Maximum Tree and Maximum Value for the Randić Index R_{-1} of Trees of Order $n \leq 102$ *

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Abstract

The Randić index $R_{-1}(G)$ of a graph G is defined as the sum of the weights $(d(u)d(v))^{-1}$ of all edges uv of G, where $d(u)$ denotes the degree of a vertex u in G. Trees with maximum Randić index R_{-1} need not be unique. Clark et al. gave the maximum values for the index of trees of order $n \leq 20$. In this paper, we determine the maximum value for the Randić index R_{-1} of all trees of order $n \leq 102$, and give one of the trees with maximum value of the index. This not only largely extends the known range of the orders n of trees with maximum index, but also gives a convincible solution for the induction initial of our previous

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paper. Because there is a huge number of trees of order $n \leq 102$, it is not possible to directly search the trees with maximum index by a computer. Our method is to first figure out the simple structure of one of the trees of order n with maximum R_{-1} for each $n \leq 102$, i.e., the branching subtree must be a star. Then from this simple structure, we can employ mathematical programming to easily calculate the maximum value of R_{-1} for each n.

1 Introduction

In 1975, Randić proposed a pair of chemical indices $R(G)$ and $R_{-1}(G)$ for a (chemical) graph G, i.e.,

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

where $d(u)$ denotes the degree of a vertex u in G. Randić himself demonstrated that his index was well correlated with a variety of physico-chemical properties of alkanes, such as boiling point, enthalpy of formation, parameters in the Antoine equation (for vapor pressure), surface area, and solubility in water. Eventually, this structure-descriptor becomes one of the most popular topological indices, and scores of its chemical and pharmacological applications have been reported. The Randić index is the only topological index to which two books are devoted [9, 10]. Like other successful chemical indices, these two indices have received considerable attention from both chemists and mathematicians. In this paper, we are only interested in the latter index R_{-1} for trees.

Until now, for trees T all the existent results are only to give lower and upper bounds for $R_{-1}(T)$, but one can not prove that the upper bound is best possible. Rautenbach [12] gave an upper bound for $R_{-1}(T)$ of trees with maximum degree 3. Li and Yang [11] gave a method to determine the sharp upper bound for R_{-1} of chemical trees (i.e., trees with maximum degree at most 4). In [7], we investigated trees with maximum value of general Randić index $R_\alpha = \sum_{uv \in E(G)} (d(u)d(v))^\alpha$, where α is an arbitrary real number, among all trees of order n. We distinguished α in several different intervals, and for most of the intervals we characterized trees with maximum general Randić index and gave the corresponding values. Only the interval $-2 < \alpha < -\frac{1}{2}$ (including the point $\alpha = -1$) is left undetermined and seems very complicated. The *Max Trees (trees with maximum Randić index)* could be not unique in this interval. So it is hard to get the maximum index and the corresponding trees. For all $n \leq 20$, Clark et al. [4] determined all trees with maximum value of R_{-1} among all trees of order n. In 2000, Clark and Moon [5] gave a lower and upper bound for $R_{-1}(T)$, i.e., $1 \leq R_{-1}(T) \leq \frac{5n+8}{18}$, where the lower bound can be attained by the star, but they could not prove that upper bound is best possible. At the end of their paper [5] they proposed two unsolved questions on the upper bound. In our recently paper [8], we gave positive answers to the two questions, and solve the sharp upper bound problem for R_{-1} of trees when n is large enough. But, we feel very unsatisfactory with the following two things:

(i) In the proof of Theorem 2.1 of [8], we used induction on the number of vertices. There the induction initial was $n \leq 71$. We simply said that "we can use a good computer to check the result for all $n \leq 71$". We feel that this cannot convince any reader(s), because there is a huge number of trees of order $n \leq 71$.

(ii) There is a small error in Section 3 of [8], which solved the second question of Clark and Moon [5]. We said there that "T_{10} defined in [5] is the Max Tree of order 71, the value of R_{-1} for T_{10} is $19 = \frac{15\times 71-1}{56}$, and so $n = 71$ can be chosen as our induction initial, and the constant C in our Theorem 2.1 of [8] can really be chosen as -1". But this is not true when we now get the maximum values of R_{-1} for all $n \leq 102$. We find that to choose $C = -1$ the smallest value (induction initial of Theorem 2.1 in [8]) of n has to be 91, but not 71.

In this paper we not only give convincible solution to (i) and correction to (ii), but also largely extend the known range of the orders n of trees with maximum index R_{-1} from $n \leq 20$ to $n \leq 102$. The first 20 values are exactly the same as those listed in

[4]. Our method is to first figure out the simple structure of one of the trees of order n with maximum R_{-1} for each $n \leq 102$. Then from this simple structure, we can employ mathematical programming to easily calculate the maximum value of R_{-1} for each n.

Throughout this paper, we use standard graph-theoretical terminology. Let T be a tree with order n. Denote by $d_T(u)$ and $N_T(u)$ the degree and neighborhood of the vertex u in T, respectively, and we omit the letter T if only one tree is under consideration. A vertex of degree 1 in a tree is called a *leaf*. A vertex of degree greater than 2 in a tree is called a *branching vertex*. A vertex of degree i is also called an *i-degree vertex*. The star of order n is denoted by S_n. Let $u_1, u_2, \cdots, u_r$ be a path and $u_i \in V(T)$, $1 \leq i \leq r$. We call $u_1 u_2 \cdots u_r$ a *suspended path* rooted at u_r, if $d(u_1) = 1$, $d(u_i) = 2$ $(i = 2, \cdots, r-1)$ and u_r is a branching vertex. $r-1$ is called the *length* of the suspended path.

2 The structure of a Max Tree of order $n \leq 102$

It is easy to see that for $n \leq 9$, $R_{-1}(T) \leq \frac{n+1}{4}$, and the equality holds when T is a path. Since for $n \geq 10$, path P_n does not have the maximum Randić index, so we assume the maximum degree $\Delta(T) \geq 3$ in the following.

