# Extremal Zeroth-Order Randić Index in Some Classes of Graphs *

Xueliang Li, Jianbin Zhang
Center for Combinatorics and LPMC-TJKLC
Nankai University, Tianjin 300071, P.R. China

(Received December 31, 2006)

**Abstract**

Let $G$ be a graph and $d(u)$ denote the degree of a vertex $u$ in $G$. The zeroth-order Randić index of $G$ is defined as ${}^0R(G) = \sum_{u \in V(G)} (d(u))^{-\frac{1}{2}}$. Let $\mathcal{W}_{n,m}$ denote the set of connected graphs of order $n$ with a maximum matching of size $m$, and $\mathcal{P}_{n,k}$ the set of connected graphs of order $n$ with exactly $k$ pendant vertices. In this paper, we first determine the graphs with minimum and maximum zeroth-order Randić index in $\mathcal{W}_{n,m}$. Then, we determine the extremal graphs in $\mathcal{P}_{n,k}$. Finally, we determine the extremal graphs for $k$-colorable graphs and hamiltonian graphs, respectively.

**Keywords:** zeroth-order Randić index, maximum matching, $k$-colorable graph, Hamiltonian graph.

## 1 Introduction

All graphs $G = (V, E)$ considered here will be finite, undirected, simple and connected. The degree of a vertex $u \in V(G)$ will be denoted by $d(u)$. The graph that arises from $G$ by deleting an edge $uv \in E(G)$ or adding an edge $xy \notin E(G)$ will be denoted by $G - uv$ and $G + xy$, respectively. The join $G_1 + G_2$ of two disjoint graphs $G_1$ and $G_2$ is obtained from

*Supported by PCSIRT, NSFC and the "973" program.

$G_1 \cup G_2$ by joining each vertex of $G_1$ to each vertex of $G_2$. The path of order $n$ is denoted by $P_n$, and the star of order $n$ is denoted by $S_n$. The complement of a graph $G$ will be denoted by $\overline{G}$.

In [10] Randić proposed a topological index, suitable for measuring the extent of branching of the carbon-atom skeleton of saturated hydrocarbons. The Randić index is defined in [10] as follows:

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d(u)d(v)}},$$

which is well correlated with a variety of physico-chemical properties of alcanes. The Randić index thus becomes one of the most popular molecular descriptors and has been widely studied (see [1, 2, 4, 5, 9]). The zeroth-order Randić index ${}^0R(G)$ is defined by Kier and Hall [6, 7] as follows:

$${}^0R(G) = \sum_{u \in V(G)} (d(u))^{-\frac{1}{2}}.$$

It is the purpose of this paper to find extremal graphs on the zeroth-order Randić index for some classes of graphs.

Let $\mathcal{W}_{n,m}$ denote the set of connected graphs of order $n$ with a maximum matching of cardinality $m$. Define a tree $A(n, m)$ of order $n$ as follows: $A(n, m)$ is obtained from the star graph $S_{n-m+1}$ with $n - m + 1$ vertices by attaching a pendant edge to each of certain $m - 1$ non-central vertices of $S_{n-m+1}$. We call $A(n, m)$ a spur and note that it has a matching of size $m$.

For $n \leq 4m$, we set

$$\mathcal{M} = \left\{ s : h(s) = \min_{1 \leq x \leq m} \left( \frac{x}{\sqrt{n-1}} + \frac{n-2m+x-1}{\sqrt{x}} + \frac{2m-2x+1}{\sqrt{2m-x}} \right) \right\}$$

In Section 2, we prove that

if $n \geq 4m + 1$, then $K_m + \overline{K_{n-m}}$ is the unique graph with minimum zeroth-order Randić index in $\mathcal{W}_{n,m}$;

if $s \in \mathcal{M}$ and $2m \leq n \leq 4m$, then $K_s + (K_{2m-2s+1} \cup \overline{K_{n-2m+s-1}})$ is the graph with minimum zeroth-order Randić index in $\mathcal{W}_{n,m}$; and

$A(n, m)$ is the unique graph with maximum zeroth-order Randić index in $\mathcal{W}_{n,m}$.

