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Research Article

Unicyclic graphs with maximum Randić indices

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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 unicyclic graphs with the third maximum for $n \geq 5$, the fourth maximum for $n \geq 7$ and the fifth maximum for $n \geq 8$. Recently, Li *et al.* [The Randić indices of trees, unicyclic graphs and bicyclic graphs, Ars Comb. 127 (2016), 409–419] obtained the n-vertex unicyclic graphs with the sixth maximum and the seventh maximum for $n \geq 9$ and the eighth maximum for $n \geq 10$. In this paper, we characterize the n-vertex unicyclic graphs with the ninth maximum, the tenth maximum, the eleventh maximum, the twelfth maximum and the thirteenth maximum of Randić values.

Keywords: Randić index, maximum values, unicyclic graphs, ordering

AMS Subject classification: 05C50

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. For more notations and terminologies not defined here, we refer to [13].

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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 $R(G)$ is defined as [11]

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

An n-vertex connected graph is known as a tree, unicyclic and bicyclic graph if it has $n+c$ edges with $c = -1, 0, 1$, respectively. A vertex u in G is called pendant if $d_u = 1$. A pendant edge is an edge incident with a pendant vertex. A path $u_1 u_2 \ldots u_r$ 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 $d_{u_r} = 1$.
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 [5]. 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 [14]. Unicyclic and bicyclic graphs with the minimum Randić indices have been obtained in [7, 12], respectively. Trees with the fifth minimum Randić index, unicyclic graph with the second, the third and the fourth minimum Randić indices, bicyclic graph with the second minimum Randić index have been determined by Du and Zhou [5]. Recent research on the relationship between Randić index and several topological indices can be referred in [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 [6, 8, 9].
Subsequently, Li *et al.* [10] obtained the n-vertex unicyclic graphs with the sixth and the seventh for $n \geq 9$, and the eighth for $n \geq 10$ maximum Randić indices. In this paper, we characterize the n-vertex unicyclic graphs with the ninth, the tenth, the eleventh, the twelfth and the thirteenth maximum Randić values.

2. Preliminaries

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 unicyclic graphs with large Randić indices.

Among the n-vertex unicyclic graphs, for $n \geq 3$, the cycle C_n is the unique graph with the maximum Randić index, which is equal to $\frac{n}{2}$, and for $n \geq 5$, the graphs with a single vertex of maximum degree three, adjacent to three vertices of degree two are the unique graphs with the second maximum Randić index, which is equal to $\frac{n-4}{2} + \frac{3}{\sqrt{6}} + \frac{1}{\sqrt{2}}$, see [2].

Du and Zhou [5] obtained the n-vertex unicyclic graphs with the third, the fourth and the fifth maximum Randić indices.

Theorem A. [5] Among the n-vertex unicyclic graphs,

(i) for $n \geq 5$, the graph with a single vertex of maximum degree three, adjacent to one vertex of degree one and two vertices of degree two is the unique graph with the third maximum Randić index, which is equal to $\frac{n-3}{2} + \frac{2}{\sqrt{6}} + \frac{1}{\sqrt{3}}$,

(ii) for $n \geq 7$, the graphs with exactly two adjacent vertices of maximum degree three, each adjacent to two vertices of degree two are the unique graphs with the fourth maximum Randić index, which is equal to $\frac{n-7}{2} + \frac{4}{\sqrt{6}} + \sqrt{2} + \frac{1}{3}$,

(iii) for $n \geq 8$, the graphs with exactly two vertices of maximum degree three, each adjacent to three vertices of degree two are the unique graphs with the fifth maximum Randić index, which is equal to $\frac{n-8}{2} + \sqrt{6} + \sqrt{2}$.

Subsequently, Li *et al.* [10] reported the n-vertex unicyclic graphs with the sixth, the seventh and the eighth maximum Randić indices.

