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ON RANDIĆ INDICES OF CHEMICAL TREES AND CHEMICAL UNICYCLIC GRAPHS

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Abstract

The fourth maximum Randić indices for the n-vertex chemical trees for $n \geq 10$ and n-vertex chemical unicyclic graphs for $n \geq 7$ are determined, respectively.

1. INTRODUCTION

For a simple graph G with vertex-set $V(G)$ and $v \in V(G)$, $\Gamma(v)$ denotes the set of its (first) neighbors in G and the degree of v is $d_v = |\Gamma(v)|$. The Randić index (also known as connectivity index) [1] $R = R(G)$ of G is defined as

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$$R = R(G) = \sum_{uv \in E(G)} \left(d_u d_v\right)^{-1/2}$$

where $E(G)$ is the edge-set of G. It is the most used molecular descriptor in QSPR and QSAR [2-6]. Mathematical properties of Randić index may be found in [7,8].

Gutman *et al.* [9], and Gutman and Miljković [10] determined the chemical trees and chemical unicyclic graphs on n vertices with the first maximum, second maximum and third maximum Randić indices, respectively. These were extended to trees and unicyclic graphs by Caporossi *et al.* [11] and Song *et al.* [12], respectively. We know that the unique n-vertex tree with the maximum Randić index is the path P_n [13], and the unique n-vertex unicyclic graph for $n \geq 3$ with the maximum Randić index is the cycle C_n [14].

In this report, we determine the n-vertex chemical trees for $n \geq 10$ and chemical unicyclic graphs for $n \geq 7$ with the fourth maximum Randić indices, respectively.

2. PRELIMINARIES

For an edge uv of the graph G (the complement of G, respectively), $G - uv$ ($G + uv$, respectively) denotes the graph resulting from G by deleting (adding, respectively) the edge uv.

For a connected graph Q with at least two vertices and $u \in V(Q)$, let G_1 be the graph obtained from Q by attaching two paths P_a and P_b to u, and G_2 the graph obtained from Q by attaching a path P_{a+b} to u, where $a \geq b \geq 1$.

Lemma 1. Let G_1 and G_2 be the two graphs depicted as above, and $d_w = d_{G_1}(w)$ for $w \in V(G_1)$. Suppose that the maximum degree of G_1 is at most four. Then $R(G_1) < R(G_2)$.

Proof. If $a = b = 1$, then

$$R(G_2) - R(G_1) = \left(\frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2(d_u - 1)}} + \sum_{xu \in E(Q)} \frac{1}{\sqrt{d_x(d_u - 1)}}\right) - \left(\frac{2}{\sqrt{d_u}} + \sum_{xu \in E(Q)} \frac{1}{\sqrt{d_x d_u}}\right)$$
$$= \left(\frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2(d_u - 1)}} - \frac{2}{\sqrt{d_u}}\right) + \sum_{xu \in E(Q)} \left(\frac{1}{\sqrt{d_x(d_u - 1)}} - \frac{1}{\sqrt{d_x d_u}}\right)$$

$$> \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2(d_u-1)}} - \frac{2}{\sqrt{d_u}} \geq \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2(3-1)}} - \frac{2}{\sqrt{3}} > 0.$$

If $a \geq 2$ and $b = 1$, then

$$R(G_2) - R(G_1) = \left(\frac{1}{2} + \frac{1}{\sqrt{2(d_u-1)}} + \sum_{xu \in E(Q)} \frac{1}{\sqrt{d_x(d_u-1)}} \right) - \left(\frac{1}{\sqrt{2d_u}} + \frac{1}{\sqrt{d_u}} + \sum_{xu \in E(Q)} \frac{1}{\sqrt{d_x d_u}} \right)$$
$$= \left(\frac{1}{2} + \frac{1}{\sqrt{2(d_u-1)}} - \frac{1}{\sqrt{2d_u}} - \frac{1}{\sqrt{d_u}} \right) + \sum_{xu \in E(Q)} \left(\frac{1}{\sqrt{d_x(d_u-1)}} - \frac{1}{\sqrt{d_x d_u}} \right)$$
$$> \frac{1}{2} + \frac{1}{\sqrt{2(d_u-1)}} - \frac{1}{\sqrt{2d_u}} - \frac{1}{\sqrt{d_u}} \geq \frac{1}{2} + \frac{1}{\sqrt{2(3-1)}} - \frac{1}{\sqrt{2 \times 3}} - \frac{1}{\sqrt{3}} > 0.$$

