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On unicycle graphs with maximum and minimum zeroth-order general randić index

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Let G be a graph and d_v denote the degree of the vertex v in G. The zeroth-order general Randić index of a graph is defined as $R_\alpha^0(G) = \sum_{v \in V(G)} d_v{}^\alpha$ where α is an arbitrary real number. In this paper, we obtained the lower and upper bounds for the zeroth-order general Randić index $R_\alpha^0(G)$ among all unicycle graphs G of order n. We give a clear picture for $R_\alpha^0(G)$ of unicycle graphs according to real number α in different intervals.

KEY WORDS: unicycle graph, zeroth-order general Randić index, minimum cardinality, maximum cardinality

1. Introduction

Let $G = (V(G), E(G))$ denote a graph whose set of vertices and set of edges are $V(G)$ and $E(G)$ respectively. For any $v \in V(G)$, we denote the neighbors of v as $N(v)$. The Randić index of G defined in [8] is

$$R(G) = \sum_{uv \in E(G)} (d_u d_v)^{-\frac{1}{2}},$$

where $d_v = d_G(v)$ denotes the degree of the vertex v in G. Randić showed that his index is well correlated with a variety of Physic-Chemical properties of an alkane. The index $R(G)$ has become one of the most popular molecular descriptors, the interesting reader is referred to [2–8, 11, 12]. The zeroth-order Randić index $R^0(G)$ of G defined by Kier and Hall [10] is $R^0(G) = \sum_{v \in V(G)} d_v{}^{-\frac{1}{2}}$. Pavlović [9] determined 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 Zagreb index [13],

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which is defined as $M_1(G) = \sum_{v \in V(G)} {d_v}^2$. Li et al. [14] defined the zeroth-order general Randić index as $R_\alpha^0(G) = \sum_{v \in V(G)} {d_v}^\alpha$. Li and Zhao [1] characterized the trees with the first three largest and smallest zeroth-order general Randić index, Wang and Deng [16] characterized the unicycle graphs with the maximum zeroth-order general Randić index, with α being equal to m, $-m$, $1/m$, $-1/m$, where $m \geqslant 2$ is an integer. In [15], Hu et al. investigated the molecular graphs having the smallest and largest zeroth-order general Randić index.

In this paper, we investigate the zeroth-order general Randić index for the unicycle graphs. All unicycle graphs having extremal (maximum or minimum) zeroth-order general Randić index are characterized.

All graphs considered here are both finite and simple. We denote, respectively, by S_n, P_n and C_n the star, path and cycle with n vertices.

Let (G_1, v_1) and (G_2, v_2) be two graphs rooted at v_1 and v_2 respectively, then $G = (G_1, v_1) \bowtie (G_1, v_2)$ denote the graph obtained by identifying v_1 with v_2 as one common vertex.

Let $V_0(T)$ denote the set of all leaves of a tree T. Let $\mathcal{U}_n$ denote the set of all unicycle graphs of order n. By $\mathcal{U}(n, k)$ we denote the set of the unicycle graphs in which the length of its cycle is k. For any graph G in $\mathcal{U}(n, k)$, we denote the unique cycle of length k in G as C_k.

Other notations and terminology not defined here will conform to those in [1].

For any graph in $\mathcal{U}(n, k)$ with $n = k$, its zeroth-order general topological index can be easily calculated. So we'll always assume that $n \geqslant k + 1$ throughout this paper.

In the following, we will investigate $R_\alpha^0(G)$ for unicycle graph according to the value of α in different intervals.

2. The case $\alpha = 1$ and $\alpha = 0$

It's easy to get the following trivial results:

When $\alpha = 0$, $R_\alpha^0(G) = \sum_{v \in V(G)} {d_v}^\alpha = n$, where n is the order of the graph G.

When $\alpha = 1$, $R_\alpha^0(G) = \sum_{v \in V(G)} {d_v}^\alpha = 2m$, where m is the number of edges of the graph G.

