Some results about a conjecture on the Randić index *

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Abstract

The Randić index $R(G)$ of a graph G is defined as the sum of the weights $(d(u)d(v))^{-\frac{1}{2}}$ of all edges uv of G, where $d(u)$ denotes the degree of a vertex u in G. Bollobás and Erdös proved that the Randić index of a graph of order n without isolated vertices is at least $\sqrt{n-1}$. They asked for the minimum value of $R(G)$ for graphs G with given minimum degree $\delta(G)$. Delorme et al answered their question for $\delta(G) = 2$ and proposed a conjecture. In this paper, we verify this conjecture for $\delta(G) = 3$, which can easily lead to the conclusion that the inequality of the conjecture holds for all chemical graphs, i.e., graphs with maximum degree at most 4. Furthermore, we prove that the conjecture is true for any graph G of order $n \geq \frac{3}{2}k^3$ (or $k \leq \sqrt[3]{\frac{2n}{3}}$) with minimum degree $\delta(G) \geq k \geq 4$.

Keywords: Randić index; minimum degree; complete bipartite graph; linear programming

AMS subject classification (2000): 05C35, 05C90, 05C07, 92E10, 90C05.

1 Introduction

The *Randić index* $R(G)$ of a graph G was introduced by the chemist Milan Randić under the name "*branching index*" in 1975 [18] as the sum of $1/\sqrt{d(u)d(v)}$ over all edges uv of G, where $d(u)$ denotes the degree of a vertex u in G, i.e.,

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

It is well known that $R(G)$ was introduced as one of the many graph-theoretical parameters derived from the graph underlying some molecule. Later, in 1998 Bollobás and Erdös [2] generalized this index by

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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 [2], [3], [18]). Recently, finding bounds for the general Randić index of a given class 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 [2], [3], [5]-[18]). For a comprehensive survey of its mathematical properties see the recent book of Li and Gutman on *Mathematical Aspects of Randić-Type Molecular Structure Descriptors* [9].

In 1998, Bollobás and Erdös [2] proved that the Randić index of a graph G of order n without isolated vertices is at least $\sqrt{n-1}$, with equality if and only if G is a star. In [6], Fajtlowicz mentioned that Bollobás and Erdös asked for the minimum value of the Randić index for graphs G with given minimum degree $\delta(G)$. In 2002, Delorme et al [5] gave a conjecture, which is also mentioned in [9].

Conjecture 1.1 *Let $G=(V,E)$ be a graph of order n with $\delta(G)\geq k$. Then*

$$R(G)\geq \frac{k(n-k)}{\sqrt{k(n-1)}}+\binom{k}{2}\frac{1}{n-1}$$

with equality if and only if $G=K^*_{k,n-k}$, where $K^*_{k,n-k}$ is obtained from a complete bipartite graph $G=K_{k,n-k}$ by joining each pair of vertices in the part with k vertices by a new edge.

They showed that the conjecture is true for $k=2$. Using linear programming, Pavlović [14] verified the conjecture for the case of $k=2$. In [1] Aouchiche and Hansen found examples showing that the conjecture is not true, and gave a modified form. In [16] Pavlović and Divnić introduced a new approach based on quadratic programming and showed that the conjecture is true for $n_k\geq n-k$ $(k\leq n/2)$, where n_i is the number of the vertices with degree i. There are many researches about this conjecture, see [13, 14, 15]. In this paper, using linear programming we verify this conjecture for $k=3$, which can easily lead to the conclusion that the inequality of the conjecture holds for all chemical graphs, i.e., graphs with maximum degree at most 4. Furthermore, we prove that for $k\geq 4$, the conjecture is true for any graph of order $n\geq\frac{3}{2}k^3$ (or $k\leq\sqrt[3]{\frac{2n}{3}}$). For convenience, we need some additional notations and terminologies. Denote by $d(u)$ and $\delta(u)$ the degree and the minimum degree of the vertex u, respectively. Denote by $x_{i,j}$ the number of edges joining the vertices of degrees i and j. Undefined notations and terminologies can be found in [4].

2 Some Lemmas

Lemma 2.1 *([2]) Let x_1x_2 be an edge of maximum weight in a graph G, then $R(G-x_1x_2)<R(G)$.* ∎

Lemma 2.2 *Let G be the graph with minimum Randić index among all simple graphs with order n and minimum degree $\delta\geq k\geq 2$. Then the minimum degree of G must be k.*

Proof. Suppose $\delta(G) > k$, we construct a new graph G' from G by deleting an edge of maximum weight of G. It is easy to see $\delta(G') \geq k$. By Lemma 2.1, we have $R(G') < R(G)$, contradicting to the choice of G. Thus, $\delta(G) = k$. ∎

From Lemma 2.2, we can rewrite Conjecture 1.1 as the following equivalent form, and consider Conjecture 2.3 only in the sequel.

Conjecture 2.3 *Let $G = (V, E)$ be a graph of order n with $\delta(G) = k$. Then*

$$R(G) \geq \frac{k(n-k)}{\sqrt{k(n-1)}} + \binom{k}{2}\frac{1}{n-1}$$

with equality if and only if $G = K^*_{k,n-k}$, where $K^*_{k,n-k}$ is obtained from a complete bipartite graph $K_{k,n-k}$ by joining each pair of vertices in the part with k vertices by a new edge.