If $b \geq 2$, then

$$R(G_2) - R(G_1) = \left(1 + \frac{1}{\sqrt{2(d_u-1)}} + \sum_{xu \in E(Q)} \frac{1}{\sqrt{d_x(d_u-1)}} \right) - \left(\frac{1}{\sqrt{2}} + \frac{\sqrt{2}}{\sqrt{d_u}} + \sum_{xu \in E(Q)} \frac{1}{\sqrt{d_x d_u}} \right)$$
$$= \left(1 - \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2(d_u-1)}} - \frac{\sqrt{2}}{\sqrt{d_u}} \right) + \left(\frac{1}{\sqrt{d_u - 1}} - \frac{1}{\sqrt{d_u}} \right) \sum_{xu \in E(Q)} \frac{1}{\sqrt{d_x}}$$
$$\geq 1 - \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2(3-1)}} - \frac{\sqrt{2}}{\sqrt{3}} + \frac{1}{2} \left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}} \right) > 0.$$

The result follows. □

3. RANDIĆ INDICES OF CHEMICAL TREES

Let **CT**(n) be the set of chemical trees with n vertices, where $n \geq 3$. A chemical tree is a graph-theoretical representation of acyclic chemical structures [15].

Lemma 2. Let $G \in \mathbf{CT}(n)$, where $n \geq 10$. If the maximum degree of G is four, or there are at least two vertices in G of maximum degree three, then

$$R(G) \leq \frac{1}{2}(n-10) + \frac{4}{\sqrt{2}} + \frac{4}{\sqrt{6}} + \frac{1}{3}$$

with equality if and only if there are exactly two adjacent vertices of maximum degree three in G each adjacent to two vertices of degree two.

Proof. Let G be a tree with maximum Randić index satisfying the given conditions. First suppose that there are at least two vertices in G of maximum degree three. If there are more than two vertices with maximum degree three, then by Lemma 1, we may get a tree in $\mathbf{CT}(n)$ with exactly two vertices of degree three with larger Randić index, a contradiction. Thus, G is a tree with exactly two vertices u and v of degree three. Suppose that u and v are non-adjacent. Let Q be the unique path joining u and v. Denote u_1 and u_2 by the two neighbors of u outside Q, and v' by the neighbor of v in Q. Then $d_G(u_1)=1,2$. Consider $G_1 = G - uu_2 + v'u_2 \in \mathbf{CT}(n)$. It is a tree with exactly two vertices of maximum degree three, and the two vertices are adjacent. But from

$$R(G_1)-R(G)=\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)\frac{1}{\sqrt{d_G(u_1)}}+\left(\frac{1}{3}-\frac{1}{\sqrt{6}}\right)\geq\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)\frac{1}{\sqrt{2}}+\left(\frac{1}{3}-\frac{1}{\sqrt{6}}\right)>0,$$

we have $R(G_1)>R(G)$, a contradiction. Therefore u and v are adjacent in G. Let a (b, respectively) be the number of neighbors of u (v, respectively) with degree two in G, where $0 \leq a,b \leq 2$. Note that $\frac{1}{\sqrt{6}}+\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}-\frac{1}{2}>0$. Then

