UNICYCLE GRAPHS WITH THE FIRST THREE EXTREMAL ZEROTH-ORDER GENERAL RANDIĆ INDICES

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Abstract

Let $G = (V, E)$ be a graph and $d_v$ the degree of the vertex $v$. The zeroth-order general Randić index of $G$ is defined as: $R_{G}^{0}(G) = \sum_{v \in V} d_v^\alpha$, where $\alpha$ is an arbitrary real number. In this paper, we characterize the unicycle graphs of order $n$ with the first three largest and the first three smallest zeroth-order general Randić indices.

1. Introduction

Let $G = (V(G), E(G))$ denote a graph with $V(G)$ as the set of vertices and $E(G)$ as the set of edges. $N_G(v_i)$ denotes the neighbors of $v_i$. The Randić index of $G$ defined in [13] is

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}.$$
where $d_v = d_G(v)$ denotes the degree of the vertex $v$ in $G$. Randić demonstrated that his index is well correlated with a variety of physicochemical properties of an alkane. The index $R(G)$ has become one of the most popular molecular descriptors. The interesting reader is referred to [1-3, 11-13]. Eventually, countless research papers are devoted. The zeroth-order Randić index $R^0(G)$ of $G$ defined by Kier and Hall [8] is given by $R^0(G) = \sum_{v \in V(G)} \frac{1}{\sqrt{d_v}}$. Pavlović [11] gave the unique graph with largest value of $R^0(G)$. In [5], Lielal investigated the same problem for the topological index $M_1(G)$, also known as the first Zagreb index [14], which is defined as $M_1(G) = \sum_{v \in V(G)} d_v^2$. Li and Zheng [10] defined the zeroth-order general Randić index of a graph $G$ as:

$$R_\alpha^0(G) = \sum_{v \in V(G)} d_v^\alpha,$$

where $\alpha$ is a real number. For $\alpha$ being one of $m, -m, \frac{1}{m}, -\frac{1}{m}$, where $m \geq 2$ is an integer, Li and Zhao [9] characterized the trees with the first three largest and smallest zeroth-order general Randić index; Wang and Deng [15] characterized the unicycle graphs with the maximum zeroth-order general Randić index. Hu et al. [6] characterized the molecular $(n, m)$-graphs with the smallest and greatest $R^0_{\alpha}$. Hua and Deng [7] characterized the unicycle graphs with the smallest and greatest $R^0_{\alpha}$.

In this paper, we investigate the zeroth-order general Randić index for the unicycle graphs. All unicycle graphs with the first three largest and the first three smallest zeroth-order general Randić index are characterized.

All graphs considered here are both finite and simple. We denote the star, path and cycle of order $n$ by $S_n$, $P_n$ and $C_n$, respectively. Let $G = (V, E)$ be an unicycle graph of order $n$ with its unique cycle $C_r = v_1v_2$.
...$v_r, v_1$ of length $r$, $T_1, T_2, \ldots, T_k (0 \leq k \leq r)$ are the all nontrivial components (they are all nontrivial trees) of $G - E(C_r)$, $u_i$ is the common vertex of $T_i$ and $C_r$, $i = 1, 2, \ldots, k$. Such an unicycle graph is denoted by $C_r^{u_1, u_2, \ldots, u_k} (T_1, T_2, \ldots, T_k)$. Let $n(T_i) = l_i + 1$ be the number of vertices in tree $T_i$, then $l = n - r = l_1 + l_2 + l_3 + \cdots + l_k$.

Specially, $u_1, u_2, \ldots, u_k$ are the centers of $S_{l_1+1}, S_{l_2+1}, \ldots, S_{l_k+1}$, respectively, in

$$G_1 = C_r^{u_1, u_2, \ldots, u_k} (S_{l_1+1}, S_{l_2+1}, \ldots, S_{l_k+1})$$

and $u_1, u_2, \ldots, u_k$ are the end-vertices of $P_{l_1+1}, P_{l_2+1}, \ldots, P_{l_k+1}$, respectively, in

$$G_2 = C_r^{u_1, u_2, \ldots, u_k} (P_{l_1+1}, P_{l_2+1}, \ldots, P_{l_k+1}).$$

We also denote $C_3 (S_{n-2})$ by $S_n + e$. $C_3 (P_{n-2})$ is simplified by $C_3 (P_{n-2})$.

$D(G) = [d_1, d_2, \ldots, d_n]$ denotes the degree sequence of a graph $G$, and $D(G) = [x_1^{q_1}, x_2^{q_2}, \ldots, x_t^{q_t}]$, $x_i^{q_i}$ means that $G$ has $a_i$ vertices of degree $x_i$, $i = 1, 2, \ldots, t$.