3. The case $0 < \alpha < 1$ and $\alpha > 1$ or $\alpha < 0$

Lemma 3.1. *Let $A = \{v \in V(C_k) : d(v) \geqslant 3\}$. If G is an unicycle graph in $\mathcal{U}(n, k)$ such that one of*

(i) *$R_\alpha^0(G)$ is as large as possible for $0 < \alpha < 1$;*

(ii) *$R_\alpha^0(G)$ is as small as possible for $\alpha > 1$ or $\alpha < 0$*

holds, then $|A| = 1$.

Proof. Assume that $|A| \geqslant 2$. $C_k = v_1 v_2 \cdots v_k v_1$. Let v_i and v_j be distinct vertices in A. By $T(v_j)$, we denote the connected component containing v_j of the graph $G - \{v_{j-1},\ v_{j+1}\}$. Obviously, $T(v_j)$ is a tree. Let y be a leaf of $T(v_j)$. Set $N(v_i) - V(C_k) = \{x_1, \ldots, x_p\}(p \geqslant 1)$.

Let $G' = G - v_i x_1 - \cdots - v_i x_p + y x_1 + \cdots + y x_p$. We have

$$\begin{aligned} R_\alpha^0(G') - R_\alpha^0(G) &= [(p+1)^\alpha - 1] + [2^\alpha - (p+2)^\alpha] \\ &= (2^\alpha - 1) - [(p+2)^\alpha - (p+1)^\alpha] \\ &= \alpha(\xi^{\alpha-1} - \eta^{\alpha-1}), \end{aligned}$$

where $1 < \xi < 2$ and $2 \leqslant p+1 < \eta < p+2$.

When $0 < \alpha < 1$, we have $R_\alpha^0(G') > R_\alpha^0(G)$, a contradiction to (i); When $\alpha < 0$ or $\alpha < 0$, we have $R_\alpha^0(G') < R_\alpha^0(G)$, a contradiction to (ii).

Consequently, we have $|A| = 1$. □

Lemma 3.2. *Let $A = \{v \in V(C_k) : d(v) \geqslant 3\}$. Suppose G is an unicycle graph in $\mathcal{U}(n,k)$ such that one of*

(i) *$R_\alpha^0(G)$ is as large as possible for $0 < \alpha < 1$;*

(ii) *$R_\alpha^0(G)$ is as small as possible for $\alpha > 1$ or $\alpha < 0$*

holds, then $d(v_i) \leqslant 4$ for $v_i \in A$.

Proof. Suppose that $d(v_i) \geqslant 5$. $C_k = v_1 v_2 \cdots v_k v_1$. Let $N(v_i) - V(C_k) = \{x_1, \ldots, x_p\}$, where $p \geqslant 3$.

Let $T(v_i, x_1)$ denote the tree containing v_i and x_1 but excluding v_{i-1}, v_{i+1}, $x_2, \ldots, x_p$. There must exist one vertex y with $d(y) = 1$ in $T(v_i, x_1)$. Set

$$G' = G - v_i x_2 - \cdots - v_i x_p + y x_2 + \cdots + y x_p.$$

We have

$$\begin{aligned} R_\alpha^0(G') - R_\alpha^0(G) &= [3^\alpha - (p+2)^\alpha] + (p^\alpha - 1) \\ &= (3^\alpha - 1) - [(p+2)^\alpha - p^\alpha] \\ &= 2\alpha(\xi^{\alpha-1} - \eta^{\alpha-1}), \end{aligned}$$

where $1 < \xi < 3$ and $3 \leqslant p < \eta < p+2$.

So, $R_\alpha^0(G') > R_\alpha^0(G)$ for $0 < \alpha < 1$ and $R_\alpha^0(G') < R_\alpha^0(G)$ for $\alpha < 0$ or $\alpha > 1$, a contradiction to i and (ii), respectively. And we have $d(v_i) \leqslant 4$ for $v_i \in A$. □

Theorem 3.3. *If G is an unicycle graph in $\mathcal{U}(n,k)$, then $R_\alpha^0(G)$ attains the largest (smallest, resp.) value if and only if $G = (C_k, v_i) \bowtie (P_{n-k+1}, v_i)$ for $0 < \alpha < 1$ ($\alpha > 1$ or $\alpha < 0$, resp.), where v_i is one end-vertex of P_{n-k+1} and any vertex of C_k.*

Proof. The proof of necessity.

