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More Results on Extremum Randić Indices of (Molecular) Trees

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Abstract. The Randić index $R(G)$ of a graph G is the sum of the weights $(d_u d_v)^{-\frac{1}{2}}$ of all edges uv in G, where d_u denotes the degree of vertex u. Du and Zhou [On Randić indices of trees, unicyclic graphs, and bicyclic graphs, Int. J. Quantum Chem. 111 (2011), 2760–2770] determined the n-vertex trees with the third for $n \geq 7$, the fourth for $n \geq 10$, the fifth and the sixth for $n \geq 11$ maximum Randić indices. Recently, Li *et al.* [The Randić indices of trees, unicyclic graphs and bicyclic graphs, Ars Comb. 127 (2016), 409–419] obtained the n-vertex trees with the seventh, the eighth, the ninth and the tenth for $n \geq 11$ maximum Randić indices. In this paper, we correct the ordering for the Randić indices of trees obtained by Li *et al.*, and characterize the trees with from the seventh to the sixteenth maximum Randić indices. The obtained extremal trees are molecular and thereby the obtained ordering also holds for molecular trees.

1. Introduction

Let G be a simple graph with vertex set $V(G)$ and edge set $E(G)$. The vertex degree of $v \in V(G)$ is denoted by d_v. A vertex u in G is called pendant if $d_u = 1$. The set of all the neighbors of $u \in V(G)$ is denoted by $N_G(u)$. For more notations and terminologies not defined here, please refer to [12].

Molecular descriptors play a significant role in mathematical chemistry, especially in the quantitative structure-property relationship and quantitative structure-activity relationship investigations. Among them, special place is reserved for the so-called topological indices [3]. The Randić index is one of the most well-known topological indices with a lot of applications in chemistry.

The Randić index [10] $R(G)$ is defined as

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}.$$

An n-vertex connected graph is known as tree, unicyclic and bicyclic if it has $n + c$ edges with $c = -1, 0, 1$, respectively.

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Trees and unicyclic graphs with the maximum and the second maximum Randić indices, and bicyclic graphs with the maximum Randić index have been determined by Caporossi *et al.* [2]. Trees with the third, the fourth, the fifth and the sixth maximum Randić indices, unicyclic graphs with the third, the fourth and the fifth maximum Randić indices, and bicyclic graphs with the second, the third, the fourth and the fifth maximum Randić indices have been determined by Du and Zhou in [4].

Bollobás and Erdös [1] showed that the star S_n is the unique n-vertex connected graph, and thus the unique n-vertex tree, with the minimum Randić index. Trees with the second, the third and the fourth minimum Randić indices have been determined by Zhao and Li [13]. Unicyclic and bicyclic graphs with the minimum Randić indices have been obtained in [6, 11], respectively. Trees with the fifth minimum Randić index, unicyclic graphs with the second, the third and the fourth minimum Randić indices, bicyclic graphs with the second minimum Randić index have been determined by Du and Zhou [4].

A connected graph with maximum degree at most four is called a chemical graph. Chemical trees and chemical unicyclic graphs with extremal Randić indices have been discussed in [5, 7, 8].

Recently, Li *et al.* [9] determined the n-vertex trees with the seventh, the eighth, the ninth and the tenth for $n \geq 11$ maximum Randić indices. In this paper, we determine all the trees with from the seventh to the sixteenth maximum Randić indices, and consequently correct the ordering reported by Li *et al.* [9].

2. Preliminaries

A pendant edge is an edge incident with a pendant vertex. A path $u_1u_2 \ldots u_r$ in a graph G is said to be a pendant path at u_1 if $d_{u_1} \geq 3$, $d_{u_i} = 2$ for $i = 2, \ldots, r-1$ and $d_{u_r} = 1$.

For an n-vertex connected graph G, it was shown in [2] that

$$R(G) = \frac{n}{2} - \frac{1}{2} f(G), \tag{1}$$

where

$$f(G) = \sum_{uv \in E(G)} \left(\frac{1}{\sqrt{d_u}} - \frac{1}{\sqrt{d_v}} \right)^2.$$

Thus for fixed n, $R(G)$ is decreasing on $f(G)$. We will use this fact to determine the trees with large Randić indices.