Undefined notations and terminology will conform to those in [9].

2. The Unicycle Graphs with the First Three Largest (Smallest) Zeroth-Order General Randić Indices for $\alpha > 1$ or $\alpha < 0$ ($0 < \alpha < 1$)

We first introduce three transfer operation.

**Transfer operation A.** Let $G$ be an unicycle graph of order $n$. If there are vertices $u$ and $v$ such that $d_u = p > 1$, $d_v = q > 1$, $p \leq q$, and $u_1, u_2, \ldots, u_k$ are the neighbors of $u$. Then $G$ is changed into $G'$ after
the transfer operation $A$, where $G' = G - \{uu_1, uu_2, \ldots, uu_k\} + \{vu_1, vu_2, \ldots, vu_k\}$, $1 \leq k \leq p$. As shown in Figure 1.

![Figure 1. Transfer operation $A$.](image)

**Lemma 2.1.** For the two graphs $G$ and $G'$ above, we have

(i) $R^0_\alpha(G') > R^0_\alpha(G)$ for $\alpha > 1$ or $\alpha < 0$;

(ii) $R^0_\alpha(G') < R^0_\alpha(G)$ for $0 < \alpha < 1$.

**Proof.** By the definition of $R^0_\alpha(G)$, we have

$$
\Delta = R^0_\alpha(G') - R^0_\alpha(G)
= [(p - k)^\alpha + (q + k)^\alpha] - [p^\alpha + q^\alpha]
= [(q + k)^\alpha - q^\alpha] - [p^\alpha - (p - k)^\alpha]
= \alpha \cdot k(\xi^{\alpha-1} - \eta^{\alpha-1}),
$$

where $\eta \in (p - k, p)$, $\xi \in (q, q + k)$. $\xi > \eta$ since $p \leq q$. Then $\Delta > 0$ when $\alpha > 1$ or $\alpha < 0$; $\Delta < 0$ when $0 < \alpha < 1$. The proof of Lemma 2.1 is completed.

**Remark.** Repeating operation $A$, any unicycle graph of order $n$ can be changed into an unicycle graph which has at most one vertex with degree greater than 2 such as $C^n_{ru_1}(T_1)$. 
Transfer operation B. Let $G$ be an unicycle graph of order $n$, $uv$ is an edge of $G$. $d_G(u) = p \geq 3$, $N_G(v)$ is the neighbors of $v$, and $N_G(v) - \{u\} = \{w_1, w_2, \ldots, w_l\}$. Then $G$ is changed into $G^*$ first and, then into $G''$ after operation $B$, where $G' = G - \{vw_1, vw_2, \ldots, vw_l\} + \{uw_1, uw_2, \ldots, uw_l\}$, $G^* = G - \{vw_2, vw_3, \ldots, vw_l\} + \{uw_2, uw_3, \ldots, uw_l\}$. As shown in Figure 2.

![Figure 2. Transfer operation B.](image)

Lemma 2.2. For the three graphs $G$, $G'$ and $G^*$ above, we have

(i) $R^0_\alpha(G') > R^0_\alpha(G^*) > R^0_\alpha(G)$ for $\alpha > 1$ or $\alpha < 0$;

(ii) $R^0_\alpha(G') < R^0_\alpha(G^*) < R^0_\alpha(G)$ for $0 < \alpha < 1$.

Proof. If $p \geq l + 1$, then

$$
\Delta = R^0_\alpha(G^*) - R^0_\alpha(G) \\
= [(p + l - 1)^\alpha + 2^\alpha] - [p^\alpha + (l + 1)^\alpha] \\
= [(p + l - 1)^\alpha - p^\alpha] - [(l + 1)^\alpha - 2^\alpha] \\
= \alpha(l - 1)(\zeta^{\alpha-1} - \eta^{\alpha-1}),
$$

where $\eta \in (2, l + 1)$, $\zeta \in (p, p + l - 1)$.

If $p \leq l + 1$, then

$$
\Delta = R^0_\alpha(G^*) - R^0_\alpha(G) \\
= [(p + l - 1)^\alpha + 2^\alpha] - [p^\alpha + (l + 1)^\alpha]
$$
where $\eta \in (2, p)$, $\xi \in (l + 1, p + l - 1)$.

And $\xi > \eta, \Delta > 0$ when $\alpha > 1$ or $\alpha < 0$; $\Delta < 0$ when $0 < \alpha < 1$. The proof of Lemma 2.2 is completed.

**Remark.** Repeating the operation $B$, any unicycle graph $G = C_{r_1, u_2, \cdots, u_k}(T_1, T_2, \cdots, T_k)$ can be changed into $C_{r_1, u_2, \cdots, u_k}(S_{i_1}, S_{i_2}, \cdots, S_{i_k})$.