Lemma 2.4 *Let k, p, n be nonnegative integers, for $k \geq 4$, $0 \leq p \leq k-1$ and $n \geq \frac{3}{2}k^3$, we have*

$$(i)\quad g(k,p,n) = (k-p)\left(\frac{n+k-2p-2}{k} - \frac{2(n-p-2)}{\sqrt{k(n-2)}} + \frac{2p}{\sqrt{k(n-1)}} - \frac{2p}{\sqrt{(n-1)(n-2)}}\right) > 0;$$

$$(ii)\quad a(k,p,n) = \frac{1}{n-2} + \frac{2p}{(n-p-2)\sqrt{(n-2)(n-1)}} - \frac{2}{n+k-2p-2}\cdot \left(\frac{p}{\sqrt{k(n-1)}} + \frac{p(k-p)}{(n-p-2)\sqrt{(n-2)(n-1)}} + \frac{k-p}{\sqrt{k(n-2)}}\right) > 0;$$

$$(iii)\quad s(k,p,n) = \frac{\binom{p}{2}}{n-1} + \frac{n-p}{n+k-2p-2}\left(\frac{p(n-p-2)}{\sqrt{k(n-1)}} + \frac{p(k-p)}{\sqrt{(n-1)(n-2)}} + \frac{(k-p)(n-p-2)}{\sqrt{k(n-2)}}\right) - \left(\binom{k}{2}\frac{1}{n-1} + \frac{\sqrt{k}(n-k)}{\sqrt{n-1}}\right) > 0.$$

Proof. (i) Let $g_1(k,p,n) = \frac{k\sqrt{(n-1)(n-2)}}{k-p} g(k,p,n)$, i.e.,

$$g_1(k,p,n) = (n+k-2p-2)\sqrt{(n-1)(n-2)} - 2(n-p-2)\sqrt{k(n-1)} + 2p\sqrt{k(n-2)} - 2pk.$$

Since $\frac{\partial g_1(k,p,n)}{\partial p} = -\sqrt{n-1}\left(\sqrt{n-2} - \sqrt{4k}\right) - \sqrt{n-2}\left(\sqrt{n-1} - \sqrt{4k}\right) - 2k$, $g_1(k,p,n)$ is a strict decreasing function in p when $n \geq \frac{3}{2}k^3$ and $k \geq 4$, and then

$$\begin{aligned} g_1(k,p,n) &> g_1(k,k,n) \\ &= (n-k-2)\sqrt{n-1}\left(\sqrt{n-2} - 2\sqrt{k}\right) + 2k\sqrt{k}\left(\sqrt{n-2} - \sqrt{k}\right) > 0, \end{aligned}$$

since when $n \geq \frac{3}{2}k^3$ and $k \geq 4$, $\sqrt{(n-2)} - \sqrt{k} > \sqrt{n-2} - \sqrt{4k} > 0$. Then $g(k,p,n) > 0$.

(ii) Let $a_1(k,p,n) = (n-2)(n+k-2p-2)(n-p-2)\sqrt{k(n-1)}\ a(k,p,n)$, i.e.,

$$\begin{aligned} a_1(k,p,n) =& (n+k-2p-2)(n-p-2)\sqrt{k(n-1)} + 2p(n+k-2p-2)\sqrt{k(n-2)} \\ & - 2p(n-2)(n-p-2) - 2p(k-p)\sqrt{k(n-2)} - 2(k-p)(n-p-2)\sqrt{(n-1)(n-2)}. \end{aligned}$$

Then we have

$$\begin{aligned} & a_1(k,p,n) \\ > & (n+k-2p-2)(n-p-2)\sqrt{k(n-2)} + 2p(n+k-2p-2)\sqrt{k(n-2)} \\ & - 2p(n-1)(n-p-2) - 2p(k-p)\sqrt{k(n-2)} - 2(k-p)(n-p-2)(n-1) \\ = & \sqrt{k(n-2)}\,((n+k-2p-2)(n+p-2) - 2p(k-p)) - 2k(n-1)(n-p-2) \\ = & (n-p-2)\left((n+k-2)\sqrt{k(n-2)} - 2k(n-1)\right) \\ > & (n-p-2)(n-1)\sqrt{k}\left(\sqrt{n-2} - \sqrt{4k}\right) > 0, \end{aligned}$$

since when $n \geq \frac{3}{2}k^3$ and $k \geq 4$, $\sqrt{n-2} - 2\sqrt{k} > 0$. So $a(k,p,n) > 0$.

(iii) Let $s_1(k,p,n) = (n-1)(n+k-2p-2)\sqrt{k(n-2)}\ s(k,p,n)$, we have

$$\begin{aligned} & s_1(k,p,n) \\ = & \binom{p}{2}(n+k-2p-2)\sqrt{k(n-2)} + p(n-p)(n-p-2)\sqrt{(n-1)(n-2)} \\ & + p(k-p)(n-p)\sqrt{k(n-1)} + (n-p-2)(k-p)(n-p)(n-1) \\ & - \binom{k}{2}(n+k-2p-2)\sqrt{k(n-2)} - k(n-k)(n+k-2p-2)\sqrt{(n-1)(n-2)}. \end{aligned}$$

$$\begin{aligned} \text{Then}\quad & s_1(k,p,n) \\ > & \frac{\sqrt{k(n-2)}}{2}[p(p-1)(n+k-2p-2) + 2p(k-p)(n-p) - k(k-1)(n+k-2p-2)] \\ & + [p(n-p)(n-p-2) - k(n-k)(n+k-2p-2)]\sqrt{(n-1)(n-2)} \\ & + (n-1)(n-p)(k-p)(n-p-2) \\ = & \frac{(k-p)\sqrt{k(n-2)}}{2}\left[(p+1-k)n + pk + 3k - 2 - k^2\right] \\ & + (k-p)[-n^2 + 2n(p+1) - p^2 - pk - 2k - 2p + k^2]\sqrt{(n-1)(n-2)} \\ & + (n-1)(n-p)(k-p)(n-p-2). \end{aligned}$$

