

Complete Solution for Unicyclic Graphs with Minimum General Randić Index *

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Abstract

The general Randić index of a (molecular) graph G is defined by $R_\alpha(G) = \sum_{uv} (d(u)d(v))^\alpha$, where $d(u)$ denotes the degree of a vertex u in G , uv runs over the edge set of G and α is an arbitrary real number. Wu and Zhang studied unicyclic graphs with minimum general Randić index. For $\alpha \geq -1$ they got the unique minimum unicyclic graph by distinguishing α into intervals $\alpha > 0$ and $-1 \leq \alpha < 0$. But, unfortunately, for $\alpha < -1$ they could not completely solve this minimum problem. At the end they figured out two classes \mathcal{G} and \mathcal{H} of possible minimum unicyclic graphs. In this paper, we completely solve this problem by showing that for $\alpha < -1$ and $n \geq 5$, the unique unicyclic graph with minimum general Randić index is either S_n^+ or $t_{\lceil \frac{n-3}{2} \rceil, \lfloor \frac{n-3}{2} \rfloor}^*$, where S_n^+ denotes the unicyclic graph obtained from the star S_n on n vertices by joining its two vertices of degree 1, whereas $t_{\lceil \frac{n-3}{2} \rceil, \lfloor \frac{n-3}{2} \rfloor}^*$ denotes the unicyclic graph that has a triangle as its unique cycle and the vertices not on the cycle are leaves that are adjacent to two vertices of the triangle such that the numbers of leaf vertices on the two branches are almost equal. Furthermore, we observe that as α approaches to -1 , if $t_{\lceil \frac{n-3}{2} \rceil, \lfloor \frac{n-3}{2} \rfloor}^*$ has the minimum value then n must

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be considerably large, that is to say, when α is near -1 , it is almost sure that S_n^+ is the unique minimum unicyclic graph, whereas when α is at a distance from -1 , it is almost sure that $t_{\lceil \frac{n-3}{2} \rceil, \lfloor \frac{n-3}{2} \rfloor}^*$ is the unique minimum unicyclic graph. In particular, for $\alpha \leq -2$, S_n^+ for $5 \leq n \leq 41$ and $t_{\lceil \frac{n-3}{2} \rceil, \lfloor \frac{n-3}{2} \rfloor}^*$ for $n \geq 42$, respectively, is the unique unicyclic graph with minimum general Randić index.

Keywords: general Randić index; unicyclic graph; star; triangle with two balanced leaf branches.

1 Introduction

For a (molecular) graph $G = (V, E)$, the *general Randić index* $R_\alpha(G)$ of G is defined as the sum of $(d(u)d(v))^\alpha$ over all edges uv of G where $d(u)$ denotes the degree of a vertex u of G , i.e.,

$$R_\alpha(G) = \sum_{uv} (d(u)d(v))^\alpha$$

where α is an arbitrary real number.

It is well known that $R_{-\frac{1}{2}}$ was introduced by Randić [17] in 1975 as one of the many graph-theoretical parameters derived from the graph underlying some molecule. Later, in 1998 Bollobás and Erdős [1] generalized this index by replacing $-\frac{1}{2}$ with any real number α , which is called the general Randić index. The research background of Randić index together with its generalization appears in chemistry or mathematical chemistry and can be found in the literature (see [1]-[12]). Recently, finding bounds for the general Randić index of graphs, as well as related problem of finding the graphs with maximum or minimum general Randić index, attracted the attention of many researchers, and many results have been obtained (see [1]-[10], [13]-[16], [18]-[20]).

A simple connected graph G is called *unicyclic* if it contains exactly one cycle. From this definition, one can see that a unicyclic graph has the same number of vertices and edges, and it is a cycle or a cycle with trees attached to its vertices. For $n \geq 3$, let S_n^+ denote the unicyclic graph obtained from the star S_n on n vertices by joining its two vertices of degree 1. For $\alpha = -\frac{1}{2}$, Gao and Lu [6] showed that for a unicyclic graph G , $R_{-\frac{1}{2}}(G) \geq$

$(n-3)(n-1)^{-\frac{1}{2}} + 2(2n-2)^{-\frac{1}{2}} + \frac{1}{2}$, and the equality holds if and only if $G \cong S_n^+$. For general α , Wu and Zhang [19] showed that among unicyclic graphs with n vertices, the cycle C_n for $\alpha > 0$ and S_n^+ for $-1 \leq \alpha < 0$, respectively, has minimum general Randić index. For $\alpha < -1$, they gave the structure of unicyclic graphs with minimum general Randić index and showed that unicyclic graphs with minimum general Randić index must fall into two classes \mathcal{G} and \mathcal{H} of graphs as shown in Figure 1.1. But, unfortunately, they could not determine which of them can achieve the minimum value.

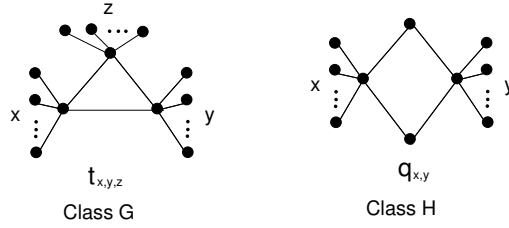


Figure 1.1

In this paper, we focus on investigating these two classes of graphs. As a first step, we show that the graphs with minimum general Randić index must fall into only one of the two classes, i.e., \mathcal{G} . Based on this we then completely determine the minimum unicyclic graphs for $\alpha < -1$. Clearly, n must be at least 3. For $\alpha = 3$, C_3 is the unique unicyclic graph and hence there is nothing to say. For $n = 4$, S_4^+ and C_4 are the only unicyclic graphs. By easy computation, we can see that when $\alpha < -3.0817$, C_4 has minimum general Randić index, whereas when $-3.0817 < \alpha < -1$, S_4^+ has minimum general Randić index. For $n \geq 5$, we will show that for $\alpha < -1$ the unique unicyclic graph with minimum general Randić index is either S_n^+ or $t_{\lceil \frac{n-3}{2} \rceil, \lfloor \frac{n-3}{2} \rfloor}^*$, where $t_{\lceil \frac{n-3}{2} \rceil, \lfloor \frac{n-3}{2} \rfloor}^*$ denotes the unicyclic graph that has a triangle as its unique cycle and the vertices not on the cycle are leaves that are adjacent to two vertices of the triangle such that the numbers of leaf vertices on the two branches are almost equal, called a *triangle with two balanced leaf branches*. Furthermore, we observe that as α approaches to -1 , if $t_{\lceil \frac{n-3}{2} \rceil, \lfloor \frac{n-3}{2} \rfloor}^*$ has the minimum value then n must be considerably large, that is to say, when α is near -1 , it is almost sure that S_n^+ is the unique minimum unicyclic graph, whereas when α is at a distance from -1 , it is almost sure that $t_{\lceil \frac{n-3}{2} \rceil, \lfloor \frac{n-3}{2} \rfloor}^*$ is the unique minimum unicyclic graph. In particular, for $\alpha \leq -2$, S_n^+ for $5 \leq n \leq 41$ and $t_{\lceil \frac{n-3}{2} \rceil, \lfloor \frac{n-3}{2} \rfloor}^*$ for

$n \geq 42$, respectively, is the unique unicyclic graph with minimum general Randić index. This property looks very much like what we did in [10] for trees with maximum general Randić index for $1 < \alpha < +\infty$.