So, an unicycle graph $G = C_{r_1, u_2, \cdots, u_k}(T_1, T_2, \cdots, T_k)$ can be changed into $G' = C_{r_1}(S_{n-r+1})$ after the operations $B$ and $A$.

**Transfer operation C.** Let $G$ be an unicycle graph of order $n$. $C_r = u_1 u_2 \cdots u_r u_1$ is the unique cycle of $G$. $e = xy$ is a pedant edge of $G$, and $d_x = 1, d_y \geq 2$. Then $G$ is changed into $G'$ after the transfer operation $C$, where $G' = G - \{xy, u_i u_{i+1}\} + \{u_i y, u_{i+1} y\}$. As shown in Figure 3.

**Figure 3.** Transfer operation C.

**Lemma 2.3.** For the two graphs $G$ and $G'$ above, we have

(i) $R_\alpha^0(G') \leq R_\alpha^0(G)$ for $\alpha > 1$ or $\alpha < 0$;

(ii) $R_\alpha^0(G') \geq R_\alpha^0(G)$ for $0 < \alpha < 1$,
with the equality if and only if $d_x = 2$.

**Proof.** By the definition of $R^0_\alpha(G)$, we have

$$\Delta = R^0_\alpha(G') - R^0_\alpha(G)$$

$$= [(d_x - 1)^\alpha + 2^\alpha] - [d_x^\alpha + 1^\alpha]$$

$$= [2^\alpha - 1^\alpha] - [d_x^\alpha - (d_x - 1)^\alpha]$$

$$= \alpha(\xi^{\alpha-1} - \eta^{\alpha-1}),$$

where $\eta \in (d_x - 1, d_x)$, $\xi \in (1, 2)$. $\xi < \eta$ since $d_x \geq 2$. $\Delta < 0$ when $\alpha > 1$ or $\alpha < 0$; $\Delta > 0$ when $0 < \alpha < 1$. The proof of Lemma 2.3 is completed.

From Lemma 2.3, we know that $R^0_\alpha(C^u_r(S_{n-r+1}))$, $3 \leq r \leq n$, is the monotone function of $r$.

If $3 \leq r \leq r' \leq n$, then

(i) $R^0_\alpha(C^u_r(S_{n-r+1})) > R^0_\alpha(C^u_{r'}(S_{n-r'+1}))$ for $\alpha > 1$ or $\alpha < 0$;

(ii) $R^0_\alpha(C^u_r(S_{n-r+1})) < R^0_\alpha(C^u_{r'}(S_{n-r'+1}))$ for $0 < \alpha < 1$.

The following result is immediate from the Lemmas above.

**Theorem 2.4 (\cite{7}).** Among all unicycle graphs of order $n$,

(i) $G = C_3(S_{n-2})$ is the unique unicycle graph with the largest zeroth-order general Randić index for $\alpha > 1$ or $\alpha < 0$;

(ii) $G = C_3(S_{n-2})$ is the unique unicycle graph with the smallest zeroth-order general Randić index for $0 < \alpha < 1$.

In the following, we consider the unicycle graphs with the second and the third largest zeroth-order general Randić index for $\alpha > 1$ or $\alpha < 0$. 
For any unicycle graph $G = C_{u_1, u_2, \ldots, u_k}(T_1, T_2, \ldots, T_k)$, by the transfer operation $B$, there is an unicycle graph $G' = C_{u_1, u_2, \ldots, u_k}(S_{i+1}, S_{l_2+1}, \ldots, S_{l+k+1})$ such that

\begin{enumerate}[(i)]
  \item $R^0_\alpha(G') \geq R^0_\alpha(G)$ for $\alpha > 1$ or $\alpha < 0$;
  \item $R^0_\alpha(G') \leq R^0_\alpha(G)$ for $0 < \alpha < 1$.
\end{enumerate}

Furthermore, if $k \geq 4$, then, by the transfer operations $A$ and $C$, there is an unicycle graph $G'' = C_{u_1, u_2, u_3}(S_{i+1}, S_{l_2+1}, S_{l_3+1})$ such that

\begin{enumerate}[(i)]
  \item $R^0_\alpha(G'') \geq R^0_\alpha(G')$ for $\alpha > 1$ or $\alpha < 0$;
  \item $R^0_\alpha(G'') \leq R^0_\alpha(G')$ for $0 < \alpha < 1$.
\end{enumerate}