First of all, Caporossi *et al.* [2] determined the trees with the maximum and the second maximum Randić indices.

Theorem A. *[2] Among the n-vertex trees,*

(i) *for $n \geq 4$, the path P_n is the unique tree with the maximum Randić index, which is equal to $\frac{n-3}{2} + \sqrt{2}$,*

(ii) *for $n \geq 7$, the trees with a single vertex of maximum degree three, adjacent to three vertices of degree two are the unique trees with the second maximum Randić index, which is equal to $\frac{n-7}{2} + \frac{3}{\sqrt{6}} + \frac{3}{\sqrt{2}}$.*

Subsequently, Du and Zhou [4] extended the ordering of Randić indices of trees to the first six maximum.

Theorem B. *[4] Among the n-vertex trees,*

(i) *for $n \geq 7$, the trees with a single vertex of maximum degree three, adjacent to one vertex of degree one and two vertices of degree two are the unique trees with the third maximum Randić index, which is equal to $\frac{n-6}{2} + \frac{2}{\sqrt{6}} + \frac{1}{\sqrt{3}} + \sqrt{2}$,*

(ii) *for $n \geq 10$, the trees with exactly two adjacent vertices of maximum degree three, each adjacent to two vertices of degree two are the unique trees with the fourth maximum Randić index, which is equal to $\frac{n-10}{2} + \frac{4}{\sqrt{6}} + \frac{4}{\sqrt{2}} + \frac{1}{3}$,*

(iii) *for $n \geq 11$, the trees with exactly two nonadjacent vertices of maximum degree three, each adjacent to three vertices of degree two are the unique trees with the fifth maximum Randić index, which is equal to $\frac{n-11}{2} + \frac{4}{\sqrt{2}} + \sqrt{6}$,* (*iv*) *for* $n \geq 11$, *the tree with a single vertex of maximum degree three, adjacent to two vertices of degree one and one vertex of degree two is the unique tree with the sixth maximum Randić index, which is equal to* $\frac{n-5}{2} + \frac{1}{\sqrt{6}} + \frac{2}{\sqrt{3}} + \frac{1}{\sqrt{2}}$.

Recently, Li *et al.* [9] reported the trees with the seventh, the eighth, the ninth and the tenth maximum Randić indices.

Theorem C. *[9] Among the n-vertex trees,*

(*i*) *for* $n \geq 11$, *the trees with exactly two adjacent vertices of maximum degree three, one is adjacent to two vertices of degree two and the other is adjacent to one vertex of degree two and one vertex of degree one are the unique trees with the seventh maximum Randić index, which is equal to* $\frac{n-9}{2} + \frac{3}{\sqrt{6}} + \frac{1}{\sqrt{3}} + \frac{3}{\sqrt{2}} + \frac{1}{3}$,

(*ii*) *for* $n \geq 11$, *the trees with no vertex of degree three and exactly one vertex of maximum degree four, which is adjacent to four vertices of degree two are the unique trees with the eighth maximum Randić index, which is equal to* $\frac{n-9}{2} + \frac{6}{\sqrt{2}}$,

(*iii*) *for* $n \geq 11$, *the trees with exactly two nonadjacent vertices of maximum degree three, one is adjacent to three vertices of degree two and the other is adjacent to two vertices of degree two and one vertex of degree one are the unique trees with the ninth maximum Randić index, which is equal to* $\frac{n-10}{2} + \frac{5}{\sqrt{6}} + \frac{1}{\sqrt{3}} + \frac{3}{\sqrt{2}}$,

(*iv*) *for* $n \geq 11$, *the trees with exactly two adjacent vertices of maximum degree three, one is adjacent to two vertices of degree two and the other is adjacent to two vertices of degree one are the unique trees with the tenth maximum Randić index, which is equal to* $\frac{n-8}{2} + \frac{2}{\sqrt{6}} + \frac{2}{\sqrt{3}} + \frac{2}{\sqrt{2}} + \frac{1}{3}$.