Since when $0 \leq p \leq k-1$ and $n \geq \frac{3}{2}k^3$,

$$-n^2+2n(p+1)-p^2-pk-2k-2p+k^2<0 \quad \text{and} \quad \sqrt{(n-1)(n-2)}\le \frac{2n-3}{2},$$

then we have

$$\begin{aligned}
&s_1(k,p,n)\\
&\ge \frac{(k-p)\sqrt{k(n-2)}}{2}\left[(p+1-k)n+pk+3k-2-k^2\right]+(k-p)\\
&\quad\cdot\left((-n^2+2n(p+1)-p^2-pk-2k-2p+k^2)\frac{2n-3}{2}+(n-1)(n-p)(n-p-2)\right)\\
&=\frac{(k-p)}{2}\big[n^2+2(k^2-pk-2k-p-1)n-3k^2+3pk+6k+p^2+2p\\
&\quad+\left((p+1-k)n+pk+3k-2-k^2\right)\sqrt{k(n-2)}\big]\\
&>\frac{(k-p)}{2}\left[n^2+2(k^2-k^2-2k-k)n-3kn+(-kn-k^2)\sqrt{kn}\right]\\
&=\frac{(k-p)\sqrt{n}}{2}\left[n\sqrt{n}-9k\sqrt{n}-(kn+k^2)\sqrt{k}\right].
\end{aligned}$$

Let $t(n,k)=(n\sqrt{n}-9k\sqrt{n})^2-\left((kn+k^2)\sqrt{k}\right)^2=n^3-(k^3+18k)n^2+(81k^2-2k^4)n-k^5$. When $n\ge \frac{3}{2}k^3$,

$$\frac{\partial t(n,k)}{\partial n}=3n^2-2k(k^2+18)n-k^2(2k^2-81)>0,$$

then when $k\ge 6$,

$$t(n,k)>t(\frac{3}{2}k^3,k)=k^5\left(\frac{9}{8}k^4-\frac{87}{2}k^2+\frac{241}{2}\right)>0.$$

This implies $s(k,p,n)>0$ for $k\ge 6$.

For the cases $k=4$ and 5, we can verify that when $0\le p\le k-1$ and $n\ge \frac{3}{2}k^3$, $s(k,p,n)>0$ by considering all possible values of p. ∎

3 Main Results

Let G be a simple graph of order n with $\delta(G)=k\ge 3$. At first, we will give some linear equalities. Mathematical description of the problem is as follows:

$$min\ R(G)=\sum_{\substack{k\le i\le n-1\\ i\le j\le n-1}}\frac{x_{i,j}}{\sqrt{ij}}$$

subject to:

$$
\begin{aligned}
2x_{k,k} + x_{k,k+1} + x_{k,k+2} + & \quad \cdots \quad + x_{k,n-1} = kn_k \\
x_{k+1,k} + 2x_{k+1,k+1} + x_{k+1,k+2} + & \quad \cdots \quad + x_{k+1,n-1} = (k+1)n_{k+1} \\
x_{k+2,k} + x_{k+2,k+1} + 2x_{k+2,k+2} + & \quad \cdots \quad + x_{k+2,n-1} = (k+2)n_{k+2} \\
& \quad \vdots \\
x_{n-1,k} + x_{n-1,k+1} + x_{n-1,k+2} + & \quad \cdots \quad + 2x_{n-1,n-1} = (n-1)n_{n-1}
\end{aligned}
\tag{3.1}
$$

and

$$
n_k + n_{k+1} + n_{k+2} + \cdots + n_{n-1} = n \tag{3.2}
$$

These constraints do not completely determine the problem. In order to have a better description for this problem we have to add the next constraints: $x_{i,n-1} = n_i n_{n-1}$ for $i = k, k+1, \cdots, n-2$ and $x_{n-1,n-1} = \binom{n_{n-1}}{2}$, which much more complicate the problem. Now the problem becomes a quadratic programming. To avoid the complexity of these quadratic inequalities, we will consider all the possible values of n_{n-1} solve the problem using linear programming.

We only consider the case of $k \leq n-2$, since the graph is unique when $k = n-1$.

Theorem 3.1 *For a given minimum degree $\delta(G) = k \geq 4$, the conjecture is true when the order of the graph $n \geq \frac{3}{2}k^3$. That is, for a given minimum degree $\delta(G) = k \geq 4$ and $n \geq \frac{3}{2}k^3$, we have*

$$
R(G) \geq \frac{k(n-k)}{\sqrt{k(n-1)}} + \binom{k}{2}\frac{1}{n-1},
$$

with equality if and only if G is a graph with $n_k = n-k$, $n_{n-1} = k$, $n_{k+1} = \cdots = n_{n-2} = 0$, $x_{k,n-1} = k(n-k)$, $x_{n-1,n-1} = \binom{k}{2}$ and all other $x_{i,j}$ and $x_{i,i}$ being equal to 0, i.e., $G \cong K^*_{k,n-k}$.

Proof. Since the minimum degree is k, we have $n_{n-1} \leq k$. So, we will consider two cases: $n_{n-1} = k$ and $n_{n-1} = p$, where p is an integer such that $0 \leq p \leq k-1$. Let G be a graph with order n and $\delta(G) = k \geq 4$. Denote G by $G^{(i)}$ if $n_{n-1}(G) = i$ $(i = 0, 1, \cdots, k)$. Let $R^{(i)} = R(G^{(i)})$.

