Research Article

Extremal Values of Randić Index among Some Classes of Graphs

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Received 18 April 2021; Accepted 31 May 2021; Published 14 June 2021

Academic Editor: Roslan Hasni

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Suppose G is a simple graph with edge set $E(G)$. The Randić index $R(G)$ is defined as $R(G) = \sum_{uv \in E(G)} (1/\sqrt{\deg_G(u)\deg_G(v)})$, where $\deg_G(u)$ and $\deg_G(v)$ denote the vertex degrees of u and v in G , respectively. In this paper, the first and second maximum of Randić index among all n -vertex c -cyclic graphs was computed. As a consequence, it is proved that the Randić index attains its maximum and second maximum on two classes of chemical graphs. Finally, we will present new lower and upper bounds for the Randić index of connected chemical graphs.

1. Mathematical Notions and Notations

In this section, we first describe some mathematical notions that will be kept throughout. A pair $G = (V, E)$ in which V is a finite nonempty set and E is a subset of 2-elements subsets of V is called a simple graph. Throughout this paper, the term graph means simple graph and the sets $V = V(G)$ and $E = E(G)$ in definition of G are called the vertex set and edge set of G , respectively.

Suppose G is a graph. For simplicity of our argument, an edge $e = \{a, b\}$ in G is simply written as $e = ab$. Choose a vertex v in G . The vertex degree of v , $\deg_G(v)$, is defined as the number of edges in the form av . A chemical graph is a graph in which all vertices have degrees less than or equal to 4 [1]. The reason for this name is from quantum chemistry in which it is convenient to model a molecule M in such a way that vertices are used to denote atoms and edges are for chemical bonds.

The set of all vertices adjacent to a vertex v is denoted by $N[v, G]$ and notations $\Delta = \Delta(G)$, $n_i = n_i(G)$, and $\varepsilon_i = \varepsilon_i(G)$ are used for the maximum degree, the number of vertices of degree i , and the number of edges of degree i in G , respectively. The number of edges connecting a vertex of degree i with a vertex of degree j in G is denoted by $m_{i,j}(G)$. A connected n -vertex graph G is called to be c -cyclic if it has $n + c - 1$ edges and the number $c = c(G)$ is said to be the cyclomatic number of G .

Suppose W is a nonempty subset of vertices in a graph G . The subgraph of G obtained by deleting the vertices of W is denoted by $G - W$, and similarly, if $F \subseteq E(G)$, then the subgraph obtained by deleting all edges in F is denoted by $G - F$. In the case that $W = \{v\}$ or $F = \{xy\}$, the subgraphs $G - W$ and $G - F$ will shortly be written as $G - v$ or $G - xy$, respectively. Furthermore, if x and y are nonadjacent vertices in G , then the notation $G + xy$ is used for the graph obtained from G by adding an edge xy .

The Randić index of a graph G is defined as

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

This topological index was proposed by Milan Randić [2] under the name “branching index.” The Randić index is suitable for measuring the extent of branching of the carbon-atom skeleton of saturated hydrocarbons. We encourage the interested readers to consult the books [3,4] for more information on this topic.

2. Background Materials

This section aims to briefly review the literature on ordering graphs concerning the Randić index. By referring to Theorems 2.2 and 2.3 in [5], among all n -vertex trees, the star S_n

has the minimum Randić index and the path P_n attains the maximum Randić index. Caporossi et al. [6] proved that among all 1-cyclic graphs of order n , the cycle C_n attains the maximum value, and the unicyclic graphs obtained by attaching a pendant path to a vertex of a cycle attain the second maximum Randić index. These are the starting point of the following problem.

Question 1. Find n -vertex c -cyclic graphs with maximum and minimum Randić index.

Shiu and Zhang [7] obtained the maximum value of Randić index in the class of all n -vertex chemical trees with k pendants such that $n < 3k - 2$. Shi [8] obtained some interesting results for chemical trees with respect to two generalizations of Randić index. Dehghan-Zadeh et al. [9, 10] obtained the first and second maximum of Randić index in the class of all n -vertex c -cyclic graphs when $c = 3, 4$.

Deng et al. [11] considered various degree mean rates of an edge and gave some tight bounds for the variation of the Randić index of a graph G in terms of its maximum and minimum degree mean rates over its edges. Gutman et al. in a recent interesting paper [12] investigated the connection between Randić index and the degree-based information content of molecular and also general graphs. This connection is based on the linear correlation between Randić index and the logarithm of the multiplicative version of the Randić index.

The aim of this paper is to proceed with Question 1. We will obtain the first and second maximum of Randić index among all c -cyclic graphs. This extends some results in [6, 9, 10].

3. Five Graph Transformations

In this section, five graph transformations will be presented which are useful in computing Randić index of graphs. The transformations I and II were introduced in [13].

- (1) *Transformation I.* Suppose that G is a graph with a given vertex w . In addition, we assume that $P: v_1, v_2, \dots, v_k$ and $Q: u_1 u_2 \dots u_l$ are two paths of lengths $k - 1$ and $l - 1$, respectively. Let G_1 be the graph obtained from G , P , and Q by attaching edges $v_1 w$ and $w u_1$. Define $G_2 = G_1 - v_1 w + u_1 v_1$. The above-referred graphs are illustrated in Figure 1.
- (2) *Transformation II.* Suppose that G is a graph with given vertices x and y such that $\deg_G(x), \deg_G(y) \geq 2$ and for all $v \in N[x, G]$, $\deg_G(x) \geq 2$. In addition, we assume that $P: v_1, v_2, \dots, v_l$ and $Q: u_1, u_2, \dots, u_k$ are two paths of lengths $l - 1$ and $k - 1$, respectively. Define G_1 be the graph obtained from G , P , and Q by attaching vertices $y v_1, u_1 x$, and $G_2 = G_1 - u_1 x + v_1 u_1$. See Figure 2 for more details.
- (3) *Transformation III.* Suppose that G is a graph with vertices x, y, w , and z such that $\{xy, wz\} \subseteq E(G)$. In

addition, we assume that G' is a trivial graph with vertex set $\{v\}$. Define $G_1 = G - \{xy\} + \{xv, vy\}$ and $G_2 = G - \{wz\} + \{wv, vz\}$. The above-referred graphs are illustrated in Figure 3.