For convenience, we need some additional notations and terminology. A vertex of degree 1 in a graph is called a *leaf vertex* (or simply, a *leaf*) and the edge incident with the leaf is called a *leaf edge*. A vertex adjacent to some leaf vertices is called a *leaf branch*. For more notations and terminology we refer to [19]. The two classes \mathcal{G} and \mathcal{H} of graphs are defined as follows: \mathcal{G} consists of the unicyclic graphs each of which has a triangle as its unique cycle, and the vertices not on the cycle are leaves. A graph in class \mathcal{G} is called a *triangle with leaves*, denoted by $t_{x,y,z}$, where x, y and z are nonnegative integers that denote the numbers of neighbors of the vertices on the triangle, respectively. Then we have $x + y + z = n - 3$. Obviously, if two of the three numbers x, y, z are zero, then the graph is S_n^+ . If the difference between two of the three numbers x, y, z is at most 1, then the graph is called a *triangle with two balanced leaf branches*, denoted by $t_{x,y,z}^*$. Particularly, if $z = 0$, a triangle with two balanced leaf branches $t_{x,y,0}^*$ is simply $t_{\lceil \frac{n-3}{2} \rceil, \lfloor \frac{n-3}{2} \rfloor}^*$. The class \mathcal{H} consists of the unicyclic graphs each of which has a 4-cycle as its unique cycle, and the vertices not on the cycle are leaves that are neighbors of two nonadjacent vertices of the cycle or neighbors of exactly one vertex of the cycle. A graph in class \mathcal{H} is called a *4-cycle with leaves*, denoted by $q_{x,y}$, where x and y are nonnegative integers that denote the numbers of neighbors of the two nonadjacent vertices on the cycle, respectively. Then we have $x + y = n - 4$.

2 Main results

In this section we always assume that $\alpha < -1$ and $n \geq 5$. First we need some inequalities and lemmas that will be used in the proof of our main results.

Lemma 2.1 *Let $f(x, \alpha) = x(x+2)^\alpha$. Then the function $f(x, \alpha)$ is monotonously decreasing for $x \geq \frac{-2}{\alpha+1}$ and $\alpha < -1$, and monotonously increasing for $x < \frac{-2}{\alpha+1}$ and $\alpha < -1$.*

Proof. Note that $\frac{\partial f(x)}{\partial x} = (x+2)^{\alpha-1}[(\alpha+1)x+2]$, which is ≤ 0 for $x \geq \frac{-2}{\alpha+1}$ and $\alpha < -1$, and > 0 for $x < \frac{-2}{\alpha+1}$ and $\alpha < -1$. The lemma thus follows. ■

Lemma 2.2 For $-5 \leq \alpha < -1$ and $1 \leq x \leq \frac{-4}{\alpha+1}$, the function

$$g(x, \alpha) = x(x+2)^\alpha - 4^\alpha > 0.$$

Proof. Note that $\frac{\partial g(x, \alpha)}{\partial x} = (x+2)^{\alpha-1}[(\alpha+1)x+2]$, where $1 \leq x \leq \frac{-4}{\alpha+1}$. If $1 \leq x < \frac{-2}{\alpha+1}$ then $\frac{\partial g(x, \alpha)}{\partial x} > 0$, and so $g(x, \alpha) > g(1, \alpha) > 0$. If $\frac{-2}{\alpha+1} \leq x \leq \frac{-4}{\alpha+1}$ then $\frac{\partial g(x, \alpha)}{\partial x} < 0$, and so

$$g(x, \alpha) > g\left(\frac{-4}{\alpha+1}, \alpha\right) = 2^\alpha \left[\frac{-4}{\alpha+1} \left(\frac{\alpha-1}{\alpha+1}\right)^\alpha - 2^\alpha \right].$$

Set the right hand side of the above formula as $h(\alpha)$. Note that the solution of the equation $\frac{\partial h(\alpha)}{\partial \alpha} = 0$ is not in the interval $[-5, 1)$ and $\frac{\partial h(\alpha)}{\partial \alpha}$ is continuous in $[-5, 1)$. Since $\lim_{\alpha \rightarrow -1} h(\alpha) = \frac{3}{4} > 0$ and $h(-5) = 3^{-5} - 4^{-5} > 0$, we know that $h(\alpha) > 0$, and so $g(x, \alpha) > h(\alpha) > 0$, the proof is thus complete. ■

Lemma 2.3 For $\alpha < -1$, if x, y are nonnegative integers such that $x + y = n - 2$, and at least one of x and y is not less than $\frac{-2}{\alpha+1}$, say $y \geq \frac{-2}{\alpha+1}$, then for any 4-cycle with leaves $q_{x,y}$ in class \mathcal{H} there is a graph $t_{x,y+1}$ in class \mathcal{G} that has a smaller general Randić index than $q_{x,y}$. Particularly, the theorem holds true for $\alpha < -1$ and $x \geq y = 1$.

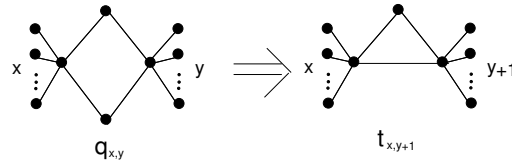


Figure 2.1

Proof. As shown in Figure 2.1, we contract one edge in the 4-cycle of $q_{x,y}$ and add one leaf vertex to the leaf branch where the number of leaf vertices is not less than $\frac{-2}{\alpha+1}$. Then, in this way we have transferred $q_{x,y}$ into $t_{x,y+1}$. Next we compare the general Randić index of the two graphs. Let R and R^* be the general Randić index of $q_{x,y}$ and $t_{x,y+1}$, respectively.

Then, we only need to show that $R - R^* > 0$. In fact, Lemma 2.1 implies

$$\begin{aligned} R - R^* &= y(y+2)^\alpha + 2^{\alpha+1}(y+2)^\alpha + 2^\alpha(x+2)^\alpha - (y+1)(y+3)^\alpha - 2^\alpha(y+3)^\alpha \\ &\quad - (x+2)^\alpha(y+3)^\alpha > 2^\alpha(y+2)^\alpha + 2^\alpha(x+2)^\alpha - (x+2)^\alpha(y+3)^\alpha > 0. \end{aligned} \quad (2.1)$$

If $x \geq y = 1$, then we transfer $q_{x,1}$ into $t_{x,2}$, and Eq.(2.1) implies

$$\begin{aligned} R - R^* &= 3^\alpha + 2 \cdot 6^\alpha - 2 \cdot 4^\alpha - 8^\alpha + 2^\alpha(x+2)^\alpha - 4^\alpha(x+2)^\alpha \\ &> 3^\alpha + 2 \cdot 6^\alpha - 8^\alpha - 2 \cdot 4^\alpha > 0. \end{aligned} \quad \blacksquare$$

Lemma 2.4 For $\alpha < -1$, if x, y are nonnegative integers and both satisfy that $2 \leq x, y < \frac{-2}{\alpha+1}$, then for any graph $q_{x,y}$ in class \mathcal{H} there is a graph $t_{x',y',z'}$ in class \mathcal{G} that has a smaller general Randić index than $q_{x,y}$.

