

Extremal $(n, n+1)$ -graphs with respected to zeroth-order general Randić index

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A $(n, n+1)$ -graph G is a connected simple graph with n vertices and $n+1$ edges. If d_v denotes the degree of the vertex v , then the zeroth-order general Randić index $R_\alpha^0(G)$ of the graph G is defined as $\sum_{v \in V(G)} d_v^\alpha$, where α is a real number. We characterize, for any α , the $(n, n+1)$ -graphs with the smallest and greatest zeroth-order general Randić index.

KEY WORDS: $(n, n+1)$ -graph, zeroth-order general Randic index, degree sequence

1. Introduction

Let $G = (V, E)$ be a simple connected graph with the vertex set V and the edge set E . For any $v \in V$, $N(v)$ denotes the neighbors of v , and $d_v = |N(v)|$ is the degree of v . The Randić index (or connectivity index) of G was introduced by Randić in 1975 and defined as [1]

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

Randić demonstrated that his index is well correlated with a variety of physico-chemical properties of various classes of organic compounds. Eventually, the index $R(G)$ has become one of the most popular molecular descriptors (see [2–4]).

In [5], generalized $R(G)$ by replacing the exponent $-1/2$ by an arbitrary real number α . This graph invariant is called the general Randić index and denoted by R_α , i.e., $R_\alpha(G) = \sum_{uv \in E} (d_u d_v)^\alpha$. Li and Yang [6] studied R_α for all graphs of order n and characterized the corresponding extremal graphs. Later, Hu et al. [7, 8] determined the trees with extremal R_α , and Li et al. [9] gave the

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lower and upper bounds for R_α of chemical (n, m) -graphs. Other results of the general Randić index can be found in [10].

The zeroth-order Randić index defined by Kier and Hall [11] is

$$R^0(G) = \sum_{v \in V(G)} d_v^{-1/2}.$$

Pavlović [12] determined the unique graph with maximum value of $R^0(G)$. Lang et al. [13] investigated the same problem for the topological index $M_1(G)$, also known as Zagreb index, which is defined as $M_1(G) = \sum_{v \in V(G)} d_v^2$. Eventually, Li and Zheng [14] defined the zeroth-order general Randić index of a graph G as

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

for any real number α . Li and Zhao [10] characterized trees with the first three largest and smallest zeroth-order general Randić indices and Wang and Deng [15] characterized the unicycle graphs with the maximum zeroth-order general Randić index with the exponent α being equal to $m, -m, 1/m, -1/m$, where $m \geq 2$ is an integer. Hua and Deng [16] characterized the unicycle graphs with the maximum and minimum zeroth-order general Randić index for any real number α .

In this paper, we investigate the zeroth-order general randić index $R_\alpha^0(G)$ of $(n, n + 1)$ -graphs G , i.e., connected simple graphs with n vertices and $n + 1$ edges. We characterize the $(n, n + 1)$ -graphs with extremal (maximum or minimum) zeroth-order general Randić index.

Note that if $\alpha = 0$ then $R_\alpha^0(G) = n$, and if $\alpha = 1$ then $R_\alpha^0(G) = 2m$. Therefore, in the following we always assume that $\alpha \neq 0, 1$.

First, we need to introduce some transformations.

Denote by $D(G) = [d_1, d_2, \dots, d_n]$ the degree sequence of the graph G , where d_i stands the degree of the i th vertex of G , and $d_1 \geq d_2 \geq \dots \geq d_n$.

If there is a graph G , such that $d_i \geq d_j + 2$. Let G' be the graph obtained from G by replacing the pair (d_i, d_j) by the pair $(d_i - 1, d_j + 1)$. In other words, if $D(G) = [d_1, d_2, \dots, d_{i-1}, d_i, d_{i+1}, \dots, d_{j-1}, d_j, d_{j+1}, \dots, d_n]$, then $D(G') = [d_1, d_2, \dots, d_{i-1}, d_i - 1, d_{i+1}, \dots, d_{j-1}, d_j + 1, d_{j+1}, \dots, d_n]$.