Theorem B. [10] Among the n-vertex unicyclic graphs,

(i) for $n \geq 9$, the graphs with exactly three pairwise adjacent vertices of maximum degree three, each adjacent to one vertex of degree two are the unique graphs with the sixth maximum Randić index, which is equal to $\frac{n-7}{2} + \frac{3}{\sqrt{2}} + \frac{3}{\sqrt{6}}$,

(ii) for $n \geq 9$, the graphs 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 graphs with the seventh maximum Randić index, which is equal to $\frac{n-4}{2} + \frac{1}{\sqrt{2}} + \frac{3}{\sqrt{6}} + \frac{1}{\sqrt{3}} - \frac{2}{3}$,

(iii) for $n \geq 10$, the graphs with exactly three vertices, say x, y, z of maximum degree three, x and y, y and z are adjacent, x and z having two vertices of degree two as adjacent vertices and y having one vertex of degree two as adjacent vertex are the unique graphs with the eighth maximum Randić index, which is equal to $\frac{n-8}{2} + \frac{3}{\sqrt{2}} + \frac{5}{\sqrt{6}} - \frac{1}{3}$.

We note that

$$\frac{n-4}{2}+\frac{3}{\sqrt{6}}+\frac{1}{\sqrt{2}}\approx\frac{n}{2}-0.0681483,$$

$$\frac{n-3}{2}+\frac{2}{\sqrt{6}}+\frac{1}{\sqrt{3}}\approx\frac{n}{2}-0.106153149,$$

$$\frac{n-7}{2}+\frac{4}{\sqrt{6}}+\sqrt{2}+\frac{1}{3}\approx\frac{n}{2}-0.119459942,$$

$$\frac{n-8}{2}+\sqrt{6}+\sqrt{2}\approx\frac{n}{2}-0.136296694,$$

$$\frac{n-7}{2}+\frac{3}{\sqrt{2}}+\frac{3}{\sqrt{6}}\approx\frac{n}{2}-0.153934785,$$

$$\frac{n-4}{2}+\frac{1}{\sqrt{2}}+\frac{3}{\sqrt{6}}+\frac{1}{\sqrt{3}}-\frac{2}{3}\approx\frac{n}{2}-0.157464744,$$

$$\frac{n-8}{2}+\frac{3}{\sqrt{2}}+\frac{5}{\sqrt{6}}-\frac{1}{3}\approx\frac{n}{2}-0.170771537.$$

3. Main results

We now present our main theorem.

Theorem 1. *Among the n-vertex unicyclic graphs,*

(*i*) *for $n\geq 10$, the graphs with exactly two non-adjacent vertices of degree three, one is adjacent to three vertices of degree two and the other is adjacent to one vertex of degree one and two vertices of degree two and all other vertices are of degree one or two, are the unique graphs with the ninth maximum Randić index, which is equal to*

$$\frac{n-7}{2}+\frac{1}{\sqrt{2}}+\frac{1}{\sqrt{3}}+\frac{5}{\sqrt{6}}\approx\frac{n}{2}-0.174301497,$$

(*ii*) *for $n\geq 11$, the graphs with exactly three vertices of degree three, say x,y,z, x and y are adjacent and each having two vertices of degree two as adjacent vertices, z is not adjacent with x and y and having three vertices of degree two as adjacent vertices, and all other vertices are of degree one or two, are the unique graphs with the tenth maximum Randić index, which is equal to*

$$\frac{n-12}{2}+\frac{3}{\sqrt{2}}+\frac{7}{\sqrt{6}}+\frac{5}{6}\approx\frac{n}{2}-0.187608289,$$

(*iii*) *for $n\geq 11$, the graphs with exactly three pairwise adjacent vertices of degree three, one is adjacent to one vertex of degree one and two other vertices are adjacent to one vertex of degree two, and all other vertices are of degree one or two, are the unique graphs with the eleventh maximum Randić index, which is equal to*

$$\frac{n-6}{2}+\frac{2}{\sqrt{2}}+\frac{1}{\sqrt{3}}+\frac{2}{\sqrt{6}}\approx\frac{n}{2}-0.191939587,$$

(*iv*) *for* $n \geq 11$*, the graphs with exactly two adjacent vertices of degree three, each is adjacent to one vertex of degree two and one, respectively, and all other vertices are of degree two, are the unique graphs with the twelfth maximum Randić index, which is equal to*

$$\frac{n-5}{2} + \frac{2}{\sqrt{3}} + \frac{2}{\sqrt{6}} + \frac{1}{3} \approx \frac{n}{2} - 0.195469547,$$