- (4) *Transformation IV.* Suppose that G is a graph with given vertex w such that $\deg_G(w) = \Delta(G) \geq 4$, $N[w, G] = \{w_1, \dots, w_{\deg_G(w)}\}$ and $\deg_G(w_1) = \deg_G(w_2) = 2$. In addition, we assume that $v \in V(G)$, $\deg_G(v) \geq 2$, and $vw_1 \in E(G)$. Define $G' = G - ww_2 + w_1 w_2$. See Figure 4 for more details.
- (5) *Transformation V.* Suppose that G is a graph with vertices $x_1, x_2, x_3, x_4, x_5, x_6$, and w such that $\{x_1 x_2, x_2 x_3, x_2 w, x_4 x_5, x_5 x_6\} \subseteq E(G)$, $\deg_G(x_1) = \deg_G(x_2) = \deg_G(x_3) = 3$, $\deg_G(x_4) = 4$, $\deg_G(x_5) = 2$, and $\deg_G(x_6) = 1$ or 2 . Define $G' = G - \{x_2 w\} + \{x_5 w\}$. The above-referred graphs are illustrated in Figure 5.

It is well-known that if the derivative $f'(x)$ of a continuous function $f(x)$ satisfies $f'(x) > 0$ on an open interval (a, b) , then $f(x)$ is increasing on (a, b) .

Lemma 1. *The following hold:*

- (1) Let G_1 and G_2 be two graphs satisfying the conditions of Transformation I. If $\deg_G(w) \geq 3$ or $\deg_G(w) = 2$ and $\min_{uw \in E(G)} \deg_G(u) \leq 168$ or $\deg_G(w) = 1$ and $\min_{uw \in E(G)} \deg_G(u) \leq 30$, then $R(G_2) > R(G_1)$.
- (2) Let G_1 and G_2 be two graphs satisfying the conditions of Transformation II and let $\deg_G(x) = a$, $N[x, G] = \{h_1, \dots, h_a\}$, $\deg_G(h_i) = d_i$, $\deg_G(h_i) = d_i$, $1 \leq i \leq a$, $d_i \leq d_{i+1}$, $1 \leq i \leq a - 1$. If $a \geq 5$ or $a = 4$ and $d_2 \leq 20$ or $a = 3$ and $d_2 \leq 6$ or $a = 2$ and $d_2 \leq 5$, then $R(G_2) > R(G_1)$.
- (3) Let G_1 and G_2 be two graphs as shown in Transformation III.
 - (a) If $\deg_G(x), \deg_G(y) \geq 3$, and $\deg_G(z) \in \{1, 2\}$, then $R(G_2) > R(G_1)$
 - (b) If $\deg_G(x) = 2$, $\deg_G(w) \geq 3$, and $\deg_G(z) = 1$, then $R(G_2) > R(G_1)$
 - (c) If $\deg_G(x) = 2$ and $\deg_G(w) = 2$, then $R(G_2) = R(G_1)$
- (4) Let G and G' be two graphs satisfying the conditions of Transformation IV. Then, $R(G') \geq R(G)$.
- (5) Let G and G' be two graphs satisfying the conditions of Transformation V. Then, $R(G') > R(G)$.

Proof

- (1) Let $x = \deg_G(w)$, $N[w, G] = \{l_1, \dots, l_x\}$, $d_G(l_i) = d_i$, $1 \leq i \leq x$, $\min_{i=1}^x d_i = d_1$, and $k, l \geq 2$. Then, by definition,

FIGURE 1: The graphs (a) G_1 and (b) G_2 in Transformation I. FIGURE 2: The graph (a) G_1 and (b) G_2 in Transformation II. FIGURE 3: The graph (a) G_1 and (b) G_2 in Transformation III. FIGURE 4: The graph (a) G and (b) G' in Transformation IV. FIGURE 5: The graph (a) G and (b) G' in Transformation V.

$$\begin{aligned}
 R(G_2) - R(G_1) &= \left(\frac{1}{\sqrt{2}(x+1)} + 1 + \sum_{i=1}^x \frac{1}{\sqrt{d_i}(x+1)} \right) - \left(\frac{2}{\sqrt{2}(x+2)} + \frac{1}{\sqrt{2}} + \sum_{i=1}^x \frac{1}{\sqrt{d_i}(x+2)} \right) \\
 &\geq \left[\frac{1}{\sqrt{2}} + \frac{1}{\sqrt{d_1}} \right] \left[\frac{1}{\sqrt{x+1}} - \frac{1}{\sqrt{x+2}} \right] - \frac{1}{\sqrt{2}} \frac{1}{\sqrt{x+2}} + 1 - \frac{1}{\sqrt{2}}.
 \end{aligned} \tag{2}$$

Now, by Equality (2),

$R(G_2) - R(G_1) \geq (1/\sqrt{2})[(1/\sqrt{x+1}) - (1/\sqrt{x+2})]$
 $+ (1/\sqrt{2})(1/\sqrt{x+2}) + 1 - (1/\sqrt{2}) > 0.013$, for $x \geq 3$,
 $R(G_2) - R(G_1) \geq 0.0000024$, for $x = 2$ and $d_1 \leq 168$,
and $R(G_2) - R(G_1) \geq 0.000086$, for $x = 1$ and

$d_1 \leq 30$. The proof of other cases of k and l is similar, and we omit them.