Lemma 1.1 ([17]). For the two graphs G and G' , specified above, we have

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

From lemma 1.1, we have immediately

Theorem 1.1. Let G_0 be a $(n, n+1)$ -graph with degree sequence $[d_1, d_2, \dots, d_n]$, such that $|d_i - d_j| \leq 1$ for any $i \neq j$. Then for $\alpha < 0$ or $\alpha > 1$, G_0 has the minimum zeroth-order general Randić index among all $(n, n+1)$ -graphs, whereas for $0 < \alpha < 1$, G_0 has the maximum zeroth-order general Randić index among all $(n, n+1)$ -graphs.

In fact, G_0 is one of the graphs in figure 1.

Transformation A: If there are two vertices u and v in G such that $d_u = p > 1$, $d_v = q > 1$, and $p \leq q$. u_1, u_2, \dots, u_k are adjacent to u , $G' = G - \{uu_1, uu_2, \dots, uu_k\} + \{vu_1, vu_2, \dots, vu_k\}$, $1 \leq k \leq p$, as shown in figure 2.

Lemma 1.2. For the two graphs G and G' above, we have

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

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

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

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 $0 < \alpha < 1$. So, the proof of lemma 1.2 is completed.

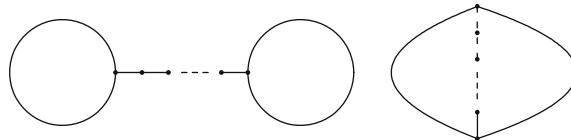


Figure 1.

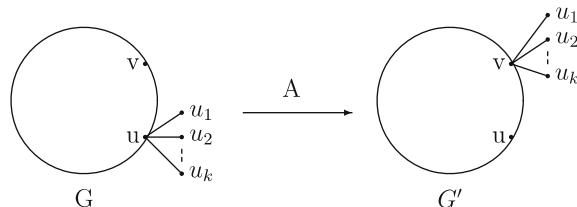


Figure 2.

Transformation B: Let uv be an edge G , the degree $d_G(u)$ of u is $p \geq 1$, $N_G(v) = \{w_1, w_2, \dots, w_l\}$ is the neighborhood of v and $N_G(v) - \{u\} = \{w_1, w_2, \dots, w_l\}$. $G' = G - \{vw_1, vw_2, \dots, vw_l\} + \{uw_1, uw_2, \dots, uw_l\}$, as shown in figure 3.

Lemma 1.3. 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. If $p \geq l + 1$, then

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

If $p \leq l + 1$, then

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

So, $\xi > \eta$ and $\Delta > 0$ when $\alpha > 1$ or $\alpha < 0$; $\Delta < 0$ when $0 < \alpha < 1$. The proof of lemma 1.3 is completed.

Note that the zeroth-order general Randić index will increase for $\alpha > 1$ or $\alpha < 0$ and decrease for $0 < \alpha < 1$ by using transformations A or B.

Now, we need to introduce some notations.

Let $\mathcal{G}(n, n+1)$ be the set of simple connected graphs with n vertices and $n+1$ edges.

For any graph $G \in \mathcal{G}(n, n+1)$, there are two cycles C_p and C_q in G .

- (1) $\mathcal{A}(p, q)$ is the set of $G \in \mathcal{G}(n, n+1)$ in which the cycles C_p and C_q have only one common vertex;
- (2) $\mathcal{B}(p, q)$ is the set of $G \in \mathcal{G}(n, n+1)$ in which the cycles C_p and C_q have no common vertex;

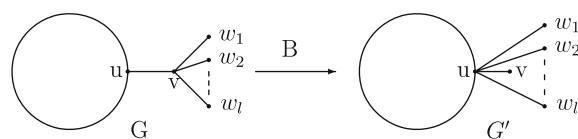


Figure 3.

