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Minimum General Randić Index on Chemical Trees with Given Order and Number of Pendent Vertices*

Xueliang Li, Yongtang Shi and Lingping Zhong
Center for Combinatorics and LPMC
Nankai University, Tianjin 300071, P.R. China

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Abstract

The general Randić index $R_\alpha(G)$ of a (chemical) graph G, which is also called the connectivity index, is defined as the sum of the weights $(d(u)d(v))^\alpha$ of all edges uv of G, where $d(u)$ denotes the degree of a vertex u in G and α is an arbitrary real number. In this paper, we consider chemical trees (with maximum degree at most 4) with a given order and number of pendent vertices and determine the extremal trees with the minimum general Randić index for arbitrary α among this class of trees. For $\alpha > 1$ we also give a sharp lower bound of the general Randić index for general trees (without degree restriction) with a given order and number of pendent vertices.

Keywords: chemical tree, pendent vertex, linear programming

1 Introduction

For a (chemical) graph $G = (V, E)$, the *general Randić index* $R_\alpha(G)$ of G is defined as the sum of $(d(u)d(v))^\alpha$ over all edges uv of G, where $d(u)$ denotes the degree of a

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vertex u of G, i.e., $R_\alpha(G) = \sum_{uv\in E}(d(u)d(v))^\alpha$, where α is an arbitrary real number. This index was extensively studied in mathematical chemistry.

In 1975, chemist Milan Randić proposed a topological index $R_{-\frac{1}{2}}$ under the name "*branching index*", suitable for measuring the extent of branching of the carbon-atom skeleton of saturated hydrocarbons. 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. The research background of Randić index together with its generalization appears in chemistry or mathematical chemistry and can be found in the literature [1]-[3], [5]-[19]. There are also many results about trees with given order and number of pendent vertices, see [1, 9, 16]. For a comprehensive survey of its mathematical properties, see the book of Li and Gutman [14].

A *chemical tree* T is a tree with maximum degree at most 4. A vertex with degree one is called a *pendent vertex*. In [8], Gutman et al characterized the chemical trees with minimum, second-minimum, third-minimum, maximum, second-maximum and third-maximum values of the Randić index. There are also some results for extremal general Randić index values of chemical trees, see [15, 17, 19]. For chemical trees with both a given order and a given number of pendent vertices, Araujo and de la Peña [1] established the lower and upper bounds for $R_{-\frac{1}{2}}(T)$, i.e., for $\alpha = -\frac{1}{2}$. Later, Hansen and Mélot [9] improved this result. In the present paper, we determine the sharp lower bound for arbitrary α and give the extremal chemical trees. In addition, for $\alpha > 1$ we give a sharp lower bound for general trees (without degree restriction) with a given order and number of pendent vertices.

Let $P_s = v_0v_1\dots v_s$ be a path of a tree T with $d(v_1) = d(v_2) = \cdots = d(v_{s-1}) = 2$ (unless $s = 1$). If $d(v_0) = 1$ and $d(v_s) \geq 3$, then P_s is called a *pendent path* of T and s is the length of this pendent path. If $d(v_0)$, $d(v_s) \geq 3$, then P_s is called an *internal path* of T. A tree T is called a *generalized star*, if there is a unique vertex $u \in V(T)$, such that $d(u) \geq 3$ and for any other vertex v, $d(v) \leq 2$. If $v \in V$, we denote $N(v) = \{u : u \text{ is the neighbor of } v\}$. Similarly, if $S \subseteq V$, we denote $N(S) = \bigcup\limits_{v\in S} N(v)$. Undefined notations and terminologies can be found in [4].

If $n_1 = 2$, T is a path; on the other hand, if $n_1 = n-1$, then T is a star. Therefore, we can always assume $3 \leq n_1 \leq n-2$.

2 For $\alpha \leq -1$

Let $3 \leq n_1 \leq n-2$ and $\alpha \leq -1$. Denote $\psi(n, n_1) := n \cdot 4^\alpha + \frac{1}{3}(8^\alpha + 3 \cdot 6^\alpha - 4^{\alpha+1})n_1 + 5 \cdot 4^\alpha - 6^{\alpha+1}$.

Lemma 1 *For $\alpha \leq -1$, $3 \cdot 9^\alpha - 8^\alpha - 3 \cdot 6^\alpha - 2 \cdot 4^\alpha + 3 \cdot 3^\alpha > 0$, $3 \cdot 6^\alpha - 8^\alpha - 5 \cdot 4^\alpha + 3 \cdot 3^\alpha > 0$, $3 \cdot 8^\alpha + 5 \cdot 2^\alpha - 2 \cdot 4^\alpha - 6 \cdot 3^\alpha$ and $2 \cdot 4^\alpha - 3 \cdot 3^\alpha + 2^\alpha \geq 0$.*

Proof. By the Lagrange mean-value theorem, there exist $\xi \in (3, 4)$ and $\zeta \in (2, 3)$ such that $3^\alpha - 4^\alpha = -\alpha\xi^\alpha$ and $2^\alpha - 3^\alpha = -\alpha\zeta^\alpha$, respectively. Hence for $\alpha \leq -1$, we have $\frac{3^\alpha - 4^\alpha}{2^\alpha - 3^\alpha} = \frac{-\alpha\xi^\alpha}{-\alpha\zeta^\alpha} = (\frac{\xi}{\zeta})^\alpha > 2^\alpha$, i.e., $3^\alpha - 4^\alpha > 2^\alpha(2^\alpha - 3^\alpha)$. Thus,