(2) Let $\deg_G(x) = a$, $N[x, G] = \{h_1, \dots, h_a\}$, $\deg_G(h_i) = d_i$, $1 \leq i \leq a$, $d_i \leq d_{i+1}$, $1 \leq i \leq a-1$ and $k, l \geq 2$. Then, by definition,

$$\begin{aligned}
R(G_2) - R(G_1) &= \left(1 + \sum_{i=1}^a \frac{1}{\sqrt{d_i a}}\right) - \left(\frac{1}{\sqrt{2(a+1)}} + \frac{1}{\sqrt{2}} + \sum_{i=1}^a \frac{1}{\sqrt{d_i(a+1)}}\right) \\
&\geq 1 - \frac{1}{\sqrt{2(a+1)}} - \frac{1}{\sqrt{2}} + \left[\frac{1}{\sqrt{d_1}} + \frac{1}{\sqrt{d_2}}\right] \left[\frac{1}{\sqrt{a}} - \frac{1}{\sqrt{a+1}}\right].
\end{aligned} \tag{3}$$

And, by last equality,

$R(G_2) - R(G_1) > 0.0042$ for $a \geq 5$, $R(G_2) - R(G_1) > 0.00027$ for $a = 4$ and $d_2 \leq 20$, $R(G_2) - R(G_1) > 0.0024$ for $a = 3$ and $d_2 \leq 6$, and $R(G_2) - R(G_1) >$

0.0007 for $a = 3$ and $d_2 \leq 5$. The proof of other cases of k and l is similar, and we omit them.

(3) Suppose $\deg_G(x) = s$, $\deg_G(y) = r$, $\deg_G(w) = l$, and $\deg_G(z) = t$. To prove (a), we note that

$$\begin{aligned}
R(G_2) - R(G_1) &= \left(\frac{1}{\sqrt{sr}} + \frac{1}{\sqrt{2l}} + \frac{1}{\sqrt{2t}}\right) - \left(\frac{1}{\sqrt{2s}} + \frac{1}{\sqrt{2r}} + \frac{1}{\sqrt{lt}}\right) \\
&= \left(\frac{1}{\sqrt{sr}} - \frac{1}{\sqrt{2s}} - \frac{1}{\sqrt{2r}}\right) + \left(\frac{1}{\sqrt{2l}} - \frac{1}{\sqrt{2t}} - \frac{1}{\sqrt{lt}}\right) > -0.48 + 0.50 > 0.
\end{aligned} \tag{4}$$

To prove (b), we first calculate the difference between $R(G_2)$ and $R(G_1)$.

$$R(G_2) - R(G_1) = \left(\frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2l}}\right) - \left(\frac{1}{2} + \frac{1}{\sqrt{l}}\right). \tag{5}$$

Let $h(x) = (1/\sqrt{2x}) - (1/\sqrt{x})$, for $x \in (0, \infty)$. Then, h is increasing on $(0, \infty)$, and hence by

equation (5), $R(G_2) - R(G_1) > 0.038$. For the proof of (c), it is enough to notice that $m_{i,j}(G_1) = m_{i,j}(G_2)$, $1 \leq i \leq j \leq n-1$. Thus, $R(G_2) = R(G_1)$, as desired.

(4) Suppose that $\deg_G(v) = s$, $\deg_G(w) = q$, and $\deg_G(w_i) = d_i$, $2 \leq i \leq q$. Then,

$$\begin{aligned}
R(G') - R(G) &= \left(\frac{1}{\sqrt{3s}} + \frac{1}{\sqrt{3(q-1)}} + \frac{1}{\sqrt{6}} + \sum_{i=3}^q \frac{1}{\sqrt{(q-1)d_i}}\right) - \left(\frac{1}{\sqrt{2s}} + \frac{2}{\sqrt{2q}} + \sum_{i=3}^q \frac{1}{\sqrt{qd_i}}\right) \\
&\geq \left(\frac{2}{\sqrt{6}} + \frac{1}{\sqrt{3(q-1)}} + \frac{q-2}{\sqrt{(q-1)q}}\right) - \left(\frac{1}{\sqrt{4}} + \frac{2}{\sqrt{2q}} - \frac{q-2}{\sqrt{q^2}}\right) > 0.02,
\end{aligned} \tag{6}$$

as desired.

(5) Suppose that $\deg_G(x_6) = r$. Then, by definition,

$$R(G') - R(G) = \left(\frac{2}{\sqrt{9}} + \frac{1}{\sqrt{8}} + \frac{1}{\sqrt{2r}}\right) - \left(\frac{2}{\sqrt{6}} + \frac{1}{\sqrt{12}} + \frac{1}{\sqrt{3r}}\right) > 0.0068. \tag{7}$$

Hence, the result.

For a graph G , its first Zagreb index $M_1(G)$ is defined as $M_1(G) = \sum_{v \in V(G)} \deg_G(v)^2$. $\square$

Lemma 2 (see [14]). *If G is a connected graph with n vertices and m edges, then*

$$\varepsilon_1(G) = 4m - M_1(G) + \sum_{i=3}^{2n-4} \varepsilon_i(G)(i-2), \tag{8}$$

$$\varepsilon_2(G) = M_1(G) - 3m - \sum_{i=3}^{2n-4} \varepsilon_i(G)(i-1).$$

Theorem 1. Let G be a connected graph with $n \geq 3$ vertices and m edges.

