general Randić index.
(3) Let T_4 be a tree with third minimum general Randić index. By the analogous proof above, we can see that T_4 contains no path with length longer than 4. Then T_4 must be one of the trees in figure 7.

For T_6, if $d(w_i) > 1$ for some $i = 1, 2, \ldots, t$, by Lemma 3.1, we can contract $w_i u_3$ to get a new tree with its general Randić index smaller than $R_\alpha(T_6)$. Hence $d(w_1) = d(w_2) = \cdots = d(w_t) = 1$. We may assume that $d(u_2) \geq d(u_4)$. □

Case 1. $-1 \leq \alpha < 0$. If $d(u_2) > 2$, we can contract u_4u_3 to get a double star $S_{p,q}$ with $3 \leq p \leq q$. By Lemma 3.1, $R_\alpha(T_6) > R_\alpha(S_{p,q}) > R_\alpha(S_{2,n-2})$, a contradiction. Hence $d(u_2) = d(u_4) = 2$. If suffices to compare $R_\alpha(T_6)$ with $R_\alpha(S_{3,n-3})$. By Lemma 3.1, we have $R_\alpha(S_{3,n-3}) < R_\alpha(P_{n,n-3})$. Hence

$$\begin{aligned}
R_\alpha(T_6) - R_\alpha(S_{3,n-3}) &> R_\alpha(T_6) - R_\alpha(P_{n,n-3}) \\
&= 2 * 2^\alpha + (n-5)(n-3)^\alpha + 2 * (2(n-3))^\alpha \\
&\quad - (2^\alpha + 4^\alpha + (n-4)(n-3)^\alpha + (2(n-3))^\alpha) \\
&= 2^\alpha - 4^\alpha - (n-3)^\alpha + (2(n-3))^\alpha \\
&= 2^\alpha - 4^\alpha - (n-3)^\alpha(1 - 2^\alpha) \\
&\geq 2^\alpha - 4^\alpha - 4^\alpha + 8^\alpha \\
&\geq 2 * \sqrt{16}^\alpha - 2 * 4^\alpha = 0.
\end{aligned}$$

Hence $S_{3,n-3}$ has a third general Randić index for $-1 \leq \alpha < 0$.

Case 2. $\alpha < -1$. Assume that the double star $S_{a,b}$ has second minimum general Randić index and $d(u_2) \neq d(u_4)$ in T_6. If $d(u_2) \neq a$ and $d(u_2) \neq b$, then we can contract u_3u_4 to get a double star $S_{p,q}$ with $R_\alpha(T_6) > R_\alpha(S_{p,q})$ and $S_{p,q} \ncong S_{a,b}$. If $d(u_2) = a$, then $d(u_4) \neq a$ and $d(u_4) \neq b$. Then we can contract u_2u_3 to get a double star $\bar{S}_{p,q}$ with $R_\alpha(T_6) > R_\alpha(\bar{S}_{p,q})$ and $\bar{S}_{p,q} \ncong S_{a,b}$. If $d(u_2) = b$, then $d(u_4) \neq b$ and $d(u_4) \neq a$. Then we can also contract u_2u_3 to get a double star $\tilde{S}_{p,q}$ with $R_\alpha(T_6) > R_\alpha(\tilde{S}_{p,q})$ and

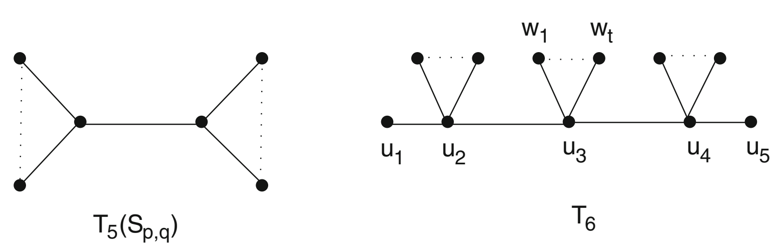

Figure 7. T_5 and T_6.

Table 1. Trees with first three smallest Randić index.

General Randić index	$\alpha > 0$	$-1 \leq \alpha < 0$	$-2 < \alpha < -1$	$\alpha \leq -2$
Minimum	Path	Star	Star	Star
Second minimum	$P_{n,3}$	$S_{2,n-2}$	One double star	Balanced double star
Third minimum	$L_{n,k,1}$ or $QS_{3,3}$	$S_{3,n-3}$	Double star or T_6 with $d(u_2) = d(u_4)$	T_6 with $d(u_2) = d(u_4)$ or double star

$\tilde{S}_{p,q} \ncong S_{a,b}$. Therefore, trees with third general Randić index for $\alpha \leq -1$ must be double stars or trees of the form T_6 with $d(u_2) = d(u_4)$.

Table 1 helps us draw the desired conclusions besides giving a clear picture.

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