$$\begin{aligned}
R(G) &= \frac{1}{3}+\frac{a}{\sqrt{6}}+\frac{a}{\sqrt{2}}+\frac{2-a}{\sqrt{3}}+\frac{b}{\sqrt{6}}+\frac{b}{\sqrt{2}}+\frac{2-b}{\sqrt{3}}+\frac{1}{2}(n-6-a-b)\\
&= \left(\frac{1}{\sqrt{6}}+\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}-\frac{1}{2}\right)a+\left(\frac{1}{\sqrt{6}}+\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}-\frac{1}{2}\right)b+\frac{1}{2}(n-6)+\frac{1}{3}+\frac{4}{\sqrt{3}}\\
&\leq 2\left(\frac{1}{\sqrt{6}}+\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}-\frac{1}{2}\right)+2\left(\frac{1}{\sqrt{6}}+\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}-\frac{1}{2}\right)+\frac{1}{2}(n-6)+\frac{1}{3}+\frac{4}{\sqrt{3}}\\
&= \frac{1}{2}(n-10)+\frac{4}{\sqrt{2}}+\frac{4}{\sqrt{6}}+\frac{1}{3}
\end{aligned}$$

with equality if and only if $a=b=2$. Now suppose that the maximum degree of G is four. Let w be a vertex of degree four. If there is another vertex different from w with degree three or four, then by Lemma 1, we may get a tree in $\mathbf{CT}(n)$ with a single vertex w of degree four and without vertices of degree three, with larger Randić index, a contradiction. Thus, G is a tree with a single vertex w of degree four and without vertices of degree three. Let k be the number of neighbors of w in G with degree two, $1 \le k \le 4$. We have

$$R(G) = \frac{3k}{2\sqrt{2}} + \frac{4-k}{2} + \frac{1}{2}(n-k-5) = \left(\frac{3}{2\sqrt{2}} - 1\right)k + \frac{1}{2}(n-1)$$
$$\le 4\left(\frac{3}{2\sqrt{2}} - 1\right) + \frac{1}{2}(n-1) < \frac{1}{2}(n-10) + \frac{4}{\sqrt{2}} + \frac{4}{\sqrt{6}} + \frac{1}{3},$$

a contradiction again. The result follows. □

Gutman *et al.* [9] showed that for $n \ge 4$, P_n is the unique tree in $\mathbf{CT}(n)$ with the maximum Randić index $\frac{1}{2}(n-3)+\sqrt{2}$, for $n \ge 7$, the trees with a single vertex of maximum degree three, adjacent to three vertices of degree two are the unique trees in $\mathbf{CT}(n)$ with the second maximum Randić index $\frac{1}{2}(n-7)+\frac{3}{\sqrt{2}}+\frac{3}{\sqrt{6}}$, and the trees with a single vertex of maximum degree three, adjacent to a vertex of degree one and two vertices of degree two are the unique trees in $\mathbf{CT}(n)$ with the third maximum Randić index $\frac{1}{2}(n-6)+\sqrt{2}+\frac{1}{\sqrt{3}}+\frac{2}{\sqrt{6}}$. The maximum part follows also from Lemma 1 and the rest follows from the arguments of the following proposition.

Proposition 1. For $n \ge 10$, the trees with exactly two adjacent vertices of maximum degree three, each adjacent to two vertices of degree two, are the unique trees in $\mathbf{CT}(n)$ with the fourth maximum Randić index $\frac{1}{2}(n-10)+\frac{4}{\sqrt{2}}+\frac{4}{\sqrt{6}}+\frac{1}{3}$.

Proof. Obviously, $R(P_n) = \frac{1}{2}(n-3)+\sqrt{2}$. Suppose that $G \in \mathbf{CT}(n)$ with $G \ne P_n$. If there is exactly one vertex, say v, of maximum degree three in G, then the degrees of the neighbors of v are 1, 1 and 2, and thus $R(G) = \frac{1}{2}(n-5)+\frac{1}{\sqrt{2}}+\frac{2}{\sqrt{3}}+\frac{1}{\sqrt{6}}$, or the degrees of the neighbors of v are 1, 2 and 2, and thus $R(G)=\frac{1}{2}(n-6)+\sqrt{2}+\frac{1}{\sqrt{3}}+\frac{2}{\sqrt{6}}$, or the degrees of the neighbors of v are 2, 2 and 2, and thus $R(G)=\frac{1}{2}(n-7)+\frac{3}{\sqrt{2}}+\frac{3}{\sqrt{6}}$. If the maximum degree of $G\in\mathbf{CT}(n)$ is four or there are at least two vertices of maximum degree three, where $n\geq 10$, then by Lemma 2, $R(G)\leq\frac{1}{2}(n-10)+\frac{4}{\sqrt{2}}+\frac{4}{\sqrt{6}}+\frac{1}{3}$ and this bound is attainable. Note that

