Conjugated trees with minimum general Randić index

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A B S T R A C T

The general Randić index $R_{\alpha}(G)$ is the sum of the weights $(d_G(u)d_G(v))^\alpha$ over all edges $uv$ of a (molecular) graph $G = (V, E)$, i.e.,

$$\chi(G) = \sum_{uv \in E(G)} (d_G(u)d_G(v))^{-\frac{1}{2}},$$

where $d_G(u)$ denotes the degree of $u \in V(G)$. Branching index is also called the connectivity index [11] or Randić index [20] and also written by $R(G)$. As demonstrated by Randić himself [19], this index is well correlated with a variety of physico-chemical properties of alkanes, such as boiling point, (experimental) Kováts index, enthalpy of formation, parameters in the Antoine equation (for vapor pressure), surface area and solubility in water, etc. In the past 30 years, Randić index has become one of the most popular molecular descriptors and has been extensively studied by both mathematicians and theoretical chemists (one can refer to a survey book written by Li and Gutman [12] for details).

Later in [1], Bollobás and Erdős generalized the Randić index by replacing $-\frac{1}{2}$ with any real number $\alpha$, i.e.,

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

The problems of finding the (upper or lower) bounds for the general Randić index and finding the corresponding extremal graphs attracted much attention of many researchers (see [1–10,13–18,21] for details). For examples, Yu [21] showed that

$$R_{\frac{1}{2}}(T) \leq \frac{n+2\sqrt{n-1}}{2}$$

for any tree $T$ of order $n$. Later, Gaporosi et al. [3] obtained the same result by using an alternative approach. Clark and Moon [4] showed that

$$1 \leq R_{-1}(T) \leq \frac{5n+4}{18}$$

and proposed two unsolved questions on the upper bound. These two questions were positively answered by Hu et al. in [8]. Others could be found in [9,10,13].
The graphical representation of the carbon-atom skeleton of an alkane is usually called a chemical tree, i.e., a tree with no vertex having degree greater than 4. In [2], Caporossi et al. fully characterized the structures of the chemical trees possessing maximal and minimal values for the Randić index $R_{\alpha}$, Li and Yuan [14] gave the best possible lower and upper bounds for $R_{-\frac{1}{2}}$ among all chemical trees. Later, Li and Zheng [15] completely characterized the structures of chemical trees with minimum and maximum general Randić index $R_{\alpha}$ for $\alpha > 0$.

In [17], Lu et al. established sharp lower bounds of $R_{\alpha}$ for conjugated trees (trees with a Kekulé structure or, equivalently, trees with a perfect matching) as well as the trees with a given size of matching. Pan et al. [18] generalized this result by extending the number $\alpha = -\frac{1}{2}$ to be in $-\frac{1}{2} < \alpha < 0$. They also gave a sharp lower bound of $R_{\alpha}$ for the trees with a given size of matching and $\alpha > 0$. In present paper, for any real number $\alpha \leq -1$, the minimum value of $R_{\alpha}$ for conjugated trees is determined and the corresponding extremal conjugated trees are characterized. These trees are also extremal over all the conjugated chemical trees.

2. Preliminaries

Lemma 1. Let $f(x) = x^\alpha \times (x - 1 \times 2^\alpha + 1)$. If $\alpha \leq -1$ then the function $f(x) - f(x - 1)$ is monotonously increasing when $x \geq 2$.

Proof. The derivative of the second order of $f(x)$ is

$$\frac{d^2 f(x)}{dx^2} = \alpha x^{\alpha - 2} (2^\alpha (\alpha + 1) + x + 2 (1 - \alpha) + \alpha - 1).$$

Consider the function $g(x) = 2^\alpha (\alpha + 1) + x + 2 (1 - \alpha) + \alpha - 1$. Since $\alpha \leq -1$, then $\frac{d^2 f(x)}{dx^2} = 2^\alpha (\alpha + 1) \leq 0$. Therefore,

$$2^\alpha (\alpha + 1)x + 2^\alpha (1 - \alpha) + \alpha - 1 \leq 2^\alpha (\alpha + 1) \times 2 + 2^\alpha (1 - \alpha) + \alpha - 1 = 2^\alpha (3 + \alpha) + \alpha - 1 \leq -1 < 0.$$

This implies that $\frac{d^2 f(x)}{dx^2} > 0$ for $\alpha \leq -1$, then $f(x) - f(x - 1)$ is monotonously increasing. The lemma follows. □

Lemma 2. The equations $4^\alpha - 3^\alpha + 2 \times (6^\alpha - 9^\alpha) = 0, 2 \times 4^\alpha - 3^\alpha - 9^\alpha = 0$ and $3 \times 4^\alpha - 3^\alpha - 2 \times 6^\alpha = 0$ have negative roots $\beta_1 \approx -1.3867$, $\beta_2 \approx -2.0684$ and $\beta_3 \approx -3.0816$, respectively. Moreover,

(i) $4^\alpha - 3^\alpha + 2 \times (6^\alpha - 9^\alpha) > 0$ if $\beta_1 < \alpha \leq -1$; $4^\alpha - 3^\alpha + 2 \times (6^\alpha - 9^\alpha) < 0$ if $\alpha < \beta_1$.

(ii) $2 \times 4^\alpha - 3^\alpha - 9^\alpha > 0$ if $\beta_2 < \alpha < \beta_1$; $2 \times 4^\alpha - 3^\alpha - 9^\alpha < 0$ if $\alpha < \beta_2$.

(iii) $3 \times 4^\alpha - 3^\alpha - 2 \times 6^\alpha > 0$ if $\beta_3 < \alpha < \beta_2$; $3 \times 4^\alpha - 3^\alpha - 2 \times 6^\alpha < 0$ if $\alpha < \beta_3$.