Case 1: $n_{n-1} = k$

Since $x_{i,n-1} = kn_i$ for $i = k, k+1, \cdots, n-2$ and $x_{n-1,n-1} = \binom{k}{2}$, the constraints in (3.1) become: $x_{j,k} + \cdots + x_{j,j-1} + 2x_{j,j} + x_{j,j+1} + \cdots + x_{j,n-2} = (j-k)n_j$, for $j = k, k+1, \cdots, n-2$. Then we have

$$R^{(k)} = \sum_{\substack{k\le i\le n-1\\ i\le j\le n-1}} \frac{x_{i,j}}{\sqrt{ij}} = \sum_{j=k}^{n-2} \frac{kn_j}{\sqrt{j(n-1)}} + \binom{k}{2}\frac{1}{n-1}$$
$$+\frac{1}{2}\sum_{j=k}^{n-2}\left(\frac{x_{j,k}}{\sqrt{jk}} + \cdots + \frac{x_{j,j-1}}{\sqrt{j(j-1)}} + \frac{2x_{j,j}}{\sqrt{jj}} + \frac{x_{j,j+1}}{\sqrt{j(j+1)}} + \cdots + \frac{x_{j,n-2}}{\sqrt{j(n-2)}}\right)$$
$$\ge \sum_{j=k}^{n-2} \frac{kn_j}{\sqrt{j(n-1)}} + \binom{k}{2}\frac{1}{n-1} + \frac{1}{2}\sum_{j=k}^{n-2}\frac{x_{j,k} + \cdots + x_{j,j-1} + 2x_{j,j} + x_{j,j+1} + \cdots + x_{j,n-2}}{\sqrt{j(n-1)}}$$
$$= \sum_{j=k}^{n-2} \frac{kn_j}{\sqrt{j(n-1)}} + \binom{k}{2}\frac{1}{n-1} + \frac{1}{2}\sum_{j=k}^{n-2}\frac{(j-k)n_j}{\sqrt{j(n-1)}}$$
$$= \binom{k}{2}\frac{1}{n-1} + \frac{1}{2\sqrt{n-1}}\sum_{j=k}^{n-2}\left(\sqrt{j} + \frac{k}{\sqrt{j}}\right)n_j$$
$$= \binom{k}{2}\frac{1}{n-1} + \frac{1}{2\sqrt{n-1}}\left(\sqrt{k} + \frac{k}{\sqrt{k}}\right)n_k + \frac{1}{2\sqrt{n-1}}\sum_{j=k+1}^{n-2}\left(\sqrt{j} + \frac{k}{\sqrt{j}}\right)n_j$$

By substituting $n_k = n - k - (n_{k+1} + n_{k+2} + \cdots + n_{n-2})$ into the last equality, we have

$$R^{(k)} \ge \binom{k}{2}\frac{1}{n-1} + \frac{\sqrt{k}(n-k)}{\sqrt{n-1}} + \frac{1}{2\sqrt{n-1}}\sum_{j=k+1}^{n-2}\left(\sqrt{j} + \frac{k}{\sqrt{j}} - 2\sqrt{k}\right)n_j.$$

Since $\sqrt{j} + \frac{k}{\sqrt{j}} - 2\sqrt{k} > 2\sqrt{k} - 2\sqrt{k} = 0$ for $k+1 \le j \le n-2$, this function attains minimum for $n_j = 0$, $j = k+1, k+2, \cdots, n-2$. Therefore, when $n_{n-1} = k$, the minimum value of the Randić index is

$$R^{*(k)} = \binom{k}{2}\frac{1}{n-1} + \frac{\sqrt{k}(n-k)}{\sqrt{n-1}}.$$

The extremal graph must have $n_k = n-k$, $n_{k+1} = n_{k+2} = \cdots = n_{n-2} = 0$, $n_{n-1} = k$, $x_{k,n-1} = k(n-k)$, $x_{n-1,n-1} = \binom{k}{2}$ and all other $x_{i,j}$ and $x_{i,i}$ are equal to 0, i.e., $G = K^*_{k,n-k}$.

Case 2: $n_{n-1} = p$ $(0 \le p \le k-1)$

By substituting $x_{i,n-1} = pn_i$ for $i = k, k+1, \cdots, n-2$ and $x_{n-1,n-1} = \binom{p}{2}$ (if $p = 0, 1$, $\binom{p}{2} = 0$) into the constraints in (3.1), they become (3.3)

$$\begin{aligned}
2x_{k,k} + x_{k,k+1} + x_{k,k+2} + \cdots + x_{k,n-2} &= (k-p)n_k\\
x_{k+1,k} + 2x_{k+1,k+1} + x_{k+1,k+2} + \cdots + x_{k+1,n-2} &= (k+1-p)n_{k+1}\\
x_{k+2,k} + x_{k+2,k+1} + 2x_{k+2,k+2} + \cdots + x_{k+2,n-2} &= (k+2-p)n_{k+2}\\
&\vdots\\
x_{n-2,k} + x_{n-2,k+1} + x_{n-2,k+2} + \cdots + 2x_{n-2,n-2} &= (n-2-p)n_{n-2}
\end{aligned} \tag{3.3}$$

Since $n_{n-1} = p$, equality (3.2) becomes (3.4)

$$n_k + n_{k+1} + n_{k+2} + \ldots + n_{n-2} = n - p. \tag{3.4}$$

We have the next problem: minimize $R^{(p)}$ subject to (3.3) and (3.4). It is easy to express n_i for $i = k+1, k+2, \cdots, n-3$ from the constraints in (3.3) as follows

$$n_i = \frac{x_{i,k} + \cdots + x_{i,i-1} + 2x_{i,i} + x_{i,i+1} + \cdots + x_{i,n-2}}{i-p} \tag{3.5}$$