Let $P_{n,k}$ be the graph obtained from $K_{n-k}$ by adding $k$ pendant vertices to it such that the vertices of $K_{n-k}$ have almost equal number pendant vertices, i.e., the difference of the numbers of pendant vertices at any two vertices is at most 1.

In Section 3, we prove that $P_{n,k}$ is the graph with minimum zeroth-order Randić index among all graphs which contains exactly $k$ pendant vertices, whereas the starlike tree with $k$ pendant vertices is the graph with maximum zeroth-order Randić index among all these kind of graphs.

In Section 4, we prove that the complete $k$-partite graph with almost equal parts and the star $S_n$ are the $k$-colorable graphs with minimum and maximum zeroth-order Randić index, respectively, and $K_n$ and $C_n$ are the Hamiltonian graphs with minimum and maximum zeroth-order Randić index, respectively.

## 2 Extremal graphs in $\mathcal{W}_{n,m}$

A component of a graph is odd or even according as it has an odd or even number of vertices. For a subset $S$ of $V(G)$, we denote by $c_0(G-S)$ the number of odd components of $G-S$. Let $M$ be a maximum matching of $G$ with order $n$ and $|M|=m$. We define the deficiency of $G$, def$(G)$, by the equation def$(G)=n-2m$. Hence def(G) is the number of vertices left unsaturated by any maximum matching. Let $S$ be a subset of $V(G)$ and $|S|=s$. Then, we have

**Lemma 1** *[8] Let $def(G)$ denote the deficiency of a graph $G$. Then, def$(G)=\max\{c_0(G-S)-s|S\subseteq V(G)\}$.*

**Lemma 2** *Let $uv\in E(G)$. Then ${}^0R(G-uv)>{}^0R(G)$.*

*Proof.* By definition, we have

$$ {}^0R(G-uv)-{}^0R(G)=\frac{1}{\sqrt{d(u)-1}}+\frac{1}{\sqrt{d(v)-1}}-\frac{1}{\sqrt{d(u)}}-\frac{1}{\sqrt{d(v)}}>0. $$

This completes the proof of the lemma. □

Apply Lemma 2, we have

**Lemma 3** *Let $T$ be a spanning tree of a graph $G$. Then ${}^0R(T)\geq{}^0R(G)$ with equality if and only if $G$ is a tree.*

**Lemma 4** *Let $s,\ x,\ y$ be positive integers and $f(x,y)=\frac{x}{\sqrt{x-1+s}}+\frac{y}{\sqrt{y-1+s}}-\frac{x-2}{\sqrt{x-3+s}}-\frac{y+2}{\sqrt{y+1+s}}$. Then $f(x,y)>0$ for $y\geq x\geq 3$.*

*Proof.* Set $t = s - 1, \sqrt{x+t} = a, \sqrt{y+t} = b$. Then $b \geq a \geq \sqrt{3}$ and

$$f(t) = \left(\frac{a^2 - t}{a} + \frac{b^2 - t}{b}\right) - \left(\frac{a^2 - t - 2}{\sqrt{a^2 - 2}} + \frac{b^2 + 2 - t}{\sqrt{b^2 + 2}}\right).$$

Let $g(b) = \frac{b^2-t}{b} - \frac{b^2+2-t}{\sqrt{b^2+2}}$. Then $g'(b) = 1 + \frac{t}{b^2} - \frac{b^3+2b+tb}{(b^2+2)^{\frac{3}{2}}}$. From this we know that $g'(b) > 0$ if and only if $(b^2+2)^3(b^2+t)^2 - (b^3+2b+bt)^2b^4 > 0$. Since

$$\begin{aligned} & (b^2+2)^3(b^2+t)^2 - (b^3+2b+bt)^2b^4 \\ = \quad & 2b^8 + 8b^6t + 6b^4t^2 + 8b^6 + 24b^4t + 12b^2t^2 + 8b^4 + 16b^2t + 8t^2 > 0, \end{aligned}$$

we have

$$f(t) \geq \left(\frac{a^2 - t}{a} - \frac{a^2 - 2 - t}{\sqrt{a^2 - 2}}\right) - \left(\frac{a^2 - t + 2}{\sqrt{a^2 + 2}} + \frac{a^2 - t}{a}\right).$$