3. Main results

3.1. Corrected version of Theorem C

In the following, we will present two classes of trees for which the ordering of Theorem C do not work, i.e., Theorem C by Li *et al.* [9] is not true.

Let G be an n-vertex tree with $n \geq 14$. Suppose that there are exactly three vertices of maximum degree 3 in G.

If there are exactly two pairs of adjacent vertices both of maximum degree three in G, and every pendant path of G is of length at least two, then

$$R(G) = \frac{n-13}{2} + \frac{5}{\sqrt{6}} + \frac{5}{\sqrt{2}} + \frac{2}{3}.$$

It is easy to check that this Randić index lies between the seventh maximum and the eighth maximum Randić indices as claimed in Theorem C, i.e.,

$$\frac{n-9}{2} + \frac{3}{\sqrt{6}} + \frac{1}{\sqrt{3}} + \frac{3}{\sqrt{2}} + \frac{1}{3} > \frac{n-13}{2} + \frac{5}{\sqrt{6}} + \frac{5}{\sqrt{2}} + \frac{2}{3} > \frac{n-9}{2} + \frac{6}{\sqrt{2}}.$$

If there is exactly one pair of adjacent vertices both of maximum degree three in G, and every pendant path of G is of length at least two, then

$$R(G) = \frac{n-14}{2} + \frac{7}{\sqrt{6}} + \frac{5}{\sqrt{2}} + \frac{1}{3}.$$

It is easy to check that this Randić index lies between the ninth maximum and the tenth maximum Randić indices as claimed in Theorem C, i.e.,

$$\frac{n-10}{2} + \frac{5}{\sqrt{6}} + \frac{1}{\sqrt{3}} + \frac{3}{\sqrt{2}} > \frac{n-14}{2} + \frac{7}{\sqrt{6}} + \frac{5}{\sqrt{2}} + \frac{1}{3} > \frac{n-8}{2} + \frac{2}{\sqrt{6}} + \frac{2}{\sqrt{3}} + \frac{2}{\sqrt{2}} + \frac{1}{3}.$$

So in the following, we would ignore the ordering as described in Theorem C, and determine from the seventh to the sixteenth maximum Randić indices, which not only extends the orderings in Theorems B and C, but also corrects the ordering in Theorem C.

3.2. Results on extremum Randić indices

We now present our main theorem.

Theorem 3.1. *Among the set of n-vertex trees,*

(*i*) *for $n \geq 11$, the trees with exactly two adjacent vertices of maximum degree three, one is adjacent to two vertices of degree two, and the other is adjacent to one vertex of degree two and one vertex of degree one, are the unique trees with the seventh maximum Randić index, which is equal to* $\frac{n-9}{2} + \frac{3}{\sqrt{6}} + \frac{1}{\sqrt{3}} + \frac{3}{\sqrt{2}} + \frac{1}{3}$,

(*ii*) *for $n \geq 13$, the trees with exactly three vertices of maximum degree three, say u, v, w, where both u and v, and v and w are adjacent, each of u, w is adjacent to two vertices of degree two, and v is adjacent to one vertex of degree two, are the unique trees with the eighth maximum Randić index, which is equal to* $\frac{n-13}{2} + \frac{5}{\sqrt{6}} + \frac{5}{\sqrt{2}} + \frac{2}{3}$,

(*iii*) *for $n \geq 13$, the trees with a single vertex of maximum degree four, adjacent to four vertices of degree two, and without vertices of degree three, are the unique trees with the ninth maximum Randić index, which is equal to* $\frac{n-9}{2} + \frac{6}{\sqrt{2}}$,

(*iv*) *for $n \geq 13$, the trees with exactly two nonadjacent vertices of maximum degree three, one is adjacent to three vertices of degree two, and the other is adjacent to two vertices of degree two and one vertex of degree one, are the unique trees with the tenth maximum Randić index, which is equal to* $\frac{n-10}{2} + \frac{5}{\sqrt{6}} + \frac{1}{\sqrt{3}} + \frac{3}{\sqrt{2}}$,

