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On the Randić index of unicyclic conjugated molecules

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The Randić index $R(G)$ of a graph G is 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 the vertex u. In this paper, we first present a sharp lower bound on the Randić index of conjugated unicyclic graphs (unicyclic graphs with perfect matching). Also a sharp lower bound on the Randić index of unicyclic graphs is given in terms of the order and given size of matching.

KEY WORDS: Randić index, unicyclic graph, given size of matching

AMS subject classification: 05C35

1. Introduction

For a (molecular) graph $G = (V, E)$, the *Randić index* $R(G)$ is defined in [12] as

$$R(G) = \sum_{uv \in E} [d(u)d(v)]^{-\frac{1}{2}}.$$

It is well known that Randić [12] introduced the index, which he called the *branching index* or *molecular connectivity index*, in his study of alkanes. The Randić index has been closely correlated with many chemical properties (see [7,8]). Recently, the Randić index attracted the attention of many researchers and many results are obtained (see [1, 4–6, 9–11, 14]). In particular, Gao and Lu [6] gave sharp lower and upper bounds for $R(G)$ of unicyclic graphs. In [10], Lu, et al. obtain sharp lower bounds on $R(G)$ of trees with a given size of matching. Here, we consider a type graph, namely that of conjugated unicyclic graphs (unicyclic graphs with perfect matching), and give sharp lower bounds on the Randić index of unicyclic graph with a given size of matching.

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We first introduce some terminologies and notations of graphs. Other undefined terminologies and notations may refer to [2]. We only consider finite, undirected and simple graphs. Denote by C_n the cycle of n vertices. For a vertex x of a graph G, we denote the neighborhood and the degree of x by $N(x)$ and $d(x)$, respectively. A *pendant vertex* is a vertex of degree 1. Denote by PV the set of pendant vertices of G. Let $d_G(x, y)$ denote the length of a shortest (x, y)-path in G. We will use $G-x$ to denote the graph that arises from G by deleting the vertex $x \in V(G)$ together with its incident edges. An edge e of G is said to be *contracted* if it is deleted and its ends are identified; the resulting graph is denoted by $G \cdot e$. A subset $M \subseteq E$ is called a *matching* in G if its elements are edges and no two are adjacent in G. A matching M *saturates* a vertex v, and v is said to be M-*saturated*, if some edge of M is incident with v. If every vertex of G is M-saturated, the matching M is *perfect*. A matching M is said to be an m-*matching*, if $|M| = m$ and for every matching M' in G, $|M'| \leqslant m$.

Let n and m be positive integers with $n \geqslant 2m$. Let $U_{n,m}$ be a graph with n vertices obtained from C_3 by attaching $n-2m+1$ pendent edges and $m-2$ paths of length 2 to one vertex of C_3 (see figure 1).

Unicyclic graphs are connected graphs with n vertices and n edges. Denote $\mathscr{U}_{n,m} = \{G : G$ is a unicyclic graph with n vertices and an m-matching$\}$.

2. Lemmas and results

We first give some lemmas that will be used in the proof of our results.

Lemma 1 [3]. Let $G \in \mathscr{U}_{2m,m}$, $m \geqslant 3$, and let T be a tree in G attached to a root r. If $v \in V(T)$ is a vertex furthest from the root r with $d_G(v, r) \geqslant 2$, then v is a pendant vertex and adjacent to a vertex u of degree 2.

Lemma 2 [13]. Let $G \in \mathscr{U}_{n,m} (n > 2m)$ and $G \ncong C_n$. Then there is an m-matching M and a pendant vertex v such that M does not saturate v.

Lemma 3 [11]. Let $G \in \mathscr{U}_{2m,m}$. If $PV \neq \emptyset$, then for any vertex $u \in V(G)$, $|N(u) \cap PV| \leqslant 1$.