Proof. Let $f_1(\alpha) = 4^\alpha - 3^\alpha + 2 \times (6^\alpha - 9^\alpha), f_2(\alpha) = 2 \times 4^\alpha - 3^\alpha - 9^\alpha$ and $f_3(\alpha) = 3 \times 4^\alpha - 3^\alpha - 2 \times 6^\alpha$. The existence of $\beta_1, \beta_2, \beta_3$ is obvious since $f_1(-2)f_1(-1) < 0, f_2(-3)f_2(-2) < 0$ and $f_3(-4)f_3(-3) < 0$. Furthermore, by using a binary search program, we have $\beta_1 \approx -1.3867, \beta_2 \approx -2.0684$ and $\beta_3 \approx -3.0816$.

(i) Let $g_1(\alpha) = \frac{1}{\beta_1} f_1(\alpha) = \left(\frac{\alpha}{\beta_1}\right)^{\alpha} - 1 + 2 \times 2^\alpha - 2 \times 3^\alpha$. Then $g_1(\alpha) = \left(\frac{\alpha}{\beta_1}\right)^{\alpha} \ln 4 + 2^\alpha \ln 4 - 3^\alpha \ln 9 > 2^\alpha \ln 4 - 3^\alpha \ln 9$ when $\alpha < 0$. Noticing that $h(\alpha) = 2^\alpha \ln 4 - 3^\alpha \ln 9 = 0$ has a unique root $r_0 = \frac{\ln(\ln 4) - \ln(\ln 9)}{\ln 2} \approx -0.6708$ and, moreover, noticing that $h(0) < 0, h(-1) = \frac{1}{\beta_1} \ln \frac{16}{9} - \frac{1}{\beta_1} \ln 9 \approx 0.1046 > 0$, we have $g_1(\alpha) > h(\alpha) > 0$ when $\alpha \leq -1 < r_0$. Hence $g_1(\alpha) > g_1(\beta_1) = 0, \text{i.e.}, f_1(\alpha) > 0$, if $\beta_1 < \alpha \leq -1$ and $g_1(\alpha) < g_1(\beta_1) = 0, \text{i.e.}, f_1(\alpha) < 0$, if $\alpha < \beta_1$.

(ii) Let $g_2(\alpha) = \frac{1}{\beta_2} f_2(\alpha) = 2 \times \left(\frac{\alpha}{\beta_2}\right)^{\alpha} - 1 - 3^\alpha$. Similar to the discussion in (i), we have $g_2(\alpha) = \left(\frac{\alpha}{\beta_2}\right)^{\alpha} \ln \frac{16}{9} - 3^\alpha \ln 3 > 0$ when $\alpha < \beta_1 < \frac{\ln(\ln 4) - \ln(\ln 3)}{\ln 2} \approx -0.7976$. Hence $g_2(\alpha) > g_2(\beta_2) = 0, \text{i.e.}, f_2(\alpha) > 0$, if $\beta_2 < \alpha < \beta_1$ and $g_2(\alpha) < g_2(\beta_2) = 0, \text{i.e.}, f_2(\alpha) < 0$, if $\alpha < \beta_2$.

(iii) Let $g_3(\alpha) = \frac{1}{\beta_3} f_3(\alpha) = 3 \times \left(\frac{\alpha}{\beta_3}\right)^{\alpha} - 1 - 2 \times 2^\alpha$. Then $g_3(\alpha) = \left(\frac{\alpha}{\beta_3}\right)^{\alpha} \ln \frac{16}{9} - 2^\alpha \ln 4 > 0$ when $\alpha < \beta_1 < \frac{\ln(\ln 4) - \ln(\ln 4)}{\ln 2} \approx -1.1688$. Hence $g_3(\alpha) > g_3(\beta_3) = 0, \text{i.e.}, f_3(\alpha) > 0$, if $\beta_3 < \alpha < \beta_2$ and $g_3(\alpha) < g_3(\beta_3) = 0, \text{i.e.}, f_3(\alpha) < 0$, if $\alpha < \beta_3$.

Thus, the proof is completed. □

Lemma 3. If $\alpha \leq -1$, then

(i) $2^\alpha + 6^\alpha - 2 \times 3^\alpha > 0$;

(ii) $2^\alpha + 4^\alpha + 3 \times 8^\alpha - 2 \times 3^\alpha - 2 \times 6^\alpha - 9^\alpha > 0$;

(iii) $2^\alpha + 2 \times 4^\alpha + 3 \times 8^\alpha - 2 \times 3^\alpha - 4 \times 6^\alpha > 0$.

Proof. (i) Let $f_1(\alpha) = \frac{\alpha + \theta_{\alpha} + 2 \times 3^\alpha}{\ln(\ln 3)} = 1 + 3^\alpha - 2 \times \left(\frac{\alpha}{\beta_1}\right)^{\alpha}$. Then $f_1(\alpha) = 3^\alpha \ln 3 - \left(\frac{\alpha}{\beta_1}\right)^{\alpha} \ln \frac{9}{4} > 0$ when $\alpha \leq -1 < \frac{\ln(\ln 4) - \ln(\ln 3)}{\ln 2} \approx -0.4380$. Hence $f_1(\alpha) \geq f_1(-1) = 0, \text{i.e.}, 2^\alpha + 6^\alpha - 2 \times 3^\alpha \geq 0, \text{if } \alpha \leq -1.$
(i) Let \( f_2(\alpha) = \frac{2^\alpha + 4^\alpha + 2 \times 8^\alpha - 2 \times 3^\alpha - 2 \times 6^\alpha}{2^\alpha} = 1 + 2^\alpha + 2 \times 4^\alpha - 2 \times \left(\frac{3}{2}\right)^\alpha - 2 \times 3^\alpha \). Then \( f_2(\alpha) = 2^\alpha \ln 2 - (\frac{3}{2})^\alpha \ln \frac{9}{4} + 4^\alpha \ln 16 - 3^\alpha \ln 9 < 4^\alpha \ln 16 - 3^\alpha \ln 9 < 0 \) when \( \alpha \leq -1 \). Therefore, \( f_2(\alpha) \geq f_2(-1) = 0 \) if \( \alpha \leq -1 \).