Using the first and the last constraint of (3.3), (3.4) and constraint (3.5), by some calculations, we can obtain

$$\begin{aligned} n_k = & \frac{(n-p-2)(n-p)}{n+k-2p-2} + \frac{2x_{k,k}}{n+k-2p-2} - \sum_{j=k+1}^{n-3} \frac{(n-j-2)x_{k,j}}{(j-p)(n+k-2p-2)} \\ & - \sum_{\substack{k+1 \le i \le n-2 \\ i \le j \le n-2}} \left(\frac{n-p-2}{i-p} + \frac{n-p-2}{j-p} \right) \frac{x_{i,j}}{n+k-2p-2}, \end{aligned} \tag{3.6}$$

$$\begin{aligned} n_{n-2} = & \frac{(n-p)(k-p)}{n+k-2p-2} - \sum_{\substack{k \le i \le n-3 \\ i \le j \le n-3}} \left(\frac{k-p}{i-p} + \frac{k-p}{j-p} \right) \frac{x_{i,j}}{n+k-2p-2} \\ & - \sum_{i=k+1}^{n-3} \left(\frac{k-p}{i-p} - 1 \right) \frac{x_{n-2,i}}{n+k-2p-2} + \frac{2x_{n-2,n-2}}{n+k-2p-2}, \end{aligned} \tag{3.7}$$

$$\begin{aligned} x_{k,n-2} = & \frac{(n-p-2)(n-p)(k-p)}{n+k-2p-2} - \sum_{j=k}^{n-3} \frac{(n-p-2)(k+j-2p)}{(j-p)(n+k-2p-2)} x_{k,j} \\ & - \sum_{\substack{k+1 \le i \le n-2 \\ i \le j \le n-2}} \left(\frac{n-p-2}{i-p} + \frac{n-p-2}{j-p} \right) \frac{(k-p)x_{i,j}}{n+k-2p-2}. \end{aligned} \tag{3.8}$$

By substituting $x_{i,n-1} = pn_i$ $(i = k, k+1, \cdots, n-2)$, $x_{n-1,n-1} = \binom{p}{2}$, (3.5), (3.6), (3.7) and (3.8) into $R^{(p)}$, we have

$$R^{(p)} = \overline{R^{(p)}} + \sum_{j=k}^{n-3} a_{k,j} x_{k,j} + \sum_{\substack{k+1 \le i \le n-2 \\ i \le j \le n-2}} a_{i,j} x_{i,j}$$

where

$$\overline{R^{(p)}} = \frac{\binom{p}{2}}{n-1} + \frac{n-p}{n+k-2p-2} \left(\frac{p(n-p-2)}{\sqrt{k(n-1)}} + \frac{p(k-p)}{\sqrt{(n-1)(n-2)}} + \frac{(k-p)(n-p-2)}{\sqrt{k(n-2)}} \right)$$

and

$$\begin{aligned} a_{i,j} = & \frac{1}{\sqrt{ij}} - \frac{p}{\sqrt{k(n-1)}} \cdot \frac{\frac{n-p-2}{i-p} + \frac{n-p-2}{j-p}}{n+k-2p-2} - \frac{p}{\sqrt{(n-1)(n-2)}} \cdot \frac{\frac{k-p}{i-p} + \frac{k-p}{j-p}}{n+k-2p-2} \\ & - \frac{k-p}{\sqrt{k(n-2)}} \cdot \frac{\frac{n-p-2}{i-p} + \frac{n-p-2}{j-p}}{n+k-2p-2} + \frac{\frac{p}{i-p}}{\sqrt{i(n-1)}} + \frac{\frac{p}{j-p}}{\sqrt{j(n-1)}}. \end{aligned}$$

We will prove that all functions $a_{i,j}$ are nonnegative for corresponding i and j.

Let $f(i,j) = (n+k-2p-2)(i-p)(j-p)a_{ij}$, then

$$\begin{aligned} f(i,j) = & \frac{(n+k-2p-2)(i-p)(j-p)}{\sqrt{ij}} - \frac{p(n-p-2)(i+j-2p)}{\sqrt{k(n-1)}} \\ & - \frac{p(k-p)(i+j-2p)}{\sqrt{(n-1)(n-2)}} - \frac{(k-p)(n-p-2)(i+j-2p)}{\sqrt{k(n-2)}} \\ & + \frac{p(n+k-2p-2)(j-p)}{\sqrt{i(n-1)}} + \frac{p(n+k-2p-2)(i-p)}{\sqrt{j(n-1)}}. \end{aligned}$$

We have

$$\begin{aligned} \partial^2 f(i,j)/\partial j^2 = & \frac{(n+k-2p-2)(i-p)}{4\sqrt{j^5}} \left(\frac{3p}{\sqrt{n-1}} - \frac{j+3p}{\sqrt{i}} \right) \\ \leq & \frac{(n+k-2p-2)(i-p)}{4\sqrt{j^5}} \left(\frac{3p}{\sqrt{n-1}} - \frac{i+3p}{\sqrt{i}} \right) \\ \leq & \frac{(n+k-2p-2)(i-p)}{4\sqrt{j^5}} \left(\frac{3p}{\sqrt{n-1}} - 2\sqrt{3p} \right) \\ = & \frac{(n+k-2p-2)(i-p)}{4\sqrt{j^5}} \cdot \frac{\sqrt{3p}}{\sqrt{n-1}} (\sqrt{3p} - 2\sqrt{n-1}) < 0, \end{aligned}$$

since $\frac{i+3p}{\sqrt{i}} = \sqrt{i} + \frac{3p}{\sqrt{i}} \geq 2\sqrt{3p}$ and $n-1 > k > p$. Thus, $f(i,j)$ is concave in j. We have to check that $a_{i,i}$ and $a_{i,n-2}$ are nonnegative in order to conclude that $a_{i,j} \geq 0$ for $k \leq i \leq n-2$ and $i \leq j \leq n-2$. Let $g(i,p,n) = (n+k-2p-2)(i-p)a_{i,i}$, then

$$\begin{aligned} g(i,p,n) = & \frac{(n+k-2p-2)(i-p)}{i} - \frac{2p(n-p-2)}{\sqrt{k(n-1)}} - \frac{2p(k-p)}{\sqrt{(n-1)(n-2)}} \\ & - \frac{2(k-p)(n-p-2)}{\sqrt{k(n-2)}} + \frac{2p(n+k-2p-2)}{\sqrt{i(n-1)}}. \end{aligned}$$