Let G be a graph in $\mathcal{U}(n,k)$ with $R_\alpha^0(G)$ taking the largest (smallest, resp.) value for $0<\alpha<1$ ($\alpha>1$ or $\alpha<0$, resp.). Suppose G is not the graph defined as above. There must exist exactly one vertex, say v_i, in $C_k=v_1v_2\cdots v_kv_1$ such that $3\leqslant d(v_i)\leqslant 4$ by lemmas 3.1 and 3.2.

We distinguish the following two cases:

Case 1. $d(v_i)=3$.

We consider the longest path v_i-y in $T(v_i)$, where $T(v_i)$ is one connected component containing v_i of the graph $G-\{v_{i-1},\ v_{i+1}\}$. By the hypothesis, there must exist at least one vertex, say v_s, in the v_i-y path with $d(v_s)\geqslant 3$. Let $N(v_s)\bigcap V_0(T(v_i))=\{z_1,\ldots,z_l\}$, where $l\geqslant 1$. Set

$$G'=G-v_sz_1-\cdots-v_sz_l+yz_1+\cdots+yz_l.$$

We have

$$\begin{aligned}R_\alpha^0(G')-R_\alpha^0(G)&=[(l+1)^\alpha-1]-[(l+2)^\alpha-2^\alpha]\\&=(2^\alpha-1)-[(l+2)^\alpha-(l+1)^\alpha]\\&=\alpha(\xi^{\alpha-1}-\eta^{\alpha-1}),\end{aligned}$$

where $1<\xi<2$ and $2\leqslant l+1<\eta<l+2$.

When $0<\alpha<1$, $R_\alpha^0(G')>R_\alpha^0(G)$; when $\alpha<0$ or $\alpha>1$, $R_\alpha^0(G')<R_\alpha^0(G)$, we have a contradiction. So, $T(v_i)$ is a path of order $n-k+1$ in this case.

Case 2. $d(v_i)=4$.

Let $N(v_i)-V(C_k)=\{u,\ w\}$. $T(v_i,u)$ (or $T(v_i,w)$) denotes the subtree of $T(v_i)$ containing u(or w) but excluding w(or u) respectively. We consider independently $T(v_i,u)$ and $(T(v_i,w))$. From the proof of case 1, it's easy to see that $T(v_i,u)$ and $T(v_i,w)$ are all paths.

Now, set $G'=G-v_iu+yu$, where y is one end vertex of $T(v_i,w)$.

We have

$$\begin{aligned}R_\alpha^0(G')-R_\alpha^0(G)&=(2^\alpha-1)-(4^\alpha-3^\alpha)\\&=\alpha(\xi^{\alpha-1}-\eta^{\alpha-1}),\end{aligned}$$

where $1<\xi<2$ and $3<\eta<4$.

When $0<\alpha<1$, $R_\alpha^0(G')>R_\alpha^0(G)$; when $\alpha<0$ or $\alpha>1$, $R_\alpha^0(G')<R_\alpha^0(G)$, we have a contradiction.

From case 1 and case 2, we know that $T(v_i)$ is P_{n-k+1}. Hence, $G=(C_k,v_i)\bowtie(P_{n-k+1},v_i)$.

The proof of sufficiency.

When $G=(C_k,v_i)\bowtie(P_{n-k+1},v_i)$, it's easy to see that the removal of any one edge of (P_{n-k+1},v_i) will decrease (increase, resp.) the value of $R_\alpha^0(G)$

for $0<\alpha<1$ ($\alpha > 1$ or $\alpha<0$, resp.). So, $R_\alpha^0(G)$ achieves the maximum (minimum, resp.) value for $0<\alpha<1$ ($\alpha > 1$ or $\alpha<0$, resp.) when $G=(C_k, v_i) \bowtie (P_{n-k+1}, v_i)$.

Therefore the proof is completed. □

Lemma 3.4. *Let* $A=\{v \in V(C_k) : d(v) \geqslant 3\}$. *If* G *is an unicycle graph in* $\mathcal{U}(n,k)$ *such that one of*

(i) $R_\alpha^0(G)$ *is as small as possible for* $0<\alpha<1$;

(ii) $R_\alpha^0(G)$ *is as large as possible for* $\alpha > 1$ *or* $\alpha<0$

holds, then $|A|=1$.