In [7], we obtained a property of Max Trees for $\alpha < -1$. If we just consider one of the structures of Max Trees, then this property also holds for $\alpha = -1$.

Property 2.1 *[7] For $\alpha \leq -1$, we can find one of the Max Trees T with the property (1) all the suspended paths of T are of length 2, except for at most one with length 3, and (2) every vertex of degree 2 must appear on a suspended path.*

Note that if T is one of the Max Trees with above property, and S_T is the subgraph obtained from T by deleting all the vertices of degrees 1 and 2, then, S_T is connected and acyclic, we call S_T the *branching subtree of T*. In the following whenever we mention a Max Tree we always mean that it has the above property.

A subtree of T is called an *(s,d)-system centered at z*, if $x_1y_1z, \cdots, x_sy_sz$ are s distinct suspended paths rooted at z with $d(z) = d \geq 3$, and $w_1, \cdots, w_{d-s}$ are the vertices of T, other than $y_1, \cdots, y_s$, adjacent to z. Clearly, $1 \leq s \leq d-1$, and if $s = d-1$ and w is the branching vertex adjacent to z, then we say that this (s,d)-system is adjacent to w.

Lemma 2.2 *Let T be a Max Tree. If there are s suspended paths rooted at a vertex z in T, then $s \leq 5$.*

Proof. By contradiction. Suppose $s \geq 6$, then $d(z) = d \geq 6$. Let $w_i (i = 1, \cdots, d-6)$ be the vertices adjacent to z, other than the vertices on the six suspended paths. Let T' be the tree obtained from T by deleting five suspended paths rooted at z and adding two $(2,3)$-systems adjacent to z. It is easy to show that T' has an index larger than T, i.e.,

$$\begin{aligned} R_{-1}(T) - R_{-1}(T') &= -\frac{1}{6} + \frac{3}{d} - \frac{1}{2(d-3)} - \frac{2}{3(d-3)} + \left(\frac{1}{d} - \frac{1}{d-3}\right)\sum_{i=1}^{d-6}\frac{1}{d(w_i)} \\ &\leq -\frac{1}{6} + \frac{3}{d} - \frac{7}{6(d-3)} = \frac{-d^2 + 14d - 54}{6d(d-3)} < 0. \end{aligned}$$

Here and in what follows, whenever we transform a tree T into another tree T', we always assume that there is no suspended path of length 3 in T. If there is a one, then instead of directly transforming T into T', we contract the leaf edge of the suspended path of length 3 to get a tree T_1 first, then transform T_1 into T_1', and finally subdivide a leaf of T_1' to get T'. ∎

Lemma 2.3 *Let T be a Max Tree and z be a leaf of the branching subtree S_T. Then there are only two or three suspended paths rooted at z, i.e., $d(z) = 3$ or 4.*

Proof. By Lemma 2.2, there are at most 5 suspended paths rooted at z in T. If there are 5 suspended paths rooted at z, and w is the branching vertex adjacent to z, suppose

$d(w) = t$, then by deleting the vertex z, adding two $(2,3)$-systems adjacent to w, and then subdividing a leaf, we get a new tree T'. Let v_i $(i = 1, \cdots, t-1)$ be the vertices adjacent to w, other than z. Then, from the property we have $d(v_i) \geq 2$. So we have

$$\begin{aligned} R_{-1}(T) - R_{-1}(T') &= \frac{1}{6t} - \frac{2}{3(t+1)} + \left(\frac{1}{t} - \frac{1}{t+1}\right) \sum_{i=1}^{t-1} \frac{1}{d(v_i)} \\ &\leq \frac{1}{6t} - \frac{2}{3(t+1)} + \frac{1}{t(t+1)} \cdot \frac{t-1}{2} \\ &= \frac{-2}{6t(t+1)} < 0, \end{aligned}$$

which is a contradiction, since T is a Max Tree.

If there are 4 suspended paths rooted at z, and w is the branching vertex adjacent to z, suppose $d(w) = t$, then, since if $t = 2$ then T is a tree with order 11 or 12, it is easy to check that T is not a Max Tree. So, we suppose $t \geq 3$. Let v_i $(i = 1, \cdots, t-1)$ be the vertices adjacent to w, other than z. We distinguish two cases to deduce contradictions.

(i) If there is a 2-degree vertex v_1 adjacent to w, then we get a new tree by deleting the vertices z and v_1, adding two $(2,3)$-systems adjacent to w, and then subdividing a leaf. Then we have

$$\begin{aligned} R_{-1}(T) - R_{-1}(T') &= \frac{4}{10} + \frac{4}{2} + \frac{1}{5t} + \frac{1}{2} + \frac{1}{2t} - \frac{4}{2} - \frac{1}{4} - \frac{4}{6} - \frac{2}{3t} \\ &= -\frac{1}{60} + \frac{1}{30t} < 0. \end{aligned}$$

(ii) If the degree of any neighbor of w is more than two, let v be a neighbor of w, other than z, with $d(v) = p \geq 3$, and $u_i (i = 1, \cdots, p-1)$ be the neighbors of v, other than w. Let y be a 2-degree vertex adjacent to z. By the property, $d(u_i) \geq 2$, for $i = 1, \cdots, p-1$. Then we get a new tree by deleting the edge yz and adding the edge yv. Then we have

$$\begin{aligned} R_{-1}(T) - R_{-1}(T') &= \frac{4}{10} + \frac{1}{5t} - \frac{3}{8} - \frac{1}{4t} - \frac{1}{2(p+1)} + \left(\frac{1}{p} - \frac{1}{p+1}\right)\left(\frac{1}{t} + \sum_{i=1}^{p-1} \frac{1}{d(u_i)}\right) \\ &\leq \frac{1}{40} - \frac{1}{20t} - \frac{1}{2(p+1)} + \left(\frac{1}{p} - \frac{1}{p+1}\right)\left(\frac{1}{t} + \frac{p-1}{2}\right) \end{aligned}$$

$$= \frac{1}{40} - \frac{1}{20t} + \frac{2-t}{2p \cdot t(p+1)} \leq \frac{1}{40} - \frac{1}{20t} + \frac{2-t}{24t} = -\frac{1}{60} + \frac{1}{30t} < 0. \qquad \blacksquare$$