We have $\partial g(i,p,n)/\partial i = \frac{p(n+k-2p-2)}{\sqrt{i^3}} \left(\frac{1}{\sqrt{i}} - \frac{1}{\sqrt{n-1}} \right) > 0$, then for $i \geq k$, $g(i,p,n) \geq g(k,p,n)$, where

$$g(k,p,n) = (k-p) \left(\frac{n+k-2p-2}{k} - \frac{2(n-p-2)}{\sqrt{k(n-2)}} + \frac{2p}{\sqrt{k(n-1)}} - \frac{2p}{\sqrt{(n-1)(n-2)}} \right).$$

By Lemma 2.4 (i), for $k \geq 4$, $0 \leq p \leq k-1$ and $n \geq \frac{3}{2}k^3$, we have $g(k,p,n) > 0$, then $a_{i,i} > 0$.

Let $q(i,p,n) = (n+k-2p-2)(i-p)a_{i,n-2}$, then

$$\begin{aligned} q(i,p,n) = & \frac{(n+k-2p-2)(i-p)}{\sqrt{(n-2)i}} - \frac{p(n-2p-2+i)}{\sqrt{k(n-1)}} - \frac{p\left(k-p+\frac{(k-p)(i-p)}{n-p-2}\right)}{\sqrt{(n-1)(n-2)}} \\ & - \frac{(k-p)(n-2p-2+i)}{\sqrt{k(n-2)}} + \frac{p(n+k-2p-2)}{\sqrt{(n-1)i}} + \frac{p(n+k-2p-2)(i-p)}{(n-p-2)\sqrt{(n-1)(n-2)}}. \end{aligned}$$

Since

$$\partial^2 q(i,p,n)/\partial i^2 = -\frac{n+k-2p-2}{4\sqrt{i^5}}\left(\frac{i+3p}{\sqrt{n-2}} - \frac{3p}{\sqrt{n-1}}\right) < 0,$$

and $q(k,p,n) = 0$, we only need to prove

$$\begin{aligned} a_{n-2,n-2} &= \frac{1}{n-2} + \frac{2p}{(n-p-2)\sqrt{(n-2)(n-1)}} - \frac{2}{n+k-2p-2} \\ &\cdot \left(\frac{p}{\sqrt{k(n-1)}} + \frac{p(k-p)}{(n-p-2)\sqrt{(n-2)(n-1)}} + \frac{k-p}{\sqrt{k(n-2)}}\right) \geq 0. \end{aligned}$$

By Lemma 2.4 (ii), for $k \geq 4$, $0 \leq p \leq k-1$ and $n \geq \frac{3}{2}k^3$, we have $a_{n-2,n-2} > 0$, then $a_{i,n-2} > 0$.

Since $a_{i,j} \geq 0$ for $k \leq i \leq n-2$ and $i \leq j \leq n-2$, then $R^{(p)}$ attains minimum if we put $x_{k,j} = 0$ for $j = k, k+1, \cdots, n-3$ and $x_{i,j} = 0$ for $k+1 \leq i \leq n-2$, $i \leq j \leq n-2$. The minimum value is $\overline{R^{(p)}}$ and

$$n_k = \frac{(n-p-2)(n-p)}{n+k-2p-2}, \quad n_{n-2} = \frac{(n-p)(k-p)}{n+k-2p-2}, \quad n_{n-1} = p, \quad n_i = 0$$

for $i = k+1, \cdots, n-3$. This solution may not correspond to any graph, and the real graphical solution $R^{*(P)} \geq \overline{R^{(p)}}$. Now we only need to show that $\overline{R^{(p)}} \geq R^{*(k)}$. Let

$$\begin{aligned} s(k,p,n) &= \overline{R^{(p)}} - R^{*(k)} \\ &= \frac{\binom{p}{2}}{n-1} + \frac{n-p}{n+k-2p-2}\left(\frac{p(n-p-2)}{\sqrt{k(n-1)}} + \frac{p(k-p)}{\sqrt{(n-1)(n-2)}} + \frac{(k-p)(n-p-2)}{\sqrt{k(n-2)}}\right) \\ &- \left(\binom{k}{2}\frac{1}{n-1} + \frac{\sqrt{k}(n-k)}{\sqrt{n-1}}\right). \end{aligned}$$

By Lemma 2.4 (iii), for $k \geq 4$, $0 \leq p \leq k-1$ and $n \geq \frac{3}{2}k^3$, we have $s(k,p,n) > 0$. The proof is thus complete. ∎

Theorem 3.2 *Let G be a simple graph of order n with minimum degree $k = 3$. Then we have*

$$R(G) \geq \frac{3(n-3)}{\sqrt{3(n-1)}} + \binom{3}{2}\frac{1}{n-1},$$

with equality if and only if $G = K^*_{k,n-k}$.

Proof. By the proof of Theorem 3.1, we only need to prove the inequalities $g(k,p,n) \geq 0$, $a_{n-2,n-2} \geq 0$ and $s(k,p,n) \geq 0$ for $k = 3$ and $0 \leq p \leq 2$. In the following we only consider $n \geq 6$, since the graph with 4 vertices and $k = 3$ is unique, the number of graphs with 5 vertices and $k = 3$ are only two (see Figure 3.1). Now we consider all the possible values of p.