(*v*) *for $n \geq 14$, the trees with exactly three vertices of maximum degree three, say u, v, w, where u and v are not adjacent, u and w are not adjacent, and v and w are adjacent, u is adjacent to three vertices of degree two, each of v, w is adjacent to two vertices of degree two, are the unique trees with the eleventh Randić index, which is equal to* $\frac{n-14}{2} + \frac{7}{\sqrt{6}} + \frac{5}{\sqrt{2}} + \frac{1}{3}$,

(*vi*) *for $n \geq 14$, the trees with exactly two adjacent vertices of maximum degree three, each adjacent to one vertex of degree two and one vertex of degree one, or one is adjacent to two vertices of degree two, and the other is adjacent to two vertices of degree one, are the unique trees with the twelfth maximum Randić index, which is equal to* $\frac{n-8}{2} + \frac{2}{\sqrt{6}} + \frac{2}{\sqrt{3}} + \frac{2}{\sqrt{2}} + \frac{1}{3}$,

(*vii*) *for $n \geq 15$, the trees with exactly three vertices of maximum degree three, say u, v, w, where u, v, w are pairwise nonadjacent, and each of u, v, w is adjacent to three vertices of degree two, are the unique trees with the thirteenth maximum Randić index, which is equal to* $\frac{n-15}{2} + \frac{9}{\sqrt{6}} + \frac{5}{\sqrt{2}}$,

(*viii*) *for $n \geq 15$, the trees with exactly three vertices of maximum degree three, say u, v, w, where both u and v, and v and w are adjacent, each of u, w is adjacent to two vertices of degree two, and v is adjacent to one vertex of degree one, or one of u, w is adjacent to two vertices of degree two, the other is adjacent to one vertex of degree two and one vertex of degree one, and v is adjacent to one vertex of degree two, are the unique trees with the fourteenth maximum Randić index, which is equal to* $\frac{n-12}{2} + \frac{4}{\sqrt{6}} + \frac{1}{\sqrt{3}} + \frac{4}{\sqrt{2}} + \frac{2}{3}$,

(*ix*) *for $n \geq 15$, the trees with exactly two nonadjacent vertices of maximum degree three, each adjacent to two vertices of degree two and one vertex of degree one, or one is adjacent to three vertices of degree two, and the other is adjacent to one vertex of degree two and two vertices of degree one, are the unique trees with the fifteenth maximum Randić index, which is equal to* $\frac{n-9}{2} + \frac{4}{\sqrt{6}} + \frac{2}{\sqrt{3}} + \frac{2}{\sqrt{2}}$,

(*x*) *for $n \geq 15$, the trees with a single vertex u of degree three and a single vertex v of maximum degree four, where u and v are adjacent, u is adjacent to two vertices of degree two, and v is adjacent to three vertices of degree two, are the unique trees with the sixteenth maximum Randić index, which is equal to* $\frac{n-12}{2} + \frac{2}{\sqrt{6}} + \frac{1}{2\sqrt{3}} + \frac{13}{2\sqrt{2}}$.

Proof. Let G be an n-vertex tree different from the trees mentioned in Theorems A and B with the first six maximum Randić indices, where $n \geq 11$.

Obviously, there are at least four pendant paths in G. Otherwise, G is the path if G has no pendant path (i.e., the graph described in Theorem A (i)), and G is a graph of the forms described in Theorem A (ii), Theorem B (i) or (iv) if G has exactly three pendant paths.

Denote by k the number of pendant paths of length one in G.

Note that every pendant path of length one contributes to $f(G)$ is at least $\left(1-\frac{1}{\sqrt{3}}\right)^2$, while every pendant path of length at least two contributes to $f(G)$ is at least $\left(1-\frac{1}{\sqrt{2}}\right)^2+\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)^2$. From

$$\left(1-\frac{1}{\sqrt{3}}\right)^2 > \left(1-\frac{1}{\sqrt{2}}\right)^2+\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)^2,$$

we may conclude that every pendant path contributes to $f(G)$ is at least $\left(1-\frac{1}{\sqrt{2}}\right)^2+\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)^2$.