Let $\Theta(u) = \frac{u^2+2-t}{\sqrt{u^2+2}} - \frac{u^2-t}{u}$. Then $f(t) \geq \Theta(\sqrt{a^2-2}) - \Theta(a)$. Since $\Theta'(u) = -g'(u) < 0$, we have $f(t) > 0$. □

**Lemma 5** *Let $s$, $n$, $m$ be positive integers satisfying $1 \leq s \leq m, 2m \leq n$ and $h(s) = \frac{s}{\sqrt{n-1}} + \frac{n-2m+s-1}{\sqrt{s}} + \frac{2m-2s+1}{\sqrt{2m-s}}$. Then $h(s) \leq h(m)$ when $n \geq 4m+1$, with equality if and only if $s = m$.*

*Proof.* It suffices to prove that $h'(s) < 0$ for $1 \leq s \leq m, 4m+1 \leq n$.

$$\begin{aligned} h'(s) &= \frac{1}{\sqrt{n-1}} + \frac{1}{\sqrt{s}} - \frac{n-2m+s-1}{2s\sqrt{s}} - \frac{2}{\sqrt{2m-s}} + \frac{2m-2s+1}{2(2m-s)\sqrt{2m-s}} \\ &\leq \frac{1}{\sqrt{n-1}} + \frac{1}{\sqrt{s}} - \frac{n-2m+s-1}{2s\sqrt{s}} - \frac{2}{\sqrt{2m-s}} + \frac{2m-2s+1}{2s\sqrt{s}} \\ &= \frac{1}{\sqrt{n-1}} - \frac{n-4m+s-2}{2s\sqrt{s}} - \frac{2}{\sqrt{2m-s}} \\ &< 0. \end{aligned}$$

We thus obtain the result. □

Let $\mathcal{M}$ be defined the same as in Section 1.

**Theorem 1** *Let $G$ be a connected graph of order $n$ with a maximum matching of size $m$.*

*(i) Let $n \geq 4m+1$. Then ${}^0R(G) \geq {}^0R(K_m + \overline{K_{n-m}})$ with equality if and only if $G \cong K_m + \overline{K_{n-m}}$;*

*(ii) Let $s \in \mathcal{M}$ and $2m \leq n \leq 4m$. Then*

$${}^0R(G) \geq {}^0R(K_s + (K_{2m-2s+1} \cup \overline{K_{n-2m+s-1}})),$$

*with equality if and only if there exists a $k$ in $\mathcal{M}$ such that $G \cong K_k + (K_{2m-2k+1} \cup \overline{K_{n-2m+k-1}})$.*

*Proof.* Let $G$ be a graph with minimum zeroth-order Randić index in $\mathcal{W}_{n,m}$. By Lemma 1, there exists a subset $S$ of $V(G)$ such that $G-S$ has $n-2m+s$ odd components. Let $G_1, G_2, \ldots, G_{n-2m+s}$ be its all odd components and $n_i = |G_i|$ for $i = 1, 2, \ldots, n-2m+s$. Without loss of generality, set $n_1 \le n_2 \le \ldots \le n_{n-2m+s}$.

**Claim 1**: $G-S$ contains no even component.

*Proof.* Suppose that there are some even components in $G-S$ and $H$ is their union. Let $G'$ be the graph obtained from $G$ by adding some edges such that $G'[V(G_1) \cup V(H)]$ is a complete graph. By Lemma 2, we have ${}^0R(G) > {}^0R(G')$, a contradiction. □

Similarly, we have

**Claim 2**: All $G[V(G_1)], G[V(G_2)], \ldots, G[V(G_{n-2m+s})]$ and $G[S]$ are complete.

By Claims 1, 2 and Lemma 2, we know that $G = K_s + (K_{n_1} \cup K_{n_2} \cup \cdots \cup K_{n_{n-2m+s}})$.