(*v*) *for* $n \geq 12$*, the graphs with exactly three non-adjacent vertices of degree three, each is adjacent to three vertices of degree two, and all other vertices are of degree one or two, are the unique graphs with the thirteenth maximum Randić index, which is equal to*

$$\frac{n-12}{2} + \frac{3}{\sqrt{2}} + \frac{9}{\sqrt{6}} \approx \frac{n}{2} - 0.204445042.$$

Proof. Let G be an n-vertex unicyclic graph different from the graphs mentioned in Theorems A and B with the first eight maximum Randić index, where $n \geq 10$. Obviously, there are at least two pendant paths in G.
If there are at least four pendant paths in G, then

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

since

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

Next we consider two cases.
Case 1. There are exactly two pendant paths in G.
In this case, there are two possible subcases.
(a) There is exactly one vertex on the cycle of G of degree four and all other vertices of G are of degrees one or two.
(b) There are exactly two vertices of degree three in G, and all other vertices of G are of degrees one or two.
If (a) holds, then since

$$\left(1-\frac{1}{\sqrt{4}}\right)^2 > \left(1-\frac{1}{\sqrt{2}}\right)^2 + \left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{4}}\right)^2,$$

we have

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

Suppose that (b) holds. Denote by u and v the two vertices of degree three in G.
If both pendant paths are of length at least two, then G is a graph of the form described in Theorem A (ii) when u and v are adjacent, and G is a graph of the form described in Theorem A (iii) when u and v are non-adjacent.
Next suppose that both pendant paths are of length one in G. If u and v are adjacent, then we have

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

If u and v are non-adjacent, then we have

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

Finally, suppose that one pendant path is of length one in G, and the other is of length at least two in G. If u and v are adjacent, then G is a graph of the form described in Theorem B (ii). If u and v are non-adjacent, then we have

$$\begin{aligned} f(G) &= \left[\left(1-\frac{1}{\sqrt{2}}\right)^2 + \left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)^2\right] + \left(1-\frac{1}{\sqrt{3}}\right)^2 + 4\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)^2 \\ &= 2\left(\frac{7}{2}-\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}-\frac{5}{\sqrt{6}}\right). \end{aligned}$$

Case 2. There are exactly three pendant paths in G.
There are three possible subcases at this time.
(i) There is exactly one vertex on the cycle of G of degree five, and all other vertices of G are of degrees one or two,
(ii) There is exactly one vertex of degree four and one vertex of degree three in G, and all other vertices of G are of degrees one or two,
(iii) There are exactly three vertices of degree three in G, and all other vertices of G are of degrees one or two.
Suppose that (i) holds. Since

$$\left(1-\frac{1}{\sqrt{5}}\right)^2 > \left(1-\frac{1}{\sqrt{2}}\right)^2 + \left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{5}}\right)^2,$$

we have

$$\begin{aligned} f(G) &\geq 3\left[\left(1-\frac{1}{\sqrt{2}}\right)^2+\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{5}}\right)^2\right]+2\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{5}}\right)^2 \\ &> 2\left(6-\frac{3}{\sqrt{2}}-\frac{9}{\sqrt{6}}\right). \end{aligned}$$

Suppose that (ii) holds. Since

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

and

$$\left(1-\frac{1}{\sqrt{4}}\right)^2 > \left(1-\frac{1}{\sqrt{2}}\right)^2+\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{4}}\right)^2,$$

we have

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

Suppose that (iii) holds. Denote by u, v, w the three vertices of degree three in G. Let k be the number of pendant paths of length one in G. Clearly, $k = 0, 1, 2, 3$. Firstly, consider no pair of vertices u, v, w are adjacent in G. If there is no pendant paths of length one, i.e., $k = 0$, then we have