Proof. If $|A| \geqslant 2$, we may assume that $A=\{v_1, \ldots, v_t\}$ where $t \geqslant 2$. Let v_i and v_j be distinct vertices in A. Set $N(v_i) - V(C_k)=\{x_1, \ldots, x_p\}$ and $N(v_j) - V(C_k)=\{y_1, \ldots, y_q\}$ where $p \geqslant 1$ and $q \geqslant 1$. We distinguish the following two cases:

Case 1. $d(v_i)=d(v_j)=p+2$, i.e., $p=q$.

Set $G'=G - v_j y_1 - \cdots - v_j y_p + v_i y_1 + \cdots + v_i y_p$, then

$$\begin{aligned} R_\alpha^0(G') - R_\alpha^0(G) &= [(2p+2)^\alpha - (p+2)^\alpha] - [(p+2)^\alpha - 2^\alpha] \\ &= \alpha(\xi^{\alpha-1} - \eta^{\alpha-1}), \end{aligned}$$

where $p+2<\xi<2p+2$ and $2<\eta<p+2$.

When $0<\alpha<1$, we have $R_\alpha^0(G')<R_\alpha^0(G)$, a contradiction to (i); When $\alpha<0$ or $\alpha>1$, we have $R_\alpha^0(G') > R_\alpha^0(G)$, a contradiction to (ii).

Case 2. $d(v_i) \neq d(v_j)$ for any $v_i,\ v_j \in A$.

We may assume that $d(v_1)<d(v_2)< \cdots <d(v_t)$. Let $N(v_1) - V(C_k)=\{x_1, \ldots, x_p\}$ where $p \geqslant 1$ and $d(v_t)=q+2$. Set $G'=G - v_1x_1 - \cdots - v_1x_p + v_tx_1 + \cdots + v_tx_p$, then

$$\begin{aligned} R_\alpha^0(G') - R_\alpha^0(G) &= [(p+q+2)^\alpha - (q+2)^\alpha] - [(p+2)^\alpha - 2^\alpha] \\ &= p\alpha(\xi^{\alpha-1} - \eta^{\alpha-1}), \end{aligned}$$

where $2<\eta<p+2<q+2<\xi<p+q+2$ since $p<q$.

When $0<\alpha<1$, we have $R_\alpha^0(G')<R_\alpha^0(G)$, a contradiction to (i); When $\alpha<0$ or $\alpha>1$, we have $R_\alpha^0(G') > R_\alpha^0(G)$, a contradiction to (ii).

From the proofs of case 1 and case 2, we have $|A|=1$. □

Lemma 3.5. *Suppose* G *is an unicycle graph in* $\mathcal{U}(n,k)$ *such that one of*

(i) $R_\alpha^0(G)$ *is as small as possible for* $0<\alpha<1$;

(ii) $R_\alpha^0(G)$*is as large as possible for* $\alpha > 1$ *or* $\alpha<0$

holds. Let v_s be any vertex in $V(G) - V(C_k)$, if $N(v_s) \bigcap V(C_k) \neq \emptyset$, then $d(v_s) \neq 2$.

Proof. Assume $d(v_s) = 2$ for some $v_s \in V(G) - V(C_k)$ such that $N(v_s) \bigcap V(C_k) \neq \emptyset$. Let $N(v_s) = \{v_i,\ v_t\}$. Suppose $v_i = N(v_s) \bigcap V(C_k)$ and $d(v_i) = p+2 (p \geqslant 1)$. Set $G' = G - v_s v_t + v_i v_t$, we have

$$\begin{aligned} R_\alpha^0(G') - R_\alpha^0(G) &= [(p+3)^\alpha - (p+2)^\alpha] - (2^\alpha - 1) \\ &= \alpha(\xi^{\alpha-1} - \eta^{\alpha-1}), \end{aligned}$$

where $p+2 < \xi < p+3$ and $1 < \eta < 2$.

When $0 < \alpha < 1$, we have $R_\alpha^0(G') < R_\alpha^0(G)$, a contradiction to (i); When $\alpha < 0$ or $\alpha > 1$, we have $R_\alpha^0(G') > R_\alpha^0(G)$, a contradiction to (ii).