Furthermore, if \( \alpha \leq -1 \), then \( (2^\alpha + 4^\alpha + 2 \times 8^\alpha - 2 \times 3^\alpha - 2 \times 6^\alpha) > (8^\alpha - 9^\alpha) \).

(ii) Let \( f(x) = x^{\alpha} \times (x^{-1} \times 2^{\alpha} + 1) \). Then by Lemma 1, we have \( 2^\alpha + 2 \times 4^\alpha + 3 \times 8^\alpha - 2 \times 3^\alpha - 4 \times 6^\alpha = (f(4) - f(3)) - (f(3) - f(2)) > 0 \).

Thus, the proof is completed. □

We now introduce some graph terminologies and notations. All trees considered in the following will be conjugated. For a positive integer \( m \), we denote by \( \mathcal{T}_{2m} \) the class of all conjugated trees of order \( 2m \). Since the cases for \( m = 1, 2 \) are trivial, we always assume \( m \geq 3 \). For a vertex \( u \) of a tree \( T \), we denote the neighborhood and the degree of \( u \) by \( N_T(u) \) and \( d_T(u) \), respectively. An edge joining two vertices \( u \) and \( v \) will be written by \( uv \). A path of \( n \) vertices is written by \( P_n \). For a vertex \( u \) (resp., an edge \( uv \)), we will use \( T - u \) (resp., \( T - uv \)) to denote the tree obtained from \( T \) by removing the vertex \( u \) (resp., the edge \( uv \)). A pendant vertex of \( T \) is a vertex of degree 1 and a pendant edge is an edge incident to a pendant vertex.

Denote by \( C_{2m}(0) \) the tree of order \( 2m \) obtained from the path \( P_m = u_1u_2 \cdots u_m \) by adding a pendant vertex \( u_i \) to the vertex \( u_i \) of \( P_m \) for each \( i \in \{1, 2, \ldots, m\} \). For any integer \( k \) with \( 0 \leq k \leq m-2 \), let \( C_{2m}(k) \) be the class of the trees of order \( 2m \) obtained from \( C_{2m}(k+1) \) by removing \( k \) pairs \( \{v_i, v_{i+1}\}, \{v_{i+1}, v_{i+2}\}, \ldots, \{v_k, v_{k+1}\} \) of the pendant vertices satisfying:

- if \( 0 \leq k \leq \left[\frac{m}{2}\right] - 2 \) then \( i_j \geq 3, i_k \leq m+k-3 \) and for any \( j \in \{1, 2, \ldots, k-1\} \), \( i_j + 2 < i_{j+1} \), where, for a real number \( x \), \([x]\) (resp., \([x]\)) is the smallest (resp., greatest) integer not smaller (resp., greater) than \( x \);
- if \( \left[\frac{m}{2}\right] - 2 < k \leq m-2 \) then \( i_1 = 2 \) or \( i_k = m+k-3 \) and for any \( j \in \{1, 2, \ldots, k-1\} \), \( i_j + 2 < i_{j+1} \), where, for a real number \( x \), \([x]\) (resp., \([x]\)) is the smallest (resp., greatest) integer not smaller (resp., greater) than \( x \);
- if \( \left[\frac{m}{2}\right] - 2 < k \leq m-2 \) then \( i_1 = 2 \) or \( i_k = m+k-3 \) and for any \( j \in \{1, 2, \ldots, k-1\} \), \( i_j + 2 < i_{j+1} \), where, for a real number \( x \), \([x]\) (resp., \([x]\)) is the smallest (resp., greatest) integer not smaller (resp., greater) than \( x \).

From the definition of \( C_{2m}(k) \), one can see that \( C_{2m}(k) \subseteq \mathcal{T}_{2m} \) and, furthermore, (I) \( C_{2m}(0) = \{C_{2m}(0)\} \). (II) If \( m \) is odd then \( C_{2m}(\frac{m+1}{2} - 2) \) consists of a unique tree; if \( m \) is even then \( C_{2m}(\frac{m}{2} - 2) \) consists of those trees in which there is exactly one pair of successive vertices of degree 3. (III) If \( m \) is even then \( C_{2m}(\frac{m}{2} - 1) \) consists of those trees satisfying: \( i_1 = 2 \) and \( i_k = m + k - 3 \) while \( i_{k+1} = i_j + 3 \) for each \( j \in \{1, 2, \ldots, k-1\} \); or \( i_1 = 3 \) and \( i_k = m + k - 2 \) while \( i_{k+1} = i_j + 3 \) for each \( j \in \{1, 2, \ldots, k-1\} \); or \( i_1 = 3 \), \( i_k = m + k - 3 \) and there is exactly one integer \( h \in \{1, 2, \ldots, k-1\} \) such that \( i_{h+1} = h + 2 \) while \( i_{h+1} = i_j + 3 \) for each \( j \in \{1, 2, \ldots, k-1\} \setminus \{h\} \). (IV) \( C_{2m}(m-2) \) consists of the unique tree \( P_{2m} = u_1u_2 \cdots u_{2m} \).

For an example, some trees in \( C_{2m}(k) \) are shown in Fig. 1, here \( C_{2m}(k) \) represents an arbitrary tree in \( C_{2m}(k) \).

Denote \( C_{2m} = \bigcup_{k=0,1}^{\left[\frac{m}{2}\right]-2} C_{2m}(k) \) and \( C_{2m}^* = \bigcup_{k=\left[\frac{m}{2}\right]-1}^{m-2} C_{2m}(k) \).

One can check easily that \( \mathcal{T}_6 = \{C_6(0), C_6(1) = P_6\}, C_6 = \{C_6(0), C_6^* = \{C_6(0), P_6\} \) and \( \mathcal{T}_8 = \{C_8(0), C_8(1), C_8(2) = P_8, F_8, F_8^*\}, C_8 = \{C_8(0), C_8^* = \{C_8(1), P_8\} \) where \( F_8, F_8^* \) are as shown in Fig. 2.