$$\begin{aligned}\frac{1}{2}(n-5)+\frac{1}{\sqrt{2}}+\frac{2}{\sqrt{3}}+\frac{1}{\sqrt{6}}<\frac{1}{2}(n-10)+\frac{4}{\sqrt{2}}+\frac{4}{\sqrt{6}}+\frac{1}{3}\\ <\frac{1}{2}(n-6)+\sqrt{2}+\frac{1}{\sqrt{3}}+\frac{2}{\sqrt{6}}\\ <\frac{1}{2}(n-7)+\frac{3}{\sqrt{2}}+\frac{3}{\sqrt{6}}<\frac{1}{2}(n-3)+\sqrt{2}.\end{aligned}$$

It follows that $\frac{1}{2}(n-10)+\frac{4}{\sqrt{2}}+\frac{4}{\sqrt{6}}+\frac{1}{3}$ is the fourth maximum Randić index of trees in $\mathbf{CT}(n)$ and then the result follows from Lemma 2. □

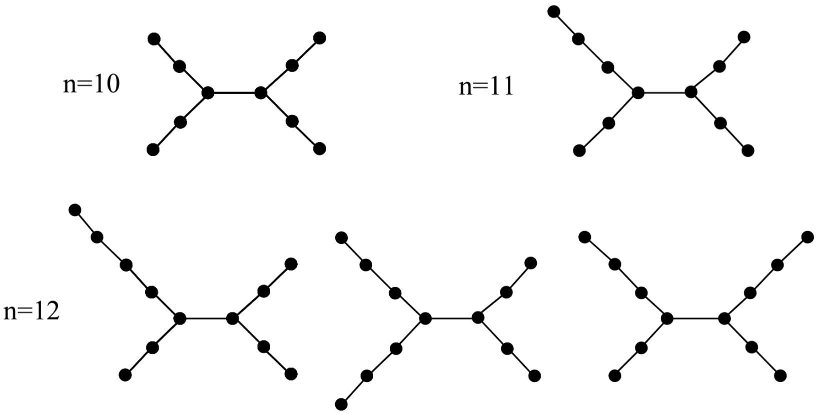

Fig. 1. The n-vertex chemical trees with the fourth maximum Randić indices for $n=10,11,12$.

4. RANDIĆ INDICES OF CHEMICAL UNICYCLIC GRAPHS

Let $\mathbf{CU}(n)$ be the set of chemical unicyclic graphs with n vertices, where $n \ge 3$. Let G be a unicyclic graph with n vertices and let $C_s = v_0 v_1 \cdots v_{s-1} v_0$ be its unique cycle. Then $G - E(C_s)$ consists of s trees $T_0, T_1, \ldots, T_{s-1}$, where $v_i \in V(T_i)$ for $i = 0, 1, \ldots, s-1$. If the degree of v_i is at least three, then the components of $T_i - v_i$ are called the branches of G (at v_i), each containing a neighbor of v_i in T_i. If T_i is a path P_{a_i+1} with an end vertex v_i, $a_i \ge 0$, for $i = 0, 1, \ldots, s-1$, then we write G as $U(a_0, \cdots, a_{s-1})$.

Lemma 3. For fixed i and j with $0 \le i < j \le s-1$ and fixed a_k with $0 \le k \le s-1$ and $k \ne i, j$, let U_{a_i, a_j} be the graph $U(a_0, \cdots, a_{s-1})$. If $a_i \ge a_j \ge 1$, then $R(U_{a_i, a_j}) < R(U_{a_i + a_j, 0})$.