- (3) $\mathcal{C}(p, q, l)$ is the set of $G \in \mathcal{G}(n, n + 1)$ in which the cycles C_p and C_q have a common path of length l .

Note that the induced subgraph of vertices on the cycles of $G \in \mathcal{A}(p, q)$ (or $\mathcal{B}(p, q)$, $\mathcal{C}(p, q, l)$) is showed in figure 4(a) (or (b),(c)) and $\mathcal{C}(p, q, l) = \mathcal{C}(p, p + q - 2l, p - l) = \mathcal{C}(p + q - 2l, q, q - l)$.

2. Extremal graphs in $\mathcal{A}(p, q)$

Let $S_n(p, q)$ be the graph in $\mathcal{A}(p, q)$ such that $n + 1 - p - q$ pendent edges attach to the common vertex of C_p and C_q .

Lemma 2.1. For any graph $G \in \mathcal{A}(p, q)$, if G is not isomorphic to $S_n(p, q)$, then

- (i) $R_\alpha^0(S_n(p, q)) > R_\alpha^0(G)$, for $\alpha > 1$ or $\alpha < 0$;
- (ii) $R_\alpha^0(S_n(p, q)) < R_\alpha^0(G)$, for $0 < \alpha < 1$.

Proof. Repeating Transformation B, any graph $G \in \mathcal{A}(p, q)$ can be changed into a graph G' in which the edges not in the cycles C_p and C_q are pendent edges, by lemma 1.3, $R_\alpha^0(G') > R_\alpha^0(G)$ (for $\alpha > 1$ or $\alpha < 0$) or $R_\alpha^0(G') < R_\alpha^0(G)$ (for $0 < \alpha < 1$). And repeating transformation A, G' can be changed into a graph G'' in which these pendent edges are attached to the same vertex u , by lemma 1.2, $R_\alpha^0(G'') > R_\alpha^0(G')$ (for $\alpha > 1$ or $\alpha < 0$) or $R_\alpha^0(G'') < R_\alpha^0(G')$ (for $0 < \alpha < 1$). If u is not the common vertex of C_p and C_q , i.e., $G'' \neq S_n(p, q)$, then $R_\alpha^0(S_n(p, q)) > R_\alpha^0(G'')$ (for $\alpha > 1$ or $\alpha < 0$) or $R_\alpha^0(S_n(p, q)) < R_\alpha^0(G'')$ (for $0 < \alpha < 1$) from

$$\begin{aligned} & R_\alpha^0(S_n(p, q)) - R_\alpha^0(G'') \\ &= [(k+4)^\alpha + 2^\alpha] - [(k+2)^\alpha + 4^\alpha] \\ &= [(k+4)^\alpha - (k+2)^\alpha] - [4^\alpha - 2^\alpha] \\ &\quad (\text{or } = [(k+4)^\alpha - 4^\alpha] - [(k+2)^\alpha - 2^\alpha]), \end{aligned}$$

where $k = n + 1 - p - q$.

Lemma 2.2 (1). If $p > 3$, then

- (i) $R_\alpha^0(S_n(p, q)) > R_\alpha^0(S_n(p - 1, q))$, for $\alpha > 1$ or $\alpha < 0$;

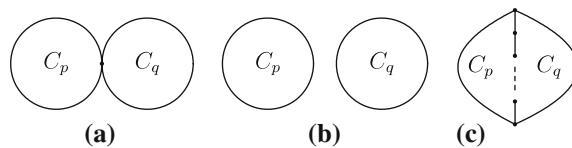


Figure 4.

- (ii) $R_\alpha^0(S_n(p, q)) < R_\alpha^0(S_n(p - 1, q))$, for $0 < \alpha < 1$;
- (2) If $q > 3$, then
- $R_\alpha^0(S_n(p, q)) > R_\alpha^0(S_n(p, q - 1))$, for $\alpha > 1$ or $\alpha < 0$;
 - $R_\alpha^0(S_n(p, q)) < R_\alpha^0(S_n(p, q - 1))$, for $0 < \alpha < 1$.