Lemma 2.4 *Let v_1u_1 and v_2u_2 be two edges of T, and T' be the tree obtained from T by deleting the edges v_1u_1 and v_2u_2 first, then adding the edges u_1v_2 and v_1u_2. If $d(u_1) \geq d(u_2)$ and $d(v_1) \leq d(v_2)$, then $R_{-1}(T) \leq R_{-1}(T')$.*

Proof.
$$\begin{aligned} R_{-1}(T) - R_{-1}(T') &= \frac{1}{d(v_1)d(u_1)} + \frac{1}{d(v_2)d(u_2)} - \frac{1}{d(v_1)d(u_2)} - \frac{1}{d(v_2)d(u_1)} \\ &= \left(\frac{1}{d(u_1)} - \frac{1}{d(u_2)}\right)\left(\frac{1}{d(v_1)} - \frac{1}{d(v_2)}\right) \leq 0. \qquad \blacksquare \end{aligned}$$

Our main result is the following, which gives the structure of a Max Tree of order $n \leq 102$.

Theorem 2.5 *For $n \leq 102$, there is a Max Tree T of order n such that the branching subtree S_T of T is a star.*

Proof. Suppose S_T is not a star, then we will transform T into another tree T' with $R_{-1}(T) \leq R_{-1}(T')$ step by step, till S_T is a star.

Let w be a maximum degree vertex of T, i.e., $d(w) = \Delta$. Since S_T is not a star, there is a branching vertex $v \in N(w)$ such that v is not a leaf of S_T, i.e., v has a neighbor u, other than w, with $d(u) \geq 3$. If w has a 2-degree neighbor v_0, then T has two edges v_0w and uv with $d(v_0) < d(u)$ and $d(w) \geq d(v)$. So by Lemma 2.4, we can assume that the neighbors of w are all branching vertices.

In the following, we always denote by v the neighbor of w which is not a leaf of S_T and the degree of v is as small as possible. Let u be the branching vertex adjacent to v, other than w, and p be a neighbor of u, other than v. Then $d(p) \leq d(w) = \Delta$. By Lemma 2.4, we can assume that $d(v) \geq d(u)$.

Now consider the two components of $T - wv$, the component with vertex v has at least 8 vertices, and the other component has at least $5(\Delta - 1) + 1$ vertices. Then

$5(\Delta-1)+9 \leq n$, so $\Delta \leq 19$, for $n \leq 102$. Denote by s the number of suspended paths rooted at v. We distinguish three cases and always assume $d(v)=t \geq 3$.

Case 1 $s \geq 2$.

By Lemma 2.2, $2 \leq s \leq min\{5, t-2\}$. Let u_i be the neighbors of v, other than w, with $d(u_i) \geq 3$ $(i=1,2,\cdots,t-s-1)$, and v_j be the neighbors of w, other than v. Then $d(v_j) \geq 3$ $(j=1,2,\cdots,\Delta-1)$. Let T' be the tree obtained from T by deleting the edges vu_i and adding the edges wu_i. Then we have

$$
\begin{aligned}
&R_{-1}(T)-R_{-1}(T') \\
=&\frac{1}{\Delta t}-\frac{1}{(s+1)(\Delta+t-s-1)}+\frac{s}{2t}-\frac{s}{2(s+1)} \\
&+\left(\frac{1}{\Delta}-\frac{1}{\Delta+t-s-1}\right)\sum_{j=1}^{\Delta-1}\frac{1}{d(v_j)}+\left(\frac{1}{t}-\frac{1}{\Delta+t-s-1}\right)\sum_{i=1}^{t-s-1}\frac{1}{d(u_i)} \qquad (2.1)\\
\leq&\frac{1}{\Delta t}-\frac{1}{(s+1)(\Delta+t-s-1)}+\frac{s}{2t}-\frac{s}{2(s+1)} \\
&+\frac{t-s-1}{\Delta(\Delta+t-s-1)}\cdot\frac{\Delta-1}{3}+\frac{\Delta-s-1}{t(\Delta+t-s-1)}\cdot\frac{t-s-1}{3}<0.
\end{aligned}
$$

This inequality holds for all $3 \leq \Delta \leq 19$, $3 \leq t \leq \Delta$, and $2 \leq s \leq min\{5, t-2\}$.

Case 2 $s=1$, *i.e., there is a suspended path xyv rooted at v.*

Consider the two components of $T-wv$, the component with vertex v has at least $5(t-2)+3$ vertices, and the other component has at least $5(\Delta-1)+1$ vertices. Then $5(\Delta+t)-11 \leq n$, so $\Delta+t \leq 22$, for $n \leq 102$.

If there is a vertex $u \in N(v) \setminus \{w, y\}$ such that u is not a leaf of S_T. Then u has a neighbor p, other than v, with $d(p) \geq 3$. Thus T has two edges yv and pu with $d(y)<d(p)$ and $d(v) \geq d(u)$. So, by Lemma 2.4 we can assume for any neighbor u_i of v, other than w and y, u_i is a leaf of S_T, i.e., $d(u_i)=3$ or 4 $(i=1,2,\cdots,t-2)$.

If there exist a vertex $u_1 \in N(v) \setminus \{w, y\}$ such that $d(u_1)=4$. Then for any $v_i \in N(w) \setminus \{v\}$, $d(v_i) \geq 4$, since, for otherwise, if there is a 3-degree vertex v_1 adjacent to w, then from Lemma 2.4, by deleting the edges wv_1 and vu_1 and adding the edges

wu_1 and vv_1, we can get a tree T' with $R_{-1}(T) \le R_{-1}(T')$.