Let

\begin{align*}
  G_1 &= \{ C_{u_1, u_2, u_3}(S_{i+1}, S_{l_2+1}, S_{l_3+1}) \mid l_i \geq 1, i = 1, 2, 3, l_1 + l_2 + l_3 = n - 3 \}, \\
  G_2 &= \{ C_{u_1, u_2}(T_1, T_2) \mid 3 \leq r \leq 4, l_i \geq 1, i = 1, 2, l_1 + l_2 = n - r \}, \\
  G_3 &= \{ C_{u_1}(T_1) \mid 3 \leq r \leq 5, l_1 = n - r \}.
\end{align*}

By the transfer operation $A$, we know that

\begin{enumerate}[(i)]
  \item the largest value of zeroth-order general Randić indices of the unicycle graphs in $G_1$ is not more than the third largest value of zeroth-order general Randić indices of all unicycle graphs for $\alpha > 1$ or $\alpha < 0$, and the smallest value of zeroth-order general Randić indices of the unicycle graphs in $G_1$ is not less than the third smallest value of zeroth-order general Randić indices of all unicycle graphs for $0 < \alpha < 1$;
  \item the largest value of zeroth-order general Randić indices of the unicycle graphs in $G_2$ is not more than the second largest value of zeroth-order general Randić indices of all unicycle graphs for $\alpha > 1$ or $\alpha < 0$,
\end{enumerate}
and the smallest value of zeroth-order general Randić indices of the unicycle graphs in \( G_2 \) is not less than the second smallest value of zeroth-order general Randić indices of all unicycle graphs for \( 0 < \alpha < 1 \).

Therefore, in order to find the unicycle graph with the second and the third largest (smallest) zeroth-order general Randić index for \( \alpha > 1 \) or \( \alpha < 0 \) \((0 < \alpha < 1)\), we only need to find

(i) the unicycle graph with the largest (smallest) zeroth-order general Randić index in \( G_1 \) for \( \alpha > 1 \) or \( \alpha < 0 \) \((0 < \alpha < 1)\); and

(ii) the unicycle graphs with the first two largest (smallest) zeroth-order general Randić index in \( G_2 \) for \( \alpha > 1 \) or \( \alpha < 0 \) \((0 < \alpha < 1)\); and

(iii) the unicycle graph with the first three largest (smallest) zeroth-order general Randić index in \( G_3 \) for \( \alpha > 1 \) or \( \alpha < 0 \) \((0 < \alpha < 1)\) and, then compare them in turn.

From the transfer operation \( A \), it is immediate that

**Lemma 2.5.** (i) The unicycle graph in \( G_1 \) with the largest (smallest) zeroth-order general Randić index for \( \alpha > 1 \) or \( \alpha < 0 \) \((0 < \alpha < 1)\) is

\[
G_1 = C_{3}^{u_{1}, u_{2}, u_{3}}(S_{2}, S_{2}, S_{n-4}) .
\]

(ii) The unicycle graph in \( G_2 \) with the largest (smallest) zeroth-order general Randić index for \( \alpha > 1 \) or \( \alpha < 0 \) \((0 < \alpha < 1)\) is

\[
G_{10} = C_{3}^{u_{1}, u_{2}}(S_{2}, S_{n-3}) .
\]

(iii) The unicycle graph in \( G_3 \) with the largest (smallest) zeroth-order general Randić index for \( \alpha > 1 \) or \( \alpha < 0 \) \((0 < \alpha < 1)\) is

\[
G_{2} = C_{3}(S_{n-2}) ,
\]

it is also the unicycle graph with the largest (smallest) zeroth-order general Randić index for \( \alpha > 1 \) or \( \alpha < 0 \) \((0 < \alpha < 1)\) among all unicycle graphs of order \( n \).
Lemma 2.6. The unicycle graph $G_2$ with the second largest (smallest) zeroth-order general Randić index for $\alpha > 1$ or $\alpha < 0$ $(0 < \alpha < 1)$ is $G_{11} = C_{3}^{u_1, u_2}(S_3, S_{n-4})$.

Proof. Let $G = C_{r}^{u_1, u_2}(T_1, T_2) \in G_2$, $3 \leq r \leq 4$, $G \neq C_{3}^{u_1, u_2}(S_2, S_{n-3})$.

Case 1. If $r = 3$, then $\{T_1, T_2\} \neq \{S_2, S_{n-3}\}$.

(1) $\{T_1, T_2\} = \{S_{l_1+1}, S_{l_2+1}\}$, where $l_1 \geq 2$, $l_2 \geq 2$, $l_1 + l_2 = n - 2$, and $u_1, u_2$ are the centers of $T_1$ and $T_2$, respectively. By the transfer operation $A$, we have

(i) $R_{\alpha}^{0}(G) \leq R_{\alpha}^{0}(G_{11})$ for $\alpha > 1$ or $\alpha < 0$;

(ii) $R_{\alpha}^{0}(G) \geq R_{\alpha}^{0}(G_{11})$ for $0 < \alpha < 1$,

where $G_{11} = C_{3}^{u_1, u_2}(S_3, S_{n-4})$, as shown in Figure 4.