- (1) If $\Delta(G) \leq 3$ or $(\Delta(G) \leq 11$ and $m_{1,4}(G) = m_{2,3}(G) = 0)$, then $R(G) \geq (4m - M_1(G)/\sqrt{2}) + (M_1(G) - 3m/2)$. The equality holds if and only if $G \cong P_n$.
- (2) If $\Delta(G) \leq 3$ and $m_{2,2}(G) = m_{1,4}(G) = m_{2,3}(G) = 0$ or $(\Delta(G) \leq 5$ and $m_{2,2}(G) = m_{1,4}(G) = m_{2,3}(G) = m_{1,5}(G) = m_{2,4}(G) = m_{3,3}(G) = 0)$, then $R(G) \geq (4m - M_1(G)/\sqrt{2}) + (M_1(G) - 3m/\sqrt{3})$, with equality if and only if $G \cong S_4$.

Proof. By definition,

$$R(G) = \sum_{1 \leq i \leq j \leq n-1} m_{i,j} \frac{1}{\sqrt{ij}} \geq m_{1,2} \frac{1}{\sqrt{2}} + m_{1,3} \frac{1}{\sqrt{3}} + m_{2,2} \frac{1}{2} + \sum_{i=3}^{2n-4} \varepsilon_i(G) \frac{1}{\Delta(G)}. \quad (9)$$

$$\begin{aligned}
 R(G) &\geq \frac{1}{\sqrt{2}} \left[4m - M_1(G) + \sum_{i=3}^4 \varepsilon_i(G) (i-2) \right] \\
 &\quad + \frac{1}{2} \left[M_1(G) - 3m - \sum_{i=3}^4 \varepsilon_i(G) (i-1) \right] + \sum_{i=3}^4 \varepsilon_i(G) \frac{1}{3} \\
 &= \frac{4m - M_1(G)}{\sqrt{2}} + \frac{M_1(G) - 3m}{2} + \left[\frac{1}{\sqrt{2}} - \frac{1}{2} \right] \sum_{i=3}^4 \varepsilon_i(G) (i-1) - \left[\frac{1}{\sqrt{2}} - \frac{1}{3} \right] \sum_{i=3}^4 \varepsilon_i(G) \\
 &\geq \frac{4m - M_1(G)}{\sqrt{2}} + \frac{M_1(G) - 3m}{2} + 2 \left[\frac{1}{\sqrt{2}} - \frac{1}{2} \right] \sum_{i=3}^4 \varepsilon_i(G) - \left[\frac{1}{\sqrt{2}} - \frac{1}{3} \right] \sum_{i=3}^4 \varepsilon_i(G) \\
 &= \frac{4m - M_1(G)}{\sqrt{2}} + \frac{M_1(G) - 3m}{2} + \left[\frac{1}{\sqrt{2}} - 1 + \frac{1}{3} \right] \sum_{i=3}^4 \varepsilon_i(G) \\
 &\geq \frac{4m - M_1(G)}{\sqrt{2}} + \frac{M_1(G) - 3m}{2}.
 \end{aligned} \quad (11)$$

Equality holds if and only if $G \cong P_n$. Let $\Delta(G) \leq 11$ and $m_{1,4}(G) = m_{2,3}(G) = 0$. Then, by Equality (9),

1. The last equality for $\Delta(G) \leq 3$ gives

$$\begin{aligned}
 R(G) &\geq m_{1,2} \frac{1}{\sqrt{2}} + \frac{1}{2} [m_{1,3} + m_{2,2}] + \sum_{i=3}^4 \varepsilon_i(G) \frac{1}{3} \\
 &= \frac{1}{\sqrt{2}} \varepsilon_1(G) + \frac{1}{2} \varepsilon_2(G) + \sum_{i=3}^4 \varepsilon_i(G) \frac{1}{3},
 \end{aligned} \quad (10)$$

and by Lemma 2,

$$\begin{aligned}
R(G) &\geq m_{1,2} \frac{1}{\sqrt{2}} + \frac{1}{2} [m_{1,3} + m_{2,2}] + \sum_{i=4}^{20} \varepsilon_i(G) \frac{1}{11} \\
&= \frac{1}{\sqrt{2}} \varepsilon_1(G) + \frac{1}{2} \varepsilon_2(G) + \sum_{i=4}^{20} \varepsilon_i(G) \frac{1}{11},
\end{aligned} \tag{12}$$

and by Lemma 2 and some simple calculations,

$$\begin{aligned}
R(G) &\geq \frac{4m - M_1(G)}{\sqrt{2}} + \frac{M_1(G) - 3m}{2} + 3 \left[\frac{1}{\sqrt{2}} - \frac{1}{2} \right] \sum_{i=4}^{20} \varepsilon_i(G) - \left[\frac{1}{\sqrt{2}} - \frac{1}{11} \right] \sum_{i=4}^{20} \varepsilon_i(G) \\
&= \frac{4m - M_1(G)}{\sqrt{2}} + \frac{M_1(G) - 3m}{2} + \left[\frac{2}{\sqrt{2}} - \frac{3}{2} + \frac{1}{11} \right] \sum_{i=4}^{20} \varepsilon_i(G) \\
&\geq \frac{4m - M_1(G)}{\sqrt{2}} + \frac{M_1(G) - 3m}{2},
\end{aligned} \tag{13}$$

with equality if and only if $G \cong P_n$.