Subcase 2.1 All the neighbors of v, other than w and y, are of degree 4.

Now, $d(v_j) \ge 4$ $(j = 1, 2, \cdots, \Delta - 1)$, and so from (2.1) we have

$$
\begin{aligned}
&R_{-1}(T) - R_{-1}(T') \\
=&\frac{1}{\Delta t} - \frac{1}{2(\Delta + t - 2)} + \frac{1}{2t} - \frac{1}{4} + \left(\frac{1}{\Delta} - \frac{1}{\Delta + t - 2}\right) \sum_{j=1}^{\Delta-1} \frac{1}{d(v_j)} \\
&+ \left(\frac{1}{t} - \frac{1}{\Delta + t - 2}\right) \sum_{i=1}^{t-2} \frac{1}{d(u_i)} \qquad (2.2) \\
\le&\frac{1}{\Delta t} - \frac{1}{2(\Delta + t - 2)} + \frac{1}{2t} - \frac{1}{4} + \frac{t-2}{\Delta(\Delta + t - 2)} \cdot \frac{\Delta - 1}{4} + \frac{\Delta - 2}{t(\Delta + t - 2)} \cdot \frac{t-2}{4} < 0.
\end{aligned}
$$

This inequality holds for all $3 \le \Delta \le 19$, $3 \le t \le \Delta$.

Subcase 2.2 There exist both a 3-degree vertex and a 4-degree vertex in the neighbors of v, other than w and y.

Obviously $t \ge 4$, therefore $\Delta \ge 4$ in this subcase. Let u_1 be a 3-degree vertex adjacent to v. Let T' be obtained from T by deleting the edge vy and adding the edge $u_1 y$, and contracting the edge wv and then subdividing a leaf. Since $d(v_j) \ge 4$ $(j = 1, 2, \cdots, \Delta - 1)$, we have

$$
\begin{aligned}
&R_{-1}(T) - R_{-1}(T') \\
=&-\frac{7}{24} + \frac{1}{\Delta t} + \frac{5}{6t} - \frac{1}{4(\Delta + t - 3)} + \left(\frac{1}{\Delta} - \frac{1}{\Delta + t - 3}\right) \sum_{j=1}^{\Delta-1} \frac{1}{d(v_j)} \\
&+ \left(\frac{1}{t} - \frac{1}{\Delta + t - 3}\right) \sum_{i=1}^{t-3} \frac{1}{d(u_i)} \qquad (2.3) \\
\le&-\frac{7}{24} + \frac{1}{\Delta t} + \frac{5}{6t} - \frac{1}{4(\Delta + t - 3)} + \frac{t-3}{\Delta(\Delta + t - 3)} \cdot \frac{\Delta - 1}{4} + \frac{\Delta - 3}{t(\Delta + t - 3)} \left(\frac{t-4}{3} + \frac{1}{4}\right) \\
<&0.
\end{aligned}
$$

This inequality holds for all $4 \le \Delta \le 19$, $4 \le t \le \Delta$, and $\Delta + t \le 22$.

Subcase 2.3 All the neighbors of v, other than w and y, are of degree 3.

Now, we have $d(v_j) \geq 3$ $(j = 1, 2, \cdots, \Delta - 1)$.

If $t = 3$, and $3 \leq \Delta \leq 5$, then from (2.2) we have

$$\begin{aligned}
& R_{-1}(T) - R_{-1}(T') \\
\leq & \frac{1}{3\Delta} - \frac{1}{2(\Delta+1)} - \frac{1}{12} + \frac{1}{\Delta(\Delta+1)} \cdot \frac{\Delta-1}{3} + \frac{\Delta-2}{3(\Delta+1)} \cdot \frac{1}{3} \\
= & \frac{\Delta^2 - 5\Delta}{36\Delta(\Delta+1)} \leq 0.
\end{aligned}$$

If $t = 3$, $\Delta \geq 6$, then let T' be the tree obtained from T by deleting the vertex v, adding a (3,4)-system adjacent to w, and then subdividing a leaf, and so we have

$$R_{-1}(T) - R_{-1}(T') = \frac{1}{12\Delta} - \frac{1}{72} \leq 0.$$

If $t = 4$, from (2.3) we have

$$\begin{aligned}
R_{-1}(T) - R_{-1}(T') &\leq -\frac{1}{12} + \frac{1}{4\Delta} - \frac{1}{4(\Delta+1)} + \frac{1}{\Delta(\Delta+1)} \cdot \frac{\Delta-1}{3} + \frac{\Delta-3}{12(\Delta+1)} \\
&= -\frac{1}{12\Delta(\Delta+1)} < 0.
\end{aligned}$$

Now we assume $t \geq 5$, and so $d \geq 5$. If there are at most two 3-degree vertices adjacent to w, other than v, then from (2.3) we have

$$\begin{aligned}
& R_{-1}(T) - R_{-1}(T') \\
& \leq -\frac{7}{24} + \frac{1}{\Delta t} + \frac{5}{6t} - \frac{1}{4(\Delta+t-3)} + \frac{t-3}{\Delta(\Delta+t-3)} \left(\frac{\Delta-3}{4} + \frac{2}{3} \right) + \frac{\Delta-3}{t(\Delta+t-3)} \cdot \frac{t-3}{3} \\
& < 0.
\end{aligned}$$

This inequality holds for all $5 \leq \Delta \leq 19$, $5 \leq t \leq \Delta$, and $\Delta + t \leq 22$.