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

If there is at least one pendant path of length one, i.e., $k = 1, 2, 3$, then

$$\begin{aligned} f(G) &\geq (3-k)(\left(1-\frac{1}{\sqrt{2}}\right)^2+(9-k)\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)^2+k\left(1-\frac{1}{\sqrt{3}}\right)^2 \\ &= \left(\frac{2}{\sqrt{2}}+\frac{2}{\sqrt{6}}-\frac{2}{\sqrt{3}}-1\right)k+12-\frac{6}{\sqrt{2}}-\frac{18}{\sqrt{6}} \\ &\geq \left(\frac{2}{\sqrt{2}}+\frac{2}{\sqrt{6}}-\frac{2}{\sqrt{3}}-1\right)1+12-\frac{6}{\sqrt{2}}-\frac{18}{\sqrt{6}} \\ &> 2\left(6-\frac{3}{\sqrt{2}}-\frac{9}{\sqrt{6}}\right). \end{aligned}$$

Next, we consider exactly one pair of vertices u, v, w is adjacent in G. If $k = 0$, then we have

$$\begin{aligned} f(G) &= 3\left[\left(1-\frac{1}{\sqrt{2}}\right)^2+\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)^2\right]+4\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)^2 \\ &= 2\left(\frac{31}{6}-\frac{3}{\sqrt{2}}-\frac{7}{\sqrt{6}}\right). \end{aligned}$$

If $k = 1, 2, 3$, then

$$\begin{aligned} f(G) &\geq (3-k)\left(1-\frac{1}{\sqrt{2}}\right)^2+(7-k)\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)^2+k\left(1-\frac{1}{\sqrt{3}}\right)^2 \\ &= \left(\frac{2}{\sqrt{2}}+\frac{2}{\sqrt{6}}-\frac{2}{\sqrt{3}}-1\right)k+\frac{31}{3}-\frac{6}{\sqrt{2}}-\frac{14}{\sqrt{6}} \\ &\geq \left(\frac{2}{\sqrt{2}}+\frac{2}{\sqrt{6}}-\frac{2}{\sqrt{3}}-1\right)1+\frac{31}{3}-\frac{6}{\sqrt{2}}-\frac{14}{\sqrt{6}} \\ &> 2\left(6-\frac{3}{\sqrt{2}}-\frac{9}{\sqrt{6}}\right). \end{aligned}$$

Now suppose that exactly two pairs of vertices u, v, w are adjacent in G. If $k = 0$, i.e., all the three pendant paths are of length at least two, then G is a graph of the form described in Theorem B (iii).
If $k = 1, 2, 3$, then

$$\begin{aligned} f(G) &\geq (3-k)\left(1-\frac{1}{\sqrt{2}}\right)^2+(5-k)\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)^2+k\left(1-\frac{1}{\sqrt{3}}\right)^2 \\ &= \left(\frac{2}{\sqrt{2}}+\frac{2}{\sqrt{6}}-\frac{2}{\sqrt{3}}-1\right)k+\frac{26}{3}-\frac{6}{\sqrt{2}}-\frac{10}{\sqrt{6}} \\ &\geq \left(\frac{2}{\sqrt{2}}+\frac{2}{\sqrt{6}}-\frac{2}{\sqrt{3}}-1\right)3+\frac{26}{3}-\frac{6}{\sqrt{2}}-\frac{10}{\sqrt{6}} \\ &> 2\left(6-\frac{3}{\sqrt{2}}-\frac{9}{\sqrt{6}}\right). \end{aligned}$$

Suppose that the vertices u, v, w are pairwise adjacent in G. Then G is a graph obtained by attaching three pendant paths each to a vertex of a triangle. If $k = 0$, then G is a graph of the form described in Theorem B (i). If $k = 1$, then we have

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

If $k = 2, 3$, then

$$\begin{aligned} f(G) &\geq (3-k)\left[\left(1-\frac{1}{\sqrt{2}}\right)^2+\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)^2\right]+k\left(1-\frac{1}{\sqrt{3}}\right)^2 \\ &= \left(\frac{2}{\sqrt{2}}+\frac{2}{\sqrt{6}}-\frac{2}{\sqrt{3}}-1\right)k+7-\frac{6}{\sqrt{2}}-\frac{6}{\sqrt{6}} \\ &\geq \left(\frac{2}{\sqrt{2}}+\frac{2}{\sqrt{6}}-\frac{2}{\sqrt{3}}-1\right)3+7-\frac{6}{\sqrt{2}}-\frac{6}{\sqrt{6}} \\ &> 2\left(6-\frac{3}{\sqrt{2}}-\frac{9}{\sqrt{6}}\right). \end{aligned}$$