Proof. (1) By the definition of $R_\alpha^0(G)$, we have

$$\begin{aligned}\Delta &= R_\alpha^0(S_n(p - 1, q)) - R_\alpha^0(S_n(p, q)) \\ &= [(n + 6 - p - q)^\alpha + 1^\alpha] - [(n + 5 - p - q)^\alpha - 2^\alpha] \\ &= [(n + 6 - p - q)^\alpha - (n + 5 - p - q)^\alpha] - [2^\alpha - 1^\alpha] \\ &= \alpha(\xi^{\alpha-1} - \eta^{\alpha-1}) \quad (\xi \in (n + 5 - p - q, n + 6 - p - q); \eta \in (1, 2)).\end{aligned}$$

Then $\Delta > 0$ when $\alpha > 1$ or $\alpha < 0$; $\Delta < 0$ when $0 < \alpha < 1$. So, the proof of lemma 2.2 is completed.

(2) It can be proved like (1).

By lemmas 2.1 and 2.2, we have

Theorem 2.1. If $\alpha > 1$ or $\alpha < 0$, then the graph in $\mathcal{A}(p, q)$ with maximum zeroth-order general Randić index is $S_n(p, q)$, and the graph in $\mathcal{A}(p, q)$ for all $p \geq 3$ and $q \geq 3$ with maximum zeroth-order general Randić index is $S_n(3, 3)$.

If $0 < \alpha < 1$, then the graph in $\mathcal{A}(p, q)$ with minimum zeroth-order general Randić index is $S_n(p, q)$, and the graph in $\mathcal{A}(p, q)$ for all $p \geq 3$ and $q \geq 3$ with minimum zeroth-order general Randić index is $S_n(3, 3)$.

3. Extremal graphs in $\mathcal{B}(p, q)$

Lemma 3.1. For any graph $G \in \mathcal{B}(p, q)$, if the length of the shortest path connecting C_p and C_q in G is r , then

- $R_\alpha^0(T_n^r(p, q)) > R_\alpha^0(G)$, for $\alpha > 1$ or $\alpha < 0$;
- $R_\alpha^0(T_n^r(p, q)) < R_\alpha^0(G)$, for $0 < \alpha < 1$,

where $T_n^r(p, q)$ is obtained from connecting C_p and C_q by a path P of length r and the other edges are all attached to the same end-vertex of P (see figure 5 (a) or (b)).

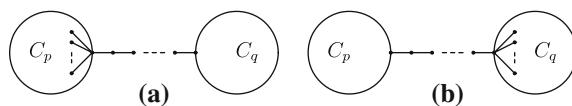


Figure 5.

Proof. Repeating transformation B, the graph $G \in \mathcal{B}(p, q)$ can be changed into a graph G' in which the edges not in the cycles C_p , C_q and P are pendent edges, by lemma 1.3, $R_\alpha^0(G') > R_\alpha^0(G)$ (for $\alpha > 1$ or $\alpha < 0$) or $R_\alpha^0(G') < R_\alpha^0(G)$ (for $0 < \alpha < 1$). And repeating transformation A, G' can be changed into a graph G'' in which these pendent edges are attached to the same vertex u , by lemma 1.2, $R_\alpha^0(G'') > R_\alpha^0(G')$ (for $\alpha > 1$ or $\alpha < 0$) or $R_\alpha^0(G'') < R_\alpha^0(G')$ (for $0 < \alpha < 1$). If u is not an end-vertex of P , then $R_\alpha^0(T_n^r(p, q)) > R_\alpha^0(G'')$ (for $\alpha > 1$ or $\alpha < 0$) or $R_\alpha^0(T_n^r(p, q)) < R_\alpha^0(G'')$ (for $0 < \alpha < 1$) from

$$\begin{aligned} & R_\alpha^0(T_n^r(p, q)) - R_\alpha^0(G'') \\ &= [(k+3)^\alpha + 2^\alpha] - [(k+2)^\alpha + 3^\alpha] \\ &= [(k+3)^\alpha - (k+2)^\alpha] - [3^\alpha - 2^\alpha], \end{aligned}$$

where $k = n + 1 - p - q - r$.