If there are at least six pendant paths in G, then

$$f(G) \geq 6\left[\left(1-\frac{1}{\sqrt{2}}\right)^2+\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)^2\right] > 12-\frac{4}{\sqrt{6}}-\frac{1}{\sqrt{3}}-\frac{13}{\sqrt{2}}.$$

Case 1. Suppose that there are exactly four pendant paths in G. Then we consider two subcases.

Subcase 1.1. There are exactly two vertices of maximum degree three in G, and all other vertices are of degrees one or two.

Subcase 1.2. There is a single vertex of maximum degree four in G, and all other vertices are of degrees one or two.

Suppose that **Subcase 1.1** holds. Denote by u and v the two vertices of maximum degree three in G.

Note that G must have at least one pendant path of length one, otherwise, G would be a tree of the forms described in Theorem B (ii) or (iii).

First suppose that there is exactly one pendant path of length one in G. If u and v are adjacent in G, then we have

$$f(G) = 3\left[\left(1-\frac{1}{\sqrt{2}}\right)^2+\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)^2\right]+\left(1-\frac{1}{\sqrt{3}}\right)^2.$$

If u and v are nonadjacent in G, then we have

$$f(G) = 3\left[\left(1-\frac{1}{\sqrt{2}}\right)^2+\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)^2\right]+\left(1-\frac{1}{\sqrt{3}}\right)^2+2\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)^2.$$

Next suppose that there are exactly two pendant paths of length one in G. If u and v are adjacent in G, then we have

$$f(G) = 2\left[\left(1-\frac{1}{\sqrt{2}}\right)^2+\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)^2\right]+2\left(1-\frac{1}{\sqrt{3}}\right)^2.$$

If u and v are nonadjacent in G, then we have

$$f(G) = 2\left[\left(1-\frac{1}{\sqrt{2}}\right)^2+\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)^2\right]+2\left(1-\frac{1}{\sqrt{3}}\right)^2+2\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)^2.$$

If there are exactly three or four pendant paths of length one in G, i.e., $k = 3, 4$, then

$$\begin{aligned} f(G) &\geq (4-k)\left[\left(1-\frac{1}{\sqrt{2}}\right)^2+\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)^2\right]+k\left(1-\frac{1}{\sqrt{3}}\right)^2 \\ &= \left(\frac{2}{\sqrt{6}}-\frac{2}{\sqrt{3}}+\frac{2}{\sqrt{2}}-1\right)k+\frac{28}{3}-\frac{8}{\sqrt{6}}-\frac{8}{\sqrt{2}} \\ &\geq \left(\frac{2}{\sqrt{6}}-\frac{2}{\sqrt{3}}+\frac{2}{\sqrt{2}}-1\right)\cdot 3+\frac{28}{3}-\frac{8}{\sqrt{6}}-\frac{8}{\sqrt{2}} \\ &> 12-\frac{4}{\sqrt{6}}-\frac{1}{\sqrt{3}}-\frac{13}{\sqrt{2}}. \end{aligned}$$

Now suppose that **Subcase 1.2** holds. If $k = 0$, then

$$f(G) = 4\left[\left(1 - \frac{1}{\sqrt{2}}\right)^2 + \left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{4}}\right)^2\right].$$

If $k \geq 1$, then

$$\begin{aligned} f(G) &= (4-k)\left[\left(1 - \frac{1}{\sqrt{2}}\right)^2 + \left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{4}}\right)^2\right] + k\left(1 - \frac{1}{\sqrt{4}}\right)^2 \\ &= \left(\frac{3}{\sqrt{2}} - 2\right)k + 9 - \frac{12}{\sqrt{2}} \\ &\geq \left(\frac{3}{\sqrt{2}} - 2\right)\cdot 1 + 9 - \frac{12}{\sqrt{2}} \\ &> 12 - \frac{4}{\sqrt{6}} - \frac{1}{\sqrt{3}} - \frac{13}{\sqrt{2}}. \end{aligned}$$

Case 2. Suppose that there are exactly five pendant paths in G. Then we consider three subcases.