Therefore the proof is completed. □

Lemma 3.6. *Suppose G is an unicycle graph in $\mathcal{U}(n, k)$ such that one of*

(i) *$R_\alpha^0(G)$ is as small as possible for $0 < \alpha < 1$;*

(ii) *$R_\alpha^0(G)$ is as large as possible for $\alpha > 1$ or $\alpha < 0$*

holds. If $N(v_i) - V(C_k) = \{x_1, \ldots, x_p\}$ and $B = \{x_j \in N(v_i) - V(C_k) : d(x_j) \geqslant 3\}$, where $v_i \in V(C_k)$, then $|B| \leqslant 1$.

Proof. Suppose to the contrary that $|B| \geqslant 2$. Without loss of generality, let $B = \{x_1, \ldots, x_w\}$ where $w \geqslant 2$. We consider the following two cases:

Case 1. $d(x_s) = d(x_t)$ for some $x_s \in B$ and $x_t \in B$.

Let $N(x_s) - \{v_i\} = \{y_1,\ \ldots,\ y_l\}$ and $N(x_t) - \{v_i\} = \{z_1,\ \ldots,\ z_l\}$, where $l \geqslant 2$. Set $G' = G - x_s y_1 - \cdots - x_s y_l + x_t y_1 + \cdots + x_t y_l$, then we have

$$\begin{aligned} R_\alpha^0(G') - R_\alpha^0(G) &= [(2l+1)^\alpha - (l+1)^\alpha] - [(l+1)^\alpha - 1] \\ &= l\alpha(\xi^{\alpha-1} - \eta^{\alpha-1}), \end{aligned}$$

where $l+1 < \xi < 2l+1$ and $1 < \eta < l+1$.

When $0 < \alpha < 1$, we have $R_\alpha^0(G') < R_\alpha^0(G)$, a contradiction to (i); When $\alpha < 0$ or $\alpha > 1$, we have $R_\alpha^0(G') > R_\alpha^0(G)$, a contradiction to (ii).

Case 2. $d(x_s) \neq d(x_t)$ for any two vertices x_s and x_t in B.

Without loss of generality, we may assume that $d(x_1) < d(x_2) < \cdots < d(x_w)$. Set $N(x_1) - \{v_i\} = \{x_{11},\ x_{12}, \ldots x_{1p'}\} (p' \geqslant 2)$ and $d(x_w) = q+1$. Let $G' = G - x_1 x_{11} - \cdots - x_1 x_{1p'} + x_w x_{11} + \cdots + x_w x_{1p'}$, then

$$\begin{aligned} R_\alpha^0(G') - R_\alpha^0(G) &= [(q+p'+1)^\alpha - (q+1)^\alpha] - [(p'+1)^\alpha - 1] \\ &= \alpha p'(\xi^{\alpha-1} - \eta^{\alpha-1}), \end{aligned}$$

where $1 < \eta < p' + 1 < q + 1 < \xi < p' + q + 1$ since $p' < q$.

When $0 < \alpha < 1$, we have $R_\alpha^0(G') < R_\alpha^0(G)$, a contradiction to (i); When $\alpha < 0$ or $\alpha > 1$, we have $R_\alpha^0(G') > R_\alpha^0(G)$, a contradiction to (ii).

From the cases 1 and 2, the desired result follows. □

Theorem 3.7. *If G is an unicycle graph in $\mathcal{U}(n, k)$, then $R_\alpha^0(G)$ attains the smallest (largest, resp.) value if and only if $G = (C_k, v_i) \bowtie (S_{n-k+1}, v_i)$ for $0 < \alpha < 1$ ($\alpha > 1$ or $\alpha < 0$, resp.), where v_i is the center of S_{n-k+1} and any vertex of C_k.*

Proof. The proof of necessity.

Let G be a graph in $\mathcal{U}(n, k)$ with $R_\alpha^0(G)$ taking the smallest value (largest value, resp.). By the lemma 3.4, we know that there exists exactly one vertex, say v_i, in $V(C_k)$ with $d(v_i) \geqslant 3$. Moreover, if $N(v_i) - V(C_k) = \{x_1, \ldots, x_p\}(p \geqslant 1)$ and $B = \{x_j \in N(v_i) - V(C_k) : d(v_j) \geqslant 3\}$, then $|B| \leqslant 1$ by the lemma 3.6.