Lemma 3.2. (1) If $p > 3$, then

- (i) $R_\alpha^0(T_n^r(p-1, q)) > R_\alpha^0(T_n^r(p, q))$, for $\alpha > 1$ or $\alpha < 0$;
- (ii) $R_\alpha^0(T_n^r(p-1, q)) < R_\alpha^0(T_n^r(p, q))$, for $0 < \alpha < 1$;

(2) If $q > 3$, then

- (i) $R_\alpha^0(T_n^r(p, q-1)) > R_\alpha^0(T_n^r(p, q))$, for $\alpha > 1$ or $\alpha < 0$;
- (ii) $R_\alpha^0(T_n^r(p, q-1)) < R_\alpha^0(T_n^r(p, q))$, for $0 < \alpha < 1$;

(3) If $r > 1$, then

- (i) $R_\alpha^0(T_n^{r-1}(p, q)) > R_\alpha^0(T_n^r(p, q))$, for $\alpha > 1$ or $\alpha < 0$;
- (ii) $R_\alpha^0(T_n^{r-1}(p, q)) < R_\alpha^0(T_n^r(p, q))$, for $0 < \alpha < 1$.

Proof. (1) By the definition of $R_\alpha^0(G)$, we have

$$\begin{aligned} \Delta &= R_\alpha^0(T_n^r(p-1, q)) - R_\alpha^0(T_n^r(p, q)) \\ &= [(n+5-p-q)^\alpha + 1^\alpha] - [(n+4-p-q)^\alpha - 2^\alpha] \\ &= [(n+5-p-q)^\alpha - (n+4-p-q)^\alpha] - [2^\alpha - 1^\alpha] \\ &= \alpha(\xi^{\alpha-1} - \eta^{\alpha-1}) \quad (\xi \in (n+4-p-q, n+5-p-q); \eta \in (1, 2)). \end{aligned}$$

Then $\Delta > 0$ when $\alpha > 1$ or $\alpha < 0$; $\Delta < 0$ when $0 < \alpha < 1$. So, the proof of lemma 3.2 is completed.

(2) and (3) can be proved like (1).

By lemmas 3.1 and 3.2, we have

Theorem 3.1. If $\alpha > 1$ or $\alpha < 0$, then the graph in $\mathcal{B}(p, q)$ with maximum zeroth-order general Randić index is $T_n^1(p, q)$, and the graph in $\mathcal{B}(p, q)$ for all $p \geq 3$ and $q \geq 3$ with maximum zeroth-order general Randić index is $T_n^1(3, 3)$.

If $0 < \alpha < 1$, then the graph in $\mathcal{B}(p, q)$ with minimum zeroth-order general Randić index is $T_n^1(p, q)$, and the graph in $\mathcal{B}(p, q)$ for all $p \geq 3$ and $q \geq 3$ with minimum zeroth-order general Randić index is $T_n^1(3, 3)$.

4. Extremal graphs in $\mathcal{C}(p, q, l)$

As in sections 3, we have the following results and omit their proofs here.

Lemma 4.1. For any graph $G \in \mathcal{C}(p, q, l)$, we have

- (i) $R_\alpha^0(\theta_n^l(p, q)) > R_\alpha^0(G)$, for $\alpha > 1$ or $\alpha < 0$;
- (ii) $R_\alpha^0(\theta_n^l(p, q)) < R_\alpha^0(G)$, for $0 < \alpha < 1$

where $\theta_n^l(p, q)$ is obtaining from the graph in figure 4(c) by attaching $n+l+1-p-q$ edges to one of its vertices with degree 3.