So there are at least three 3-degree vertices adjacent to w, other than v. By the choice of v, all the 3-degree vertices adjacent to w must be leaves of S_T. Let T' be the tree obtained from T by deleting the three (2,3)-systems adjacent to w and two (2,3)-systems adjacent to v and the suspended path adjacent to v, then contracting the edge wv to a new vertex w' and adding four (3,4)-systems adjacent to w'. Then

$$\begin{aligned}
&R_{-1}(T)-R_{-1}(T')\\
=&-\frac{1}{3}+\frac{1}{\Delta t}+\frac{3}{3\Delta}+\frac{2}{3t}+\frac{1}{2t}-\frac{4}{4(\Delta+t-4)}+\left(\frac{1}{\Delta}-\frac{1}{\Delta+t-4}\right)\sum_{j=1}^{\Delta-4}\frac{1}{d(v_j)}\\
&+\left(\frac{1}{t}-\frac{1}{\Delta+t-4}\right)\sum_{i=1}^{t-4}\frac{1}{d(u_i)}\\
\leq&-\frac{1}{3}+\frac{1}{\Delta t}+\frac{1}{\Delta}+\frac{7}{6t}-\frac{1}{\Delta+t-4}+\frac{t-4}{\Delta(\Delta+t-4)}\cdot\frac{\Delta-4}{3}+\frac{\Delta-4}{t(\Delta+t-4)}\cdot\frac{t-4}{3}\\
<&0.
\end{aligned}$$

This inequality holds for all $5\leq\Delta\leq 19$, $5\leq t\leq\Delta$, and $\Delta+t\leq 22$.

Case 3 $s=0$, i.e., there is no suspended path rooted at any of v and w.

Subcase 3.1 There is a vertex $u\in N(v)\setminus\{w\}$ such that u is not a leaf of S_T.

If $t\leq 4$, T' is obtained from T by contracting the edge wv and subdividing a leaf, then

$$\begin{aligned}
&R_{-1}(T)-R_{-1}(T')\\
=&\frac{1}{\Delta t}-\frac{1}{4}+\left(\frac{1}{\Delta}-\frac{1}{\Delta+t-2}\right)\sum_{j=1}^{\Delta-1}\frac{1}{d(v_j)}+\left(\frac{1}{t}-\frac{1}{\Delta+t-2}\right)\sum_{i=1}^{t-1}\frac{1}{d(u_i)} \qquad (2.4)\\
\leq&\frac{1}{\Delta t}-\frac{1}{4}+\frac{t-2}{\Delta(\Delta+t-2)}\cdot\frac{\Delta-1}{3}+\frac{\Delta-2}{t(\Delta+t-2)}\cdot\frac{t-1}{3}<0.
\end{aligned}$$

This inequality holds for all $3\leq\Delta\leq 19$, $t\leq 4$. So we assume $t\geq 5$ in the following. By the choice of v, for any neighbor v_i of w, v_i is either a leaf of S_T or $d(v_i)\geq 5$.

If there is a vertex $v_1\in N(w)\setminus\{v\}$ such that $d(v_1)=3$, then v_1 is a leaf of S_T, and $d(v_1)\leq d(u)$. By Lemma 2.4, we can get a tree T' with $R_{-1}(T)\leq R_{-1}(T')$.

So for any vertex $v_i\in N(w)\setminus\{v\}$, $d(v_i)\geq 4$ $(i=1,2,\cdots,\Delta-1)$. Consider the two components of $T-wv$, the component with vertex v has at least $5(t-1)+1$ vertices, and the other component has at least $7(\Delta-1)+1$ vertices. Then $7\Delta+5t-10\leq n$, so $7\Delta+5t\leq 112$ and $\Delta\leq 12$, for $n\leq 102$ and $t\geq 5$. Then, from (2.4) we have

$$R_{-1}(T)-R_{-1}(T') \leq \frac{1}{\Delta t}-\frac{1}{4}+\frac{t-2}{\Delta(\Delta+t-2)}\cdot\frac{\Delta-1}{4}+\frac{\Delta-2}{t(\Delta+t-2)}\cdot\frac{t-1}{3}<0.$$

This inequality holds for all $3 \leq \Delta \leq 12$, $5 \leq t \leq d$ and $7\Delta+5t \leq 112$.

Subcase 3.2 For any $u_i \in N(v)\setminus\{w\}$, u_i is a leaf of S_T, i.e., $d(u_i)=3$ or 4 $(i=1,2,\cdots t-1)$.

Consider the two components of $T-wv$, the component containing vertex v has at least $5(t-1)+1$ vertices, and the other component has at least $5(\Delta-1)+1$ vertices. Then $5(\Delta+t)-8 \leq n$, so $\Delta+t \leq 22$, for $n \leq 102$.

If $t=3$, then by (2.4) we have

$$R_{-1}(T)-R_{-1}(T') \leq \frac{1}{3\Delta}-\frac{1}{4}+\frac{1}{\Delta(\Delta+1)}\cdot\frac{\Delta-1}{3}+\frac{\Delta-2}{3(\Delta+1)}\cdot\frac{2}{3}=-\frac{1}{36}<0.$$

Now we assume $4 \leq t \leq 7$, therefore $d \geq 4$.

If there are at most three 3-degree vertices adjacent to v, then by (2.4) we have

$$\begin{aligned}
& R_{-1}(T)-R_{-1}(T') \\
\leq\ & \frac{1}{\Delta t}-\frac{1}{4}+\frac{t-2}{\Delta(\Delta+t-2)}\cdot\frac{\Delta-1}{3}+\frac{\Delta-2}{t(\Delta+t-2)}\cdot\left(\frac{3}{3}+\frac{t-4}{4}\right) \\
=\ & \frac{1}{\Delta t}-\frac{1}{4}+\frac{t-2}{\Delta(\Delta+t-2)}\cdot\frac{\Delta-1}{3}+\frac{\Delta-2}{t(\Delta+t-2)}\cdot\frac{t}{4}<0.
\end{aligned}$$

This inequality holds for all $4 \leq \Delta \leq 19$, $4 \leq t \leq 7$ and $\Delta+t \leq 22$.