- (2) A similar argument as the case 1, it can be proved that for $\Delta(G) \leq 3$ and $m_{2,2}(G) = m_{1,4}(G) = m_{2,3}(G) = 0$,

$$\begin{aligned}
R(G) &\geq \frac{4m - M_1(G)}{\sqrt{2}} + \frac{M_1(G) - 3m}{\sqrt{3}} + \left[\frac{2}{\sqrt{2}} - \frac{3}{\sqrt{3}} + \frac{1}{3} \right] \varepsilon_4(G) \\
&\geq \frac{4m - M_1(G)}{\sqrt{2}} + \frac{M_1(G) - 3m}{\sqrt{3}},
\end{aligned} \tag{14}$$

with equality if and only if $G \cong S_4$. For $\Delta(G) \leq 5$ and $m_{2,2}(G) = m_{1,4}(G) = m_{2,3}(G) = m_{1,5}(G) = m_{2,4}(G) = m_{3,3}(G) = 0$,

$$\begin{aligned}
R(G) &\geq \frac{4m - M_1(G)}{\sqrt{2}} + \frac{M_1(G) - 3m}{\sqrt{3}} + \left[\frac{3}{\sqrt{2}} - \frac{4}{\sqrt{3}} + \frac{1}{5} \right] \sum_{i=5}^8 \varepsilon_i(G) \\
&\geq \frac{4m - M_1(G)}{\sqrt{2}} + \frac{M_1(G) - 3m}{\sqrt{3}},
\end{aligned} \tag{15}$$

with equality if and only if $G \cong S_4$. This completes the proof. $\square$

Theorem 2 (see [6]). Let G be a graph with n vertices. Then,

$$R(G) = \frac{n}{2} - \frac{1}{2} \sum_{uv \in E(G)} \left(\frac{1}{\sqrt{\deg_G(u)}} - \frac{1}{\sqrt{\deg_G(v)}} \right)^2. \tag{16}$$

Lemma 3 (see [15]). If G is a connected graph with n vertices and cyclomatic number c , then $n_1(G) = 2 - 2c + \sum_{i=3}^{\Delta(G)} (i - 2)n_i$ and $n_2(G) = 2c + n - 2 - \sum_{i=3}^{\Delta(G)} (i - 1)n_i$.

Corollary 1. Let G be a connected graph with n vertices and cyclomatic number c .

- (1) If $c = 5$, then $n_1(G) = \sum_{i=3}^{\Delta(G)} (i - 2)n_i - 8$ and $n_2(G) = n + 8 - \sum_{i=3}^{\Delta(G)} (i - 1)n_i$
- (2) If $c = 6$, then $n_1(G) = \sum_{i=3}^{\Delta(G)} (i - 2)n_i - 10$ and $n_2(G) = n + 10 - \sum_{i=3}^{\Delta(G)} (i - 1)n_i$

Define $Y_1(n) = \{G | n_3 = 8, n_2 = n - 8\}$, $Y_2(n) = \{G | n_1 = 1, n_3 = 9, n_2 = n - 10\}$, $Y_3(n) = \{G | n_3 = 10, n_2 = n - 10\}$, and $Y_4(n) = \{G | n_1 = 1, n_3 = 11, n_2 = n - 12\}$.

Lemma 4. Let G be a connected graph with n vertices, m edges, and cyclomatic number c .

- (1) Suppose $n_1 = 0$ and $0 < n_i < n$ for some $3 \leq i \leq n-1$. Then, $m_{i,i}(G) \leq n_i(G) - 2 + c$.
- (2) Suppose $n_1 \geq 1$ and $0 < n_i < n$ for some $3 \leq i \leq n-1$. Then, $m_{i,i}(G) \leq n_i(G) - 1 + c$.

Proof. Since $n_1 = 0$, $c(G-v) \leq c(G) - 1$, for all $v \in V(G)$. Now, the proof follows from this fact that $m = n - 1 + c$. The part (2) is similar.

Let n be a positive integer. Define

$$\begin{aligned}\Omega_1(n) &= \{G \in Y_1(n) | m_{3,3} = 11, m_{2,3} = 2, m_{2,2} = n - 9\}, \\ \Omega_2(n) &= \{G \in Y_2(n) | m_{3,3} = 13, m_{2,3} = 1, m_{1,2} = 1, m_{2,2} = n - 11\}, \\ \Omega_3(n) &= \{G \in Y_3(n) | m_{3,3} = 14, m_{2,3} = 2, m_{2,2} = n - 11\}, \\ \Omega_4(n) &= \{G \in Y_4(n) | m_{3,3} = 16, m_{2,3} = 1, m_{1,2} = 1, m_{2,2} = n - 13\}.\end{aligned}\tag{17}$$

If $G_i \in \Omega_i(n)$ for $1 \leq i \leq 4$, then $R(G_1) = (1/2)n - (5 - 2\sqrt{6}/6)$, $R(G_2) = (1/2)n - (7 - (\sqrt{6} + 3\sqrt{2})/6)$, $R(G_3) = (1/2)n - (5 - 2\sqrt{6}/6)$, and $R(G_4) = (1/2)n - (7 - (\sqrt{6} + 3\sqrt{2})/6)$. $\square$

Theorem 3. The following hold:

- (1) Let G be a connected graph with $n \geq 9$ vertices and cyclomatic number 5. Then, $R(G) \leq (1/2)n - (5 - 2\sqrt{6}/6)$, with equality if and only if $G \in \Omega_1(n)$.
- (2) Let G be a connected graph with $n \geq 11$ vertices and cyclomatic number 6. Then, $R(G) \leq (1/2)n - (5 - 2\sqrt{6}/6)$, with equality if and only if $G \in \Omega_3(n)$.