At the end, it is easy to check that

$$\begin{aligned} & 2\left(\frac{7}{2}-\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}-\frac{5}{\sqrt{6}}\right) \\ < \; & 2\left(\frac{31}{6}-\frac{3}{\sqrt{2}}-\frac{7}{\sqrt{6}}\right) \\ < \; & 2\left(3-\frac{2}{\sqrt{2}}-\frac{1}{\sqrt{3}}-\frac{2}{\sqrt{6}}\right) \\ < \; & 2\left(\frac{13}{6}-\frac{2}{\sqrt{2}}-\frac{2}{\sqrt{6}}\right) \\ < \; & 2\left(6-\frac{3}{\sqrt{2}}-\frac{9}{\sqrt{6}}\right). \end{aligned}$$

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

$$f(G) > 2\left(6-\frac{3}{\sqrt{2}}-\frac{9}{\sqrt{6}}\right).$$

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

The unicyclic graphs in Theorem 1 with the smallest numbers of vertices are listed in Appendix.

4. Conclusions

In this paper, we presented a further ordering for the Randić index of unicyclic graphs, and determined the ninth, the tenth, the eleventh, the twelfth and the thirteenth maximum Randić values. In particular, in our proof, we mainly investigated the Randić index of unicyclic graphs with exactly two or three pendant paths. If one wants to order more unicyclic graphs with large Randić index, it needs only to consider such graphs with more pendant paths, i.e., the unicyclic graphs with exactly four or five pendant paths.

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5. Appendix

In what follows, we present some examples to illustrate the unicyclic graphs with the smallest numbers of vertices in Theorem 1.

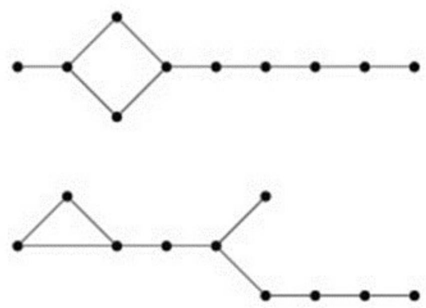

Figure 1. **The unicyclic graphs in Theorem 1 (i) with $n = 10$.**

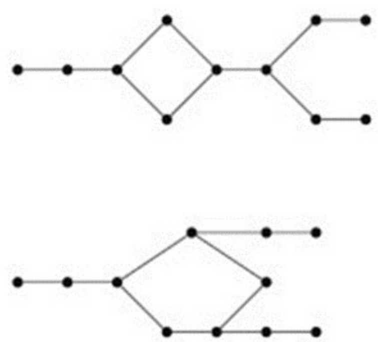

Figure 2. **The unicyclic graphs in Theorem 1 (ii) with $n = 11$.**

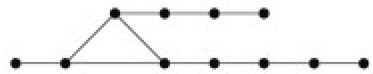

Figure 3. **The unicyclic graphs in Theorem 1 (iii) with $n = 11$.**

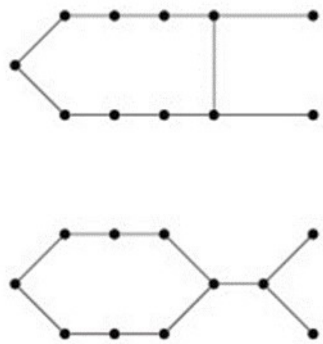

Figure 4. **The unicyclic graphs in Theorem 1 (iv) with $n = 11$.**

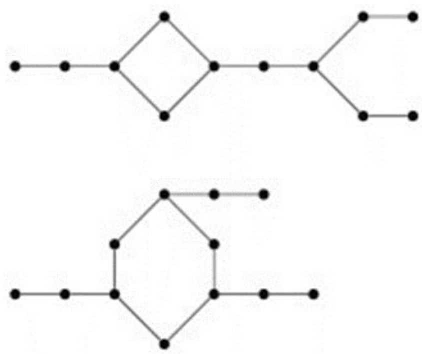

Figure 5. **The unicyclic graphs in Theorem 1 (v) with $n = 12$.**