By Lemmas 2 and 3, the following corollary is immediate.

**Corollary.** (i) If \( \beta_2 < \alpha \leq -1 \), then \( R_\alpha(C_6(0)) \subseteq R_\alpha(P_6); R_\alpha(C_8(0)) \subseteq R_\alpha(C_8(1)); R_\alpha(F_8) \subseteq R_\alpha(F_8^*) \).

(ii) If \( \alpha < \beta_2 \), then \( R_\alpha(C_6(1)) \subseteq R_\alpha(C_6(0)); R_\alpha(F_8^*); R_\alpha(C_8(0)) \subseteq R_\alpha(F_8) \).

(iii) If \( \alpha = \beta_2 \) then \( R_\alpha(C_6(0)) = R_\alpha(C_6(1)) \subseteq R_\alpha(P_6); R_\alpha(F_8) \subseteq R_\alpha(F_8^*) \).
3. The main result

Let

$$\phi_0(m) = (m - 2) \times 3^\alpha + (m - 3) \times 9^\alpha + 2^{\alpha+1} + 2 \times 6^\alpha;$$

$$\phi_1(m) = \begin{cases} 
(m - 1) \times 3^\alpha + (m - 3) / 2 \times 4^\alpha + (m - 1) \times 6^\alpha + 2^{\alpha+1}, & \text{if } m \text{ is odd} \\
2 \times 3^\alpha + (m - 4) / 2 \times 4^\alpha + (m - 2) \times 6^\alpha + 2^{\alpha+1} + 9^\alpha, & \text{if } m \text{ is even};
\end{cases}$$

$$\phi_2(m) = \begin{cases} 
(m - 1) \times 3^\alpha + (m - 3) / 2 \times 4^\alpha + (m - 1) \times 6^\alpha + 2^{\alpha+1}, & \text{if } m \text{ is odd} \\
2 \times 3^\alpha + (m - 4) / 2 \times 4^\alpha + (m - 2) \times 6^\alpha + 2^{\alpha+1}, & \text{if } m \text{ is even};
\end{cases}$$

$$\rho(m) = (2m - 3) \times 4^\alpha + 2^{\alpha+1}. $$

From the definition of $C_{2m}(k)$, for $T \in C_{2m}(k)$, one can verify that

$$R_\alpha(T) = \begin{cases} 
\phi_0(m) + k \times (4^\alpha - 3^\alpha + 2 \times (6^\alpha - 9^\alpha)), & \text{if } 0 \leq k \leq \left\lfloor \frac{m}{2} \right\rfloor - 2, \\
\rho(m) + (m - k - 2) \times (3^\alpha + 2 \times 6^\alpha - 3 \times 4^\alpha), & \text{if } \left\lfloor \frac{m}{2} \right\rfloor - 1 \leq k \leq m - 2.
\end{cases} \quad (1)$$

**Theorem.** If $\alpha \leq -1$, then the minimum value of $R_\alpha(T)$ over all the conjugated trees and the corresponding extremal conjugated trees are listed in Table 1.

**Proof.** Let $T$ be a minimum (with respect to $R_\alpha(T)$ and, herein after) conjugated tree and $P_k = u_1u_2 \cdots u_k$ be a longest path of $T$ (recalling that $m \geq 3$, we have $k \geq 5$). Since $T$ has a perfect matching, then $d_T(u_1) = 1$ and $d_T(u_2) = 2$. Let $d_T(u_3) = d$ and $N_T(u_3) \setminus \{u_2, u_4\} = \{v_1, v_2, \ldots, v_{d-2}\}$ (see Fig. 3).

**Claim 1.** If $d \geq 3$, then there is exactly one pendent vertex in $\{v_1, v_2, \ldots, v_{d-2}\}$.

Since $T$ has a perfect matching and $P_k$ is a longest path, we have $d_T(v_i) = 1$ or 2 for each $i \in \{1, 2, \ldots, d-2\}$, and furthermore, there is at most one $v_i \in \{v_1, v_2, \ldots, v_{d-2}\}$ such that $d_T(v_i) = 1$. For the sake of contradiction, suppose that $d_T(v_i) = 2$ for all $i = 1, 2, \ldots, d-2$ and let $x$ be the pendent vertex adjacent to $v_1$. Observe that $T_0 = T - xv_1 + xu_4$ also has a perfect matching. Let $N_T(u_4) \setminus \{u_3, u_5\} = \{w_1, w_2, \ldots, w_{d_T(u_4) - 2}\}$. Then by Lemma 3(i) and noticing that $d \geq 3, \alpha \leq -1$ and $d_T(u_4) \geq 2$, we have

$$R_\alpha(T) - R_\alpha(T_0) = 2^\alpha - (d_T(u_4) + 1)^\alpha + (2^\alpha - 1) \times d^\alpha + (d_T(u_4)^\alpha - (d_T(u_4) + 1)^\alpha) \times (d^\alpha + d_T(u_5)^\alpha)$$

\[+ \sum_{i=1}^{d_T(u_4) - 2} d_T(w_i)^\alpha. \]
which contradicts the fact that $T$ is minimum. Our claim follows. □

By Claim 1, if $d \geq 3$, then without loss of generality, we may assume $d_T(v_1) = 1$ and $d_T(v_i) = 2$ for $i = 2, 3, \ldots, d - 2$. Let $T' = T - u_1 - u_2$. Then $T' \in \mathcal{T}_{2(m-1)}$ and, furthermore,

$$R_{\alpha}(T) = R_{\alpha}(T') + 2^\alpha + (2d)^{\alpha} + (d^\alpha - (d - 1)^\alpha) \left( \sum_{i=1}^{d-2} d_T(v_i)^{\alpha} + d_T(u_4)^{\alpha} \right)$$

$$= \begin{cases} 
R_{\alpha}(T') + 2^\alpha + (2d)^{\alpha} + (d^\alpha - (d - 1)^\alpha)(1 + 2^\alpha(d - 3) + d_T(u_4)^{\alpha}), & \text{if } d \geq 3, \\
R_{\alpha}(T') + 2^\alpha + 4^\alpha + (2^\alpha - 1)d_T(u_4)^{\alpha}, & \text{if } d = 2.
\end{cases} \quad (2)

Now we have three cases to discuss.