Proof. Let d_1, d_2 be the degrees of the two neighbors of v_j on C_s in U_{a_i, a_j}, where $d_1, d_2 = 2$ or 3. If $a_i = a_j = 1$, then

$$\begin{aligned} R(U_{a_i+a_j,0}) - R(U_{a_i,a_j}) &= \left(\frac{1}{\sqrt{2d_1}} + \frac{1}{\sqrt{2d_2}} + \frac{1}{\sqrt{6}} + \frac{1}{\sqrt{2}} \right) - \left(\frac{1}{\sqrt{3d_1}} + \frac{1}{\sqrt{3d_2}} + \frac{2}{\sqrt{3}} \right) \\ &= \left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}} \right) \left(\frac{1}{\sqrt{d_1}} + \frac{1}{\sqrt{d_2}} \right) + \frac{1}{\sqrt{6}} + \frac{1}{\sqrt{2}} - \frac{2}{\sqrt{3}} \\ &\ge \left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}} \right) \left(\frac{1}{\sqrt{3}} + \frac{1}{\sqrt{3}} \right) + \frac{1}{\sqrt{6}} + \frac{1}{\sqrt{2}} - \frac{2}{\sqrt{3}} > 0. \end{aligned}$$

If $a_i \ge 2$ and $a_j = 1$, then

$$\begin{aligned} R(U_{a_i+a_j,0}) - R(U_{a_i,a_j}) &= \left(\frac{1}{\sqrt{2d_1}} + \frac{1}{\sqrt{2d_2}} + \frac{1}{\sqrt{2}} + \frac{1}{2} \right) - \left(\frac{1}{\sqrt{3d_1}} + \frac{1}{\sqrt{3d_2}} + \frac{1}{\sqrt{3}} + \frac{1}{\sqrt{2}} \right) \\ &= \left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}} \right) \left(\frac{1}{\sqrt{d_1}} + \frac{1}{\sqrt{d_2}} \right) + \frac{1}{2} - \frac{1}{\sqrt{3}} \\ &\ge \left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}} \right) \left(\frac{1}{\sqrt{3}} + \frac{1}{\sqrt{3}} \right) + \frac{1}{2} - \frac{1}{\sqrt{3}} > 0. \end{aligned}$$

If $a_j \geq 2$, then

$$R(U_{a_i+a_j,0}) - R(U_{a_i,a_j}) = \left(\frac{1}{\sqrt{2d_1}} + \frac{1}{\sqrt{2d_2}} + 1\right) - \left(\frac{1}{\sqrt{3d_1}} + \frac{1}{\sqrt{3d_2}} + \frac{1}{\sqrt{6}} + \frac{1}{\sqrt{2}}\right)$$
$$= \left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}}\right)\left(\frac{1}{\sqrt{d_1}} + \frac{1}{\sqrt{d_2}}\right) + 1 - \frac{1}{\sqrt{6}} - \frac{1}{\sqrt{2}}$$
$$\geq \left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}}\right)\left(\frac{1}{\sqrt{3}} + \frac{1}{\sqrt{3}}\right) + 1 - \frac{1}{\sqrt{6}} - \frac{1}{\sqrt{2}} > 0.$$

The result follows. □

Lemma 4. Let $G \in \mathbf{CU}(n)$, where $n \geq 7$. If the maximum degree of G is four, or there are at least two vertices in G of maximum degree three, then

$$R(G) \leq \frac{1}{2}(n-7) + \sqrt{2} + \frac{4}{\sqrt{6}} + \frac{1}{3}$$

with equality if and only if there are exactly two adjacent vertices of maximum degree three in G each adjacent to two vertices of degree two.