(2) Otherwise, by the transfer operations $A$ and $B$, we have

(i) $R_{\alpha}^{0}(G) \leq R_{\alpha}^{0}(G')$ for $\alpha > 1$ or $\alpha < 0$;

(ii) $R_{\alpha}^{0}(G) \geq R_{\alpha}^{0}(G')$ for $0 < \alpha < 1$,

where $G' = G_{11}$ or $G_{12}$, as shown in Figure 4.

Case 2. If $r = 4$, then by the transfer operations $A$ and $B$, we have

(i) $R_{\alpha}^{0}(G) \leq R_{\alpha}^{0}(G')$ for $\alpha > 1$ or $\alpha < 0$;

(ii) $R_{\alpha}^{0}(G) \geq R_{\alpha}^{0}(G')$ for $0 < \alpha < 1$,

where $G' = G_{13}$ or $G_{14}$, as shown in Figure 4. Continuing the transfer operation $C$, we have

(i) $R_{\alpha}^{0}(G') \leq R_{\alpha}^{0}(G_{11})$ for $\alpha > 1$ or $\alpha < 0$;

(ii) $R_{\alpha}^{0}(G') \geq R_{\alpha}^{0}(G_{11})$ for $0 < \alpha < 1$. 
Finally, comparing the zeroth-order general Randić indices of $G_{11}$ and $G_{12}$ we have

(i) $R_{\alpha}^0(G_{12}) < R_{\alpha}^0(G_{11})$ for $\alpha > 1$ or $\alpha < 0$;

(ii) $R_{\alpha}^0(G_{12}) > R_{\alpha}^0(G_{11})$ for $0 < \alpha < 1$.

The proof of Lemma 2.6 is completed.

Similarly, the unicycle graph in $G_{3}$ with the second largest (smallest) zeroth-order general Randić index for $\alpha > 1$ or $\alpha < 0$ $(0 < \alpha < 1)$ is $G_{3}$ and $G_{7}$. The unicycle graph in $G_{3}$ with the third largest (smallest) zeroth-order general Randić index for $\alpha > 1$ or $\alpha < 0$ $(0 < \alpha < 1)$ is one of $G_{4}$, $G_{5}$ and $G_{6}$. Comparing the zeroth-order general Randić indices of $G_{4}$, $G_{5}$ and $G_{6}$, we have

**Lemma 2.7.** (i) The unicycle graph in $G_{3}$ with the second largest (smallest) zeroth-order general Randić index for $\alpha > 1$ or $\alpha < 0$ $(0 < \alpha < 1)$ is $G_{3}$ or $G_{7}$;

(ii) The unicycle graph in $G_{3}$ with the third largest (smallest) zeroth-order general Randić index for $\alpha > 1$ or $\alpha < 0$ $(0 < \alpha < 1)$ is $G_{5}$.

Comparing the zeroth-order general Randić indices of $G_{3}$, $G_{7}$, $G_{1}$, $G_{10}$ and $G_{11}$, we have

**Theorem 2.8.** Among all unicycle graphs of order $n$,

(i) The unicycle graph with the second largest (smallest) zeroth-order general Randić index for $\alpha > 1$ or $\alpha < 0$ $(0 < \alpha < 1)$ is $G_{10}$;

(ii) The unicycle graph with the third largest (smallest) zeroth-order general Randić index for $\alpha > 1$ or $\alpha < 0$ $(0 < \alpha < 1)$ is $G_{3}$ or $G_{7}$. 
Figure 4.
3. The Unicycle Graphs with the First Three Smallest (Largest) Values of Zeroth-Order Randić Index for \( \alpha > 1 \) or \( \alpha < 0 \) \((0 < \alpha < 1)\)

For convenience, we introduce some new transfer operations.

Transfer operation \( D \). Let \( G = C_{r}^{u_{1},u_{2},\ldots,u_{k}}(T_{1},\ldots,T_{i},\ldots,T_{k}) \), \( k \geq 1 \). If \( T_{i} \) is not a path, or \( T_{i} \) is a path and \( u_{i} \) is not the end-vertex of the path, then \( G \) can be changed into \( G' = C_{r}^{u_{1},\ldots,u_{i},\ldots,u_{k}}(T_{1},\ldots,P_{i+1}^{l_{i}}),\ldots,T_{k}) \) after the transfer operation \( D \), where \( l_{i} + 1 = n(T_{i}) \) and \( u_{i} \) is the end-vertex of \( P_{i+1}^{l_{i}} \), as shown in Figure 5.