Proof. We distinguish the following cases.

Case 1. If one of the two variables x and y is less than $\frac{-(2+2^{\alpha+1}\alpha)}{\alpha+1}$, note that $\frac{-2}{\alpha+1} > 2$ only if $-2 < \alpha < -1$. Suppose $2 \leq x < \frac{-(2+2^{\alpha+1}\alpha)}{\alpha+1}$, then contract one edge in the 4-cycle of $q_{x,y}$ and move the leaf branch where the number of leaf vertices is y to the leaf branch where the number of leaf vertices is x , as shown in Figure 2.2. In this way we have transferred $q_{x,y}$ into S_{x+y+4}^+ . Next we compare the general Randić index of the two graphs. Let R and R^* be the general Randić index of $q_{x,y}$ and S_{x+y+4}^+ , respectively. Then, we only need to show that $R - R^* > 0$. In fact,

$$\begin{aligned} R - R^* &= x(x+2)^\alpha + y(y+2)^\alpha + 2^{\alpha+1}(x+2)^\alpha + 2^{\alpha+1}(y+2)^\alpha \\ &\quad - (x+y+1)(x+y+3)^\alpha - 2^{\alpha+1}(x+y+3)^\alpha - 4^\alpha. \end{aligned}$$

Set the right hand side as $f(x, y, \alpha)$. We want to show it is > 0 . By calculation,

$$\begin{aligned} \frac{\partial f(x, y, \alpha)}{\partial x} &= (x+2)^{\alpha-1}(x+2 + \alpha x + \alpha 2^{\alpha+1}) \\ &\quad - (x+y+3)^{\alpha-1}[x+y+3 + (x+y+1)\alpha + \alpha 2^{\alpha+1}]. \end{aligned}$$

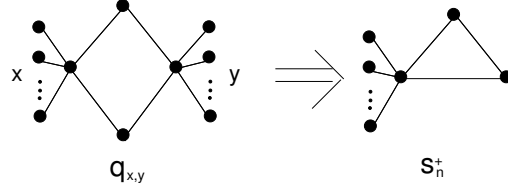


Figure 2.2

Let $\beta = -\alpha$. If $x + y + 3 + (x + y + 1)\alpha + 2^{\alpha+1}\alpha \leq 0$, then $\frac{\partial f(x,y,a)}{\partial x} > 0$. If $x + y + 3 + (x + y + 1)\alpha + 2^{\alpha+1}\alpha > 0$, then $0 < x + y + 3 + (x + y + 1)\alpha + 2^{\alpha+1}\alpha < x + 2 + x\alpha + 2^{\alpha+1}\alpha$ since $\alpha < -1$. Thus, $\frac{\partial f(x,y,a)}{\partial x} > 0$, and so, $f(x,y,\alpha) \geq f(2,y,\alpha) = 2 \cdot 4^\alpha + y(y+2)^\alpha + 2^{\alpha+1}4^\alpha + 2^{\alpha+1}(y+2)^\alpha - (y+3)(y+5)^\alpha - 2^{\alpha+1}(y+5)^\alpha - 4^\alpha > 4^\alpha + 2 \cdot 8^\alpha - 3(y+5)^\alpha > 4^\alpha - 7^\alpha + 2(8^\alpha - 7^\alpha) = \frac{(14^\beta - 8^\beta) - 2(8^\beta - 7^\beta)}{56^\beta} > 0$.

Case 2. If $\max\{2, \frac{-(2+2^{\alpha+1}\alpha)}{\alpha+1}\} \leq x < \frac{-2}{\alpha+1}$ and $\max\{2, \frac{-(2+2^{\alpha+1}\alpha)}{\alpha+1}\} \leq y < \frac{-2}{\alpha+1}$, note that $\frac{-2}{\alpha+1} \geq 2$ only if $-2 \leq \alpha < -1$. Contract one edge in the 4-cycle of $q_{x,y}$ and add one leaf vertex to the leaf branch where the number of leaf vertices is y , as shown in Figure 2.1. In this way we have transferred $q_{x,y}$ into $t_{x,y+1}$. Next we compare the general Randić index of the two graphs. Let R and R^* be the general Randić index of $q_{x,y}$ and $t_{x,y+1}$, respectively. Then, we only need to show that $R - R^* > 0$. In fact, for $-2 \leq \alpha < -1$,

$$R - R^* > (y + 2^\alpha)(y + 2)^\alpha - (y + 1)(y + 3)^\alpha.$$

Set the right hand side as $f(y,\alpha)$. We want to show it is > 0 . Note that

$$\frac{\partial f(y,\alpha)}{\partial y} = (y + 2)^{\alpha-1}[(\alpha + 1)y + 2 + 2^\alpha\alpha] - (y + 3)^{\alpha-1}[(\alpha + 1)y + 2 + 1 + \alpha].$$

If $-1.5 \leq \alpha < -1$, let $g(\alpha) = \alpha + 1 - 2^\alpha\alpha$. Note that $g'(\alpha) = 1 - 2^\alpha - \alpha 2^\alpha \ln 2$, $g''(\alpha) = -2^\alpha \ln 2 [2 + \ln 2] < 0$. Since $-1.5 < \alpha < -1$, $g'(\alpha) > g'(-1) = \frac{1 - \ln 2}{2} > 0$. Note that $g(-1.5) = 0.03 > 0$, and so, for $-1.5 < \alpha < -1$, $g(\alpha) > g(-1.5) > 0$, hence $2^\alpha\alpha < \alpha + 1 < 0$. Therefore, $\frac{\partial f(y,\alpha)}{\partial y} < 0$. Thus, $f(x,\alpha) > f(\frac{-2}{\alpha+1}, \alpha) = (\frac{-2}{\alpha+1} + 2^\alpha)(\frac{-2}{\alpha+1} + 2)^\alpha - (\frac{-2}{\alpha+1} + 1)(\frac{-2}{\alpha+1} + 3)^\alpha$. Denote the right hand side by $t(\alpha)$, and we want to find the solution of the equation $\frac{dt(\alpha)}{d\alpha} = 0$ for $-1.5 < \alpha < -1$. We have the only solution $\alpha \approx -1.433143$ in the interval $[-1.5, -1]$. Then, we determine the minimum value of the function $f(\frac{-2}{\alpha+1}, \alpha)$ for

$-1.5 < \alpha < -1$. Since $f_{\alpha \approx -1.433143}(\frac{-2}{\alpha+1}, \alpha) > 0$, $t(-1.5) = 0.026 > 0$, $\lim_{\alpha \rightarrow -1} t(\alpha) = 0$, then $f(x, \alpha) > 0$.

If $-2 \leq \alpha < -1.5$, note that $x \geq 2$, then x should only be 2 or 3. By calculation, both $f(2, \alpha)$ and $f(3, \alpha)$ are greater than 0 for $-2 \leq \alpha < -1.5$. Thus the lemma follows. ■

To sum up the above Lemmas 2.3 and 2.4, we have the following result.