Proof

- (1) If $n_1(G) = 0$, then by Corollary 1 and Theorem 2, $R(G) \leq (1/2)n - (5 - 2\sqrt{6}/6)$, with equality if and

only if $G \in \Omega_1(n)$. For $n_1(G) = 1$, $R(G) \leq (1/2)n - (7 - (\sqrt{6} + 3\sqrt{2})/6) < (1/2)n - (5 - 2\sqrt{6}/6)$. Let $n_1(G) \geq 2$. Then, again by Corollary 1 and Theorem 2, $R(G) \leq (1/2)n - (3 - 2\sqrt{2}/2) < (1/2)n - (5 - 2\sqrt{6}/6)$.

- (2) Proof is similar to the last case, and we omit it. $\square$

Remark 1

- (1) Let G be a connected graph with $n = 8$ vertices and cyclomatic number 5. Then, $R(G) \leq 4$, with equality if and only if G is a 3-regular graph.
- (2) Let G be a connected graph with $n = 10$ vertices and cyclomatic number 6. Then, $R(G) \leq 5$, with equality if and only if G is a 3-regular graph.

For a positive number $c \geq 3$, we define

$$\begin{aligned}\Lambda_c^1(n) &= \{G | m_{3,3} = 3c - 4, m_{2,3} = 2, m_{2,2} = n - (2c - 1)\}, \\ \Gamma_c^1(n) &= \{G | m_{3,3} = 3c - 2, m_{2,3} = 1, m_{1,2} = 1, m_{2,2} = n - (2c + 1)\}.\end{aligned}\tag{18}$$

If $G_1 \in \Lambda_c^1(n)$ and $G_2 \in \Gamma_c^1(n)$, then $R(G_1) = (1/2)n - (5 - 2\sqrt{6}/6)$ and $R(G_2) = (1/2)n - (7 - (\sqrt{6} + 3\sqrt{2})/6)$.

Proposition 1. Let G be a connected graph with n vertices, m edges, and cyclomatic number c , where $c \geq 3$ is a positive integer. If $n \geq 2c - 1$ and $n_1(G) = 0$, then $n_2(G) \geq 1$.

Proof. Those are well-known that $c = m - n + 1$ and $\sum_{i=1}^n n_i(G)i = 2m$. Therefore, $2c = 2n_2(G) + \sum_{i=3}^n n_i(G)i - 2n + 2$. Thus, $2c \geq 2n_2(G) + 3(n - n_2(G)) - 2n + 2 = n - n_2(G) + 2$, and this implies that $n_2(G) \geq n - 2c + 2$. Now, since $n \geq 2c - 1$, $n_2(G) \geq 1$.

By Proposition 1 and a similar argument as the proof of Theorem 3, we will have the following general result. $\square$

Theorem 4. Let G be a connected graph with n vertices and cyclomatic number c , where $c \geq 3$ is a positive integer.

- (1) If $n \geq 2c - 1$, then $R(G) \leq (1/2)n - (5 - 2\sqrt{6}/6)$, with equality if and only if $G \in \Lambda_c^1(n)$.
- (2) If $n = 2c - 2$, then $R(G) \leq (1/2)n$, with equality if and only if G is a 3-regular graph.

Let n be a positive number, $Y_5(n) = \{G | n_1 = 0, n_4 = 1, n_3 = 6, n_2 = n - 7\}$ and $Y_6(n) = \{G | n_1 = 0, n_4 = 1, n_3 = 8, n_2 = n - 9\}$. Define

$$\begin{aligned}
\Omega_5(n) &= \{G \in Y_5(n) | m_{4,3} = 4, m_{3,3} = 6, m_{2,3} = 2, m_{2,2} = n - 8\}, \\
\Omega_6(n) &= \{G \in Y_1(n) | m_{3,3} = 10, m_{2,3} = 4, m_{2,2} = n - 10\}, \\
\Omega_7(n) &= \{G \in Y_6(n) | m_{4,3} = 4, m_{3,3} = 9, m_{2,3} = 2, m_{2,2} = n - 10\}, \\
\Omega_8(n) &= \{G \in Y_3(n) | m_{3,3} = 13, m_{2,3} = 4, m_{2,2} = n - 12\}.
\end{aligned} \tag{19}$$

If $G_i \in \Omega_5(n)$ for $1 \leq i \leq 4$, then $R(G_1) = (1/2)n - (6 - (2\sqrt{3} + \sqrt{6})/3)$, $R(G_2) = (1/2)n - (5 - 2\sqrt{6}/3)$, $R(G_3) = (1/2)n - (6 - (2\sqrt{3} + \sqrt{6})/3)$ and $R(G_4) = (1/2)n - (5 - 2\sqrt{6}/3)$.

Theorem 5. *The following hold:*

- (1) Let G be a connected graph with $n \geq 9$ vertices and cyclomatic number 5. If $G \notin \Omega_1(n)$, then $R(G) \leq (1/2)n - (6 - (2\sqrt{3} + \sqrt{6})/3)$, with equality if and only if $G \in \Omega_5(n)$.
- (2) Let G be a connected graph with $n \geq 11$ vertices and cyclomatic number 6. If $G \notin \Omega_3(n)$, then $R(G) \leq (1/2)n - (6 - (2\sqrt{3} + \sqrt{6})/3)$, with equality if and only if $G \in \Omega_7(n)$.