**Lemma 3.1.** For the two graphs \( G \) and \( G' \) above, we have

(i) \( R_{0}^{0}(G') < R_{0}^{0}(G) \) for \( \alpha > 1 \) or \( \alpha < 0 \);

(ii) \( R_{0}^{0}(G') > R_{0}^{0}(G) \) for \( 0 < \alpha < 1 \).

**Proof.** By the definition of \( R_{0}^{0}(G) \), we have

\[
\Delta = R_{0}^{0}(G) - R_{0}^{0}(G')
\]

\[
= R_{0}^{0}(T_{i}) - R_{0}^{0}(P_{i+1}^{l_{i}}) + [(p + 2)^{\alpha} - 3^{\alpha}] - [p^{\alpha} - 1^{\alpha}]
\]
= R^0_\alpha(T_i) - R^0_\alpha(P_{i+1}) + [(p + 2)^\alpha - p^\alpha] - [3^\alpha - 1^\alpha] \\
= R^0_\alpha(T_i) - R^0_\alpha(P_{i+1}) + 2\alpha(\xi^{\alpha-1} - \eta^{\alpha-1}),

where \( \xi \in (p, p + 2), \eta \in (1, 3) \) (or \( \xi \in (3, p + 2), \eta \in (1, p) \)).

Let \( \Delta_1 = f(T_i) - f(P_{i+1}), \Delta_2 = \alpha(\xi^{\alpha-1} - \eta^{\alpha-1}). \)

If \( \alpha > 1 \) or \( \alpha < 0 \), then \( \Delta_2 \geq 0 \); and \( \Delta_1 \geq 0 \) from [9]. And at least one of the equalities strictly holds. So, \( \Delta > 0 \).

If \( 0 < \alpha < 1 \), then \( \Delta_2 < 0 \); and \( \Delta_1 < 0 \) from [9]. And at least one of the inequalities strictly holds. So, \( \Delta < 0 \).

The proof of Lemma 3.1 is completed.

**Remark.** Repeating the operations \( D \), any unicycle graph
\[ G = C_{r_1, r_2, \ldots, r_k} (T_1, T_2, \ldots, T_k) \]
can be changed into
\[ C_{r_1, r_2, \ldots, r_k} (P_{1+1}, P_{2+1}, \ldots, P_{k+1}). \]

For any unicycle graph \( G = C_{r_1, r_2, \ldots, r_k} (T_1, T_2, \ldots, T_k) \), we can see from Lemma 3.1 that

(i) \( R^0_\alpha(G) \geq R^0_\alpha(C_{r_1, r_2, \ldots, r_k} (P_{1+1}, P_{2+1}, \ldots, P_{k+1})) \) for \( \alpha > 1 \) or \( \alpha < 0 \);

(ii) \( R^0_\alpha(G) \leq R^0_\alpha(C_{r_1, r_2, \ldots, r_k} (P_{1+1}, P_{2+1}, \ldots, P_{k+1})) \) for \( 0 < \alpha < 1 \).

And the equality holds if and only if
\[ G = C_{r_1, r_2, \ldots, r_k} (P_{1+1}, P_{2+1}, \ldots, P_{k+1}). \]

**Transfer operation** \( F \). Let \( G = C_{r_1, r_2, \ldots, r_k} (P_{1+1}, P_{2+1}, \ldots, P_{k+1}) \).

If \( k > 1 \), then \( G \) can be changed into
\[ G' = C_{r_1, \ldots, r_{k-1}} (P_{1+1}, P_{2+1}, \ldots, P_{k-1}+l_{k+1}). \]
Lemma 3.2. For the two graphs $G$ and $G'$ above, we have

(i) $R_{\alpha}^0(G') < R_{\alpha}^0(G)$ for $\alpha > 1$ or $\alpha < 0$;

(ii) $R_{\alpha}^0(G') > R_{\alpha}^0(G)$ for $0 < \alpha < 1$.

Proof. By the definition of $R_{\alpha}^0(G)$, we have

$$\Delta = R_{\alpha}^0(G') - R_{\alpha}^0(G)$$

$$= [2^\alpha + 2^\alpha] - [3^\alpha + 1^\alpha]$$

$$= [2^\alpha - 1^\alpha] - [3^\alpha - 2^\alpha]$$

$$= \alpha(\zeta\alpha^{-1} - \eta\alpha^{-1}),$$

where $\zeta \in (1, 2)$, $\eta \in (2, 3)$. And $\xi < \eta$, $\Delta < 0$ for $\alpha > 1$ or $\alpha < 0$, $\Delta > 0$ for $0 < \alpha < 1$. The proof of Lemma 3.2 is completed.