Lemma 2.5 *We can always transfer a graph $q_{x,y}$ in class \mathcal{H} into a graph $t_{x',y',z'}$ in class \mathcal{G} , where $x' + y' + z' = x + y - 1$, such that for $\alpha < -1, n \geq 5$, $t_{x',y',z'}$ has a smaller general Randić index than $q_{x,y}$.*

From the above discussion, we conclude that if $\alpha < -1$ and $n \geq 5$, then for any graph $q_{x,y}$ in class \mathcal{H} there is a graph $t_{x',y',z'}$ in class \mathcal{G} that has a smaller general Randić index than $q_{x,y}$. So, to find the unicyclic graphs with minimum general Randić index, we only need to investigate the graphs $t_{x,y,z}$ in class \mathcal{G} , where $x \geq y \geq z$ and x, y and z are nonnegative integers.

Lemma 2.6 *For $\alpha < -1$ and $n \geq 5$, among the graphs $t_{x,y,z}$, triangles with leaves, on n vertices in class \mathcal{G} , where x, y, z are nonnegative integers such that $x \geq y \geq z$ and $x + y + z = n - 3$, if $x \geq y \geq \frac{-4}{1+\alpha}$, then $t_{x'',y'',z}^*$, triangle with two balanced leaf branches, where $x + y = x'' + y'' = n - 3 - z$ and $|x'' - y''| \leq 1$, has a smaller general Randić index than $t_{x,y,z}$. Particularly, if one of the three leaf branches has no leaves, say $z = 0$, then $t_{\lceil \frac{n-3}{2} \rceil, \lfloor \frac{n-3}{2} \rfloor}^*$ has a smaller general Randić index.*

Proof. Note that x, y, z are nonnegative integers, and $x \geq y \geq z$ and $x + y + z = n - 3$. We distinguish the following cases.

Case 1. If $x + y = 2k$ and $|x - y| > 1$, let $x = k + t, y = k - t$, where $k > t \geq 1$. Let R be the general Randić index of $t_{x,y,z}$, triangle with leaf branches. Transfer this graph into $t_{x'',y'',z}^*$, triangle with two balanced leaf branches, such that x'' and y'' are equal. Let R^* be the general Randić index of $t_{x'',y'',z}^*$, where $x'' = y'' = k$. Then, we only need to show that

$R - R^* > 0$. In fact,

$$\begin{aligned}
R - R^* &= (k-t)(k-t+2)^\alpha + (k+t)(k+t+2)^\alpha + (k+t+2)^\alpha(k-t+2)^\alpha \\
&\quad - k(k+2)^\alpha - k(k+2)^\alpha - (k+2)^\alpha(k+2)^\alpha + (k-t+2)^\alpha(z+2)^\alpha \\
&\quad + (k+t+2)^\alpha(z+2)^\alpha - (k+2)^\alpha(z+2)^\alpha - (k+2)^\alpha(z+2)^\alpha \\
&> (k-t)(k-t+2)^\alpha + (k+t)(k+t+2)^\alpha + (k+t+2)^\alpha(k-t+2)^\alpha \\
&\quad - 2k(k+2)^\alpha - (k+2)^\alpha(k+2)^\alpha \\
&> 2\left[\frac{1}{2}(k-t)(k-t+2)^\alpha + \frac{1}{2}(k+t)(k+t+2)^\alpha - k(k+2)^\alpha\right].
\end{aligned}$$

Let $f(t) = t(t+2)^\alpha$, then $\frac{d^2 f(t)}{dt^2} = \alpha(t+2)^{\alpha-2}[(\alpha+1)t+4]$. If $t \geq \frac{-4}{1+\alpha}$, then $\frac{d^2 f(t)}{dt^2} \geq 0$. Since $y = k-t \geq \frac{-4}{\alpha+1}$, $R - R^* > 2\left[\frac{1}{2}(k-t)(k-t+2)^\alpha + \frac{1}{2}(k+t)(k+t+2)^\alpha - k(k+2)^\alpha\right] \geq 0$.

Case 2. If $x = k+t+1$, $y = k-t$, $k > t \geq 1$, let R be the general Randić index of $t_{x,y,z}$, triangle with leaf branches, and transfer this graph into $t_{x'',y'',z}^*$, triangle with two balanced leaf branches. Let R^* be the general Randić index of $t_{x'',y'',z}^*$, where $x'' = k+1$, $y'' = k$. Then, we only need to show that $R - R^* > 0$. In fact,

$$\begin{aligned}
R - R^* &= (k-t)(k-t+2)^\alpha + (k+t+1)(k+t+3)^\alpha + (k+t+3)^\alpha(k-t+2)^\alpha \\
&\quad - k(k+2)^\alpha - (k+1)(k+3)^\alpha - (k+2)^\alpha(k+3)^\alpha + (k-t+2)^\alpha(z+2)^\alpha \\
&\quad + (k+t+3)^\alpha(z+2)^\alpha - (k+2)^\alpha(z+2)^\alpha - (k+3)^\alpha(z+2)^\alpha \\
&> [(k-t)(k-t+2)^\alpha - k(k+2)^\alpha] - [(k+1)(k+3)^\alpha - (k+t+1)(k+t+3)^\alpha] \\
&= (-t)\{(k+\xi_1+2)^{\alpha-1}[(\alpha+1)(k+\xi_1)+2] - (k+\xi_2+3)^{\alpha-1}[(\alpha+1)(k+\xi_2+1)+2]\},
\end{aligned}$$

where $-k < -t < \xi_1 < 0, 0 < \xi_2 < t < k$, and thus, $R - R^* > 0$. ■

Lemma 2.7 For $\alpha < -1$ and $n \geq 5$, among graphs $t_{x,y,z}$, triangles with leaves, on n vertices in class \mathcal{G} , where x, y, z are nonnegative integers such that $x \geq y \geq z$, $x \geq y \geq \frac{-4}{1+\alpha}$ and $x + y + z = n - 3$, the graph $t_{\lceil \frac{n-3}{2} \rceil, \lfloor \frac{n-3}{2} \rfloor}^*$, triangle with two balanced leaf branches, has a smaller general Randić index than $t_{x,y,z}$.

Proof. To show the lemma, it suffices to discuss the two cases $z = 2c$ and $z = 2c - 1$, where c is a nonnegative integer. The above Lemma 2.6 implies that among graphs $t_{x,y,z}$ in class \mathcal{G} , $t_{x'',y'',z}^*$, triangle with two balanced leaf branches, where $x + y = x'' + y'' = n - 3 - z$ and

$|x'' - y''| \leq 1$, has a smaller general Randić index than $t_{x,y,z}$ for $x \geq y \geq \frac{-4}{1+\alpha}$ and $x \geq y \geq z$. Next, transfer the graph $t_{x'',y'',z}^*$, triangle with two balanced leaf branches, by moving the leaves in the branch whose number of leaves is z to the remaining two branches such that the numbers of leaves in the remaining branches are almost equal, as shown in Figure 2.3. Then, this resultant new graph is $t_{\lceil \frac{n-3}{2} \rceil, \lfloor \frac{n-3}{2} \rfloor}^*$. Let R and R^* be the general Randić index of $t_{x'',y'',z}^*$ and $t_{\lceil \frac{n-3}{2} \rceil, \lfloor \frac{n-3}{2} \rfloor}^*$, respectively. Then, we only need to show that $R - R^* > 0$.