Case 1. $d = 2$.
Since $d_T(u_4) \geq 2$ and $\alpha \leq -1$, then by (2) we have

$$R_{\alpha}(T) \geq R_{\alpha}(T') + 2 \times 4^\alpha,$$  \hspace{1cm} (3)

and the equality holds if and only if $d_T(u_4) = 2$.

Case 2. $d = 3$.
Again by (2), if $d_T(u_4) \geq 3$ then

$$R_{\alpha}(T) = R_{\alpha}(T') + 2^\alpha + 6^\alpha + (3^\alpha - 2^\alpha) \times (1 + d_T(u_4)^{\alpha})$$

$$\geq R_{\alpha}(T') + 3^\alpha + 9^\alpha,$$  \hspace{1cm} (4)

and the equality holds if and only if $d_T(u_4) = 3$.

If $d_T(u_4) = 2$, let $T'' = T' - v_1 - u_3$, then $T'' \in \mathcal{T}_{2(m-2)}$, we have

$$R_{\alpha}(T) = R_{\alpha}(T'') + 2^\alpha + 3^\alpha + 2 \times 6^\alpha + (2^\alpha - 1) \times d_T(u_5)^{\alpha}.$$  \hspace{1cm} (5)

If $m \geq 5$, then $d_T(u_5) \geq 2$, we have

$$R_{\alpha}(T) \geq R_{\alpha}(T'') + 3^\alpha + 4^\alpha + 2 \times 6^\alpha,$$

and the equality holds if and only if $d_T(u_5) = 2$.

Case 3. $d \geq 4$.
Let $f(x) = x^{\alpha} \times ((x - 1) \times 2^\alpha + 1)$, by Lemma 1 we have $f(d) - f(d - 1) \geq f(4) - f(3)$. Then by (2), we have

$$R_{\alpha}(T) \geq R_{\alpha}(T') + 2^\alpha + d^\alpha \times ((d - 1) \times 2^\alpha + 1) - (d - 1)^\alpha \times ((d - 2) \times 2^\alpha + 1)$$

$$\geq R_{\alpha}(T') + 2^\alpha + f(d) - f(d - 1)$$

$$\geq R_{\alpha}(T') + 2^\alpha + f(4) - f(3)$$

$$= R_{\alpha}(T') + 2^\alpha + 4^\alpha + 3 \times 8^\alpha - 3^\alpha - 2 \times 6^\alpha.$$  \hspace{1cm} (6)

**Claim 2.** If $\beta_2 < \alpha \leq -1$, then $T \in \mathcal{C}_{2m}$.

We prove the claim by induction on $m$. By Corollary 1(i), it is easy to verify that $\mathcal{C}_6(0)$ and $\mathcal{C}_6(0)$ are the unique minimum trees in $\mathcal{T}_6$ and $\mathcal{T}_6$, respectively. The claim follows when $m = 3, 4$. Now assume $m \geq 5$.

Let $T_{2(m-1)}$ be a minimum tree of $2(m - 1)$ vertices. Then $R_{\alpha}(T') \geq R_{\alpha}(T_{2(m-1)})$. By the induction hypothesis, we have $T_{2(m-1)} \in \mathcal{C}_{2(m-1)}$ and furthermore, if $R_{\alpha}(T') = R_{\alpha}(T_{2(m-1)})$ then $T' \in \mathcal{C}_{2(m-1)}$. Let $T_{2m}$ be obtained from $T_{2(m-1)}$ by adding an edge between a vertex of path $P_T$ and a vertex of degree 2 of $T_{2(m-1)}$ which is adjacent to a pendant vertex. In view of the definition of $\mathcal{C}_{2m}(k)$ and the construction of $T_{2m}$, one can see that if $T_{2(m-1)} \in \mathcal{C}_{2(m-1)}(k)$, $k \in \{0, 1, \ldots, m - 2\}$, then $T_{2m} \in \mathcal{C}_{2m}(k)$. On the other hand, recall that

$$\mathcal{C}_{2m} = \bigcup_{k=0,1,\ldots,[\frac{m-1}{2}]-2} \mathcal{C}_{2m}(k)$$

and $T_{2(m-1)} \in \mathcal{C}_{2(m-1)}$, say $T_{2(m-1)} = \mathcal{C}_{2(m-1)}(k) \in \mathcal{C}_{2(m-1)}(k)$. Then we have $k \leq [\frac{m-1}{2}] - 2$ and, therefore, $k \leq [\frac{m}{2}] - 2$. This implies that $T_{2m} \in \mathcal{C}_{2m}(k) \subseteq \mathcal{C}_{2m}$. Moreover,

$$R_{\alpha}(T_{2m}) = R_{\alpha}(T_{2(m-1)}) + 3^\alpha + 9^\alpha.$$  \hspace{1cm} (7)
Case 1. \( d = 2. \)

In view of (3), (7) and Lemma 2(ii), for \( \beta_2 < \alpha \leq -1, \) we have
\[
R_\alpha(T) \geq R_\alpha(T_2(m-1)) + 2 \times 4^\alpha
= R_\alpha(T_{2m}) + 2 \times 4^\alpha - 3^\alpha - 9^\alpha > R_\alpha(T_{2m}),
\]
which is a contradiction to the fact that \( T \) is minimum.