$$\begin{aligned}
& 3 \cdot 9^\alpha - 8^\alpha - 3 \cdot 6^\alpha - 2 \cdot 4^\alpha + 3 \cdot 3^\alpha > 3[(3^\alpha - 4^\alpha) - 3^\alpha(2^\alpha - 3^\alpha)] \\
> \; & 3[2^\alpha(2^\alpha - 3^\alpha) - 3^\alpha(2^\alpha - 3^\alpha)] = 3(2^\alpha - 3^\alpha)^2 > 0. \\
& 3 \cdot 6^\alpha - 8^\alpha - 5 \cdot 4^\alpha + 3 \cdot 3^\alpha > 3(3^\alpha - 4^\alpha) - 2^{\alpha+1}(2^\alpha - 3^\alpha) \\
> \; & 3 \cdot 2^\alpha(2^\alpha - 3^\alpha) - 2^{\alpha+1}(2^\alpha - 3^\alpha) = 2^\alpha(2^\alpha - 3^\alpha) > 0. \\
& 3 \cdot 8^\alpha + 5 \cdot 2^\alpha - 2 \cdot 4^\alpha - 6 \cdot 3^\alpha = (2^\alpha - 3^\alpha)(5 - 3 \cdot 2^\alpha) - (3^\alpha - 4^\alpha)(3 \cdot 2^\alpha + 1) \\
> \; & (2^\alpha - 3^\alpha)(5 - 3 \cdot 2^\alpha) - (2^\alpha - 3^\alpha)(3 \cdot 2^\alpha + 1) = 2(2^\alpha - 3^\alpha)(2 - 3 \cdot 2^\alpha) > 0. \\
& 2 \cdot 4^\alpha - 3 \cdot 3^\alpha + 2^\alpha = \frac{1}{2}(4^{\alpha+1} - 2 \cdot 3^{\alpha+1} + 2^{\alpha+1}) \\
= \; & \frac{1}{2}\left((2^{\alpha+1} - 3^{\alpha+1}) - (3^{\alpha+1} - 4^{\alpha+1})\right) \geq 0.
\end{aligned}$$

∎

Theorem 1 *For $\alpha \leq -1$ and $3 \leq n_1 \leq n-2$, let T be a chemical tree of order n with n_1 pendent vertices. Then $R_\alpha(T) \geq \psi(n, n_1)$.*

Proof. We give our proof by induction on n_1.

If $n_1 = 3$, by easy calculations we can get the result. We assume that the result is valid for smaller values of $n_1 \geq 4$. Let u be a pendent vertex of T and $uv \in E(T)$. Then $d(v) \geq 2$.

Case 1. $d(v) = 2$.

We assume $N(v) = \{u, v_1\}$. Let $P = v_{-1}v_0v_1 \ldots v_s w$ $(u = v_{-1},\ v = v_0)$ be a pendent path with $d(w) = t \geq 3$. Let $T' = T \setminus \{v_{-1}, v_0, v_1, \ldots, v_{s-1}\}$. Then T is a chemical tree of order $n-s-1$ with n_1 pendent vertices, thus

$$\begin{aligned} R_\alpha(T) &= R_\alpha(T')+2^\alpha+s\cdot 4^\alpha+(2^\alpha-1)t^\alpha \\ &\geq (n-s-1)4^\alpha+\frac{1}{3}(8^\alpha+3\cdot 6^\alpha-4^{\alpha+1})n_1+5\cdot 4^\alpha-6^{\alpha+1} \\ &\quad +2^\alpha+s\cdot 4^\alpha+(2^\alpha-1)t^\alpha=\psi(n,n_1)+(1-2^\alpha)(2^\alpha-t^\alpha)>\psi(n,n_1). \end{aligned}$$

Case 2. $d(v)=3$.

Let $N(v)=\{u,x,y\}$ and $1=d(u)\leq d(x)\leq d(y)\leq 4$.

Subcase 2.1. $d(x)=1$, $d(y)\geq 3$.

Let $T'=T\setminus\{u,x\}$ and $d(y)=t$. Then T' is a chemical tree of order $n-2$ with n_1-1 pendent vertices, thus we have

$$\begin{aligned} & R_\alpha(T)=R_\alpha(T')+2\cdot 3^\alpha+(3^\alpha-1)t^\alpha \\ \geq\ & (n-2)4^\alpha+\frac{1}{3}(8^\alpha+3\cdot 6^\alpha-4^{\alpha+1})(n_1-1)+5\cdot 4^\alpha-6^{\alpha+1}+2\cdot 3^\alpha+(3^\alpha-1)t^\alpha \\ \geq\ & (n-2)4^\alpha+\frac{1}{3}(8^\alpha+3\cdot 6^\alpha-4^{\alpha+1})(n_1-1)+5\cdot 4^\alpha-6^{\alpha+1}+2\cdot 3^\alpha+(3^\alpha-1)3^\alpha \\ =\ & \psi(n,n_1)+\frac{1}{3}(3\cdot 9^\alpha-8^\alpha-3\cdot 6^\alpha-2\cdot 4^\alpha+3\cdot 3^\alpha)>\psi(n,n_1). \end{aligned}$$

The latter inequality follows from Lemma 1.

Subcase 2.2. $d(x)=1$, $d(y)=2$.

Let $P=v_0v_1\ldots v_{s-1}v_s$ be an internal path of T with $v=v_0, y=v_1$ and $d(v_s)=t\geq 3$ and let $T'=T\setminus\{u,x,v_0,v_1,\ldots,v_{s-2}\}$. Then T' is a chemical tree of order $n-s-1$ with n_1-1 pendent vertices, thus we have

$$\begin{aligned} R_\alpha(T) &= R_\alpha(T')+2\cdot 3^\alpha+6^\alpha+(s-2)4^\alpha+(2^\alpha-1)t^\alpha \\ &\geq (n-s-1)4^\alpha+\frac{1}{3}(8^\alpha+3\cdot 6^\alpha-4^{\alpha+1})(n_1-1)+5\cdot 4^\alpha-6^{\alpha+1} \\ &\quad +2\cdot 3^\alpha+6^\alpha+(s-2)4^\alpha+(2^\alpha-1)3^\alpha \\ &= \psi(n,n_1)+\frac{1}{3}(3\cdot 6^\alpha-8^\alpha-5\cdot 4^\alpha+3\cdot 3^\alpha)>\psi(n,n_1). \end{aligned}$$

The latter inequality follows from Lemma 1.