Lemma 4.2. (1) If $p > 3$, then

- (i) $R_\alpha^0(\theta_n^l(p-1, q)) > R_\alpha^0(\theta_n^l(p, q))$, for $\alpha > 1$ or $\alpha < 0$;
- (ii) $R_\alpha^0(\theta_n^l(p-1, q)) < R_\alpha^0(\theta_n^l(p, q))$, for $0 < \alpha < 1$;

(2) If $q > 3$, then

- (i) $R_\alpha^0(\theta_n^l(p, q-1)) > R_\alpha^0(\theta_n^l(p, q))$, for $\alpha > 1$ or $\alpha < 0$;
- (ii) $R_\alpha^0(\theta_n^l(p, q-1)) < R_\alpha^0(\theta_n^l(p, q))$, for $0 < \alpha < 1$;

(3) If $l > 1$, then

- (i) $R_\alpha^0(\theta_n^{l-1}(p, q)) > R_\alpha^0(\theta_n^l(p, q))$, for $\alpha > 1$ or $\alpha < 0$;
- (ii) $R_\alpha^0(\theta_n^{l-1}(p, q)) < R_\alpha^0(\theta_n^l(p, q))$, for $0 < \alpha < 1$.

Theorem 4.2. If $\alpha > 1$ or $\alpha < 0$, then the graph in $\mathcal{C}(p, q, l)$ with maximum zeroth-order general Randić index is $\theta_n^l(p, q)$, and the graph in $\mathcal{C}(p, q, l)$ for all $p \geq 3$, $q \geq 3$ and $l > 1$ with maximum zeroth-order general Randić index is $\theta_n^1(3, 3)$.

If $0 < \alpha < 1$, then the graph in $\mathcal{C}(p, q, l)$ with minimum zeroth-order general Randić index is $\theta_n^l(p, q)$, and the graph in $\mathcal{C}(p, q, l)$ for all $p \geq 3$, $q \geq 3$ and $l > 1$ with minimum zeroth-order general Randić index is $\theta_n^1(3, 3)$.

5. Extremal graphs in $\mathcal{G}(n, n+1)$

Theorem 5.1. (1). $\theta_n^1(3, 3)$ is the graph with maximum zeroth-order general Randić index in $\mathcal{G}(n, n+1)$ for $\alpha > 1$ or $\alpha < 0$;

(2) $\theta_n^1(3, 3)$ is also the graph with minimum zeroth-order general Randić index in $\mathcal{G}(n, n+1)$ for $0 < \alpha < 1$.

Proof. By theorems in sections 2–4, we only need compare the zeroth-order general Randić indices of $S_n(3, 3)$, $T_n^1(3, 3)$, and $\theta_n(3, 3)$.

$$\begin{aligned}\Delta_1 &= R_\alpha^0(\theta_n^1(3, 3)) - R_\alpha^0(S_n(3, 3)) \\ &= [(n-1)^\alpha + 3^\alpha + 2 \times 2^\alpha + (n-4)] - [(n-l)^\alpha + 4 \times 2^\alpha + (n-5)] \\ &= [3^\alpha - 2^\alpha] - [2^\alpha - 1^\alpha] \\ &= \alpha(\xi^{\alpha-1} - \eta^{\alpha-1}) \quad (\xi \in (2, 3), \eta \in (1, 2)),\end{aligned}$$

$$\begin{aligned}\Delta_2 &= R_\alpha^0(\theta_n^1(3, 3)) - R_\alpha^0(T_n^1(3, 3)) \\ &= [(n-1)^\alpha + 3^\alpha + 2 \times 2^\alpha + (n-4)] - [(n-3)^\alpha + 4 \times 2^\alpha + 3^\alpha + (n-6)] \\ &= [(n-1)^\alpha - (n-3)^\alpha] - 2[2^\alpha - 1^\alpha] \\ &= 2\alpha(\xi^{\alpha-1} - \eta^{\alpha-1}) \quad (\xi \in (n-3, n-1), \eta \in (1, 2)),\end{aligned}$$