Subcase 2.1. There are exactly three vertices of maximum degree three, and all other vertices are of degrees one or two.

Subcase 2.2. There is exactly one vertex of degree three, one vertex of maximum degree four, and all other vertices are of degrees one or two.

Subcase 2.3. There is a single vertex of maximum degree five in G, and all other vertices are of degrees one or two.

Suppose that **Subcase 2.1** holds. Note that there are at most two pairs of adjacent vertices both of maximum degree three.

First suppose that there are exactly two pairs of adjacent vertices both of maximum degree three. If $k = 0$, i.e., the five pendant paths of G are all of length at least two, then

$$f(G) = 5\left[\left(1 - \frac{1}{\sqrt{2}}\right)^2 + \left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}}\right)^2\right].$$

If $k = 1$, i.e., there is exactly one pendant path of length one in G, then

$$f(G) = 4\left[\left(1 - \frac{1}{\sqrt{2}}\right)^2 + \left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}}\right)^2\right] + \left(1 - \frac{1}{\sqrt{3}}\right)^2.$$

If $k \geq 2$, then

$$\begin{aligned} f(G) &= (5-k)\left[\left(1 - \frac{1}{\sqrt{2}}\right)^2 + \left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}}\right)^2\right] + k\left(1 - \frac{1}{\sqrt{3}}\right)^2 \\ &= \left(\frac{2}{\sqrt{6}} - \frac{2}{\sqrt{3}} + \frac{2}{\sqrt{2}} - 1\right)k + \frac{35}{3} - \frac{10}{\sqrt{6}} - \frac{10}{\sqrt{2}} \\ &\geq \left(\frac{2}{\sqrt{6}} - \frac{2}{\sqrt{3}} + \frac{2}{\sqrt{2}} - 1\right)\cdot 2 + \frac{35}{3} - \frac{10}{\sqrt{6}} - \frac{10}{\sqrt{2}} \\ &> 12 - \frac{4}{\sqrt{6}} - \frac{1}{\sqrt{3}} - \frac{13}{\sqrt{2}}. \end{aligned}$$

Next suppose that there is exactly one pair of adjacent vertices both of maximum degree three. If $k = 0$, i.e., the five pendant paths of G are all of length at least two, then

$$f(G) = 5\left[\left(1 - \frac{1}{\sqrt{2}}\right)^2 + \left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}}\right)^2\right] + 2\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}}\right)^2.$$

If $k \geq 1$, then

$$\begin{aligned}
f(G) &= (5-k)\left[\left(1-\frac{1}{\sqrt{2}}\right)^2+\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)^2\right]+k\left(1-\frac{1}{\sqrt{3}}\right)^2 \\
&\quad +2\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)^2 \\
&= \left(\frac{2}{\sqrt{6}}-\frac{2}{\sqrt{3}}+\frac{2}{\sqrt{2}}-1\right)k+\frac{40}{3}-\frac{14}{\sqrt{6}}-\frac{10}{\sqrt{2}} \\
&\geq \left(\frac{2}{\sqrt{6}}-\frac{2}{\sqrt{3}}+\frac{2}{\sqrt{2}}-1\right)\cdot 1+\frac{40}{3}-\frac{14}{\sqrt{6}}-\frac{10}{\sqrt{2}} \\
&> 12-\frac{4}{\sqrt{6}}-\frac{1}{\sqrt{3}}-\frac{13}{\sqrt{2}}.
\end{aligned}$$

Now suppose that any two vertices of maximum degree three are not adjacent. If $k = 0$, i.e., the five pendant paths in G are all of length at least two, then

$$f(G) = 5\left[\left(1-\frac{1}{\sqrt{2}}\right)^2+\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)^2\right]+4\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)^2.$$