Subcase 2.3. $d(x)=r\geq 2$, $d(y)=t\geq 2$.

Let $T' = T - u$. Then T' is a chemical tree of order $n-1$ with $n_1 - 1$ pendent vertices, thus we have

$$\begin{aligned}R_\alpha(T) =& R_\alpha(T') + 3^\alpha + (3^\alpha - 2^\alpha)(r^\alpha + t^\alpha) \geq (n-1)4^\alpha + \frac{1}{3}(8^\alpha + 3\cdot 6^\alpha - 4^{\alpha+1})(n_1 - 1)\\ &+ 5\cdot 4^\alpha - 6^{\alpha+1} + 3^\alpha + (3^\alpha - 2^\alpha)(2^\alpha + 2^\alpha)\\ =& \psi(n, n_1) + \frac{1}{3}(3\cdot 6^\alpha - 8^\alpha - 5\cdot 4^\alpha + 3\cdot 3^\alpha) > \psi(n, n_1).\end{aligned}$$

The latter inequality follows from Lemma 1.

Case 3. $d(v) = 4$.

Let $N(v) = \{x, y, z, u\}$ and $1 = d(u) \leq d(x) \leq d(y) \leq d(z) \leq 4$.

Subcase 3.1. $d(x) = d(y) = 1, d(z) \geq 2$.

If $d(z) = 2$, let $P = v_0 v_1 \ldots v_{s-1} v_s$ be an internal path of T with $v = v_0, z = v_1$ and $d(v_s) \geq 3$. Now we consider two cases:

(a) If $d(v_s) = 3$, by Case 2 we can assume that $N(v_s) = \{v_{s-1}, w_1, w_2\}$ with $d(w_1) = r \geq 2, d(w_2) = t \geq 2$. Construct $T' = T \setminus \{u, x, y, v_0, v_1, \ldots, v_{s-1}\}$. Then T' is a chemical tree of order $n-s-3$ with $n_1 - 3$ pendent vertices, so we have

$$\begin{aligned}R_\alpha(T) &= R_\alpha(T') + (s+1)4^\alpha + 8^\alpha + 6^\alpha + (3^\alpha - 2^\alpha)(r^\alpha + t^\alpha)\\ &\geq (n-s-3)4^\alpha + \frac{1}{3}(8^\alpha + 3\cdot 6^\alpha - 4^{\alpha+1})(n_1 - 3) + 5\cdot 4^\alpha - 6^{\alpha+1}\\ &\quad +(s+1)4^\alpha + 8^\alpha + 6^\alpha + (3^\alpha - 2^\alpha)(2^\alpha + 2^\alpha) = \psi(n, n_1).\end{aligned}$$

(b) If $d(v_s) = 4$, let $T' = T \setminus \{u, x, y, v_0, v_1, \ldots, v_{s-2}\}$, then T' is a chemical tree of order $n-s-2$ with $n_1 - 2$ pendent vertices, thus we have

$$\begin{aligned}R_\alpha(T) &= R_\alpha(T') + 3\cdot 4^\alpha + 8^\alpha + (s-2)4^\alpha + 8^\alpha - 4^\alpha\\ &\geq (n-s-2)4^\alpha + \frac{1}{3}(8^\alpha + 3\cdot 6^\alpha - 4^{\alpha+1})(n_1 - 2) + 5\cdot 4^\alpha - 6^{\alpha+1}\\ &\quad +3\cdot 4^\alpha + 8^\alpha + (s-2)4^\alpha + 8^\alpha - 4^\alpha\\ &\geq \psi(n, n_1) + \frac{1}{3}\cdot 2^{\alpha+1}(2\cdot 4^\alpha - 3\cdot 3^\alpha + 2^\alpha) \geq \psi(n, n_1).\end{aligned}$$

The latter inequality follows from Lemma 1.

If $d(z) = 3$, by Case 2 we can assume that $N(z) = \{v, w_1, w_2\}$ with $d(w_1) = r \geq 2, d(w_2) = t \geq 2$. Let $T' = T \setminus \{u, v, x, y\}$, then

$$\begin{aligned} R_\alpha(T) &= R_\alpha(T') + 3 \cdot 4^\alpha + 12^\alpha + (3^\alpha - 2^\alpha)(r^\alpha + t^\alpha) \\ &\geq (n-4)4^\alpha + \frac{1}{3}(8^\alpha + 3 \cdot 6^\alpha - 4^{\alpha+1})(n_1 - 3) + 5 \cdot 4^\alpha - 6^{\alpha+1} \\ &\quad +3 \cdot 4^\alpha + 12^\alpha + (3^\alpha - 2^\alpha)(2^\alpha + 2^\alpha) \\ &\geq \psi(n, n_1) + 2^\alpha(1 - 2^\alpha)(2^\alpha - 3^\alpha) > \psi(n, n_1). \end{aligned}$$

If $d(z) = 4$, construct $T' = T \setminus \{x, y, u\}$, then

$$\begin{aligned} R_\alpha(T) =& R_\alpha(T') + 3 \cdot 4^\alpha + 16^\alpha - 4^\alpha \\ \geq& (n-3)4^\alpha + \frac{1}{3}(8^\alpha + 3 \cdot 6^\alpha - 4^{\alpha+1})(n_1 - 2) + 5 \cdot 4^\alpha - 6^{\alpha+1} + 2 \cdot 4^\alpha + 16^\alpha \\ \geq& \psi(n, n_1) + \frac{2^\alpha}{3}(3 \cdot 8^\alpha + 5 \cdot 2^\alpha - 2 \cdot 4^\alpha - 6 \cdot 3^\alpha) > \psi(n, n_1). \end{aligned}$$

The latter inequality follows from Lemma 1.