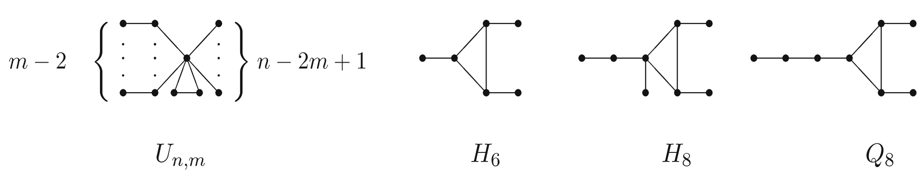


Figure 1.

Denote

$$h(x, y) = \frac{y}{\sqrt{x}} + \frac{x-y}{\sqrt{2x}}, \quad 0 \leqslant y \leqslant x-1, \tag{1}$$

and

$$f(x) = \frac{1}{\sqrt{x+1}} + \frac{x}{\sqrt{2(x+1)}}, \quad x \geqslant 1,$$

where x and y are integers.

Lemma 4 [10,11]. (i) The function $h(x-1, y) - h(x, y+1)$ are monotonously increasing in $x \geqslant 2$ and $y \geqslant 0$, respectively;
(ii) the function $f(x) - f(x+1)$ is monotonously increasing in $x \geqslant 1$.

Lemma 5. Let $g(x) = \dfrac{2}{\sqrt{x}} + \dfrac{x-2}{\sqrt{2x}}, x \geqslant 3$. Then the function $g(x) - g(x+1)$ is monotonously increasing in $x \geqslant 3$.

Proof. Note that $\dfrac{d^2 g(x)}{dx^2} = -\dfrac{1}{2}x^{-\frac{5}{2}}\left(\dfrac{\sqrt{2}}{4}x + \dfrac{3\sqrt{2}}{2} - 3\right) < 0$, and hence the lemma holds. □

Lemma 6 [9]. Let G be a simple connected graph of order n. Then

$$R(G) \leqslant \frac{n}{2}$$

with equality if and only if G is a regular graph.

Denote

$$\psi(n, m) = \frac{n-2m+1}{\sqrt{n-m+1}} + \frac{m}{\sqrt{2(n-m+1)}} + \frac{m}{\sqrt{2}} + \frac{1-2\sqrt{2}}{2},$$

where n and m are positive integers and $n \geqslant 2m$.

Lemma 7. If $m \geqslant 3$, then $\psi(2m-1, m-1) + 1 > \psi(2m+1, m)$, $\psi(2m-2, m-1) + \dfrac{1}{\sqrt{3}} + \dfrac{2}{\sqrt{6}} - \dfrac{1}{2} > \psi(2m, m)$ and $\psi(2m-2, m-1) + \dfrac{1}{\sqrt{3}} + \dfrac{1}{3} > \psi(2m, m)$.

Proof. First we have

$$\begin{aligned}
&\psi(2m-1, m-1) - \psi(2m+1, m) + 1 \\
&= \frac{2}{\sqrt{m+1}} + \frac{m-1}{\sqrt{2(m+1)}} - \frac{2}{\sqrt{m+2}} - \frac{m}{\sqrt{2(m+2)}} - \frac{1}{\sqrt{2}} + 1 \\
&\geqslant 1 + \frac{2}{\sqrt{8}} - \frac{2}{\sqrt{5}} - \frac{3}{\sqrt{10}} - \frac{1}{\sqrt{2}} + 1 > 0,
\end{aligned}$$

where the last second inequality follows by lemma 5.

Similarly,

$$\begin{aligned}
&\psi(2m-2, m-1) - \psi(2m, m) + \frac{1}{\sqrt{3}} + \frac{2}{\sqrt{6}} - \frac{1}{2} \\
&= \frac{m-1}{\sqrt{2m}} + \frac{1}{\sqrt{m}} - \frac{m}{\sqrt{2(m+1)}} - \frac{1}{\sqrt{m+1}} - \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{3}} + \frac{2}{\sqrt{6}} - \frac{1}{2} \\
&\geqslant \frac{2}{\sqrt{6}} + \frac{1}{\sqrt{3}} - \frac{3}{\sqrt{8}} - \frac{1}{2} - \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{3}} + \frac{2}{\sqrt{6}} - \frac{1}{2} \\
&= \frac{4}{\sqrt{6}} + \frac{2}{\sqrt{3}} - \frac{3}{\sqrt{8}} - \frac{1}{\sqrt{2}} - 1 > 0,
\end{aligned}$$

where the last second inequality follows by lemma 4(ii).