If $|B| = 0$, we have $d(x_j) = 1$ for any $x_j \in N(v_i) - V(C_k)$, since $d(x_j) \neq 2$ for any vertex $x_j \in N(v_j) - V(C_k)$ by the lemma 3.5. So $T(v_i)$ is a star of order $n - k + 1$ and $G = (C_k, v_i) \bowtie (S_{n-k+1}, v_i)$, where $T(v_i)$ is defined as before.

If $|B| = 1$, we assume that $B = \{x_1\}$. Suppose $N(x_1) - \{v_i\} = \{y_1, \ldots, y_q\}(q \geqslant 2)$, we consider the following two cases:

Case 1. $p + 2 \geqslant q + 1$.

Set $G' = G - x_1y_1 - \cdots - x_1y_q + v_iy_1 + \cdots + v_iy_q$, we have

$$\begin{aligned} R_\alpha^0(G') - R_\alpha^0(G) &= [(p + q + 2)^\alpha - (p + 2)^\alpha] - [(q + 1)^\alpha - 1] \\ &= q\alpha(\xi^{\alpha-1} - \eta^{\alpha-1}), \end{aligned}$$

where $1 < \eta < q + 1 \leqslant p + 2 < \xi < p + q + 2$.

So, $R_\alpha^0(G') < R_\alpha^0(G)$ for $0 < \alpha < 1$; or $R_\alpha^0(G') > R_\alpha^0(G)$ for $\alpha < 0$ or $\alpha > 1$, a contradiction to the minimality or maximality of $R_\alpha^0(G)$ respectively.

Case 2. $p + 2 < q + 1$.

We consider the following two subcases:

Subcase 2.1. $3 = p + 2 < q + 1$.

Set $G' = G - v_iv_{i-1} - v_iv_{i+1} + x_1v_{i-1} + x_1v_{i+1}$, we have

$$\begin{aligned} R_\alpha^0(G') - R_\alpha^0(G) &= [(q + 3)^\alpha - (q + 1)^\alpha] - (3^\alpha - 1) \\ &= 2\alpha(\xi^{\alpha-1} - \eta^{\alpha-1}), \end{aligned}$$

where $1 < \eta < 3 = p + 2 < q + 1 < \xi < q + 3$.

So, $R_\alpha^0(G') < R_\alpha^0(G)$ for $0 < \alpha < 1$; or $R_\alpha^0(G') > R_\alpha^0(G)$ for $\alpha < 0$ or $\alpha > 1$, a contradiction to the minimality or maximality of $R_\alpha^0(G)$ respectively once again.

Subcase 2.2. $4 \leqslant p + 2 < q + 1$.

Set $G' = G - v_i x_2 - \cdots - v_i x_p + x_1 x_2 + \cdots + x_1 x_p$, we have

$$R^0_\alpha(G') - R^0_\alpha(G) = [3^\alpha - (p+2)^\alpha] + [(p+q)^\alpha - (q+1)^\alpha]$$
$$= (p-1)\alpha(\xi^{\alpha-1} - \eta^{\alpha-1}),$$

where $3 < \eta < p+2 < q+1 < \xi < p+q$.

So, $R^0_\alpha(G') < R^0_\alpha(G)$ for $0 < \alpha < 1$; or $R^0_\alpha(G') > R^0_\alpha(G)$ for $\alpha < 0$ or $\alpha > 1$, a contradiction to the minimality or maximality of $R^0_\alpha(G)$ respectively.

Therefore, $|B| \neq 1$ and $G = (C_k, v_i) \bowtie (S_{n-k+1}, v_i)$, where v_i is the center of S_{n-k+1} and any vertex of C_k respectively.

The proof of sufficiency.

If $G = (C_k, v_i) \bowtie (S_{n-k+1}, v_i)$, where v_i is the center of S_{n-k+1}, the removal of any one edge of (S_{n-k+1}, v_i) will increase (decrease, resp.) the value of $R^0_\alpha(G)$ for $0 < \alpha < 1$ ($\alpha < 0$ or $\alpha > 1$, resp.), so $R^0_\alpha(G)$ attains the smallest (largest, resp.) value for $0 < \alpha < 1$ ($\alpha < 0$ or $\alpha > 1$, resp.).