Remark. Repeating the operation $F$, any unicycle graph $G = C_{r_1, u_2, \ldots, u_k}(P_{l_1 + 1}, P_{l_2 + 1}, \ldots, P_{l_k + 1})$ can be changed into $C_{r}^{u_1}(P_{n-r+1})$, as shown in Figure 6.

Therefore, any unicycle graph $G = C_{r_1, u_2, \ldots, u_k}(T_1, T_2, \ldots, T_k)$ can be changed into $C_{r}^{u_1}(P_{n-r+1})$ after the operations $D$ and $F$.

Figure 6. $C_{r}^{u_1}(P_{n-r+1})$. 
Lemma 3.3. If $3 \leq r < n$, then

(i) $R_{\alpha}^{0}(C_{r}^{\text{un}}(P_{n-r+1})) > R_{\alpha}^{0}(C_{n})$ for $\alpha > 1$ or $\alpha < 0$;

(ii) $R_{\alpha}^{0}(C_{r}^{\text{un}}(P_{n-r+1})) < R_{\alpha}^{0}(C_{n})$ for $0 < \alpha < 1$.

Proof. If $3 \leq r < n$, then the degree sequence of $C_{r}^{\text{un}}(P_{n-r+1})$ is $[1, 2, \ldots, 2 \cdots, 3]$. The degree sequence of $C_{n}$ is $[2, 2, \ldots, 2 \cdots, 2]$. By the definition of $R_{\alpha}^{0}(G)$, we have

$$\Delta = R_{\alpha}^{0}(C_{r}^{\text{un}}(P_{n-r+1})) - R_{\alpha}^{0}(C_{n})$$

$$= [1^{\alpha} + 3^{\alpha}] - [2^{\alpha} + 2^{\alpha}]$$

$$= [3^{\alpha} - 2^{\alpha}] - [2^{\alpha} - 1^{\alpha}]$$

$$= \alpha(\xi^{\alpha-1} - \eta^{\alpha-1}),$$

where $\xi \in (2, 3)$, $\eta \in (1, 2)$. And $\Delta > 0$ for $\alpha > 1$ or $\alpha < 0$, $\Delta < 0$ for $0 < \alpha < 1$. The proof of Lemma 3.3 is completed.

From Lemmas 3.1 and 3.2, the following result is immediate.

Theorem 3.4. Among all unicycle graphs,

(i) $C_{n}$ is the unique unicycle graph with the smallest (largest) zeroth-order general Randić index for $\alpha > 1$ or $\alpha < 0$ ($0 < \alpha < 1$);

(ii) the unicycle graphs with the second smallest (largest) zeroth-order general Randić index for $\alpha > 1$ or $\alpha < 0$ ($0 < \alpha < 1$) are $C_{r}^{\text{un}}(P_{n-r+1})$, $3 \leq r \leq n-1$, their degree sequences are $[1, 2, \ldots, 2 \cdots, 3]$.

In the following, we consider the unicycle graph with third smallest (largest) zeroth-order general Randić index for $\alpha > 1$ or $\alpha < 0$ ($0 < \alpha < 1$).
Let

\[ \mathcal{F}_1 = \{ C_{r_1}^{u_1, u_2}(P_{l_1 + 1}, P_{l_2 + 1}) | l_1, l_2 \geq 1, l_1 + l_2 = n - r, r \geq 3 \} \]

\[ \mathcal{F}_2 = \{ C_{r_1}^{u_1}(T_1) | 3 \leq r \leq n - 1 \}. \]

For any unicycle \( G = C_{r_1}^{u_1, u_2, \ldots, u_k}(T_1, \ldots, T_1, \ldots, T_k) \), if \( k \geq 3 \), then by the operations \( D \) and \( F \), there is \( G' \in \mathcal{F}_1 \) such that

(i) \( R^0_{\alpha}(G) > R^0_{\alpha}(G') \) for \( \alpha > 1 \) or \( \alpha < 0 \);

(ii) \( R^0_{\alpha}(G) < R^0_{\alpha}(G') \) for \( 0 < \alpha < 1 \).

Similarly, for any unicycle graph \( G \in \mathcal{F}_1 \), there is \( G' \in \mathcal{F}_2 \) such that

(i) \( R^0_{\alpha}(G) > R^0_{\alpha}(G') \) for \( \alpha > 1 \) or \( \alpha < 0 \);

(ii) \( R^0_{\alpha}(G) < R^0_{\alpha}(G') \) for \( 0 < \alpha < 1 \).

Therefore, the smallest value of zeroth-order general Randić indices of the unicycle graphs in \( \mathcal{F}_1 \) is not less than the third smallest value of zeroth-order general Randić indices of all unicycle graphs for \( \alpha > 1 \) or \( \alpha < 0 \); and the largest value of zeroth-order general Randić indices of the unicycle graphs in \( \mathcal{F}_1 \) is not more than the third largest value of zeroth-order general Randić indices of all unicycle graphs for \( 0 < \alpha < 1 \).