Case 1: $p = 0$

We have

$$
\begin{aligned}
g(3,0,n) &= n+1-\frac{6(n-2)}{\sqrt{3n-6}} \geq g(3,0,6)>0;\\
a_{n-2,n-2} &= \frac{1}{n-2}-\frac{6}{(n+1)\sqrt{3(n-2)}}=\frac{1}{\sqrt{n-2}}\left(\frac{1}{\sqrt{n-2}}-\frac{2\sqrt{3}}{n+1}\right)\geq 0;\\
s(3,0,n) &= \frac{\sqrt{3}n(n-1)\sqrt{n-2}-3(n+1)-\sqrt{3}(n-3)(n+1)\sqrt{n-1}}{(n+1)(n-1)}.
\end{aligned}
$$

$$
\begin{aligned}
\text{Let}\quad s_0(n) &= \sqrt{3}n(n-1)\sqrt{n-2}-3(n+1)-\sqrt{3}(n-3)(n+1)\sqrt{n-1}\\
&= \sqrt{3}n\left((n-1)\sqrt{n-2}-\sqrt{3}-(n-2)\sqrt{n-1}\right)+3\sqrt{3}\sqrt{n-1}-3.
\end{aligned}
$$

By simple calculation, we can prove that $3\sqrt{3}\sqrt{n-1}-3>0$ and $(n-1)\sqrt{n-2}-\sqrt{3}-(n-2)\sqrt{n-1}>0$ for $n\geq 14$, i.e., $s_0(n)\geq 0$ for $n\geq 14$. We can directly verify that $s_0(n)\geq 0$ for $6\leq n\leq 13$.

Case 2: $p=1$

We have

$$
g(3,1,n)=\frac{2\sqrt{n-1}\left((n-1)\sqrt{n-2}-2\sqrt{3}(n-3)\right)+4\sqrt{3}\left(\sqrt{n-2}-\sqrt{3}\right)}{3\sqrt{(n-1)(n-2)}}
$$

For $n\geq 6$, we have $\sqrt{n-2}-\sqrt{3}>0$. Let $g_1(n)=(n-1)\sqrt{n-2}-2\sqrt{3}(n-3)$, we have $g_1'(n)=\frac{1}{2\sqrt{n-2}}+\frac{3}{2}\sqrt{n-2}-2\sqrt{3}>\frac{1}{2\sqrt{n-2}}>0$ for $n\geq 9$, then $g_1(n)$ is a strictly increasing function in $n\geq 9$. So $g_1(n)>g_1(9)=8\sqrt{7}-12\sqrt{3}>0$. By some calculations we obtain that $g(3,1,n)>0$ for $6\leq n\leq 8$.

$$
\begin{aligned}
a_{n-2,n-2} &= \frac{1}{n-2}-\frac{2}{\sqrt{3}(n-1)}\left(\frac{1}{\sqrt{n-1}}+\frac{2}{\sqrt{n-2}}\right)+\frac{2}{(n-1)\sqrt{(n-1)(n-2)}}\\
&\geq \frac{1}{n-2}-\frac{2}{\sqrt{3}(n-1)}\cdot\frac{3}{\sqrt{n-2}}=\frac{1}{\sqrt{n-2}}\left(\frac{1}{\sqrt{n-2}}-\frac{2\sqrt{3}}{n-1}\right)
\end{aligned}
$$

For $n\geq 12$, $\frac{1}{\sqrt{n-2}}-\frac{2\sqrt{3}}{n-1}>0$, i.e., $a_{n-2,n-2}>0$. For smaller n, we can verify it easily.

Let $s_1(n)=\sqrt{3}(n-1)\sqrt{n-2}\ s(3,1,n)$, i.e.,

$$
s_1(n)=-2(n-3)\sqrt{(n-1)(n-2)}+2\sqrt{3}\sqrt{n-1}+2(n-3)(n-1)-3\sqrt{3}\sqrt{n-2}.
$$

By some calculations, we have

$$
\begin{aligned}
s_1(n) &> 2(n-3)\left(n-1-\sqrt{(n-1)(n-2)}\right)-\sqrt{3}\sqrt{n-2}\\
&> \sqrt{3(n-2)}\left[\sqrt{n-2}\left(n-1-\sqrt{(n-1)(n-2)}\right)-1\right]>0,
\end{aligned}
$$

since $2(n-3) > \sqrt{3}(n-2)$ and $\sqrt{n-2}\left(n-1-\sqrt{(n-1)(n-2)}\right)-1 > 0$ for $n \geq 10$. Thus, $s(3,1,n) > 0$ for $n \geq 10$. We can directly verify that $s(3,1,n) \geq 0$ for $6 \leq n \leq 9$.

Case 3: $p = 2$

Suppose $n \geq 8$. We have

$$\begin{aligned} g(3,2,n) &= \frac{(n-3)\sqrt{(n-1)(n-2)} - 2\sqrt{3}(n-4)\sqrt{n-1} + 4\sqrt{3}\sqrt{n-2} - 12}{3\sqrt{(n-1)(n-2)}} \\ &\geq \frac{(n-3)(n-2) - 2\sqrt{3}(n-4)\sqrt{n-1} + 4\sqrt{3}\sqrt{n-2} - 12}{3\sqrt{(n-1)(n-2)}} = \frac{g_2(n)}{3\sqrt{(n-1)(n-2)}}, \end{aligned}$$

where $g_2(n) = (n-3)(n-2) - 2\sqrt{3}(n-4)\sqrt{n-1} + 4\sqrt{3}\sqrt{n-2} - 12$. Since

$$\begin{aligned} g_2'(n) &= n-2+n-3-2\sqrt{3}\sqrt{n-1} - \frac{\sqrt{3}(n-4)}{\sqrt{n-1}} + \frac{2\sqrt{3}}{\sqrt{n-2}} \\ &> 2n-5-2\sqrt{3}\sqrt{n-1} - \sqrt{3}\sqrt{n-1} = 2n-5-3\sqrt{3}\sqrt{n-1}, \end{aligned}$$

and for $n \geq 11$, $g_2'(n) \geq g_2'(11) > 0$, we have $g_2(n) \geq g_2(11) = 60 + 12\sqrt{3} - 14\sqrt{30} > 0$. By some calculations for smaller n, we have $g(3,2,n) > 0$ for $n \geq 8$.