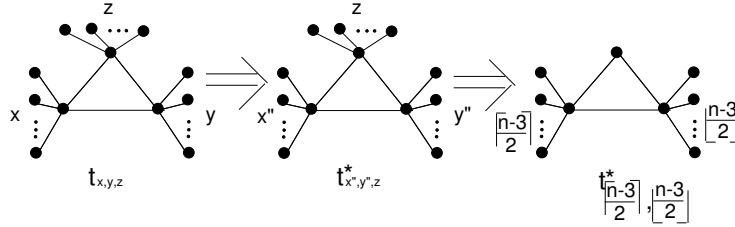


Figure 2.3

Case 1. For $z = 2c$, transfer the graph $t_{x'',y'',2c}^*$ into $t_{x''+c,y''+c,0}^*$. Then,

$$\begin{aligned}
R - R^* &= x''(x'' + 2)^\alpha + y''(y'' + 2)^\alpha + 2c(2c + 2)^\alpha + (2c + 2)^\alpha(x'' + 2)^\alpha \\
&\quad + (2c + 2)^\alpha(y'' + 2)^\alpha + (x'' + 2)^\alpha(y'' + 2)^\alpha - (x'' + c)(x'' + c + 2)^\alpha \\
&\quad - (y'' + c)(y'' + c + 2)^\alpha - (x'' + c + 2)^\alpha(y'' + c + 2)^\alpha \\
&\quad - 2^\alpha(x'' + c + 2)^\alpha - 2^\alpha(y'' + c + 2)^\alpha \\
&> 2c(2c + 2)^\alpha - 2^\alpha(x'' + c + 2)^\alpha - 2^\alpha(y'' + c + 2)^\alpha \\
&> 0.
\end{aligned}$$

Case 2. For $z = 2c - 1$, transfer the graph $t_{x'',y'',2c-1}^*$ into $t_{x''+c-1,y''+c,0}^*$. Then,

$$\begin{aligned}
R - R^* &= x''(x'' + 2)^\alpha + y''(y'' + 2)^\alpha + (2c - 1)(2c + 1)^\alpha + (2c + 1)^\alpha(x'' + 2)^\alpha \\
&\quad + (2c + 1)^\alpha(y'' + 2)^\alpha + (x'' + 2)^\alpha(y'' + 2)^\alpha - (x'' + c - 1)(x'' + c + 1)^\alpha \\
&\quad - (y'' + c)(y'' + c + 2)^\alpha - (x'' + c + 1)^\alpha(y'' + c + 2)^\alpha \\
&\quad - 2^\alpha(x'' + c + 1)^\alpha - 2^\alpha(y'' + c + 2)^\alpha \\
&> (2c - 1)(2c + 1)^\alpha - 2^\alpha(x'' + c + 1)^\alpha - 2^\alpha(y'' + c + 2)^\alpha \\
&> 0.
\end{aligned}$$

■

Lemma 2.8 For $\alpha < -1$ and $n \geq 5$, among the graphs $t_{x,y,z}$, triangles with leaves, on n vertices in class \mathcal{G} , where x, y, z are nonnegative integers such that $x + y + z = n - 3$. If $x \geq y \geq z$ and $z \leq y < \frac{-4}{\alpha+1}$, then S_n^+ has a smaller general Randić index than $t_{x,y,z}$.

Proof. First, note that $\frac{-4}{\alpha+1} \geq 1$ for $-5 \leq \alpha < -1$. Then we only need to show the lemma for $-5 \leq \alpha < -1$.

We transfer the graph $t_{x,y,z}$ into the graph S_n^+ , where $x + y + z = n - 3$, as shown in Figure 2.4. Let R and R^* be the general Randić index of $t_{x,y,z}$ and S_n^+ , respectively. Then, it remains to show that $R - R^* > 0$.

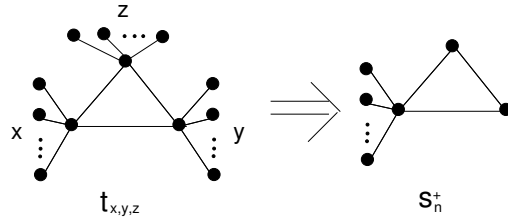


Figure 2.4

Case 1. $z = 0$, $y < \frac{-4}{\alpha+1}$ and $y \leq x$.

If $x \geq \frac{-2}{\alpha+1}$ and $2 \leq y \leq x$, then Lemmas 2.1 and 2.2 imply

$$\begin{aligned} R - R^* &= x(x+2)^\alpha + y(y+2)^\alpha + (x+2)^\alpha(y+2)^\alpha \\ &\quad + (x+2)^\alpha 2^\alpha + 2^\alpha(y+2)^\alpha \\ &\quad - (x+y)(x+y+2)^\alpha - 4^\alpha - 2^{\alpha+1}(x+y+2)^\alpha > 0. \end{aligned}$$

If $2 \leq y \leq x < \frac{-2}{\alpha+1}$, then Lemma 2.2 implies

$$\begin{aligned} R - R^* &= x(x+2)^\alpha + y(y+2)^\alpha + (x+2)^\alpha(y+2)^\alpha + (x+2)^\alpha 2^\alpha \\ &\quad + 2^\alpha(y+2)^\alpha - (x+y)(x+y+2)^\alpha - 4^\alpha - 2^{\alpha+1}(x+y+2)^\alpha \\ &> (x+2^{\alpha+1})(x+2)^\alpha - (x+y+2^{\alpha+1})(x+y+2)^\alpha. \end{aligned}$$

Let $f(t, \alpha) = (t+2^{\alpha+1})(t+2)^\alpha$, then $\frac{\partial f(t, \alpha)}{\partial t} = (t+2)^{\alpha-1}[(\alpha+1)t+2+\alpha 2^{\alpha+1}]$. If $\frac{-2-\alpha 2^{\alpha+1}}{\alpha+1} \leq x < \frac{-2}{\alpha+1}$ ($2 \leq y \leq x$), then $\frac{\partial f(x, \alpha)}{\partial x} < 0$, and so $R - R^* > f(x, \alpha) - f(x+y, \alpha) > 0$. If

$2 \leq y \leq x \leq \frac{-2-\alpha 2^{\alpha+1}}{\alpha+1}$, let $g(x, y, \alpha) = x(x+2)^\alpha + y(y+2)^\alpha + 2^{\alpha+1}(x+2)^\alpha - (x+y)(x+y+2)^\alpha - 4^\alpha - 2^{\alpha+1}(x+y+2)^\alpha$. Since $\frac{\partial g(x, y, \alpha)}{\partial y} = (y+2)^{\alpha-1}[(\alpha+1)y+2] - (x+y+2)^{\alpha-1}[(\alpha+1)(x+y)+2+\alpha 2^{\alpha+1}] > 0$, we have

$$\begin{aligned} R - R^* &> x(x+2)^\alpha + y(y+2)^\alpha + 2^{\alpha+1}(x+2)^\alpha \\ &\quad - (x+y)(x+y+2)^\alpha - 4^\alpha - 2^{\alpha+1}(x+y+2)^\alpha = g(x, y, \alpha) \\ &> g(x, 2, \alpha) = x(x+2)^\alpha + 2^{\alpha+1}(x+2)^\alpha \\ &\quad - (x+2)(x+4)^\alpha - 2^{\alpha+1}(x+4)^\alpha + 4^\alpha. \end{aligned}$$

Since $\frac{\partial g(x, 2, \alpha)}{\partial x} = (x+2)^{\alpha-1}[(\alpha+1)x+2+\alpha \cdot 2^{\alpha+1}] - (x+4)^{\alpha-1}[(\alpha+1)(x+2)+2+\alpha \cdot 2^{\alpha+1}] > 0$, we have $R - R^* \geq g(x, y, \alpha) > g(x, 2, \alpha) > g(2, 2, \alpha) > 3 \cdot 4^\alpha - 4 \cdot 6^\alpha > 0$.