**Claim 3**: $n_1 = n_2 = \ldots = n_{n-2m+s-1} = 1$.

*Proof.* Suppose that there are two odd components $G_i$, $G_j$ such that $3 \le n_i \le n_j$. Let $G''$ be the graph obtained from $G$ by moving two vertices from $G_i$ to $G_j$, that is, $G'' = K_s + (K_{n_1} \cup \cdots \cup K_{n_i-2} \cup \cdots \cup K_{n_j+2} \cup \cdots \cup K_{n_{n-2m+s}})$. For simplicity, we set $n_i = x, n_j = y$. Then

$${}^0R(G) - {}^0R(G'') = \frac{x}{\sqrt{x-1+s}} + \frac{y}{\sqrt{y-1+s}} - \frac{x-2}{\sqrt{x-3+s}} - \frac{y+2}{\sqrt{y+1+s}}.$$

By Lemma 4, we have ${}^0R(G) > {}^0R(G'')$, again a contradiction. □

By Claims 1,2 and 3, $G \cong K_s + (K_{2m-2s+1} \cup \overline{K_{n-2m+s-1}})$ and ${}^0R(G) = \frac{s}{\sqrt{n-1}} + \frac{n-2m+s-1}{\sqrt{s}} + \frac{2m-2s+1}{\sqrt{2m-s}}$, where $1 \le s \le m$.

If $n \ge 4m+1$, by Lemma 5 we obtain the result.

If $2m \le n \le 4m$, by choosing $s \in \mathcal{M}$, we also obtain the result.

This completes the proof of the theorem. □

**Corollary 1** *Let $G \in \mathcal{W}_{n,m}$.*

*If $n \ge 4m+1$, then ${}^0R(G) \ge \frac{m}{\sqrt{n-1}} + \frac{n-m}{\sqrt{m}}$ with equality if and only if $G \cong K_m + (\overline{K_{n-m}})$;*

*If $s \in \mathcal{M}$ and $2m \le n \le 4m$, then*

$${}^0R(G) \ge \frac{s}{\sqrt{n-1}} + \frac{n-2m+s-1}{\sqrt{s}} + \frac{2m-2s+1}{\sqrt{2m-s}}$$

*with equality if and only if there exists a $k$ in $\mathcal{M}$ such that* $G \cong K_k + (K_{2m-2k+1} \cup \overline{K_{n-2m+k-1}})$

Let $M$ be a maximum matching of $G$. A vertex $v$ of $G$ is said to be $M$-saturated if $v$ is incident with an edge in $M$; otherwise, $v$ is $M$-unsaturated. An $M$-alternating path in $G$ is a path whose edges are alternately in $E \setminus M$ and $M$. An $M$-augmenting path is an $M$-alternating path whose origin and terminus are $M$-unsaturated.

**Lemma 6** *[3] A matching $M$ in $G$ is maximum if and only if $G$ contains no $M$-augmenting path.*

**Lemma 7** $f(d_1, d_2) = \frac{1}{\sqrt{d_1+d_2-2}} + \frac{1}{\sqrt{2}} - \frac{1}{\sqrt{d_1}} - \frac{1}{\sqrt{d_2}} > 0 \, (d_2 \geq d_1 \geq 3)$.

*Proof.* Since $\frac{\partial f(d_1,d_2)}{\partial d_1} = -\frac{1}{2(d_1+d_2-2)\sqrt{d_1+d_2-2}} + \frac{1}{2d_1\sqrt{d_1}} > 0$, we have $f(d_1, d_2) \geq f(3, 3) > 0$. □

A tree is said to be starlike if it possesses exactly one vertex of degree greater than two, which can also be obtained from some paths by identifying its one pendant vertices. These paths is said to pendant paths of it.

**Theorem 2** *Let $G$ be a graph of order $n \, (n \geq 6)$ with a maximum matching of size $m$. Then ${}^0R(G) \leq {}^0R(A(n, m))$, with equality if and only if $G$ is isomorphic to $A(n, m)$.*

*Proof.* Let $M$ be a maximum matching of $G$. Then $G$ must contain a spanning tree that contains all edges of $M$. By Lemma 3, we have ${}^0R(T) \geq {}^0R(G)$. It suffices to find the tree with maximum zeroth-order Randić index in $\mathcal{W}_{n,m}$.