Subcase 3.2. $d(x) = 1$, $d(y) = r \geq 2$, $d(z) = t \geq 2$.

Let $T' = T \setminus \{u, x\}$. Then T' is a chemical tree of order $n - 2$ with $n_1 - 2$ pendent vertices, thus we have

$$\begin{aligned} R_\alpha(T) &= R_\alpha(T') + 2 \cdot 4^\alpha + (4^\alpha - 2^\alpha)(r^\alpha + t^\alpha) \\ &\geq (n-2)4^\alpha + \frac{1}{3}(8^\alpha + 3 \cdot 6^\alpha - 4^{\alpha+1})(n_1 - 2) + 5 \cdot 4^\alpha - 6^{\alpha+1} \\ &\quad +2 \cdot 4^\alpha + (4^\alpha - 2^\alpha)(r^\alpha + t^\alpha) \\ &\geq (n-2)4^\alpha + \frac{1}{3}(8^\alpha + 3 \cdot 6^\alpha - 4^{\alpha+1})(n_1 - 2) + 5 \cdot 4^\alpha - 6^{\alpha+1} \\ &\quad +2 \cdot 4^\alpha + (4^\alpha - 2^\alpha)(2^\alpha + 2^\alpha) \\ &= \psi(n, n_1) + \frac{1}{3} \cdot 2^{\alpha+1}(2 \cdot 4^\alpha - 3 \cdot 3^\alpha + 2^\alpha) > \psi(n, n_1). \end{aligned}$$

The latter inequality follows from Lemma 1.

Subcase 3.3. $d(x) = r \geq 2$, $d(y) = t \geq 2$, $d(z) = \ell \geq 2$.

Let $T' = T - u$. Then T' is a chemical tree of order $n-1$ with $n_1 - 1$ pendent vertices, thus we have

$$\begin{aligned}
R_\alpha(T) &= R_\alpha(T') + 4^\alpha + (4^\alpha - 3^\alpha)(r^\alpha + t^\alpha + \ell^\alpha) \\
&\geq (n-1)4^\alpha + \frac{1}{3}(8^\alpha + 3\cdot 6^\alpha - 4^{\alpha+1})(n_1 - 1) + 5\cdot 4^\alpha - 6^{\alpha+1} \\
&\quad +4^\alpha + (4^\alpha - 3^\alpha)(r^\alpha + t^\alpha + \ell^\alpha) \\
&\geq (n-1)4^\alpha + \frac{1}{3}(8^\alpha + 3\cdot 6^\alpha - 4^{\alpha+1})(n_1 - 1) + 5\cdot 4^\alpha - 6^{\alpha+1} \\
&\quad +4^\alpha + (4^\alpha - 3^\alpha)(2^\alpha + 2^\alpha + 2^\alpha) \\
&= \psi(n, n_1) + \frac{1}{3}\cdot 2^{\alpha+2}(2\cdot 4^\alpha - 3\cdot 3^\alpha + 2^\alpha) > \psi(n, n_1).
\end{aligned}$$

The latter inequality follows from Lemma 1. The proof is now complete. ∎

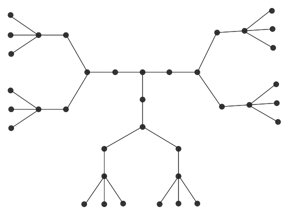

Figure 2.1 An extremal chemical tree for Theorem 1.

Remark. In Figure 2.1, we give a graph for showing that the bound in Theorem 1 is sharp.

3 For $\alpha \geq 1$

Let $\mathcal{T}_{n,n_1}$={T: T is a tree with n vertices and n_1 pendent vertices, $3 \leq n_1 \leq n-2$}. Denote $\mathcal{T}_{n_1}$={T: $T \in \mathcal{T}_{n,n_1}$ and T is a generalized star}. A *comet* $CS(n, n_1)$ of order n with n_1 pendent vertices is a tree formed by a path P_{n-n_1} of which one end vertex coincides with a pendent vertex of a star S_{n_1+1}.

For $T \in \mathcal{T}_{n,n_1}$, denote $V_0(T) := \{v : v$ is a pendent vertex of $T\}$. Let $\mathcal{P}(T)$ be the set of pendent paths in T. Let $\mathcal{T}^3_{n_1}$:={T is a tree with n_1 pendent vertices and for any vertex v in $V(T)\backslash V_0(T)$, $d_T(v) = 3$}. Denote by $\mathcal{T}^3_{n,n_1}$ the set of trees of order n

obtained from $T \in \mathcal{T}_{n_1}^3$ by replacing each non-pendent edge by a path of length at least 2.

Lemma 2 *For $\alpha \geq 1$, if $T \in \mathcal{T}_{n,n_1}$ and $R_\alpha(T)$ is as small as possible, then $|\mathcal{P}(T)| \leq 1$.*

Proof. Assume $P = u_0u_1 \dots u_s$ and $Q = v_0v_1 \dots v_t$ $(s, t \geq 2)$ are two pendent paths of T with $u_0, v_0 \in V_0(T)$. Let $T' = T - u_{s-1}u_{s-2} + u_0v_0$. Then $T' \in \mathcal{T}_{n,n_1}$. Let $d(u_s) = r \geq 3$, then

$$R_\alpha(T') - R_\alpha(T) = (1 - 2^\alpha)(r^\alpha - 2^\alpha) < 0,$$

a contradiction. ∎

Lemma 3 *For $\alpha \geq 1$, if $T \in \mathcal{T}_{n,n_1} \backslash \mathcal{T}_{n_1}$ and $R_\alpha(T)$ is as small as possible, then $\mathcal{P}(T) = \emptyset$.*