If $x \geq y = 1$ and $z = 0$, we transfer $t_{x,1,0}$ into S_n^+ , where $n = x + 4$. Let R and R^* be general Randeć index of $t_{x,1,0}$ and S_n^+ , respectively. Then, we only need to show that $R - R^* > 0$. First, let $g(x, \alpha) = (3x+6)^\alpha - (x+3)^\alpha - (2x+6)^\alpha$. Then, $\frac{\partial g(x, \alpha)}{\partial x} = \alpha[3(3x+6)^{\alpha-1} - 2(2x+6)^{\alpha-1} - (x+3)^{\alpha-1}] \geq 0$ for $x \geq 2$. So, by setting $\beta = -\alpha$, we have for $x \geq 2$,

$$\begin{aligned} R - R^* &= x(x+2)^\alpha + 3^\alpha + 3^\alpha 2^\alpha + 3^\alpha(x+2)^\alpha + 2^\alpha(x+2)^\alpha \\ &\quad - (x+1)(x+3)^\alpha - (x+3)^\alpha 2^{\alpha+1} - 4^\alpha \\ &> 3^\alpha + 6^\alpha + (3x+6)^\alpha - (x+3)^\alpha - (2x+6)^\alpha - 4^\alpha \\ &= 3^\alpha + 6^\alpha + g(x, \alpha) - 4^\alpha > 3^\alpha + 6^\alpha + 12^\alpha - 5^\alpha - 10^\alpha - 4^\alpha \\ &= \frac{20^\beta + 10^\beta + 5^\beta - 12^\beta - 6^\beta - 15^\beta}{60^\beta} > 0. \end{aligned}$$

For $x = 1$, it is not difficult to see that $R - R^* > 0$.

Case 2. $1 \leq z \leq y < \frac{-4}{\alpha+1}$. Then,

$$\begin{aligned} R - R^* &= x(x+2)^\alpha + y(y+2)^\alpha + z(z+2)^\alpha + (x+2)^\alpha(y+2)^\alpha \\ &\quad + (x+2)^\alpha(z+2)^\alpha + (z+2)^\alpha(y+2)^\alpha \\ &\quad - (x+y+z)(x+y+z+2)^\alpha - 4^\alpha - 2^{\alpha+1}(x+y+z+2)^\alpha \\ &\geq (x+y-1)(x+2)^\alpha - (x+y+z)(x+y+z+2)^\alpha + (x+2)^\alpha \\ &\quad - 2^{\alpha+1}(x+y+z+2)^\alpha + z(z+2)^\alpha - 4^\alpha \end{aligned}$$

$$> (x + y - 1)(x + 2)^\alpha - (x + y + z)(x + y + z + 2)^\alpha.$$

To show the above is > 0 , let $f(x, y, \alpha) = (x + y - 1)(x + 2)^\alpha$, then $\frac{\partial f}{\partial x}(x, y, \alpha) = (x + 2)^\alpha + \alpha(x + 2)^{\alpha-1}(x + y - 1) = (x + 2)^{\alpha-1}[x + 2 + \alpha(x + y - 1)]$. If $y \geq 3$, $\frac{\partial f}{\partial x}(x, y, \alpha) < 0$, then

$$\begin{aligned} f(x, y, \alpha) &= (x + y - 1)(x + 2)^\alpha > [x + (z + 1) + y - 1][x + (z + 1) + 2]^\alpha \\ &= (x + y + z)(x + z + 3)^\alpha > (x + y + z)(x + y + z + 2)^\alpha. \end{aligned}$$

If $x \geq y = 2$ and $z = 2$, we transfer $t_{x,2,2}$ into S_n^+ , where $n = x + 7$. Let R and R^* be the general Randeć index of $t_{x,2,2}$ and S_n^+ , respectively. Then, we only need to show that $R - R^* > 0$. First, let $g(x, \alpha) = 2 \cdot 4^\alpha(x + 2)^\alpha - 4(x + 6)^\alpha - 2^{\alpha+1}(x + 6)^\alpha$. Since $x \geq 2$, we have $2x + 4 \geq x + 6$, and hence

$$\frac{\partial g}{\partial x}(x, y, \alpha) = \alpha[4 \cdot (4x + 8)^{\alpha-1} - 4 \cdot (2x + 12)^{\alpha-1} - 4(x + 6)^{\alpha-1}] > 0.$$

Then, by setting $\beta = -\alpha$ we have

$$\begin{aligned} R - R^* &= x(x + 2)^\alpha + 3 \cdot 4^\alpha + 2 \cdot 4^\alpha(x + 2)^\alpha 16^\alpha - (x + 4)(x + 6)^\alpha - (x + 6)^\alpha 2^{\alpha+1} \\ &> 3 \cdot 4^\alpha + 16^\alpha + 2 \cdot 4^\alpha(x + 2)^\alpha - 4(x + 6)^\alpha - 2^{\alpha+1}(x + 6)^\alpha \\ &= 3 \cdot 4^\alpha + 16^\alpha + g(x, \alpha) > 3 \cdot 4^\alpha + 16^\alpha + g(2, \alpha) = \frac{3 \cdot 4^\beta + 1 - 4 \cdot 2^\beta}{16^\beta} > 0. \end{aligned}$$

If $x \geq y = 2$ and $z = 1$, we transfer $t_{x,2,1}$ into S_n^+ , where $n = x + 6$. Let R and R^* be the general Randeć index of $t_{x,2,1}$ and S_n^+ , respectively. Then, we only need to show that $R - R^* > 0$. First, let $g(x, \alpha) = 4^\alpha(x + 2)^\alpha + 3^\alpha(x + 2)^\alpha - 3(x + 5)^\alpha - 2^{\alpha+1}(x + 5)^\alpha$, and so, $\frac{\partial g}{\partial x}(x, y, \alpha) = \alpha[4 \cdot (4x + 8)^{\alpha-1} + 3 \cdot (3x + 6)^{\alpha-1} - 3 \cdot (x + 5)^{\alpha-1} - 4 \cdot (2x + 10)^{\alpha-1}] > 0$. Then,

$$\begin{aligned} R - R^* &= x(x + 2)^\alpha + 2 \cdot 4^\alpha + 3^\alpha + 3^\alpha 4^\alpha + 4^\alpha(x + 2)^\alpha + 3^\alpha(x + 2)^\alpha \\ &\quad - (x + 3)(x + 5)^\alpha - (x + 5)^\alpha 2^{\alpha+1} - 4^\alpha > 4^\alpha + 3^\alpha + 3^\alpha 4^\alpha \\ &\quad + 4^\alpha(x + 2)^\alpha + 3^\alpha(x + 2)^\alpha - 3(x + 5)^\alpha - 2^{\alpha+1}(x + 5)^\alpha \\ &= 4^\alpha + 3^\alpha + 3^\alpha 4^\alpha + g(x, \alpha) > 4^\alpha + 3^\alpha + 3^\alpha 4^\alpha + g(2, \alpha) \\ &> 4^\alpha + 3^\alpha + 12^\alpha + 16^\alpha + 12^\alpha - 3 \cdot 7^\alpha - 2 \cdot 14^\alpha > 0. \end{aligned}$$