If $k \geq 1$, then

$$\begin{aligned}
f(G) &= (5-k)\left[\left(1-\frac{1}{\sqrt{2}}\right)^2+\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)^2\right]+k\left(1-\frac{1}{\sqrt{3}}\right)^2 \\
&\quad +4\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)^2 \\
&= \left(\frac{2}{\sqrt{6}}-\frac{2}{\sqrt{3}}+\frac{2}{\sqrt{2}}-1\right)k+15-\frac{18}{\sqrt{6}}-\frac{10}{\sqrt{2}} \\
&\geq \left(\frac{2}{\sqrt{6}}-\frac{2}{\sqrt{3}}+\frac{2}{\sqrt{2}}-1\right)\cdot 1+15-\frac{18}{\sqrt{6}}-\frac{10}{\sqrt{2}} \\
&> 12-\frac{4}{\sqrt{6}}-\frac{1}{\sqrt{3}}-\frac{13}{\sqrt{2}}.
\end{aligned}$$

Suppose that **Subcase 2.2** holds. Denote by u the unique vertex in G of degree three, and k_1 the number of pendant paths of length one attached to u, and denote by v the unique vertex in G of degree four, and k_2 the number of pendant paths of length one attached to v. Clearly, $0 \leq k_1 \leq 2$ and $0 \leq k_2 \leq 3$.

Suppose that $k_1 = k_2 = 0$, i.e., the five pendant paths in G are all of length at least two. If u and v are adjacent, then

$$\begin{aligned}
f(G) &= 2\left[\left(1-\frac{1}{\sqrt{2}}\right)^2+\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)^2\right]+3\left[\left(1-\frac{1}{\sqrt{2}}\right)^2+\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{4}}\right)^2\right] \\
&\quad +\left(\frac{1}{\sqrt{3}}-\frac{1}{\sqrt{4}}\right)^2.
\end{aligned}$$

If u and v are nonadjacent, then

$$\begin{aligned} f(G) &= 2\left[\left(1-\frac{1}{\sqrt{2}}\right)^2+\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)^2\right]+3\left[\left(1-\frac{1}{\sqrt{2}}\right)^2+\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{4}}\right)^2\right] \\ &\quad +\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)^2+\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{4}}\right)^2 \\ &> 12-\frac{4}{\sqrt{6}}-\frac{1}{\sqrt{3}}-\frac{13}{\sqrt{2}}. \end{aligned}$$

Suppose that $k_1 \geq 1$ or $k_2 \geq 1$. Then

$$\begin{aligned} f(G) &> (2-k_1)\left[\left(1-\frac{1}{\sqrt{2}}\right)^2+\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)^2\right]+k_1\left(1-\frac{1}{\sqrt{3}}\right)^2 \\ &\quad +(3-k_2)\left[\left(1-\frac{1}{\sqrt{2}}\right)^2+\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{4}}\right)^2\right]+k_2\left(1-\frac{1}{\sqrt{4}}\right)^2 \\ &= \left[\left(\frac{2}{\sqrt{6}}-\frac{2}{\sqrt{3}}+\frac{2}{\sqrt{2}}-1\right)k_1+\frac{14}{3}-\frac{4}{\sqrt{6}}-\frac{4}{\sqrt{2}}\right]+\left[\left(\frac{3}{\sqrt{2}}-2\right)k_2+\frac{27}{4}-\frac{9}{\sqrt{2}}\right]. \end{aligned}$$

In particular, when $k_1 \geq 1$, we have

$$\begin{aligned} f(G) &> \left[\left(\frac{2}{\sqrt{6}}-\frac{2}{\sqrt{3}}+\frac{2}{\sqrt{2}}-1\right)\cdot 1+\frac{14}{3}-\frac{4}{\sqrt{6}}-\frac{4}{\sqrt{2}}\right]+\left(\frac{27}{4}-\frac{9}{\sqrt{2}}\right) \\ &> 12-\frac{4}{\sqrt{6}}-\frac{1}{\sqrt{3}}-\frac{13}{\sqrt{2}}, \end{aligned}$$

and when $k_2 \geq 1$, we have

$$\begin{aligned} f(G) &> \left(\frac{14}{3}-\frac{4}{\sqrt{6}}-\frac{4}{\sqrt{2}}\right)+\left[\left(\frac{3}{\sqrt{2}}-2\right)\cdot 1+\frac{27}{4}-\frac{9}{\sqrt{2}}\right] \\ &> 12-\frac{4}{\sqrt{6}}-\frac{1}{\sqrt{3}}-\frac{13}{\sqrt{2}}. \end{aligned}$$