Proof

- (1) Let $n_1(G) = 0$ and $G \notin \Omega_1(n)$. For $\Delta(G) = 3$, $m_{2,3} \geq 4$ and Corollary 1 and Theorem 2 give $R(G) \leq (1/2)n - (5 - 2\sqrt{6}/3) < (1/2)n - (6 - (2\sqrt{3} + \sqrt{6})/3)$. For $\Delta(G) \geq 4$, $R(G) \leq (1/2)n - (6 - (2\sqrt{3} + \sqrt{6})/3)$, with equality if and only if $G \in \Omega_5(n)$. If $n_1(G) \geq 1$,

then $R(G) \leq (1/2)n - (7 - (\sqrt{6} + 3\sqrt{2})/6) < (1/2)n - (6 - (2\sqrt{3} + \sqrt{6})/3)$.

(2) Proof is similar to Case 1, and we omit it.

By a simple calculation, one can easily see that Theorem 5 (1) holds for $n = 8$ and Theorem 5 (2) holds for $n = 10$. On the other hand, Theorems 3 and 5 imply the following result. $\square$

Corollary 2. *The following hold:*

- (1) Suppose $n \geq 9$. The connected graphs with cyclomatic number 5 in the sets $\Omega_1(n)$ and $\Omega_5(n)$ have the first and second maximum Randić index among all n -vertex connected graphs with cyclomatic number 5, respectively.
- (2) Suppose $n \geq 11$. The connected graphs with cyclomatic number 6 in the sets $\Omega_7(n)$ and $\Omega_8(n)$ have the first and second maximum Randić index among all n -vertex connected graphs with cyclomatic number 6, respectively.

Suppose $c \geq 4$ is a positive integer. Define

$$\begin{aligned}
\Lambda_c^2(n) &= \{G | m_{3,3} = 3c - 5, m_{2,3} = 4, m_{2,2} = n - 2c\}, \\
\Gamma_c^2(n) &= \{G | m_{4,3} = 4, m_{3,3} = 3c - 9, m_{2,3} = 2, m_{2,2} = n - (2c - 2)\}.
\end{aligned} \tag{20}$$

If $H_1 \in \Lambda_c^2(n)$ and $H_2 \in \Gamma_c^2(n)$, then $R(H_1) = (1/2)n - (5 - 2\sqrt{6}/3)$ and $R(H_2) = (1/2)n - (6 - (2\sqrt{3} + \sqrt{6})/3)$.

Theorem 6. *Let G be a connected graph with n vertices and cyclomatic number $c \geq 4$.*

- (1) If $n \geq 2c - 1$ and $G \notin \Lambda_c^1(n)$, then $R(G) \leq (1/2)n - (6 - (2\sqrt{3} + \sqrt{6})/3)$, with equality if and only if $G \in \Gamma_c^2(n)$.
- (2) If $n = 2c - 2$ and G is not a 3-regular graph, then $R(G) \leq (1/2)n - (6 - (2\sqrt{3} + \sqrt{6})/3)$, with equality if and only if $G \in \Gamma_c^2(n)$.

Proof. The result follows from Proposition 1 and a similar argument as Theorem 3.

We end this section with the following result that follows from Theorems 4 and 6. $\square$

Theorem 7. *Let G be a connected graph with n vertices and cyclomatic number $c \geq 4$.*

- (1) If $n \geq 2c - 1$, then the connected graphs with cyclomatic number c in the sets $\Lambda_c^1(n)$ and $\Gamma_c^2(n)$ have the first and second maximum Randić index among all n -vertices connected graphs with cyclomatic number c , respectively.
- (2) If $n = 2c - 2$, then the 3-regular connected graphs and the connected graphs in the set $\Gamma_c^2(n)$ with cyclomatic number c have the first and second maximum Randić index among all n -vertices connected graphs with cyclomatic number c , respectively.

4. Connected Chemical Graphs

Let G be a connected chemical graph with n vertices and m edges. By Lemma 3,

$$\begin{aligned} n_1 &= 2n - 2m + n_3 + 2n_4, \\ n_2 &= 2m - n - 2n_3 - 3n_4, \end{aligned} \quad (21)$$

and by Lemma 2,

$$\begin{aligned} \varepsilon_1(G) &= 4m - [n_1 + 4n_2 + 9n_3 + 16n_4] + \varepsilon_3(G) + 2\varepsilon_4(G) + 3\varepsilon_5(G) + 4\varepsilon_6(G), \\ \varepsilon_2(G) &= n_1 + 4n_2 + 9n_3 + 16n_4 - 3m - [2\varepsilon_3(G) + 3\varepsilon_4(G) + 4\varepsilon_5(G) + 5\varepsilon_6(G)]. \end{aligned} \quad (22)$$

Now, by some calculations, we have

$$\begin{aligned} \varepsilon_1(G) &= 2n - 2m - 2n_3 - 6n_4 + \varepsilon_3(G) + 2\varepsilon_4(G) + 3\varepsilon_5(G) + 4\varepsilon_6(G), \\ \varepsilon_2(G) &= 3m - 2n + 2n_3 + 6n_4 - [2\varepsilon_3(G) + 3\varepsilon_4(G) + 4\varepsilon_5(G) + 5\varepsilon_6(G)]. \end{aligned} \quad (23)$$

Suppose $M_k = \{m_{i,j} | 1 \leq i \leq j \leq 4 \text{ and } i + j = k + 2\}$, $1 \leq k \leq 4$. Since $\varepsilon_k = \sum_{x \in M_k} x$, $1 \leq k \leq 4$,

$$\begin{aligned} m_{1,2} &= 2n - 2m - 2n_3 - 6n_4 + m_{1,4} + m_{2,3} + 2m_{2,4} + 2m_{3,3} + 3m_{3,4} + 4m_{4,4}, \\ m_{2,2} &= 3m - 2n + 2n_3 + 6n_4 - [m_{1,3} + 2m_{1,4} + 2m_{2,3} + 3m_{2,4} + 3m_{3,3} + 4m_{3,4} + 5m_{4,4}], \end{aligned} \quad (24)$$

and since $m_{1,3} = 3n_3 - m_{2,3} - 2m_{3,3} - m_{3,4}$ and $m_{1,4} = 4n_4 - m_{2,4} - m_{3,4} - 2m_{4,4}$,