Case 2. \( d = 3. \)

If \( d_T(u_4) \geq 3, \) then by (4) and (7), we have
\[
R_\alpha(T) \geq R_\alpha(T_2(m-1)) + 3^\alpha + 9^\alpha = R_\alpha(T_{2m}),
\]
and if the equality holds then \( T' \in C_{2(m-1)}^2 \) and \( d_T(u_4) = 3, \) that is \( T \in C_{2m}. \)

If \( d_T(u_4) = 2, \) by the induction hypothesis, there is \( T_{2(m-2)} \in C_{2(m-2)}^2 \) such that \( R_\alpha(T'') \geq R_\alpha(T_{2(m-2)}) \) and if the equality holds then \( T'' \in C_{2(m-2)}. \) Let \( T_{2m} \) be obtained from \( T_{2(m-2)} \) by adding an edge between a vertex of degree 2 of path \( P_4 \) and a pendant vertex of \( T_{2(m-2)} \) which is adjacent to a vertex of degree 2. By the construction of \( C_{2m} \) we can observe that \( T_{2m} \in C_{2m}. \) Moreover,
\[
R_\alpha(T_{2m}) = R_\alpha(T_{2(m-2)}) + 3^\alpha + 4^\alpha + 2 \times 6^\alpha.
\]
Together with (5) and (8), we have
\[
R_\alpha(T) \geq R_\alpha(T_{2(m-2)}) + 3^\alpha + 4^\alpha + 2 \times 6^\alpha = R_\alpha(T_{2m}),
\]
and if the equality holds then \( T'' \in C_{2(m-2)}^2 \) and \( d_T(u_5) = 2, \) that is \( T \in C_{2m}. \)

Case 3. \( d \geq 4. \)

From (6) and (7) and Lemma 3(ii), if \( \alpha \leq -1 \) then
\[
R_\alpha(T) \geq R_\alpha(T_2(m-1)) + 2^\alpha + 4^\alpha + 3 \times 8^\alpha - 3^\alpha - 2 \times 6^\alpha
= R_\alpha(T_{2m}) + 2^\alpha + 4^\alpha + 3 \times 8^\alpha - 2 \times 3^\alpha - 2 \times 6^\alpha - 9^\alpha > R_\alpha(T_{2m}),
\]
which is also a contradiction. The claim follows. \( \square \)

From Claim 2, if \( \beta_2 < \alpha \leq -1 \) then \( T \in C_{2m}, \) say \( T \in C_{2m}(k), \) \( 0 \leq k \leq \lceil \frac{m}{3} \rceil - 2. \) Further, if \( \beta_1 < \alpha \leq -1, \) then by Lemma 2(i), we have \( 4^\alpha - 3^\alpha + 2 \times (6^\alpha - 9^\alpha) > 0. \) Since \( T \) is minimum, then by (1) we have \( k = 0, \) i.e., \( T = C_{2m}(0). \) Similarly, if \( \beta_2 \leq \beta_1 < \alpha, \) again by (1) and Lemma 2(i) we have \( 4^\alpha - 3^\alpha + 2 \times (6^\alpha - 9^\alpha) < 0, \) which implies that \( k = \lceil \frac{m}{3} \rceil - 2, \) i.e., \( T \in C_{2m}(\lceil \frac{m}{3} \rceil - 2). \) Notice that all the trees in \( C_{2m}(\lceil \frac{m}{3} \rceil - 2) \) have the same value of \( R_\alpha, \) which implies that \( T \) is minimum if and only if \( T \in C_{2m}(\lceil \frac{m}{3} \rceil - 2). \) If \( \alpha = \beta_1, \) we have \( 4^\alpha - 3^\alpha + 2 \times (6^\alpha - 9^\alpha) = 0, \) which implies that all the trees in \( C_{2m} \) have the same value of \( R_\alpha. \) Therefore, each tree in \( C_{2m} \) is minimum. This completes the proof for the case that \( \beta_2 < \alpha \leq -1. \)

Claim 3. If \( \alpha < \beta_2, \) then \( T \in C_{2m}^*: \)

Apply induction on \( m. \) When \( m = 3, \) the claim follows directly since \( C_6 = C_6^*. \) When \( m = 4, \) since \( T \) is minimum, then by Corollary 1(ii) we have \( T = C_5(1) \) or \( T = P_8. \) The claim again follows. Now we assume \( m \geq 5. \)

By the induction hypothesis, there is \( T_2(m-1) \in C_{2(m-1)}^2 \) such that \( R_\alpha(T') \geq R_\alpha(T_{2(m-1)}) \) and if the equality holds then \( T' \in C_{2(m-1)}^2. \) Let \( T_{2m} \) be obtained from \( T_{2(m-1)} \) by adding an edge between a vertex of path \( P_2 \) and a pendant vertex of \( T_{2(m-1)} \) which is adjacent to a vertex of degree 2. Then it is clear that \( T_{2m} \in C_{2m}^* \) and
\[
R_\alpha(T_{2m}) = R_\alpha(T_{2(m-1)}) + 2 \times 4^\alpha.
\]

Case 1. \( d = 2. \)

By (3) and (9), we have
\[
R_\alpha(T) \geq R_\alpha(T_{2(m-1)}) + 2 \times 4^\alpha = R_\alpha(T_{2m}),
\]
and if the equality holds then \( T' \in C_{2(m-1)}^* \) and \( d_T(u_4) = 2, \) that is \( T \in C_{2m}^*. \)

Case 2. \( d = 3. \)

Recall that \( \alpha < \beta_2. \) So if \( d_T(u_4) \geq 3, \) then by (4), (9) and Lemma 2(ii), we have
\[
R_\alpha(T) \geq R_\alpha(T_{2(m-1)}) + 3^\alpha + 9^\alpha
= R_\alpha(T_{2m}) + 3^\alpha + 9^\alpha - 2 \times 4^\alpha > R_\alpha(T_{2m}),
\]
a contradiction.

If \( d_T(u_4) = 2, \) similar to the discussion of Claim 2, there is \( T_{2m} \in C_{2m}^* \) such that \( R_\alpha(T) \geq R_\alpha(T_{2m}) \) and if the equality holds then \( T'' \in C_{2(m-2)}^* \) and \( d_T(u_5) = 2, \) that is \( T \in C_{2m}^*. \)
Case 3. $d \geq 4$.