Next note that $\psi(2m-2, m-1) - \psi(2m, m) + \frac{1}{\sqrt{3}} + \frac{1}{3} > \psi(2m-2, m-1) - \psi(2m, m) + \frac{1}{\sqrt{3}} + \frac{2}{\sqrt{6}} - \frac{1}{2} > 0$, and hence the lemma holds. □

We first obtain the following result.

Theorem 8. Let $G \in \mathscr{U}_{2m,m} \backslash \{H_6, H_8\} (m \geqslant 2)$. Then

$$R(G) \geqslant \psi(2m, m). \tag{2}$$

Furthermore, equality in (2) holds if and only if $G \cong U_{2m,m}$.

Proof. First we note that if $G \cong U_{2m,m}$, then equality in (2) holds clearly.

Now we prove that if $G \in \mathscr{U}_{2m,m}$, then (2) holds and equality in (2) holds only if $G \cong U_{2m,m}$.

If $m = 2$, then either $G \cong C_4$ or $G \cong U_{4,2}$. Note that $R(C_4) = 2 > R(U_{4,2}) = \frac{1}{2} + \frac{1}{\sqrt{3}} + \frac{1}{\sqrt{6}} = 1.8939$. Thus the theorem holds for $m = 2$.

We now suppose that $m \geqslant 3$ and proceed by induction on m.

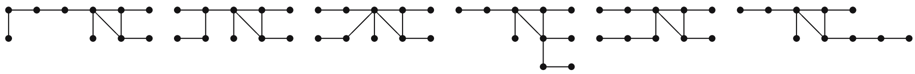
If $G \cong C_{2m}$, by the induction hypothesis and lemma 7, then

$$\begin{aligned}
R(G) = R(C_{2(m-1)}) + 1 > \psi(2m-2, m-1) + 1 > \psi(2m-2, m-1) + \frac{1}{\sqrt{3}} \\
+ \frac{1}{3} > \psi(2m, m).
\end{aligned}$$

So in the following proof, we can assume that $G \ncong C_{2m}$.

By lemmas 1 and 3, we only consider the following two cases.

Case 1. G has a pendant vertex v which is adjacent to a vertex w of degree 2.



4.6260 4.5478 4.4983 4.5260 4.6867 4.6640

G_1 G_2 G_3 G_4 G_5 G_6

Figure 2.

In this case, there is a unique vertex $u \neq v$ such that $uw \in E(G)$. Denote $N(u) \cap PV = \{v_1, \ldots, v_{r-1}, v_r\}$ and $N(u) \setminus PV = \{x_1, \ldots, x_{t-r-1}, x_{t-r} = w\}$. Then $t \leqslant m+1$ and all $d(x_j) = d_j \geqslant 2$.

Let $G' = G - v - w$. Then $G' \in \mathscr{U}_{2(m-1),m-1}$.

If $G' \cong H_6$, then $G \cong Q_8$ and $R(Q_8) = 3.7701 > \psi(8,4) = 3.6263$.

If $G' \cong H_8$, then $G \in \{G_i | 1 \leqslant i \leqslant 6\}$, where G_i $(1 \leqslant i \leqslant 6)$ are illustrated in figure 2.

By $\psi(10,5) = 4.4729$, it is easy to verify that $U_{10,5}$ has the minimum Randić index among all unicyclic graphs in $\{G_i | 1 \leqslant i \leqslant 6\} \cup \{U_{10,5}\}$ (see figure 2).