Let $T$ be a tree of order $n$ with a maximum matching $M$ of size $m$, $V^*(T) = \{v \in V(T) : d(v) \geq 3\}$. If $V^* = \phi$, $T$ is a path on $n$ vertices. Assume that $V^* \neq \phi$. If there are two vertices that belong to it, say $u, v$, and $d(u) \geq d(v) \geq 3$. Suppose there exists no vertex that belongs to $V^*(T)$ in the unique path connecting $u, v$. We obtain a new tree $T_1$ by moving $d(v) - 2$ edges from $v$ to $u$ and leaving the edge of $M$ that incident to $v$ if it has. Clearly, $T_1$ has a $M$-augmenting path if and only if $T$ has, too. By Lemma 6, we have $T_1 \in \mathcal{W}_{n,m}$; and

$${}^0R(T_1) - {}^0R(T) = \frac{1}{\sqrt{d(u) + d(v) - 2}} + \frac{1}{\sqrt{2}} - \frac{1}{\sqrt{d(u)}} - \frac{1}{\sqrt{d(v)}},$$

by Lemma 7, we have ${}^0R(T_1) \geq {}^0R(T)$. Beside it we have $V^*(T_1) = V^*(T) - 1$. Repeating this process, we finally obtain a tree $T_2$ such that ${}^0R(T_2) \geq {}^0R(T)$ and $V^*(T_2) = 1$, that is, $T_2$ is a starlike tree that has larger zeroth-order Randić index than $T$. Moreover, $M$ is still a maximum matching of it. Assume that $u$ is the center vertex and $d(u) = k \geq 3$. If there is a pendant path $P = uv_1v_2v_3 \cdots v_l$ $(l \geq 3)$, letting $T_3 = T - v_2v_3 + uv_3$, then $T_3 \in \mathcal{W}_{n,m}$ and

$$^0R(T_3) - {}^0R(T_2) = \frac{1}{\sqrt{k+1}} + 1 - \frac{1}{\sqrt{2}} - \frac{1}{\sqrt{k}} \geq \frac{1}{2} + 1 - \frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}} > 0.$$

Repeating this process, we finally obtain the tree $A(n, m)$. In the following, we will compare the zeroth-order Randić indices of $A(n, m)$ and $P_n$ when $n = 2m$ and $n = 2m + 1$. By simple computation, we obtain

$$\begin{aligned} ^0R(P_n) &= 2 + \tfrac{n-2}{\sqrt{2}} \\ ^0R(A(n, m)) &= \tfrac{1}{\sqrt{n-m}} + \tfrac{m-1}{\sqrt{2}} + n - m \end{aligned}$$

When $n = 2m$,

$$^0R(A(2m, m)) - {}^0R(P_{2m}) = \frac{1}{\sqrt{m}} + \frac{m-1}{\sqrt{2}} + m - 2 - \frac{2m-2}{\sqrt{2}} = \begin{cases} a = 0 & m = 1, 2, \\ a > 0 & m \geq 3. \end{cases}$$

When $n = 2m + 1$,

$$^0R(A(2m + 1, m)) - {}^0R(P_{2m+1}) = \tfrac{1}{\sqrt{m+1}} + \tfrac{m}{\sqrt{2}} + m + 1 - 2 - \tfrac{2m-1}{\sqrt{2}} > 0.$$

This completes this proof of the theorem. $\square$

By Theorem 2 we thus have

**Corollary 2** *Let $G \in \mathcal{W}_{n,m} (n \geq 6)$. Then $^0R(G) \leq \frac{1}{\sqrt{n-m}} + \frac{m-1}{\sqrt{2}} + n - m$, with equality if and only if $G \cong A(n, m)$.*

## 3 Extremal graphs in $\mathcal{P}_{n,k}$

Let $\mathcal{P}_{n,k}$ be the set of connected graphs of order $n$ with exactly $k$ pendant vertices.

**Lemma 8** *Let $x$, $k$, $d$ be nonnegative integers and $0 \leq x \leq \frac{k}{2}$. Then*

$$\frac{1}{\sqrt{d+x}} + \frac{1}{\sqrt{d+k-x}} \geq \frac{1}{\sqrt{d + \lfloor \frac{k}{2} \rfloor}} + \frac{1}{\sqrt{d + \lceil \frac{k}{2} \rceil}}.$$

*Proof.* Let $f(x) = \frac{1}{\sqrt{d+x}} + \frac{1}{\sqrt{d+k-x}}$. $f'(x) = -\frac{1}{2(d+x)\sqrt{d+x}} + \frac{1}{2(d+k-x)\sqrt{d+k-x}}$. When $x \leq \frac{k}{2}$, $f'(x) \leq 0$, which completes the proof of the lemma. $\square$

Let $P_{n,k}$ be the graph obtained from $K_{n-k}$ by adding $k$ pendant vertices to it such that the vertices of $K_{n-k}$ have almost equal number pendant vertices.