Since $\alpha < \beta_2 < -1$, then by (6), (9) and Lemma 2(ii), Lemma 3(ii), we have
\[
R_\alpha(T) \geq R_\alpha(T_{(2m-1)}) + 2^{\alpha} + 4^\alpha + 3 \times 8^\alpha - 3^{\alpha} - 2 \times 6^\alpha
\]
\[
= R_\alpha(T_{2m}) + 2^{\alpha} + 4^\alpha + 3 \times 8^\alpha - 3^{\alpha} - 2 \times 6^\alpha - 2 \times 4^\alpha
\]
\[
> R_\alpha(T_{2m}) + 2^{\alpha} + 4^\alpha + 3 \times 8^\alpha - 2 \times 3^{\alpha} - 2 \times 6^\alpha - 9^\alpha > R_\alpha(T_{2m}).
\]
again a contradiction. The claim follows. \qed

By Claim 3, if $\alpha < \beta_2$ then $T \in C_{2m}^*$, say $T \in C_{2m}(k)$ for some $k$, $\lceil \frac{m}{2} \rceil - 1 \leq k \leq m - 2$. In view of (1) and Lemma 2(iii), if $\beta_3 < \alpha < \beta_2$ then $k = \lfloor \frac{m}{2} \rfloor - 1$, i.e., $T$ is minimum if and only if $T \in C_{2m}(\lfloor \frac{m}{2} \rfloor - 1)$; if $\alpha < \beta_3$ then $k = m - 2$, i.e., $T = P_{2m}$; if $\alpha = \beta_3$ then each tree in $C_{2m}^*$ is minimum. This completes the proof for the case that $\alpha < \beta_2$.

Claim 4. If $\alpha = \beta_2$ then $T \in C_{2m}(\lfloor \frac{m}{2} \rfloor - 2) \cup C_{2m}(\lfloor \frac{m}{2} \rfloor - 1)$.

Again apply induction on $m$. In view of Corollary 1(iii), it is easy to verify that the claim holds when $m = 3$ or $m = 4$. We now suppose $m \geq 5$.

Assume firstly $m$ is odd. Notice that $\lceil \frac{m}{2} \rceil - 2 = \lfloor \frac{m}{2} \rfloor - 1$ and $C_{2m}(\lfloor \frac{m}{2} \rfloor - 2)$ consists of the unique tree $C_{2m}(\lfloor \frac{m}{2} \rfloor - 2)$. So we need only to prove that $R_\alpha(T) \geq R_\alpha(C_{2m}(\lceil \frac{m}{2} \rceil - 2))$ for any $T \in P_{2m}$ and if the equality holds then $T = C_{2m}(\lfloor \frac{m}{2} \rfloor - 2)$.

By the induction hypothesis, there is $T_{(2m-1)} \in C_{2m-1}(\lceil \frac{m-1}{2} \rceil - 2) \cup C_{2m-1}(\lfloor \frac{m-1}{2} \rfloor - 1)$ such that $R_\alpha(T_{(2m-1)}) \geq R_\alpha(T_{(2m-1)})$ and if the equality holds then $T_{(2m-1)} \in C_{2m-1}(\lceil \frac{m-1}{2} \rceil - 2) \cup C_{2m-1}(\lfloor \frac{m-1}{2} \rfloor - 1)$. In view of Lemma 2(ii), if $\alpha = \beta_2$ then $R_\alpha(T_{(2m-1)}) = \phi_1(m) - \phi_2(m - 1)$. Therefore,
\[
R_\alpha \left( C_{2m} \left( \lfloor \frac{m}{2} \rceil - 2 \right) \right) - R_\alpha(T_{(2m-1)}) = \phi_1(m) - \phi_2(m - 1) = 3^{\alpha} + 2 \times 6^\alpha - 4^\alpha.
\] (10)

Case 1. $d = 2$.

Since $\beta_3 < \alpha = \beta_2 < 0$, then by (3), (10) and Lemma 2(iii), we have
\[
R_\alpha(T) \geq R_\alpha(T_{(2m-1)}) + 2 \times 4^\alpha
\]
\[
= R_\alpha \left( C_{2m} \left( \lfloor \frac{m}{2} \rceil - 2 \right) \right) + 3 \times 4^\alpha - 3^{\alpha} - 2 \times 6^\alpha > R_\alpha \left( C_{2m} \left( \lfloor \frac{m}{2} \rceil - 2 \right) \right).
\]

Case 2. $d = 3$.

Since $d_T(u_4) \geq 2$, then by (2) and (10), we have
\[
R_\alpha(T) = R_\alpha(T') + 2^{\alpha} + 6^\alpha + (3^{\alpha} - 2^{\alpha}) \times (1 + d_T(u_4)^\alpha)
\]
\[
\geq R_\alpha(T_{(2m)}) + 3^{\alpha} + 2 \times 6^\alpha - 4^\alpha = R_\alpha \left( C_{2m} \left( \lfloor \frac{m}{2} \rceil - 2 \right) \right),
\]
and if the equality holds then $T' \in C_{2m-1}(\lceil \frac{m-1}{2} \rceil - 2) \cup C_{2m-1}(\lfloor \frac{m-1}{2} \rfloor - 1)$ and $d_T(u_4) = 2$. Notice that the degrees of $v_1, u_3$ and $u_4$ in $T'$ are $d_T(v_1) = 1$, $d_T(u_3) = 2$ and $d_T(u_4) = 2$, respectively. Thus, in view of the construction of $C_{2m-1}(\lceil \frac{m-1}{2} \rceil - 2)$, $T' \not\in C_{2m-1}(\lfloor \frac{m-1}{2} \rfloor - 1)$ and therefore, $T' \in C_{2m-1}(\lfloor \frac{m-1}{2} \rfloor - 1)$. Furthermore, $T'$ has the unique form as shown in Fig. 4. That is, $T = C_{2m}(\lfloor \frac{m}{2} \rceil - 2)$.

Case 3. $d \geq 4$.