Therefore, the proof is completed. □

Theorem 3.8. *Let G be an unicycle graph in* $\mathcal{U}(n,k)$*. For* $0 < \alpha < 1$*, we have* $(n-k+2)^\alpha + (k-1)2^\alpha + n - k \leqslant R^0_\alpha(G) \leqslant (n-2)2^\alpha + 3^\alpha + 1$*, with the left equality holds if and only if* $G = (C_k, v_i) \bowtie (S_{n-k+1}, v_i)$ *and with the right equality holds if and only if* $G = (C_k, v_i) \bowtie (P_{n-k+1}, v_i)$.

Proof. For $0 < \alpha < 1$, by an elementary calculation, we can easily get that $R^0_\alpha(G) = (n-k+2)^\alpha + (k-1)2^\alpha + n - k$ when $G = (C_k, v_i) \bowtie (S_{n-k+1}, v_i)$ and $R^0_\alpha(G) = (n-2)2^\alpha + 3^\alpha + 1$ when $G = (C_k, v_i) \bowtie (P_{n-k+1}, v_i)$. By theorems 3.3 and 3.7, we have $(n-k+2)^\alpha + (k-1)2^\alpha + n - k \leqslant R^0_\alpha(G) \leqslant (n-2)2^\alpha + 3^\alpha + 1$ with the left equality holds if and only if $G = (C_k, v_i) \bowtie (S_{n-k+1}, v_i)$ and with the right equality holds if and only if $G = (C_k, v_i) \bowtie (P_{n-k+1}, v_i)$. □

Theorem 3.9. *Let G be an unicycle graph in* $\mathcal{U}(n,k)$*. For* $\alpha > 1$ *or* $\alpha < 0$*, we have* $(n-2)2^\alpha + 3^\alpha + 1 \leqslant R^0_\alpha(G) \leqslant (n-k+2)^\alpha + (k-1)2^\alpha + n - k$*, with left equality holds if and only if* $G = (C_k, v_i) \bowtie (P_{n-k+1}, v_i)$ *and with right equality holds if and only if* $G = (C_k, v_i) \bowtie (S_{n-k+1}, v_i)$.

The proof of theorem 3.9 is omitted here since it can be proved in a similar way as that of theorem 3.8.

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References

[1] X. Li and H. Zhao, MATCH Commun. Math. Comput. Chem. 51 (2004) 205.
[2] O. Araujo and J. Rada, J. Math. Chem. 27 (2000) 19.
[3] E. Esrrada, Chem. Phs. Lett. 336 (2001) 248.
[4] M. Fishermann, I. Gutman, A. Hoffmann, D. Rautenbach, D. Vidoić and L. Volkmann, Z. Naturforsch 57a (2002) 49.
[5] P. Hansen and H. Mélot, J. Chem. Inf. Comput. Sci. 43 (2003) 1.
[6] I. Gutman and O. Miljković, Chem. Phs. Lett. 306 (1999) 366.
[7] M. Randić, J. Am. Chem. Soc. 97 (1975) 6609.
[8] M. Randić, J. Math. Chem. 24 (1998) 345.
[9] L. Pavlovič, Discrete Applied Mathematics 127 (2003) 615.
[10] L.B. Kier and L. Hall, Molecular Connectivity in Structure Activity Analysis, (Research Studies Press, Wiley UK, 1986).
[11] P. Yu, J. Math. Study (Chinese) 31 (1998) 225.
[12] B. Bollobás and P. Erdös, Ars Combin. 5 (1998) 225.
[13] X. Li and Y. Yang, MATCH Commun. Math. Comput. Chem. 51 (2004) 155.
[14] X. Li and J. Zheng, MATCH Commun. Math. Comput. Chem. 51 (2005) 195.
[15] Y. Hu et al., On molecular graphs with smallest and greatest zeroth-order general Randić index, *Manuscript*.
[16] H. Wang and H. Deng, Accepted by J. Math. Chem.