$$\begin{aligned} a_{n-2,n-2} &= \frac{1}{n-2} - \frac{2}{\sqrt{3}(n-3)}\left(\frac{2}{\sqrt{n-1}} + \frac{1}{\sqrt{n-2}}\right) + \frac{4}{(n-3)\sqrt{(n-1)(n-2)}} \\ &\geq \frac{1}{n-2} - \frac{2}{\sqrt{3}(n-3)}\,\frac{3}{\sqrt{n-2}} = \frac{1}{\sqrt{n-2}}\left(\frac{1}{\sqrt{n-2}} - \frac{2\sqrt{3}}{n-3}\right) \end{aligned}$$

For $n \geq 16$, $\frac{1}{\sqrt{n-2}} - \frac{2\sqrt{3}}{n-3} > 0$, i.e., $a_{n-2,n-2} > 0$. For smaller n, we can verify it easily.

Let $s_2(n) = \sqrt{3}(n-1)(n-3)\sqrt{n-2}\; s(3,2,n)$, where

$$\begin{aligned} s_2(n) &= (n-2)(n-1)(n-4) + 2\sqrt{3}(n-2)\sqrt{n-1} - 2\sqrt{3}(n-3)\sqrt{n-2} \\ &\quad - (n^2-6n+11)\sqrt{(n-1)(n-2)}. \end{aligned}$$

Since $2\sqrt{3}(n-2)\sqrt{n-1} - 2\sqrt{3}(n-3)\sqrt{n-2} > 0$ for $n \geq 8$, we have

$$s_2(n) \geq (n-2)(n-1)(n-4) - (n^2-6n+11)\sqrt{(n-1)(n-2)}.$$

Then we only need to prove

$$((n-2)(n-1)(n-4))^2 > \left((n^2-6n+11)\sqrt{(n-1)(n-2)}\right)^2,$$

i.e., $(n-1)(n-2)\big((n-3)(n^2-13n+29)-2\big) > 0$. By some calculations, we have $(n-3)(n^2-13n+29)-2 > 0$ when $n \geq 11$. Thus, $s(3,2,n) > 0$ for $n \geq 8$, since we can verify easily for $8 \leq n \leq 10$.

For $6 \le n \le 7$, all the graphs with minimum degree 3 and $2 \le p \le 3$ and the values of their Randić Index are shown in Figure 3.1. By easy comparisons, we can check the result of the theorem. The proof is now complete. ∎

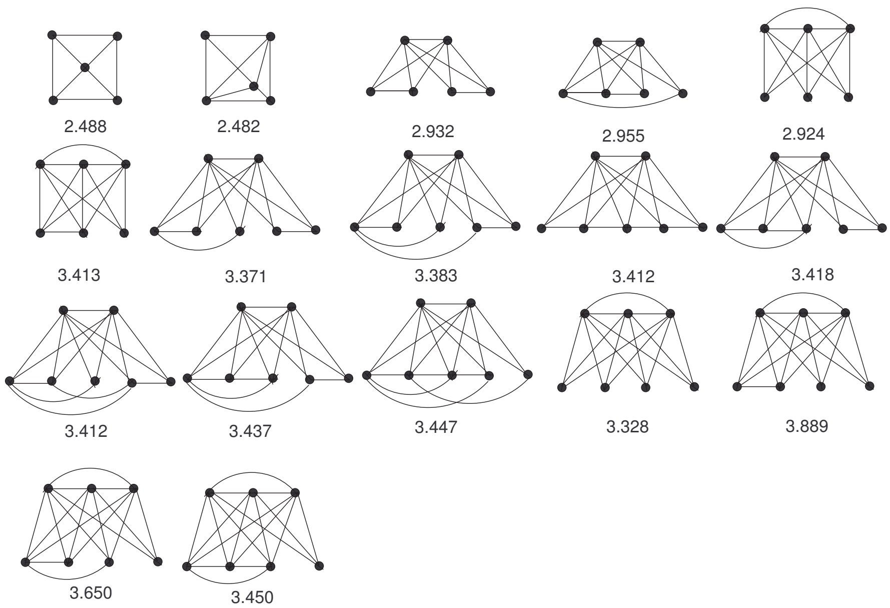

Figure 3.1 The graphs of order $5 \le n \le 7$ with minimum degree $k = 3$ and $2 \le p \le 3$.

Theorem 3.3 *The inequality of the conjecture holds for all chemical graphs, i.e., graphs with maximum degree at most 4.*

Proof. From the the result of Delorme et al for minimum degree $k = 2$ and the above Theorem 3.2 for minimum degree $k = 3$, we know that we only need to check the inequality of the conjecture for 4-regular graphs. It is easy to see that a 4-regular graph of order n has $2n$ edges, and each edge has a weight equal to $\frac{1}{4}$. So, any 4-regular graph G has a Randić index equal to $\frac{n}{2}$. It is then not difficult to check that

$$R(G) = \frac{n}{2} \ge \frac{4(n-4)}{\sqrt{4(n-1)}} + \binom{4}{2}\frac{1}{n-1} = \frac{2(n-4)}{\sqrt{(n-1)}} + \frac{6}{n-1}.$$

The proof is complete. ∎

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