In view of (6), (10) and Lemma 3(iii), for $\alpha = \beta_2 < -1$, we have
\[
R_\alpha(T) \geq R_\alpha(T_{(2m-1)}) + 2^{\alpha} + 4^\alpha + 3 \times 8^\alpha - 3^{\alpha} - 2 \times 6^\alpha
\]
\[
= R_\alpha(T_{2m}) + 2^{\alpha} + 2 \times 4^\alpha + 3 \times 8^\alpha - 2 \times 3^{\alpha} - 4 \times 6^\alpha > R_\alpha \left( C_{2m} \left( \lfloor \frac{m}{2} \rceil - 2 \right) \right).
\]

Now we assume that $m$ is even and $m \geq 6$. Since $m - 1$ is odd, then $\lceil \frac{m-1}{2} \rceil - 2 = \lfloor \frac{m-1}{2} \rfloor - 1$ and $C_{2m-1}(\lfloor \frac{m-1}{2} \rfloor - 2)$ contains exactly one tree $C_{2m-1}(\lfloor \frac{m-1}{2} \rfloor - 2)$. By the induction hypothesis, we have $R_\alpha(T') \geq R_\alpha(C_{2m-1}(\lceil \frac{m-1}{2} \rceil - 2))$ and if the equality holds then $T' = C_{2m-1}(\lceil \frac{m-1}{2} \rceil - 2)$. Choose $T_{2m} \in C_{2m}(\lfloor \frac{m}{2} \rceil - 2) \cup C_{2m}(\lfloor \frac{m}{2} \rfloor - 1)$. Recalling that $\beta_2$ is a root of $2 \times 4^\alpha - 3^{\alpha} - 9^\alpha = 0$, we have
\[
R_\alpha(T_{2m}) - R_\alpha \left( C_{2m-1} \left( \lceil \frac{m-1}{2} \rceil - 2 \right) \right) = 3^{\alpha} + 9^\alpha = 2 \times 4^\alpha.
\] (11)
Case 1. $d = 2$.

By (3) and (11), we have
\[
R_\alpha(T) \geq R_\alpha \left( C_{2(m-1)} \left( \left\lceil \frac{m-1}{2} \right\rceil - 2 \right) \right) + 2 \times 4^\alpha = R_\alpha(T_{2m}).
\]

If the equality holds then $T' = C_{2(m-1)} \left( \left\lceil \frac{m-1}{2} \right\rceil - 2 \right)$ and $d_7(u_4) = 2$, then $T \in C_{2m}(\left\lfloor \frac{m}{2} \right\rfloor - 1)$.

Case 2. $d = 3$.

If $d_7(u_4) \geq 3$, then by (4) and (11), we have
\[
R_\alpha(T) \geq R_\alpha \left( C_{2(m-1)} \left( \left\lceil \frac{m-1}{2} \right\rceil - 2 \right) \right) + 3^\alpha + 9^\alpha = R_\alpha(T_{2m}).
\]

If the equality holds then $T' = C_{2(m-1)} \left( \left\lceil \frac{m-1}{2} \right\rceil - 2 \right)$ and $d_7(u_4) = 3$. Thus, $T \in C_{2m}(\left\lfloor \frac{m}{2} \right\rfloor - 2)$.

If $d_7(u_4) = 2$, similar to the proof of Claim 2, there is $T_{2m} \in C_{2m}(\left\lfloor \frac{m}{2} \right\rfloor - 2) \cup C_{2m}(\left\lceil \frac{m}{2} \right\rceil - 1)$ and if the equality holds then $T'' \in C_{2(m-2)} \left( \left\lceil \frac{m-2}{2} \right\rceil - 2 \right) \cup C_{2(m-2)} \left( \left\lfloor \frac{m-2}{2} \right\rfloor - 1 \right)$ and $d_7(u_4) = 2$, i.e., $T \in C_{2m}(\left\lfloor \frac{m}{2} \right\rfloor - 2) \cup C_{2m}(\left\lfloor \frac{m}{2} \right\rceil - 1)$. Case 3. $d \geq 4$.

Combining Lemma 3(ii) with (6) and (11), we have
\[
R_\alpha(T) \geq R_\alpha \left( C_{2(m-1)} \left( \left\lceil \frac{m-1}{2} \right\rceil - 2 \right) \right) + 2\alpha + 4^\alpha + 3 \times 8^\alpha - 3^\alpha - 2 \times 6^\alpha
\]
\[
= R_\alpha(T_{2m}) + 2\alpha + 4^\alpha + 3 \times 8^\alpha - 2^\alpha - 2 \times 6^\alpha - 9^\alpha > R_\alpha(T_{2m}).
\]

A contradiction. The claim follows. 

When $\alpha = \beta_2$, by (1) and Lemma 2 one can check that each tree in $C_{2m}(\left\lfloor \frac{m}{2} \right\rceil - 2) \cup C_{2m}(\left\lfloor \frac{m}{2} \right\rceil - 1)$ has the same value $\phi_1(m) (= \phi_2(m))$ of $R_\alpha$. Thus, by Claim 4, a tree $T$ is minimum if and only if $T \in C_{2m}(\left\lfloor \frac{m}{2} \right\rceil - 2) \cup C_{2m}(\left\lfloor \frac{m}{2} \right\rceil - 1)$. Theorem follows.

4. Final remarks

Observe that the trees listed in Table 1 are all chemical trees and hence, they are also extremal over all the conjugated chemical trees.

So far, the structure(s) of conjugated trees with minimum general Randić index still remain open for $-1 < \alpha < -\frac{1}{2}$. In fact, by using the method in [17], we can generalize the result of Pan et al. in [18] by extending $\alpha$ to be $\beta_0 \leq \alpha < 0$, where $\beta_0$ ($\approx -0.6705$) is a negative root of the equation $(4 + 2x) \times 2^x + x - 1 = 0$. Then a natural question arises: what about the case where $-1 < \alpha < \beta_0$?

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