Proof. By Lemma 2, $|\mathcal{P}(T)| \leq 1$. Suppose $|\mathcal{P}(T)| = 1$, and let $P = v_0v_1 \dots v_s (s \geq 2)$ be a pendent path of T such that $v_0 \in V_0(T)$ and $d(v_s) = r \geq 3$. Since $T \notin \mathcal{T}_{n_1}$, there must exist a vertex $w \in V(T) \backslash \{v_s\}$ with $d(w) \geq 3$. Further, let P' be the unique path between v_s and w. If u is the vertex of P' adjacent to v_s, let $d(u) = t \geq 2$ and set $T' = T - v_su - v_0v_1 + v_0v_s + v_1u$, then

$$R_\alpha(T') - R_\alpha(T) = r^\alpha + 2^\alpha t^\alpha - 2^\alpha - r^\alpha t^\alpha = (r^\alpha - 2^\alpha)(1 - t^\alpha) < 0,$$

contradicting to the choice of T. ∎

Lemma 4 *Let $T \in \mathcal{T}_{n_1}$ and $\alpha \geq 1$. Then*

$$R_\alpha(T) \geq (n_1 + 2^\alpha - 1)n_1^\alpha + (n - n_1 - 2)4^\alpha + 2^\alpha$$

with equality if and only if $T \cong CS(n, n_1)$.

Proof. Note that if $T \cong CS(n, n_1)$, then the inequality holds.

We choose $T' \in \mathcal{T}_{n_1}$ so that $R_\alpha(T')$ is as small as possible. Since $T' \ncong K_{1,n_1}$, we have $\mathcal{P}(T') \neq \emptyset$. By Lemma 2, $|\mathcal{P}(T')| = 1$. Therefore, $T' \cong CS(n, n_1)$ since T' is a generalized star. Then, for any $T \in \mathcal{T}_{n_1}$,

$$R_\alpha(T) \geq R_\alpha(T') \geq (n_1 + 2^\alpha - 1)n_1^\alpha + (n - n_1 - 2)4^\alpha + 2^\alpha.$$ ∎

Let $3 \leq n_1 \leq n - 2$ and $\alpha \geq 1$, and denote $\varphi(n, n_1) := n \cdot 4^\alpha + (3^\alpha + 2 \cdot 6^\alpha - 3 \cdot 4^\alpha)n_1 + 5 \cdot 4^\alpha - 6^{\alpha+1}$.

Theorem 2 *Let $3 \leq n_1 \leq n-2$ and $\alpha \geq 1$. If $T \in \mathcal{T}_{n,n_1}$, then*

$$R_\alpha(T) \geq \begin{cases} n \cdot 4^\alpha + 6^\alpha - 5 \cdot 4^\alpha + 2 \cdot 3^\alpha + 2^\alpha & if\ n_1 = 3 \\ \varphi(n, n_1) & if\ 4 \leq n_1 \leq n-2 \end{cases} \tag{1}$$

In (1), if $n_1 = 3$, the equality holds if and only if $T \cong CS(n,3)$; if $4 \leq n_1 \leq n-2$, the equality holds if and only if $n \geq 3n_1 - 5$ and $T \in \mathcal{T}^3_{n,n_1}$.

Proof. Let $T \in \mathcal{T}_{n_1}$, by Lemma 4 we have

$$R_\alpha(T) \geq (n_1 + 2^\alpha - 1)n_1^\alpha + (n - n_1 - 2)4^\alpha + 2^\alpha,$$

so if $n_1 = 3$,

$$R_\alpha(T) \geq 4^\alpha n + 6^\alpha - 5 \cdot 4^\alpha + 2 \cdot 3^\alpha + 2^\alpha$$

with equality holds if and only if $T \cong CS(n,3)$.

If $4 \leq n_1 \leq n-2$, then by some calculations we can prove

$$\begin{aligned} & R_\alpha(T) \geq (n_1 + 2^\alpha - 1)n_1^\alpha + (n - n_1 - 2)4^\alpha + 2^\alpha \\ = \ & \varphi(n, n_1) + (n_1 + 2^\alpha - 1)n_1^\alpha + (-2 \cdot 6^\alpha - 3^\alpha + 2 \cdot 4^\alpha)n_1 + (6^{\alpha+1} - 7 \cdot 4^\alpha + 2^\alpha). \end{aligned}$$

Denote $f(n_1, \alpha) = (n_1 + 2^\alpha - 1)n_1^\alpha + (-2 \cdot 6^\alpha - 3^\alpha + 2 \cdot 4^\alpha)n_1 + (6^{\alpha+1} - 7 \cdot 4^\alpha + 2^\alpha)$, then

$$\begin{aligned} \frac{\partial f(n_1, \alpha)}{\partial n_1} &= (\alpha+1)n_1^\alpha + \alpha n_1^{\alpha-1}(2^\alpha - 1) + (-2 \cdot 6^\alpha - 3^\alpha + 2 \cdot 4^\alpha) \\ &\geq (\alpha+1)4^\alpha + \alpha(2^\alpha - 1)4^{\alpha-1} + (-2 \cdot 6^\alpha - 3^\alpha + 2 \cdot 4^\alpha) \\ &= \left(\frac{3}{4}\alpha + 3\right)4^\alpha + \frac{\alpha}{4} \cdot 8^\alpha - 2 \cdot 6^\alpha - 3^\alpha > 3 \cdot 4^\alpha + \frac{\alpha}{4} \cdot 8^\alpha - 2 \cdot 6^\alpha > 0, \end{aligned}$$

i.e., $f(n_1, \alpha)$ is increasing in n_1. Therefore $f(n_1, \alpha) \geq f(4, \alpha) = (8^\alpha - 6^\alpha) - (6^\alpha - 4^\alpha) + 3(4^\alpha - 3^\alpha) - (3^\alpha - 2^\alpha) > 0$. So we have $R_\alpha(T) > \varphi(n, n_1)$.

In view of this, we assume that $T \in \mathcal{T}_{n,n_1} \backslash \mathcal{T}_{n_1}$ and $4 \leq n_1 \leq n-2$.