In order to find the unicycle graph with the third smallest (largest) zeroth-order general Randić index for \( \alpha > 1 \) or \( \alpha < 0 \) (\( 0 < \alpha < 1 \)), we only need to find

(i) the unicycle graph with the smallest (largest) zeroth-order general Randić index in \( \mathcal{F}_1 \) for \( \alpha > 1 \) or \( \alpha < 0 \) (\( 0 < \alpha < 1 \)); and

(ii) the unicycle graphs with the second smallest (largest) zeroth-order general Randić index in \( \mathcal{F}_2 \) for \( \alpha > 1 \) or \( \alpha < 0 \) (\( 0 < \alpha < 1 \)) and, then compare them in turn.

Note that the degree sequences of graphs in \( \mathcal{F}_1 \) are \([1, 1, 2, \ldots, 2, 3, 3]\), and their zeroth-order general Randić indices are the same value:
$R^0_\alpha(G) = 2 + 2^\alpha(n - 4) + 2 \cdot 3^\alpha$. 

So, we only need to find the unicycle graphs with the second smallest (largest) zeroth-order general Randić index in $F_2$ for $\alpha > 1$ or $\alpha < 0$ ($0 < \alpha < 1$).

Let $D(G) = [d_1, d_2, \ldots, d_n]$ be the degree sequence of unicycle graph $G$ with order $n$, where $d_i \geq d_j + 2$. $G'$ is obtained by replacing $(d_i, d_j)$ with $(d_i - 1, d_j + 1)$ in $D(G)$, i.e.,

$$D(G') = [d_1, \ldots, d_{i-1}, d_i - 1, d_{i+1}, \ldots, d_{j-1}, d_j + 1, d_{j+1}, \ldots, d_n].$$

**Lemma 3.4** ([9]). For the two graphs $G$ and $G'$ above, we have

(i) $R^0_\alpha(G) > R^0_\alpha(G')$ for $\alpha > 1$ or $\alpha < 0$;

(ii) $R^0_\alpha(G) < R^0_\alpha(G')$ for $0 < \alpha < 1$.

**Lemma 3.5.** The graphs in $F_2$ with the degree sequence $D(G) = [1, 1, 2, \ldots, 2, 3, 3]$ are the unicycle graphs with the second smallest (largest) zeroth-order general Randić index in $F_2$ for $\alpha > 1$ or $\alpha < 0$ ($0 < \alpha < 1$).

**Proof.** Let $G = C^m_n(T_1)$ be the unicycle graph in $F_2$ with the second smallest (largest) for $\alpha > 1$ or $\alpha < 0$ ($0 < \alpha < 1$). Since $r \leq n - 1$, $G$ must have at least one vertex with degree more than 2.

If $F_0$ is the unicycle graph with the smallest (largest) zeroth-order general Randić index in $F_2$ for $\alpha > 1$ or $\alpha < 0$ ($0 < \alpha < 1$), then, by Theorem 3.1, the degree sequence of $F_0$ is $[1, 2, \ldots, 2, 3]$.

Therefore, $G$ must have at least two vertices with degree more than 2.

If the degree sequence of $G$ is not $[1, 1, 2, \ldots, 2, 3, 3]$, then, by Lemma 3.4, there is an unicycle graph $G' \in F_2$ such that $D(G') = [1, 1, 2, \ldots, 2, 3, 3]$, and
(i) $R_\alpha^0(G) > R_\alpha^0(G') > R_\alpha^0(F_0)$ for $\alpha > 1$ or $\alpha < 0$;

(ii) $R_\alpha^0(G) < R_\alpha^0(G') < R_\alpha^0(F_0)$ for $0 < \alpha < 1$.

This contradicts that $G$ is the unicycle graph in $F_2$ with the second smallest (largest) for $\alpha > 1$ or $\alpha < 0$ ($0 < \alpha < 1$). So, the degree sequence of $G$ is $D(G) = [1, 1, 2, \ldots, 2, 3, 3]$.

Since the degree sequence of the graph in $F_1$ is $[1, 1, 2, \ldots, 2, 3, 3]$, combining Lemma 3.5 and the above, we have

**Theorem 3.2.** Among all the unicycle graphs of order $n$, the unicycle graphs with the third smallest (largest) zeroth-order general Randić index for $\alpha > 1$ or $\alpha < 0$ ($0 < \alpha < 1$) are the graphs whose degree sequences are $[1, 1, 2, \ldots, 2, 3, 3]$.

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**References**