Proof. Let G be a unicyclic graph with maximum Randić index satisfying the given conditions. First suppose that G has at least two branches. If the maximum degree is four, or there are at least three vertices of maximum degree three, then by Lemmas 1 and 3, we may get a graph in $\mathbf{CU}(n)$ with exactly two branches and two vertices of maximum degree three, with larger Randić index, a contradiction. Thus, G is a unicyclic graph with exactly two branches and two vertices, say u and v, of maximum degree three. Suppose that u and v are non-adjacent. Denote u' by the unique neighbor of u outside the unique cycle of G, and v' by a neighbor of v on the cycle. Consider $G_1 = G - uu' + v'u' \in \mathbf{CU}(n)$. It is a unicyclic graph with exactly two adjacent vertices of maximum degree three but $R(G_1) - R(G) = \frac{5}{6} - \frac{2}{\sqrt{6}} > 0$, a contradiction. Thus, u and v are adjacent in G. Now suppose that G has exactly one branch, say at x of G. Suppose that $d_G(x)=4$. If there exist some vertices of degree more than two outside the cycle of G, then by Lemma 1, we may get a graph in **CU**(n) with vertices of degree one or two different from x with larger Randić index, a contradiction. Thus, G is a graph with vertices of degree one or two different from x. Denote x_1 and x_2 by the two neighbors of x outside the cycle, and x' by a neighbor of x on the cycle. Then $d_G(x_1), d_G(x_2)=1,2$. Consider $G_2 = G - xx_1 + x'x_1 \in \mathbf{CU}(n)$. It is a graph with exactly two adjacent vertices of maximum degree three. But

$$R(G_2)-R(G)=\left(\frac{1}{\sqrt{3}}-\frac{1}{2}\right)\left(\frac{1}{\sqrt{d_G(x_1)}}+\frac{1}{\sqrt{d_G(x_2)}}\right)+\frac{2}{\sqrt{6}}-\frac{1}{6}-\frac{1}{\sqrt{2}}$$
$$\geq\left(\frac{1}{\sqrt{3}}-\frac{1}{2}\right)\left(\frac{1}{\sqrt{2}}+\frac{1}{\sqrt{2}}\right)+\frac{2}{\sqrt{6}}-\frac{1}{6}-\frac{1}{\sqrt{2}}>0,$$

which is a contradiction. Thus $d_G(x)=3$. If there are more than one vertex of maximum degree three outside the cycle, or the maximum degree is four, then by Lemma 1, we may get a graph in **CU**(n) with exactly one vertex of maximum degree three outside the cycle with larger Randić index, a contradiction. Thus, G is a graph with exactly one vertex, y of maximum degree three outside the cycle. Suppose that x and y are non-adjacent. Let Q be the unique path joining x and y. Denote x_3 by the unique neighbor of x outside the cycle, and y_1 and y_2 by the two neighbors of y outside Q. Then $d_G(y_1)=1,2$. Consider $G_3 = G - yy_2 + x_3y_2 \in \mathbf{CU}(n)$. It is a graph with exactly two adjacent vertices of maximum degree three. But

$$R(G_3)-R(G)=\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)\frac{1}{\sqrt{d_G(y_1)}}+\frac{1}{3}-\frac{1}{\sqrt{6}}\geq\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)\frac{1}{\sqrt{2}}+\frac{1}{3}-\frac{1}{\sqrt{6}}>0,$$

which is a contradiction. Therefore x and y are adjacent in G.

Now we have showed that G has exactly two adjacent vertices of maximum degree three. Then G has exactly two vertices p and q of degree one. If p and q are both adjacent to vertices of degree three, then $R(G)=\frac{1}{2}(n-5)+\frac{2}{\sqrt{3}}+\frac{1}{3}+\frac{2}{\sqrt{6}}$. If only one of p and q is adjacent to a vertex of degree two, then $R(G)=\frac{1}{2}(n-6)+\frac{1}{\sqrt{3}}+\frac{1}{\sqrt{2}}+\frac{1}{3}+\frac{3}{\sqrt{6}}$. If p and q are both adjacent to vertices of degree two, then $R(G)=\frac{1}{2}(n-7)+\sqrt{2}+\frac{4}{\sqrt{6}}+\frac{1}{3}$. Obviously, $\frac{1}{2}(n-5)+\frac{2}{\sqrt{3}}+\frac{1}{3}+\frac{2}{\sqrt{6}}<\frac{1}{2}(n-6)+\frac{1}{\sqrt{3}}+\frac{1}{\sqrt{2}}+\frac{1}{3}+\frac{3}{\sqrt{6}}<\frac{1}{2}(n-7)+\sqrt{2}+\frac{4}{\sqrt{6}}+\frac{1}{3}$ for $n\geq 7$. The result follows. □