Note that if $T \in \mathcal{T}^3_{n,n_1}$, then $n \geq 3n_1 - 5$ and the theorem is verified by elementary calculations. We will prove that if $T \in \mathcal{T}_{n,n_1} \backslash \mathcal{T}_{n_1}$, then the theorem holds by induction on n_1. We choose T such that $R_\alpha(T)$ is as small as possible.

If $n_1 = 4$, then by Lemma 3, $T \in \mathcal{T}^3_4$ for $n = 6$ or $T \in \mathcal{T}^3_{n,4}$ for $n \geq 7$. Hence

$$R_\alpha(T) = \begin{cases} 4 \cdot 3^\alpha + 9^\alpha > \varphi(n, n_1) & if\ n = 6 \\ 4 \cdot 3^\alpha + 2 \cdot 6^\alpha + (n-7)4^\alpha = \varphi(n, n_1) & if\ n \geq 7 \end{cases}$$

Therefore, we assume that $n_1 \geq 5$ and the result holds for smaller values of n_1. Let $u \in N(V_0(T))$ and $d(u) = t$, and let $v_1, \ldots, v_r$ and $v_{r+1}, \ldots, v_t$ be the pendent and non-pendent neighbors of u, respectively. Then $t - r \geq 1$ (because $T \not\cong K_{1,n-1}$).

Case 1. $t \geq 4$.

Let $T' = T - v_1$. Then $T' \in \mathcal{T}_{n-1,n_1-1}$. Suppose $d(v_i) = d_i$ for $i = r+1, \ldots, t$. Then

$$\begin{aligned}
R_\alpha(T) &= R_\alpha(T') + t^\alpha + (r-1)[t^\alpha - (t-1)^\alpha] + [t^\alpha - (t-1)^\alpha]\sum_{i=1}^{t-r} d_i^\alpha \\
&\geq \varphi(n-1, n_1-1) + t^\alpha + (r-1)[t^\alpha - (t-1)^\alpha] + 2^\alpha(t-r)[t^\alpha - (t-1)^\alpha] \\
&= \varphi(n, n_1) - 3^\alpha - 2\cdot 6^\alpha + 2\cdot 4^\alpha + t^\alpha + [t^\alpha - (t-1)^\alpha][2^\alpha(t-r) + r - 1] \\
&\geq \varphi(n, n_1) - 3^\alpha - 2\cdot 6^\alpha + 2\cdot 4^\alpha + 4^\alpha + (4^\alpha - 3^\alpha)(3^\alpha + 2) \\
&= \varphi(n, n_1) + (4^\alpha - 3^\alpha)(3^\alpha + 3) - 2^{\alpha+1}(3^\alpha - 2^\alpha) \\
&\geq \varphi(n, n_1) + (3^\alpha - 2^\alpha)(3^\alpha + 3 - 2^{\alpha+1}) > \varphi(n, n_1).
\end{aligned}$$

Case 2. $t = 3$.

Subcase 2.1. $r = 1$.

Let $N(u)\backslash\{v_1\} = \{x_1, x_2\}$ and $d(x_i) = d_i$. Let $T' = T - v_1$, then $T' \in \mathcal{T}_{n-1,n_1-1}$ and

$$\begin{aligned}
R_\alpha(T) &= R_\alpha(T') + 3^\alpha + (d_1^\alpha + d_2^\alpha)(3^\alpha - 2^\alpha) \\
&\geq \varphi(n-1, n_1-1) + 3^\alpha + 2^{\alpha+1}(3^\alpha - 2^\alpha) = \varphi(n, n_1)
\end{aligned}$$

Equality holds only if $d_1 = d_2 = 2$ and $R_\alpha(T') = \varphi(n-1, n_1-1)$. By the induction hypothesis, $T' \in \mathcal{T}^3_{n-1,n_1-1}$. Since $d_1 = d_2 = 2$, there is an internal path of length at least 4 which connects x_1 and x_2 in T' and $|V(T')| \geq 3(n_1-1) + 2 - 5$.

Thus, $n = |V(T')| + 1 \geq 3n_1 - 5$ and $T \in \mathcal{T}^3_{n,n_1}$.

Subcase 2.2. $r = 2$.

Let $N(u)\backslash\{v_1, v_2\} = \{x_1\}$. Suppose $P = u_0u_1\ldots u_t, u = u_0$ $(x_1 = u_1)$ be an internal path of T with $d(u) = 3$ and $d(u_t) = s \geq 3$, where $t \geq 1$.

If $t = 1$, let $T' = T \setminus \{v_1, v_2\}$, $T' \in \mathcal{T}_{n-2,n_1-1}$, then

$$\begin{aligned} R_\alpha(T) &= R_\alpha(T') + 2 \cdot 3^\alpha + (3^\alpha - 1)s^\alpha \\ &\geq \varphi(n-2, n_1-1) + 2 \cdot 3^\alpha + (3^\alpha - 1)s^\alpha \\ &= \varphi(n, n_1) + 3^\alpha + 4^\alpha - 2 \cdot 6^\alpha + (3^\alpha - 1)s^\alpha \\ &\geq \varphi(n, n_1) + 9^\alpha + 4^\alpha - 2 \cdot 6^\alpha > \varphi(n, n_1). \end{aligned}$$

If $t \geq 2$, let $T' = T \setminus \{v_1, v_2, u_0, u_1, \ldots, u_{t-2}\}$, $T' \in \mathcal{T}_{n-t-1,n_1-1}$, then

$$\begin{aligned} R_\alpha(T) &= R_\alpha(T') + 4^\alpha(t-2) + 6^\alpha + 2 \cdot 3^\alpha + (2^\alpha - 1)s^\alpha \\ &\geq \varphi(n-t-1, n_1-1) + 4^\alpha(t-2) + 6^\alpha + 2 \cdot 3^\alpha + (2^\alpha - 1)s^\alpha \\ &= \varphi(n, n_1) + 3^\alpha - 6^\alpha + (2^\alpha - 1)s^\alpha \\ &= \varphi(n, n_1) + (2^\alpha - 1)(s^\alpha - 3^\alpha) \geq \varphi(n, n_1). \end{aligned}$$

Equality holds only if $R_\alpha(T') = \varphi(n-t-1, n_1-1)$ and $s = 3$. By the induction hypothesis, $T' \in \mathcal{T}^3_{n-t-1,n_1-1}$ and $|V(T')| \geq 3(n_1-1) - 5$. Thus, $n = |V(T')| + t + 1 \geq 3n_1 - 5$ and $T \in \mathcal{T}^3_{n,n_1}$. The proof is complete. ∎

For $T = CS(n,3)$ or $T \in \mathcal{T}^3_{n,n_1}$, the maximum degree of T is 3, then Theorem 2 also holds for chemical trees.