If $x \geq y = 1$ and $z = 1$, we transfer $t_{x,1,1}$ into S_n^+ , where $n = x + 5$. Let R and R^* be the general Randić index of $t_{x,1,1}$ and S_n^+ , respectively. Then, we only need to show that $R - R^* > 0$. First, let $f(x, \alpha) = 3^\alpha(x+2)^\alpha - (x+4)^\alpha - 2^\alpha(x+4)^\alpha$. Then, $\frac{\partial f(x, \alpha)}{\partial x} = \alpha[(3^\alpha(x+2)^{\alpha-1} - 2^\alpha(x+4)^{\alpha-1} - (x+4)^{\alpha-1})] \geq 0$ for $x \geq 2$. So, we have for $x \geq 2$,

$$\begin{aligned} R - R^* &= x(x+2)^\alpha + 2 \cdot 3^\alpha + 3^\alpha 3^\alpha + 2 \cdot 3^\alpha(x+2)^\alpha \\ &\quad - (x+2)(x+4)^\alpha - (x+4)^\alpha 2^{\alpha+1} - 4^\alpha \\ &> 3^\alpha + 9^\alpha + 2 \cdot 3^\alpha(x+2)^\alpha - 2(x+4)^\alpha - 2^{\alpha+1}(x+4)^\alpha \\ &= 3^\alpha + 9^\alpha + 2f(x, \alpha) \geq 3^\alpha + 9^\alpha + 2 \cdot 12^\alpha - 2 \cdot 6^\alpha - 2 \cdot 12^\alpha > 0. \end{aligned}$$

For $x = 1$, it is not difficult to see that $R - R^* > 0$.

In conclusion, for $\alpha < -1$ and $n \geq 5$, among the graphs $t_{x,y,z}$, triangles with leaves, where $z \leq y \leq x$ and $z \leq y < \frac{-4}{\alpha+1}$, S_n^+ has a smaller general Randić index than $t_{x,y,z}$, where $x + y + z = n - 3$. ■

From Theorems 2.7 and 2.8, we arrive at our following main result.

Theorem 2.9 For $\alpha < -1$ and $n \geq 5$, among unicyclic graphs with n vertices, either S_n^+ or $t_{\lceil \frac{n-3}{2} \rceil, \lfloor \frac{n-3}{2} \rfloor}^*$ is the unique one with minimum general Randić index. ■

Theorem 2.10 Particularly, for $\alpha \leq -2$, if $n \geq 42$ then $t_{\lceil \frac{n-3}{2} \rceil, \lfloor \frac{n-3}{2} \rfloor}^*$ is the unique unicyclic graph with minimum general Randić index. If $5 \leq n < 42$ then S_n^+ is the unique unicyclic graph with minimum general Randić index.

Proof. Theorem 2.9 implies that for $\alpha < -1$ and $n \geq 5$, among unicyclic graphs with n vertices, either S_n^+ or $t_{\lceil \frac{n-3}{2} \rceil, \lfloor \frac{n-3}{2} \rfloor}^*$ has minimum general Randić index. For $n \geq 64$, we have $4^\alpha > n(\frac{n}{2})^\alpha$, and hence

$$\begin{aligned} R_\alpha(S_n^+) &= (n-3+2^{\alpha+1})(n-1)^\alpha + 4^\alpha > (n-4)(n-1)^\alpha + 4^\alpha > 4^\alpha > n(\frac{n}{2})^\alpha \\ &> R_\alpha(t_{\lceil \frac{n-3}{2} \rceil, \lfloor \frac{n-3}{2} \rfloor}^*) = \lceil \frac{n-3}{2} \rceil (\lceil \frac{n-3}{2} \rceil + 2)^\alpha + \lfloor \frac{n-3}{2} \rfloor (\lfloor \frac{n-3}{2} \rfloor + 2)^\alpha \\ &\quad + 2^\alpha (\lfloor \frac{n-3}{2} \rfloor + 2)^\alpha + 2^\alpha (\lceil \frac{n-3}{2} \rceil + 2)^\alpha + (\lfloor \frac{n-3}{2} \rfloor + 2)^\alpha (\lceil \frac{n-3}{2} \rceil + 2)^\alpha. \end{aligned}$$

Table 1 the approximate values of γ for different n

n	9	10	11	12	15	18	20
γ	-7.9265	-6.3314	-4.9428	-4.4095	-3.3710	-2.9268	-2.7307
n	25	30	35	40	41	42	43
γ	-2.4185	-2.2372	-2.1129	-2.0240	-2.0084	-1.9944	-1.9804
n	50	10^2	10^3	10^4	10^7	10^{10}	10^{15}
γ	-1.9008	-1.6491	-1.2124	-1.1036	-3.9036	-1.0684	-1.0437

By using a computer to exhaust the values of general Randić index for S_n^+ and $t_{\lceil \frac{n-3}{2} \rceil, \lfloor \frac{n-3}{2} \rfloor}^*$, we get that for $42 \leq n < 64$, $t_{\lceil \frac{n-3}{2} \rceil, \lfloor \frac{n-3}{2} \rfloor}^*$ has minimum general Randić index, and for $5 \leq n < 42$, S_n^+ has minimum general Randić index. ■

In fact, for any given n there is a critical value $\gamma \in (-\infty, -1)$ such that for $\alpha \geq \gamma$, S_n^+ has minimum general Randić index among unicyclic graphs, whereas for $\alpha < \gamma$, the graph $t_{\lceil \frac{n-3}{2} \rceil, \lfloor \frac{n-3}{2} \rfloor}^*$, triangle with two balance leaf branches, has minimum general Randić index. For some $n \geq 9$, we list the approximate values of γ in Table 1.

Table 1 tells us that γ increases with the increasing of n . Indeed, let $\alpha = -1 - \epsilon$, $\epsilon > 0$. Since $4^\alpha > n(\frac{n}{2})^\alpha$, we have $\frac{1}{4^{1+\epsilon}} > \frac{n \cdot 2^{1+\epsilon}}{n^{1+\epsilon}} \Rightarrow \frac{n^\epsilon}{8^{1+\epsilon}} > 1 \Rightarrow n^\epsilon > 8^{1+\epsilon} \Rightarrow n > e^{(1+\frac{1}{\epsilon})\ln 8}$. We can see that as $\alpha \rightarrow -1$ (i.e., $\epsilon \rightarrow 0$), if $t_{\lceil \frac{n-3}{2} \rceil, \lfloor \frac{n-3}{2} \rfloor}^*$, the triangle with two balance leaf branches, has minimum general Randić index among unicyclic graphs then n must be considerably large.