Gutman and Miljković [10] showed that for $n\geq 3$, C_n is the unique graph in $\mathbf{CU}(n)$ with the maximum Randić index $\frac{n}{2}$, 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 in $\mathbf{CU}(n)$ with the second maximum Randić index $\frac{1}{2}(n-4)+\frac{1}{\sqrt{2}}+\frac{3}{\sqrt{6}}$, and the graph with a single vertex of maximum degree three, adjacent to a vertex of degree one and two vertices of degree two is the unique graph in $\mathbf{CU}(n)$ with the third maximum Randić index $\frac{1}{2}(n-3)+\frac{1}{\sqrt{3}}+\frac{2}{\sqrt{6}}$. These follow also from the arguments of the following proposition.

Proposition 2. 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 in $\mathbf{CU}(n)$ with the fourth maximum Randić index $\frac{1}{2}(n-7)+\sqrt{2}+\frac{4}{\sqrt{6}}+\frac{1}{3}$.

Proof. It is easily seen that $R(C_n)=\frac{n}{2}$. Suppose that $G\in\mathbf{CU}(n)$ with $G\neq C_n$. Note that the maximum degree of G is three or four. If G has exactly one vertex, say v, of maximum degree three, then either $R(G)=\frac{1}{2}(n-3)+\frac{1}{\sqrt{3}}+\frac{2}{\sqrt{6}}$ when v is adjacent to one vertex of degree one and two vertices of degree two for $n\geq 4$, or $R(G)=\frac{1}{2}(n-4)+\frac{1}{\sqrt{2}}+\frac{3}{\sqrt{6}}$ when v is adjacent to three vertices of degree two for $n\geq 5$. If the maximum degree of G is four or there are at least two vertices of maximum degree three, where $n \geq 7$, then by Lemma 4, $R(G) \leq \frac{1}{2}(n-7)+\sqrt{2}+\frac{4}{\sqrt{6}}+\frac{1}{3}$ and this bound is attainable. Obviously,

$$\frac{1}{2}(n-7)+\sqrt{2}+\frac{4}{\sqrt{6}}+\frac{1}{3}<\frac{1}{2}(n-3)+\frac{1}{\sqrt{3}}+\frac{2}{\sqrt{6}}<\frac{1}{2}(n-4)+\frac{1}{\sqrt{2}}+\frac{3}{\sqrt{6}}<\frac{n}{2}.$$

Then $\frac{1}{2}(n-7)+\sqrt{2}+\frac{4}{\sqrt{6}}+\frac{1}{3}$ is the fourth maximum Randić index of graphs in $\mathbf{CU}(n)$. Now the result follows from Lemma 4. □

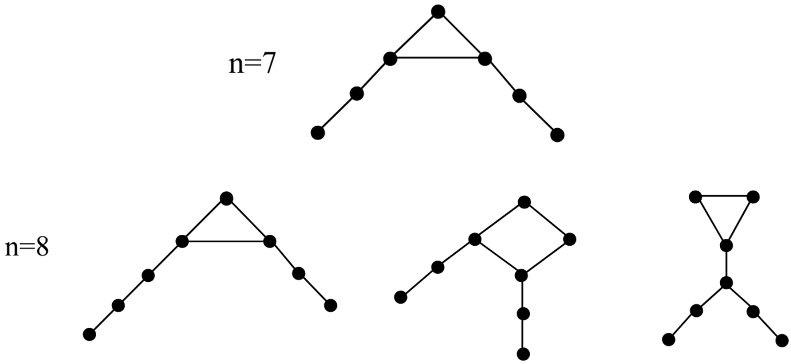

Fig. 2. The *n*-vertex chemical unicyclic graphs with the fourth maximum Randić indices for $n = 7, 8$.

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