On the other hand,

$$\begin{aligned} m_{1,2} &= 2n - 2m - 2n_3 - 2n_4 + m_{2,3} + m_{2,4} + 2m_{3,3} \\ &\quad + 2m_{3,4} + 2m_{4,4}, \end{aligned} \quad (25)$$

$$\begin{aligned} m_{2,2} &= 3m - 2n - n_3 - 2n_4 - m_{2,3} - m_{2,4} - m_{3,3} \\ &\quad - m_{3,4} - m_{4,4}. \end{aligned} \quad (26)$$

$$R(G) = \frac{1}{\sqrt{2}}m_{1,2} + \frac{1}{\sqrt{3}}m_{1,3} + \frac{1}{2}m_{1,4} + \frac{1}{2}m_{2,2} + \frac{1}{\sqrt{6}}m_{2,3} + \frac{1}{\sqrt{8}}m_{2,4} + \frac{1}{3}m_{3,3} + \frac{1}{\sqrt{12}}m_{3,4} + \frac{1}{4}m_{4,4}. \quad (27)$$

By equations (25)–(27), we have

$$\begin{aligned} R(G) &= \frac{1}{2}(3 - 2\sqrt{2})(m + 2\sqrt{2}n + 2n) - \frac{1}{2}(1 - 2\sqrt{3} + 2\sqrt{2})n_3 \\ &\quad - (\sqrt{2} - 1)n_4 + \frac{1}{6}(\sqrt{3}\sqrt{2} + 3\sqrt{2} - 2\sqrt{3} - 3)m_{2,3} + \frac{1}{4}(3\sqrt{2} - 4)m_{2,4} \\ &\quad + \frac{1}{6}(6\sqrt{2} - 4\sqrt{3} - 1)m_{3,3} + \frac{1}{6}(6\sqrt{2} - \sqrt{3} - 6)m_{3,4} + \frac{1}{4}(4\sqrt{2} - 5)m_{4,4}. \end{aligned} \quad (28)$$

Theorem 8. Let G be a connected chemical graph with $n > 5$ vertices and m edges. Then,

(1) $R(G) \leq (1/2)(3 - 2\sqrt{2})(m + 2\sqrt{2}n + 2n)$, with equality if and only if $G \cong P_n$ or C_n

$$(2) R(G) \geq (1/6)(2\sqrt{2} - 3)((\sqrt{3}\sqrt{2} + 2\sqrt{3} - 3\sqrt{2} - 3)n - \sqrt{3}\sqrt{2} - 2\sqrt{3} + 3\sqrt{2} - 3m + 3)$$

Proof. It is easy to see that $n_3 \geq (1/3)(m_{2,3} + 2m_{3,3} + m_{3,4})$ and $n_4 \geq (1/4)(m_{2,4} + m_{3,4} + 2m_{4,4})$. Therefore, by equation (28), we have

$$\begin{aligned} R(G) &\leq \frac{1}{2}(3 - 2\sqrt{2})(m + 2\sqrt{2}n + 2n) - \frac{1}{6}(4 - \sqrt{3}\sqrt{2} - \sqrt{2})m_{2,3} \\ &\quad - \frac{1}{4}(3 - 2\sqrt{2})m_{2,4} - \frac{1}{6}(3 - 2\sqrt{2})m_{3,3} - \frac{1}{12}(11 - 2\sqrt{3} - 5\sqrt{2})m_{3,4} \\ &\quad - \frac{1}{4}(3 - 2\sqrt{2})m_{4,4} \leq \frac{1}{2}(3 - 2\sqrt{2})(m + 2\sqrt{2}n + 2n), \end{aligned} \quad (29)$$

with equality if and only if $G \cong P_n$ or C_n . On the other hand, $n_3 + n_4 \leq n$ and $m_{2,3} + m_{2,4} + m_{3,3} + m_{3,4} + m_{4,4} \geq n_3 + n_4 - 1$. Therefore, by equation (28),

$$\begin{aligned} R(G) &\geq \frac{1}{2}(3 - 2\sqrt{2})(m + 2\sqrt{2}n + 2n) - (\sqrt{2} - 1)(n_3 + n_4) \\ &\quad + \frac{1}{6}(\sqrt{3}\sqrt{2} + 3\sqrt{2} - 2\sqrt{3} - 3)(n_3 + n_4 - 1) \\ &\geq \frac{1}{2}(3 - 2\sqrt{2})(m + 2\sqrt{2}n + 2n) - \frac{1}{6}(3\sqrt{2} + 2\sqrt{3} - 3 - \sqrt{3}\sqrt{2})(n_3 + n_4 + 5 - 2\sqrt{3}\sqrt{2}) \\ &\geq \frac{1}{6}(2\sqrt{2} - 3)((\sqrt{3}\sqrt{2} + 2\sqrt{3} - 3\sqrt{2} - 3)n - \sqrt{3}\sqrt{2} - 2\sqrt{3} + 3\sqrt{2} - 3m + 3). \end{aligned} \quad (30)$$

This completes the proof. $\square$

Data Availability

All data generated or analyzed during this study are included in this published article. There are no experimental data in this article.

Conflicts of Interest

The authors declare that there are no conflicts of interest regarding the publication of this article.

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