Corollary 1 *Let $3 \leq n_1 \leq n-2$ and $\alpha \geq 1$. If T is a chemical tree with n_1 pendent vertices, then*

$$R_\alpha(T) \geq \begin{cases} n \cdot 4^\alpha + 6^\alpha - 5 \cdot 4^\alpha + 2 \cdot 3^\alpha + 2^\alpha & if\ n_1 = 3 \\ \varphi(n, n_1) & if\ 4 \leq n_1 \leq n-2 \end{cases} \tag{2}$$

In (2), if $n_1 = 3$, the equality holds if and only if $T \cong CS(n,3)$; if $4 \leq n_1 \leq n-2$, the equality holds if and only if $n \geq 3n_1 - 5$ and $T \in \mathcal{T}^3_{n,n_1}$.

4 For $-1 < \alpha < 0$ and $0 < \alpha < 1$

In [9], the authors introduced one class of chemical trees $L_e(n, n_1)$, which were founded by the system *AutoGraphix (AGX)* of Caporossi and Hansen (further papers describing mathematical applications of *AGX* are in [6], [7]). The structure of $L_e(n, n_1)$ (n_1 is even) is depicted in Figure 4.1. These trees are composed of subgraphs that are

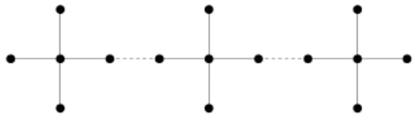

Figure 4.1 Structure of $L_e(n, n_1)$.

stars S_5 , and these stars are connected by paths (the dotted lines in the figure), whose lengths can be 0. The Randić index of $L_e(n, n_1)$ is

$$R(L_e(n, n_1)) = \frac{n}{2} + \frac{n_1}{2}\left(\frac{1}{\sqrt{2}} - 1\right) + \frac{3}{2} - \sqrt{2}\ .$$

Let T be a chemical tree with n vertices and n_1 pendent vertices. Denote by $x_{i,j}$ the number of edges joining the vertices of degrees i and j, and n_i the number of vertices of degree i in T. Then, we have another description for the Randić index of T,

$$R_\alpha(T) = \sum_{1 \le i \le j \le 4} x_{ij} \cdot (ij)^\alpha\ . \tag{1}$$

Note that $x_{11} = 0$ whenever $n \ge 3$, and therefore the case $i = j = 1$ needs not be considered any further. Consequently, the right-hand side of (1) is a linear function of the following nine variables $x_{12}\, , x_{13}\, , x_{14}\, , x_{22}\, , x_{23}\, , x_{24}\, , x_{33}\, , x_{34}\, , x_{44}$. Then

$$n_1 + n_2 + n_3 + n_4 = n\ . \tag{2}$$

Counting the edges terminating at vertices of degree i , we obtain for $i = 1, 2, 3, 4$

$$x_{12} + x_{13} + x_{14} = n_1 \tag{3}$$

$$x_{12} + 2x_{22} + x_{23} + x_{24} = 2n_2 \tag{4}$$

$$x_{13} + x_{23} + 2x_{33} + x_{34} = 3n_3 \tag{5}$$

$$x_{14} + x_{24} + x_{34} + 2x_{44} = 4n_4\ . \tag{6}$$

Another linearly independent relation of this kind is

$$n_1 + 2n_2 + 3n_3 + 4n_4 = 2m = 2(n-1)\ . \tag{7}$$

Now we will solve the linear programming

$$min\ \ R_\alpha(T) = \sum_{1 \le i \le j \le 4} x_{ij} \cdot (ij)^\alpha$$

with constraints (2) – (7).

Theorem 3 *Let T be a chemical tree of order n with $n_1 \geq 5$ pendent vertices. Then for $-1 < \alpha < 0$,*

$$R_\alpha(T) \geq n \cdot 4^\alpha + (8^\alpha - 4^\alpha)n_1 + 3 \cdot 4^\alpha - 4 \cdot 8^\alpha$$

with equality if and only if n_1 is even and $T \cong L_e(n, n_1)$.

Proof. By some calculations, we have

$$x_{22} = \frac{2n - 5n_1 + 6}{2} - \frac{1}{2}x_{12} + \frac{1}{6}x_{13} + \frac{1}{2}x_{14} - \frac{1}{3}x_{23} + \frac{1}{3}x_{33} + \frac{2}{3}x_{34} + x_{44} \qquad (8)$$

$$x_{24} = 2n_1 - 4 - \frac{2}{3}x_{13} - x_{14} - \frac{2}{3}x_{23} - \frac{4}{3}x_{33} - \frac{5}{3}x_{34} - 2x_{44} \qquad (9)$$