3 Concluding remarks

In this paper, we discuss unicyclic graphs with minimum general Randić index. We completely solve the case for $\alpha < -1$, which was left unsolved by Wu and Zhang [19]. Now we can use the following table to give a clear picture for unicyclic graphs with minimum general Randić index, including the results of Wu and Zhang.

α	extremal unicyclic graph	minimum value
$(-\infty, -2]$	$t_{\lceil \frac{n-3}{2} \rceil, \lfloor \frac{n-3}{2} \rfloor}^*$ for $n \geq 42$, S_n^+ for $5 \leq n \leq 41$	for $n \geq 42$, $\lceil \frac{n-3}{2} \rceil (\lceil \frac{n-3}{2} \rceil + 2)^\alpha + \lfloor \frac{n-3}{2} \rfloor (\lfloor \frac{n-3}{2} \rfloor + 2)^\alpha + 2^\alpha (\lfloor \frac{n-3}{2} \rfloor + 2)^\alpha + 2^\alpha (\lceil \frac{n-3}{2} \rceil + 2)^\alpha + (\lfloor \frac{n-3}{2} \rfloor + 2)^\alpha (\lceil \frac{n-3}{2} \rceil + 2)^\alpha$; for $5 \leq n \leq 41$, $(n-3)(n-1)^\alpha + 2(2n-2)^\alpha + 4^\alpha$
$(-2, -1)^*$	$t_{\lceil \frac{n-3}{2} \rceil, \lfloor \frac{n-3}{2} \rfloor}^*$ or S_n^+ for $n \geq 9$; S_n^+ for $5 \leq n \leq 8$	for $n \geq 9$, $\lceil \frac{n-3}{2} \rceil (\lceil \frac{n-3}{2} \rceil + 2)^\alpha + \lfloor \frac{n-3}{2} \rfloor (\lfloor \frac{n-3}{2} \rfloor + 2)^\alpha + 2^\alpha (\lfloor \frac{n-3}{2} \rfloor + 2)^\alpha + 2^\alpha (\lceil \frac{n-3}{2} \rceil + 2)^\alpha + (\lfloor \frac{n-3}{2} \rfloor + 2)^\alpha (\lceil \frac{n-3}{2} \rceil + 2)^\alpha$ or $(n-3)(n-1)^\alpha + 2(2n-2)^\alpha + 4^\alpha$; for $5 \leq n \leq 8$, $(n-3)(n-1)^\alpha + 2(2n-2)^\alpha + 4^\alpha$.
$[-1, 0)$	S_n^+	$(n-3)(n-1)^\alpha + 2(2n-2)^\alpha$
$(0, +\infty)$	C_n	$n \cdot 4^\alpha$

The interval $(-2, -1)^*$ means that for $n \geq 9$, the unicyclic graph with minimum Randić index depends on α . There is a critical value $\gamma \in (-\infty, -1)$ for each n , such that for $\alpha > \gamma$ and $\alpha < \gamma$, the corresponding unique minimum unicyclic graph is S_n^+ and $t_{\lceil \frac{n-3}{2} \rceil, \lfloor \frac{n-3}{2} \rfloor}^*$, and the corresponding minimum value is $(n-3)(n-1)^\alpha + 2(2n-2)^\alpha + 4^\alpha$ and $\lceil \frac{n-3}{2} \rceil (\lceil \frac{n-3}{2} \rceil + 2)^\alpha + \lfloor \frac{n-3}{2} \rfloor (\lfloor \frac{n-3}{2} \rfloor + 2)^\alpha + 2^\alpha (\lfloor \frac{n-3}{2} \rfloor + 2)^\alpha + 2^\alpha (\lceil \frac{n-3}{2} \rceil + 2)^\alpha + (\lfloor \frac{n-3}{2} \rfloor + 2)^\alpha (\lceil \frac{n-3}{2} \rceil + 2)^\alpha$, respectively. Note that for $\alpha < -1$ and $n = 4$, when $\alpha < -3.0817$, C_4 has minimum general Randić index, whereas when $-3.0817 < \alpha < -1$, S_4^+ has minimum general Randić index. The above property looks very much like what we did in [10] for trees with maximum general Randić index for α in the interval $(1, \infty)$.

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References

- [1] B. Bollobás and P. Erdős, Graphs of extremal weights, *Ars Combin.* 50(1998), 225-233.
- [2] B. Bollobás, P. Erdős and A. Sarkar, Extremal graphs for weights, *Discrete Math.* 200(1999), 5-19.

- [3] G. Caporossi, I. Gutman, P. Hansen and L. Pavlović, Graphs with maximum connectivity index, *Comput. Biol and Chem.* 27(2003), 85-90.
- [4] L.H. Clark and J.W. Moon, On the general Randić index for certain families of trees, *Ars Combin.* 54(2000), 223-235.
- [5] C. Delorme, O. Favaron and D. Rautenbach, On the Randić index, *Discrete Math.* 257(2002), 29-38.
- [6] J. Gao and M. Lu, On the Randić index of unicyclic graphs, *MATCH Commun. Math. Comput. Chem.* 53(2)(2005), 377-384.
- [7] I. Gutman, O. Miljković, G. Caporossi and P. Hansen, Alkanes with small and large Randić connectivity index, *Chem. Phys. Lett.* 306(1999), 366-372.
- [8] Y. Hu, X. Li and Y. Yuan, Solutions to two unsolved questions on the best upper bound for the Randić index R_{-1} of trees, *MATCH Commun. Math. Comput. Chem.* 54(2)(2005), 441-454.
- [9] Y. Hu, X. Li and Y. Yuan, Trees with minimum general Randić index, *MATCH Commun. Math. Comput. Chem.* 52(2004), 119-128
- [10] Y. Hu, X. Li and Y. Yuan, Trees with maximum general Randić index, *MATCH Commun. Math. Comput. Chem.* 52(2004), 129-146.
- [11] L.B. Kier and L.H. Hall, *Molecular Connectivity in Chemistry and Drug Research*, Academic Press, San Francisco, 1976.
- [12] L.B. Kier and L.H. Hall, *Molecular Connectivity in Structure-Activity Analysis*, Wiley, 1986.
- [13] X. Li, X. Wang and B. Wei, On the lower and upper bounds for general Randić index of chemical (n,m) -graphs, *MATCH Commun. Math. Comput. Chem.* 52(2004), 157-166.
- [14] X. Li and Y. Yang, Best lower and upper bounds for the Randić index R_{-1} of chemical trees, *MATCH Commun. Math. Comput. Chem.* 51(2004), 147-156.

- [15] X. Li and Y. Yang, Sharp bounds for the general Randić index, MATCH Commun. Math. Comput. Chem. 51(2004), 157-166.
- [16] M. Lu, H. Liu and F. Tian, The connectivity index, MATCH Commun. Math. Comput. Chem. 51(2004), 149-154.
- [17] M. Randić, On characterization of molecular branching, J. Amer. Chem. Soc. 97(1975), 6609-6615.
- [18] D. Rautenbach, A note on trees of maximum weight and restricted degrees, Discrete Math. 271(2003), 335-342.
- [19] B. Wu and L. Zhang, Unicyclic graphs with minimum general Randić index, MATCH Commun. Math. Comput. Chem. 54(2)(2005), 455-464.
- [20] P. Yu, An upper bound for the Randić indices of trees, J. Math. Study (Chinese) 31(1998), 225-230.