$$\begin{aligned}\Delta_3 &= R_\alpha^0(S_n(3, 3)) - R_\alpha^0(T_n^1(3, 3)) \\ &= [(n-1)^\alpha + 4 \times 2^\alpha + (n-5)] - [(n-3)^\alpha + 4 \times 2^\alpha + 3^\alpha + (n-6)] \\ &= [(n-1)^\alpha - (n-3)^\alpha] - [3^\alpha - 1^\alpha] \\ &= 2\alpha(\xi^{\alpha-1} - \eta^{\alpha-1}) \quad (\xi \in (n-3, n-1), \eta \in (1, 3)).\end{aligned}$$

Then $\Delta_i > 0$ when $\alpha > 1$ or $\alpha < 0$; $\Delta_i < 0$ when $0 < \alpha < 1$ ($i = 1, 2, 3$). So, the proof of theorem 5.1 is completed.

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References

- [1] M. Randić, On the characterization of molecular branching, *J. Am. Chem. Soc.* 97 (1975) 6609–6615.
- [2] L.B. Kier, L.H. Hall, *Molecular Connectivity in Chemistry and Drug Research* (Academic Press, New York, 1976).
- [3] L.B. Kier, L.H. Hall, *Molecular Connectivity in Structure-analysis* (Research Studies Press, Wiley, Chichester, UK, 1986).
- [4] M. Randić, The connectivity index 25 years after, *J. Mol. Graphics Modell.* 20 (2001) 19–35.
- [5] B. Bollobás and P. Erdős, Graphs of extremal weights, *Ars Combin.* 50 (1998) 225–233.
- [6] X. Li and Y. Yang, Sharp bounds for the general Randić indices, *MATCH Commun. Math. Comput. Chem.* 51 (2004) 155–166.
- [7] Y. Hu, X. Li and Y. Yuan, Trees with minimum general Randić indices, *MATCH Commun. Math. Comput. Chem.* 52 (2004) 119–128.

- [8] Y. Hu, X. Li and Y. Yuan, Trees with maximum general Randić indices, *MATCH Commun. Math. Comput. Chem.* 52 (2004) 129–146.
- [9] X. Li, X.Q. Wang and B. Wei, On the lower and upper bounds for general Randić indices of chemical(n,m)-graphs, *MATCH Commun. Math. Comput. Chem.* 52 (2004) 157–166.
- [10] X. Li and H. Zhao, Trees with the first three smallest and largest generalized topological indices, *MATCH Commun. Math. Comput. Chem.* 51 (2004) 205–210.
- [11] L.B. Kier, L.H. Hall, The nature of structure-activity relationships and their relation to molecular connectivity, *Eur. J. Med. Chem.* 12 (1977) 307–312.
- [12] L. Pavlović, Maximal value of the zeroth-order Randić index, *Discrete Appl. Math.* 127 (2003) 615–626.
- [13] R. Lang, X. Li and S. Zhang, Inverse problem for Zagreb index of molecular graphs, *Appl. Math. J. Chinese Univ.* 18 (A) (2003) 487–493 (in Chinese).
- [14] X. Li and J. Zheng, A unified approach to the extremal trees for different indices, *MATCH Commun. Math. Comput. Chem.* 54 (2005) 195–208.
- [15] H. Wang and H. Deng, Unicycle graphs with maximum generalized topological indices, Accepted by *J. Math. Chem.*
- [16] H. Hua and H. Deng, Unicycle graphs with maximum and minimum zeroth-order general Randić indices, Accepted by *J. Math. Chem.*
- [17] Y. Hu, X. Li, Y. Shi, T. Xu and I. Gutman, on molecular graphs with smallest and greatest zeroth-order general Randić index, *MATCH Commun. Math. Comput. Chem.* 54 (2005) 425–434.