**Theorem 3** *Let $G$ be a graph with exactly $k$ pendant vertices. Then ${}^0R(G) \geq {}^0R(P_{n,k})$, with equality if and only if $G \cong P_{n,k}$.*

*Proof.* Let $G$ be a graph with minimum zeroth-order Randić index in $\mathcal{P}_{n,k}$. Let $V_0(G) = \{v \in V(G) : d(v) = 1\}$ and $V'(G) = V(G) \setminus V_0(G)$. Then $G[V'(G)]$ must be isomorphic to $K_{n-k}$. Otherwise, adding some edges will decrease the value of the zeroth-order Randić index of $G$ by Lemma 2. Since there are $k$ pendant vertices in $G$, $G$ is also viewed as planting $k$ pendant edges at $K_{n-k}$. Let $u, v \in V'(G)$, planted $x, y$ pendant edges, respectively. Without loss of generality, let $x + y = k$ and $y = k - x \geq x \geq 0$. Then

$$ {}^0R(G) = \sum_{w \in (V(G) - \{u,v\})} \frac{1}{\sqrt{d(w)}} + \frac{1}{\sqrt{n-k-1+x}} + \frac{1}{\sqrt{n-k-1+k-x}}. $$

By Lemma 8, we know that $x, y$ must be almost equal. This completes the proof of the theorem. □

Let $k = \lfloor \frac{k}{n-k} \rfloor (n-k) + r$. By simple computation, we have

**Corollary 3** *Let $G \in \mathcal{P}_{n,k}$. Then ${}^0R(G) \geq k + \frac{n-k-r}{\sqrt{n-k-1+\lfloor \frac{k}{n-k} \rfloor}} + \frac{r}{\sqrt{n-k+\lfloor \frac{k}{n-k} \rfloor}}$, with equality if and only if $G \cong P_{n,k}$.*

Let $S(n,k) = \{G \in \mathcal{P}_{n,k} : G$ is a starlike tree and the degree of its center is exactly $k\}$. Then we have

**Theorem 4** *Let $G$ be a graph of order $n$ with exactly $k$ pendant vertices. Then ${}^0R(G) \leq k + \frac{n-k-1}{\sqrt{2}} + \frac{1}{\sqrt{k}}$, with equality if and only if $G \in S(n,k)$.*

*Proof.* In the proof of Theorem 2, the first transform does not change the number of pendant vertices. Applying it to graph $G$ repeatedly, we thus obtain the result. □

## 4 Extremal graphs in other classes of graphs

A $k$-vertex coloring of $G$ is an assignment of $k$ colors $1, 2, \ldots, k$ to the vertices of $G$. The coloring is proper if no two distinct adjacent vertices have the same color. We call a graph $k$-colorable if $G$ has a proper $k$-vertex coloring. Let $K(n_1, n_2, \ldots, n_k)$ be a complete $k$-partite graph and the number of vertices in each part are $n_1, n_2, \ldots, n_k$, respectively. If the numbers of vertices in any two parts are almost equal, we denote it by $K_n^k$. Let $\mathcal{C}_{n,k}$ denote the set of all $k$-colorable graphs.

**Lemma 9** *Let $n \geq x \geq y \geq 1$ be three positive integers and $x \geq y+2$. Then*

$$\frac{x}{\sqrt{n-x}} + \frac{y}{\sqrt{n-y}} \geq \frac{x-1}{\sqrt{n-x+1}} + \frac{y+1}{\sqrt{n-y-1}}.$$

*Proof.* Let $x+y=k, 1 \leq y = k-x \leq x-2$ and $\omega(x) = \frac{x}{\sqrt{n-x}} + \frac{k-x}{\sqrt{n-k+x}}$. Then

$$\omega'(x) = \frac{1}{\sqrt{n-x}} + \frac{x}{2(n-x)\sqrt{n-x}} - \frac{1}{\sqrt{n-k+x}} - \frac{k-x}{2(n-k+x)\sqrt{n-k+x}}.$$

Since $x > k-x$, we have $n-x < n-k+x$. Thus $\omega'(x) > 0$. This completes the proof. □

**Theorem 5** *Let $G$ be a proper $k$-colorable graph. Then ${}^0R(K_n^k) \leq {}^0R(G) \leq {}^0R(S_n)$, and $K_n^k$, $S_n$ are the unique graphs obtaining the low and upper bounds, respectively.*

*Proof.* Similar to the proof of Theorem 2, we easily obtain the upper bound.