So there are at least four 3-degree vertices adjacent to v (now $t \geq 5$), say u_1, u_2, u_3, u_4, i.e., there are at least four (2,3)-systems adjacent to v. We obtain T' from T by deleting these four (2,3)-systems, contracting the edge wv to a new vertex w', and then adding three (3,4)-systems adjacent to w'. Then we have

$$\begin{aligned}
& R_{-1}(T)-R_{-1}(T') \\
=\ & \frac{1}{\Delta t}+\frac{4}{3t}+\frac{16}{3}-\frac{45}{8}-\frac{3}{4(\Delta+t-3)} \\
& +\left(\frac{1}{\Delta}-\frac{1}{\Delta+t-3}\right)\sum_{j=1}^{\Delta-1}\frac{1}{d(v_j)}+\left(\frac{1}{t}-\frac{1}{\Delta+t-3}\right)\sum_{i=5}^{t-1}\frac{1}{d(u_i)}
\end{aligned}$$

$$\leq \frac{1}{\Delta t} - \frac{7}{24} + \frac{4}{3t} - \frac{3}{4(\Delta+t-3)} + \frac{t-3}{\Delta(\Delta+t-3)} \cdot \frac{\Delta-1}{3} + \frac{\Delta-3}{t(\Delta+t-3)} \cdot \frac{t-5}{3} < 0.$$

This inequality holds for all $4 \leq \Delta \leq 19$, $4 \leq t \leq 7$ and $\Delta + t \leq 22$.

Note that for $t \geq 8$, $\Delta \geq 8$, and if there is another neighbor v' of w, which is not a leaf of S_T, since v is the smallest degree vertex among the neighbors of w which are not the leaves of S_T, then $d(v') = t' \geq 8$. Now T has at least $5(d-2)+5(t-1)+5(t'-1)+3 \geq 103$ vertices, which is out of the scope of our discussion. So for $n \leq 102$, all the neighbors of w, other than v, are the leaves of S_T, i.e., S_T is a double star.

For $\Delta + t \leq 19$, if there is at most one 3-degree vertex adjacent to w, then from (2.4) we have

$$R_{-1}(T) - R_{-1}(T') \leq \frac{1}{\Delta t} - \frac{1}{4} + \frac{t-2}{\Delta(\Delta+t-2)} \left(\frac{1}{3} + \frac{\Delta-2}{4}\right) + \frac{\Delta-2}{t(\Delta+t-2)} \cdot \frac{t-1}{3} < 0.$$

This inequality holds for all $8 \leq \Delta \leq 19$, $8 \leq t \leq d$ and $\Delta + t \leq 19$.

And if there is at most one 3-degree vertex adjacent to v, then from (2.4) we have

$$R_{-1}(T) - R_{-1}(T') \leq \frac{1}{\Delta t} - \frac{1}{4} + \frac{t-2}{\Delta(\Delta+t-2)} \cdot \frac{\Delta-1}{3} + \frac{\Delta-2}{t(\Delta+t-2)} \left(\frac{1}{3} + \frac{t-2}{4}\right) < 0.$$

This inequality holds for all $8 \leq \Delta \leq 19$, $8 \leq t \leq d$ and $\Delta + t \leq 19$.

For $\Delta + t = 20$, denote by x_4 the number of 4-degree vertices among the leaves of S_T. Since $7x_4 + 5(\Delta + t - x_4 - 2) + 2 \leq n$, we have $x_4 \leq 5$, for $n \leq 102$. Since $\Delta \geq 8$, and $t \geq 8$, from above discussion, for $\Delta + t \leq 20$, both w and v have at least two 3-degree neighbors, i.e., both w and v have at least two (2,3)-systems adjacent to them. Let T' be obtained from T by deleting these four (2,3)-systems, contracting the edge wv to a new vertex w', and then adding three (3,4)-systems adjacent to w'. Then we have

$$\begin{aligned} & R_{-1}(T) - R_{-1}(T') \\ = \; & \frac{1}{\Delta t} + \frac{2}{3t} + \frac{2}{3\Delta} + \frac{16}{3} - \frac{45}{8} - \frac{3}{4(\Delta+t-3)} \\ & + \left(\frac{1}{\Delta} - \frac{1}{\Delta+t-3}\right) \sum_{j=3}^{\Delta-1} \frac{1}{d(v_j)} + \left(\frac{1}{t} - \frac{1}{\Delta+t-3}\right) \sum_{i=3}^{t-1} \frac{1}{d(u_i)} \end{aligned}$$

$$
\begin{aligned}
&\leq \frac{1}{\Delta t}-\frac{7}{24}+\frac{2}{3t}+\frac{2}{3\Delta}-\frac{3}{4(\Delta+t-3)}+\frac{t-3}{\Delta(\Delta+t-3)}\cdot\frac{\Delta-3}{3}+\frac{\Delta-3}{t(\Delta+t-3)}\cdot\frac{t-3}{3}\\
&< 0.
\end{aligned}
$$

This inequality holds for all $8 \leq \Delta \leq 19$, $8 \leq t \leq d$ and $\Delta + t \leq 20$.

Now only the case that $21 \leq \Delta+t \leq 22$ is left. Since $5(\Delta+t-x_4-2)+7x_4+2 \leq n$, we have $x_4 \leq 2$, for $n \leq 102$. Since $\Delta \geq 8$ and $t \geq 8$, there are at least five (2,3)-systems adjacent to v and at least six (2,3)-systems adjacent to w. Let T' be obtained from T by deleting these 11 (2,3)-systems, contracting the edge wv to a new vertex w', and then adding 8 (3,4)-systems adjacent to w'. Then we have

$$
\begin{aligned}
& R_{-1}(T)-R_{-1}(T')\\
={}& \frac{1}{\Delta t}+\frac{5}{3t}+\frac{6}{3\Delta}+\frac{2\times 22}{3}-\frac{5\times 24}{8}-\frac{8}{4(\Delta+t-5)}\\
& +\left(\frac{1}{\Delta}-\frac{1}{\Delta+t-5}\right)\sum_{j=7}^{\Delta-1}\frac{1}{d(v_j)}+\left(\frac{1}{t}-\frac{1}{\Delta+t-5}\right)\sum_{i=6}^{t-1}\frac{1}{d(u_i)}\\
\leq{}& \frac{1}{\Delta t}-\frac{1}{3}+\frac{5}{3t}+\frac{2}{\Delta}-\frac{2}{(\Delta+t-5)}+\frac{t-5}{\Delta(\Delta+t-5)}\cdot\frac{\Delta-7}{3}+\frac{\Delta-5}{t(\Delta+t-5)}\cdot\frac{t-6}{3}\\
<{}& 0.
\end{aligned}
$$

This inequality holds for all $8 \leq \Delta \leq 19$, $8 \leq t \leq d$ and $\Delta + t \leq 22$.