Suppose that **Subcase 2.3** holds. Then

$$\begin{aligned} f(G) &= (5-k)\left[\left(1-\frac{1}{\sqrt{2}}\right)^2+\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{5}}\right)^2\right]+k\left(1-\frac{1}{\sqrt{5}}\right)^2 \\ &= \left(\frac{2}{\sqrt{10}}-\frac{2}{\sqrt{5}}+\frac{2}{\sqrt{2}}-1\right)k+11-\frac{10}{\sqrt{10}}-\frac{10}{\sqrt{2}} \\ &\geq 11-\frac{10}{\sqrt{10}}-\frac{10}{\sqrt{2}} \\ &> 12-\frac{4}{\sqrt{6}}-\frac{1}{\sqrt{3}}-\frac{13}{\sqrt{2}}. \end{aligned}$$

Finally, it is easy to check that

$$\begin{aligned}
& 3\left[\left(1-\frac{1}{\sqrt{2}}\right)^2+\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)^2\right]+\left(1-\frac{1}{\sqrt{3}}\right)^2 \\
< \ & 5\left[\left(1-\frac{1}{\sqrt{2}}\right)^2+\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)^2\right] \\
< \ & 4\left[\left(1-\frac{1}{\sqrt{2}}\right)^2+\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{4}}\right)^2\right] \\
< \ & 3\left[\left(1-\frac{1}{\sqrt{2}}\right)^2+\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)^2\right]+\left(1-\frac{1}{\sqrt{3}}\right)^2+2\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)^2 \\
< \ & 5\left[\left(1-\frac{1}{\sqrt{2}}\right)^2+\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)^2\right]+2\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)^2 \\
< \ & 2\left[\left(1-\frac{1}{\sqrt{2}}\right)^2+\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)^2\right]+2\left(1-\frac{1}{\sqrt{3}}\right)^2 \\
< \ & 5\left[\left(1-\frac{1}{\sqrt{2}}\right)^2+\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)^2\right]+4\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)^2 \\
< \ & 4\left[\left(1-\frac{1}{\sqrt{2}}\right)^2+\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)^2\right]+\left(1-\frac{1}{\sqrt{3}}\right)^2 \\
< \ & 2\left[\left(1-\frac{1}{\sqrt{2}}\right)^2+\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)^2\right]+2\left(1-\frac{1}{\sqrt{3}}\right)^2+2\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)^2 \\
< \ & 2\left[\left(1-\frac{1}{\sqrt{2}}\right)^2+\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)^2\right]+3\left[\left(1-\frac{1}{\sqrt{2}}\right)^2+\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{4}}\right)^2\right] \\
& +\left(\frac{1}{\sqrt{3}}-\frac{1}{\sqrt{4}}\right)^2 \\
= \ & 12-\frac{4}{\sqrt{6}}-\frac{1}{\sqrt{3}}-\frac{13}{\sqrt{2}}.
\end{aligned}$$

From the above arguments, if $f(G)$ is not equal to one of the above ten values, then

$$f(G) > 12-\frac{4}{\sqrt{6}}-\frac{1}{\sqrt{3}}-\frac{13}{\sqrt{2}}.$$

Now the result follows from Eq. (1) easily. □

4. Conclusions

In this paper, we extend the existing ordering for the Randić indices of trees, and determine all the trees with from the seventh to the sixteen maximum Randić indices. In particular, in our proof, we mainly investigate the Randić indices of trees with exactly four or five pendant paths.

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