Substituting (8) and (9) into (1), we have

$$\begin{aligned} R(T) &= \left(n - \frac{5}{2}n_1 + 3\right)4^\alpha + (2n_1 - 4)8^\alpha + c_{12}x_{12} + c_{13}x_{13} + c_{14}x_{14} \\ &\quad + c_{23}x_{23} + c_{33}x_{33} + c_{34}x_{34} + c_{44}x_{44} \\ &= \left(n - \frac{5}{2}n_1 + 3\right)4^\alpha + (2n_1 - 4)8^\alpha + \left(2^\alpha - \frac{1}{2}4^\alpha\right)x_{12} + \left(3^\alpha + \frac{1}{6}4^\alpha - \frac{2}{3}8^\alpha\right)x_{13} \\ &\quad + \left(\frac{3}{2}4^\alpha - 8^\alpha\right)x_{14} + \left(6^\alpha - \frac{1}{3}4^\alpha - \frac{2}{3}8^\alpha\right)x_{23} + \left(9^\alpha + \frac{1}{3}4^\alpha - \frac{4}{3}8^\alpha\right)x_{33} \\ &\quad + \left(12^\alpha + \frac{2}{3}4^\alpha - \frac{5}{3}8^\alpha\right)x_{34} + (16^\alpha + 4^\alpha - 2 \cdot 8^\alpha)x_{44} \qquad (10) \end{aligned}$$

Because all coefficients c_{ij} on the right-hand side of (10) are positive-valued for $-1 < \alpha < 0$, it is clear that for fixed n and n_1, $R(T)$ will be minimum if the parameters x_{12}, x_{13}, x_{14}, x_{23}, x_{33}, x_{34} and x_{44} are all equal to zero (provided this is possible). However, a tree must have at least two pendent vertices, and so we have

$$x_{12} + x_{13} + x_{14} > 0. \qquad (11)$$

Since $c_{14} < c_{13} < c_{12}$, considering the minimum of $R(T)$, the best solution of (11) is that all pendent vertices are adjacent to vertices with degree 4, i.e., $x_{14} = n_1$.

Thus, we get

$$\begin{aligned} R(T) &\geq \left(n - \frac{5}{2}n_1 + 3\right)4^\alpha + (2n_1 - 4)8^\alpha + \left(\frac{3}{2}4^\alpha - 8^\alpha\right)n_1 \\ &= 4^\alpha n + (8^\alpha - 4^\alpha)n_1 + 3 \cdot 4^\alpha - 4 \cdot 8^\alpha \end{aligned}$$

with equality if and only if $x_{12} = x_{13} = x_{23} = x_{33} = x_{34} = x_{44} = 0$, $x_{14} = n_1$ and $n_3 = 0$. The proof is complete. ∎

Theorem 4 *Let T be a chemical tree of order n with $n_1 \geq 5$ pendent vertices. Then for $0 < \alpha < 1$,*

$$R_\alpha(T) \geq n \cdot 4^\alpha + (3^\alpha + 2 \cdot 6^\alpha - 3 \cdot 4^\alpha)n_1 + 5 \cdot 4^\alpha - 6^{\alpha+1},$$

with equality if and only if $T \in \mathcal{T}^3_{n,n_1}$.

Proof. By some calculations, we have

$$x_{22} = n - n_1 + 5 - 3x_{12} - 2x_{13} - \frac{3}{2}x_{14} + \frac{1}{2}x_{24} + x_{33} + \frac{3}{2}x_{34} + 2x_{44} \tag{12}$$

$$x_{23} = -6 + 3x_{12} + 2x_{13} + \frac{3}{2}x_{14} - \frac{3}{2}x_{24} - 2x_{33} - \frac{5}{2}x_{34} - 3x_{44} \tag{13}$$

Substituting (12) and (13) into (1), we have

$$\begin{aligned} R(T) &= (n - n_1 + 5)4^\alpha - 6^{\alpha+1} + c_{12}x_{12} + c_{13}x_{13} + c_{14}x_{14} \\ &\quad + c_{23}x_{23} + c_{33}x_{33} + c_{34}x_{34} + c_{44}x_{44} \\ &= (n - n_1 + 5)4^\alpha - 6^{\alpha+1} + (2^\alpha - 3 \cdot 4^\alpha + 3 \cdot 6^\alpha)x_{12} + (3^\alpha - 2 \cdot 4^\alpha + 2 \cdot 6^\alpha)x_{13} \\ &\quad + \left(-\frac{1}{2}4^\alpha + \frac{3}{2}6^\alpha\right)x_{14} + \left(\frac{1}{2}4^\alpha - \frac{3}{2}6^\alpha + 8^\alpha\right)x_{24} + (4^\alpha - 2 \cdot 6^\alpha + 9^\alpha)x_{33} \\ &\quad + \left(\frac{3}{2}4^\alpha - \frac{5}{2}6^\alpha + 12^\alpha\right)x_{34} + (2 \cdot 4^\alpha - 3 \cdot 6^\alpha + 16^\alpha)x_{44}. \end{aligned} \tag{14}$$

Because all coefficients c_{ij} on the right-hand side of (14) are positive-valued for $0 < \alpha < 1$, it is clear that for fixed n and n_1, $R(T)$ will be minimum if the parameters x_{12}, x_{13}, x_{14}, x_{24}, x_{33}, x_{34} and x_{44} are all equal to zero (provided this is possible). However, a tree must have at least two pendent vertices, and so we have

$$x_{12} + x_{13} + x_{14} > 0. \tag{15}$$

Since $c_{13} < c_{12}$ and $c_{13} < c_{14}$, considering the minimum of $R(T)$, the best solution of (15) is that all pendent vertices are adjacent to vertices with degree 3, i.e., $x_{13} = n_1$.

Thus, we get

$$\begin{aligned} R(T) &\geq (n - n_1 + 5)4^\alpha - 6^{\alpha+1} + (3^\alpha - 2 \cdot 4^\alpha + 2 \cdot 6^\alpha)n_1 \\ &= n \cdot 4^\alpha + (3^\alpha + 2 \cdot 6^\alpha - 3 \cdot 4^\alpha)n_1 + 5 \cdot 4^\alpha - 6^{\alpha+1} \end{aligned}$$

with equality if and only if $x_{12} = x_{14} = x_{24} = x_{33} = x_{34} = x_{44} = 0$, $x_{13} = n_1$ and $n_4 = 0$. The proof is complete. ∎

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