The proof is now complete. ∎

Remark 2.6 *One might be able to get the same or similar structure(s) for Max Trees of order larger than 102 by improving our above proof. But, the really interesting problem is how to drop the restriction on the orders of trees.*

3 Maximum value and maximum tree for R_{-1} of trees of order $n \leq 102$

By Lemmas 2.2, 2.3 and Theorem 2.5, we can conclude that there is a Max Tree T such that the branching subtree S_T of T is a star. Let w be the maximum degree vertex of S_T, i.e., $d(w) = \Delta$. Suppose that there are r 2-degree vertices adjacent to w, p (2,3)-systems adjacent to w, and q (3,4)-systems adjacent to w, and there is at most one suspended path of length 3. Then the following theorem is straightforward.

Theorem 3.1 *Denote by $f(n)$ the maximum value of R_{-1} among all trees of order n. Then, for $n \leq 102$ we have*

$$f(n) = max\ R_{-1}(T) = \begin{cases} \frac{r}{2} + \frac{4p}{3} + \frac{15q}{8} + \frac{r}{2\Delta} + \frac{p}{3\Delta} + \frac{q}{4\Delta} & n - \Delta + r - 1 \equiv 0\ (mod\ 2); \\ \frac{r}{2} + \frac{4p}{3} + \frac{15q}{8} + \frac{r}{2\Delta} + \frac{p}{3\Delta} + \frac{q}{4\Delta} + \frac{1}{4} & n - \Delta + r - 1 \equiv 1\ (mod\ 2). \end{cases}$$

$$s.t. \begin{cases} p + q + r = \Delta \\ 2p + 3q + r = \lfloor \frac{n-\Delta+r-1}{2} \rfloor \\ 0 \leq r \leq 5,\ 0 \leq p \leq \Delta - r,\ 0 \leq q \leq \Delta - r \end{cases}$$

Now we can easily compile a Maple program and use a computer to calculate it. The maximum value for Randić index R_{-1} of trees of order n and the corresponding maximum tree are shown in the following table.

n	10	11*	12	13	14	15	16	17
$f(n)$	$\frac{25}{9}$	$\frac{109}{36}$	$\frac{79}{24}$	$\frac{32}{9}$	$\frac{61}{16}$	$\frac{49}{12}$	$\frac{13}{3}$	$\frac{221}{48}$
(p,q,r)	(1,0,2)	(1,0,2)	(0,1,2)	(2,0,1)	(0,1,3)	(2,0,2)	(3,0,0)	(1,1,2)
n	18	19*	20	21	22	23	24*	25
$f(n)$	$\frac{39}{8}$	$\frac{41}{8}$	$\frac{27}{5}$	$\frac{17}{3}$	$\frac{237}{40}$	$\frac{31}{5}$	$\frac{129}{20}$	$\frac{269}{40}$
(p,q,r)	(3,0,1)	(3,0,1)	(3,0,2)	(4,0,0)	(2,1,2)	(4,0,1)	(4,0,1)	(3,1,1)
n	26	27*	28	29*	30	31	32*	33
$f(n)$	7	$\frac{29}{4}$	$\frac{271}{36}$	$\frac{70}{9}$	$\frac{145}{18}$	$\frac{25}{3}$	$\frac{103}{12}$	$\frac{319}{36}$
(p,q,r)	(5,0,0)	(5,0,0)	(5,0,1)	(5,0,1)	(4,1,1)	(6,0,0)	(6,0,0)	(5,1,0)
n	34*	35	36	37	38	39*	40	41
$f(n)$	$\frac{82}{9}$	$\frac{169}{18}$	$\frac{29}{3}$	$\frac{119}{12}$	$\frac{571}{56}$	$\frac{585}{56}$	$\frac{901}{84}$	11
(p,q,r)	(5,1,0)	(4,2,0)	(7,0,0)	(3,3,0)	(6,1,0)	(6,1,0)	(5,2,0)	(8,0,0)

n	42	43	44	45	46	47	48	49
$f(n)$	$\frac{1891}{168}$	$\frac{369}{32}$	$\frac{165}{14}$	$\frac{193}{16}$	$\frac{37}{3}$	$\frac{403}{32}$	$\frac{2779}{216}$	$\frac{105}{8}$
(p,q,r)	(4,3,0)	(7,1,0)	(3,4,0)	(6,2,0)	(9,0,0)	(5,3,0)	(8,1,0)	(4,4,0)

n	50	51	52	53	54	55	56	57
$f(n)$	$\frac{1447}{108}$	$\frac{41}{3}$	$\frac{1003}{72}$	$\frac{71}{5}$	$\frac{781}{54}$	$\frac{221}{15}$	15	$\frac{229}{15}$
(p,q,r)	(7,2,0)	(10,0,0)	(6,3,0)	(9,1,0)	(5,4,0)	(8,2,0)	(11,0,0)	(7,3,0)

n	58	59	60	61	62	63	64	65
$f(n)$	$\frac{1367}{88}$	$\frac{79}{5}$	$\frac{707}{44}$	$\frac{49}{3}$	$\frac{1461}{88}$	$\frac{2429}{144}$	$\frac{377}{22}$	$\frac{1253}{72}$
(p,q,r)	(10,1,0)	(6,4,0)	(9,2,0)	(5,5,0)	(8,3,0)	(11,1,0)	(7,4,0)	(10,2,0)