Let $G$ be a graph with minimum zeroth-order Randić index in $\mathcal{C}_{n,k}$. Then $G$ has a partition $(V_1, V_2, \ldots, V_k)$ of $V(G)$ into $k$ independent sets. Let $n_i = |V_i|$ $(i = 1, 2, \ldots, k)$. By Lemma 2 $G$ must be a complete $k$ partite graph. Moreover, the numbers of vertices in any two parts are almost equal. Otherwise, assume $n_i \geq n_j + 2$. Let $G'$ be the graph obtained from $G$ by moving 2 vertices from $V_i$ to $V_j$. Then

$${}^0R(G) - {}^0R(G') = \frac{n_i}{\sqrt{n-n_i}} + \frac{n_j}{\sqrt{n-n_j}} - \frac{n_i-1}{\sqrt{n-n_i+1}} - \frac{n_j+1}{\sqrt{n-n_j-1}}.$$

By Lemma 9, ${}^0R(G) > {}^0R(G')$, a contradiction.

This completes the proof of the theorem. □

Let $n = \lfloor \frac{n}{k} \rfloor k + r$. Then we have

**Corollary 4** *Let $G \in \mathcal{C}_{n,k}$. Then*

$$\frac{(k-r)\lfloor \frac{n}{k} \rfloor}{\sqrt{n - \lfloor \frac{n}{k} \rfloor}} + \frac{r\lceil \frac{n}{k} \rceil}{\sqrt{n - \lceil \frac{n}{k} \rceil}} \leq {}^0R(G) \leq n-1+\frac{1}{\sqrt{n-1}},$$

*and $K_n^k$, $S_n$ are the unique graphs obtaining the low and upper bounds, respectively.*

A Hamiltonian cycle of $G$ is a cycle that contains every vertex of $G$. A graph is Hamiltonian if it contains a Hamiltonian cycle. By Lemma 2, we easily obtain

**Theorem 6** *Let $G$ be a Hamiltonian graph. Then*

$$\frac{n}{\sqrt{n-1}} \leq {}^0R(G) \leq \frac{n}{\sqrt{2}},$$

*and $K_n$, $C_n$ are the unique graphs obtaining the low and upper bounds, respectively.*

## References


[1] B. Bollob$\acute{a}$s and P. Erd$\ddot{o}$s, Graphs of extremal weights, Ars Combin. 50(1998), 225-33.

[2] B. Bollob$\acute{a}$s, P. Erd$\ddot{o}$s and A. Sarkar, Extremal graphs for weights, Discrete Math. 200(1999), 5-19.

[3] J.A. Bondy and U.S.R. Murty, Graph Theory with Applications, Macmillan Press Ltd., London, 1976.

[4] G. Caporossi, I. Gutman and P. Hansen, Variable neighborhood search for extremal graphs 4: Chemical trees with extremal connectivity index, Comput. Chem. 23(1999), 469-477.

[5] Y. Hu, X. Li, Y. Shi and T. Xu, Connected $(n, m)$-graphs with minimum and maximum zeroth-order general Randić index, Discrete Appl. Math. 8(155)(2007), 1044-1054.

[6] L.N. Kier and L.H. Hall, The nature of structure-activety relationships and their relation to molecular connectivity, J. Med. Chem. 12(1977b), 307-312.

[7] L.N. Kier and L.H. Hall, Moleclar Connectivity in Structure-Activity Analysis, Research Studies Press, Wiley, Chichester, UK, 1986.

[8] L. Lov́sz and M.D. Plummer, Matching Theory, Ann. Discrete Math. (29)(1986).

[9] L. Pavlović, Maximal value of the zeroth-order Randić index, Discrete Appl. Math. 127(2003), 615-626.

[10] M. Randić, On characterization of molecular branching, J. Amer. Chem. Soc. 97(1975), 6609-6615.