n	66	67	68	69	70	71	72	73
$f(n)$	$\frac{1555}{88}$	$\frac{287}{16}$	$\frac{801}{44}$	$\frac{665}{36}$	$\frac{1649}{88}$	$\frac{2737}{144}$	$\frac{212}{11}$	$\frac{469}{24}$
(p,q,r)	(6,5,0)	(9,3,0)	(5,6,0)	(8,4,0)	(4,7,0)	(7,5,0)	(3,8,0)	(6,6,0)

n	74	75	76	77	78	79	80	81
$f(n)$	$\frac{515}{26}$	$\frac{2891}{144}$	$\frac{6347}{312}$	$\frac{371}{18}$	$\frac{3257}{156}$	$\frac{1015}{48}$	$\frac{2227}{104}$	$\frac{1561}{72}$
(p,q,r)	(9,4,0)	(5,7,0)	(8,5,0)	(4,8,0)	(7,6,0)	(3,9,0)	(6,7,0)	(2,10,0)

n	82	83	84	85	86	87	88	89
$f(n)$	$\frac{856}{39}$	$\frac{3199}{144}$	$\frac{7015}{312}$	$\frac{91}{4}$	$\frac{1197}{52}$	$\frac{163}{7}$	$\frac{7349}{312}$	$\frac{667}{28}$
(p,q,r)	(5,8,0)	(1,11,0)	(4,9,0)	(0,12,0)	(3,10,0)	(6,8,0)	(2,11,0)	(5,9,0)

n	90	91	92	93	94	95	96	97
$f(n)$	$\frac{1879}{78}$	$\frac{341}{14}$	$\frac{197}{8}$	$\frac{697}{28}$	$\frac{3019}{120}$	$\frac{178}{7}$	$\frac{925}{36}$	$\frac{727}{28}$
(p,q,r)	(1,12,0)	(4,10,0)	(0,13,0)	(3,11,0)	(6,9,0)	(2,12,0)	(5,10,0)	(1,13,0)

n	98	99	100	101	102			
$f(n)$	$\frac{9443}{360}$	$\frac{53}{2}$	$\frac{803}{30}$	$\frac{865}{32}$	$\frac{9829}{360}$			
(p,q,r)	(4,11,0)	(0,14,0)	(3,12,0)	(6,10,0)	(2,13,0)			

where n^* means that there is a suspended path of length 3 in the Max Tree of order n.

Remark 3.2 *Note that in Theorem 2.1 of [8], we showed by induction that for any* *tree T of order $n \geq 3$, $R_{-1}(T) \leq \frac{15n+C}{56}$. Since for $91 \leq n \leq 102$, $f(n) \leq \frac{15n-1}{56}$, we have enough n's as our induction initial in Theorem 2.1 of [8]. So, we can say that $R_{-1}(T) \leq \frac{15n-1}{56}$, for $n \geq 91$. This corrects a small error in Section 3 of [8]. On the other hand, since for the infinitely many trees T_r (obtained from the star S_r by appending three internally-disjoint paths of length 2 to each leaf of S_r), $R_{-1}(T_r) = \frac{15n-1}{56}$, we know that $\frac{15n-1}{56}$ is a sharp upper bound for infinitely many values of n.*

In fact, we can prove that $r \leq 2$ for $n \geq 21$, and then the computer search can be faster. However, since the search is fast enough even without this improvement, it might be not worthy of showing. And by observing the table, one can find that $r = 0$ for $n \geq 31$, and so we propose the following conjecture.

Conjecture 3.3 *For a pair of integers (p, q), $T_{p,q}$ denotes the tree obtained from the star S_m (where $m = p + q + 1$) by appending two internally-disjoint paths of length 2 to p leaves of S_m, and appending three internally-disjoint paths of length 2 to q leaves of S_m. Then, for $n \geq 103$ there is a pair (p, q) such that $T_{p,q}$ has the maximum Randić index R_{-1}.*

References

[1] B. Bollobás and P. Erdös, Graphs of extremal weights, Ars Combin. 50(1998) 225–233.

[2] G. Caporossi, I. Gutman and P. Hansen, Variable neighborhood search for extremal graphs IV: Chemical trees with extremal connectivity index, Comput. Chem. 23 (1999) 469–477.

[3] G. Caporossi, I. Gutman, P. Hansen and L. Pavlović, Graphs with maximum connectivity index, Comput. Biol. Chem. 27 (2003) 85–90.

[4] L.H. Clark, I. Gutman, M. Lepović and D. Vidović, Exponent-dependent properties of the connectivity index, Indian J. Chem. 41 A (2002) 457–461.

[5] L.H. Clark and J.W. Moon, On the general Randić index for certain families of trees, Ars Combin. 54 (2000) 223–235.

[6] Y. Hu, X. Li and Y. Yuan, Trees with minimum general Randić index, MATCH Commun. Math. Comput. Chem. 52(2004) 119–128.

[7] Y. Hu, X. Li and Y. Yuan, Trees with maximum general Randić index, MATCH Commun. Math. Comput. Chem. 52(2004) 129–146.

[8] Y. Hu, X. Li and Y. Yuan, Solutions to two unsolved questions on the best upper bound for the Randic index R_{-1} of trees MATCH Commun. Math. Comput. Chem. 54(2)(2005).

[9] L.B. Kier, L.H. Hall, Molecular Connectivity in Chemistry and Drug Research, Academic Press, New York, 1976.

[10] L.B. Kier, L.H. Hall, Molecular Connectivity in Structure-Analysis, Research Studies Press, Wiley, Chichester, UK, 1986.

[11] X. Li and Y. Yang, Best lower and upper bounds for the Randić index R_{-1} of chemical trees, MATCH Commun. Math. Comput. Chem. 52(2004) 147–156.

[12] D. Rautenbach, A note on trees of maximum weight and restricted degrees, Discrete Math. 271(2003) 335–342.