Otherwise, if $G' \notin \{H_6, H_8\}$, by the induction hypothesis, then

$$
\begin{aligned}
R(G) &= R(G') + \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2t}} + r\left(\frac{1}{\sqrt{t}} - \frac{1}{\sqrt{t-1}}\right) + \sum_{i=1}^{t-r-1} \frac{1}{\sqrt{d_i}}\left(\frac{1}{\sqrt{t}} - \frac{1}{\sqrt{(t-1)}}\right) \\
&\geqslant R(G') + \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2t}} + r\left(\frac{1}{\sqrt{t}} - \frac{1}{\sqrt{t-1}}\right) + (t-r-1)\left(\frac{1}{\sqrt{2t}} - \frac{1}{\sqrt{2(t-1)}}\right) \\
&\geqslant \psi(2m-2, m-1) + \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2t}} + r\left(\frac{1}{\sqrt{t}} - \frac{1}{\sqrt{t-1}}\right) \\
&\quad + (t-r-1)\left(\frac{1}{\sqrt{2t}} - \frac{1}{\sqrt{2(t-1)}}\right) \\
&= \psi(2m, m) + \frac{m-1}{\sqrt{2m}} + \frac{1}{\sqrt{m}} - \frac{m}{\sqrt{2(m+1)}} - \frac{1}{\sqrt{m+1}} \\
&\quad + \frac{1}{\sqrt{2t}} + r\left(\frac{1}{\sqrt{t}} - \frac{1}{\sqrt{t-1}}\right) + (t-r-1)\left(\frac{1}{\sqrt{2t}} - \frac{1}{\sqrt{2(t-1)}}\right).
\end{aligned} \tag{3}
$$

Note that $r \leqslant 1$ by lemma 3. If $r = 1$, by (3), then

$$
\begin{aligned}
R(G) &\geqslant \psi(2m, m) + \frac{m-1}{\sqrt{2m}} + \frac{1}{\sqrt{m}} - \frac{m}{\sqrt{2(m+1)}} - \frac{1}{\sqrt{m+1}} \\
&\quad + \frac{t-1}{\sqrt{2t}} + \frac{1}{\sqrt{t}} - \frac{t-2}{\sqrt{2(t-1)}} - \frac{1}{\sqrt{t-1}} \\
&= \psi(2m, m) + [f(m-1) - f(m)] - [f(t-2) - f(t-1)] \\
&\geqslant \psi(2m, m),
\end{aligned}
$$

where $f(x)$ is defined in (1) and the last inequality follows by lemma 4 as $m-1 \geqslant t-2$. In order for the equality to hold, all inequalities in the above argument should be equalities. Thus we have

$$R(G') = \psi(2m-2, m-1), \quad m = t-1, \quad r = 1 \text{ and } d_1 = \cdots = d_{t-1} = 2.$$

By the induction hypothesis, $G' \cong U_{2m-2,m-1}$. Note that $U_{2m-2,m-1}$ has a unique vertex of degree greater than 2, and hence $G \cong U_{2m,m}$.

If $r = 0$, by (3), then

$$\begin{aligned} R(G) \geqslant\ & \psi(2m, m) + \left(\frac{1}{\sqrt{2}} - 1\right)\left(\frac{1}{\sqrt{t}} - \frac{1}{\sqrt{t-1}}\right) \\ & + [f(m-1) - f(m)] - [f(t-2) - f(t-1)] \\ >\ & \psi(2m, m). \end{aligned}$$

Case 2. G is a cycle C together with some pendant edges attached to some vertices on C. For convenience, we label the vertices of C with $u_1, u_2, \ldots, u_p$ one by one clockwise.

If each vertex of C is attached by a pendant edges, then $m \geqslant 4$ as $G \ncong H_6$. If $m = 4$, then $R(G) = 4 \cdot \left(\frac{1}{3} + \frac{1}{\sqrt{3}}\right) = 3.6427 > \psi(8, 4) = 3.6263$. If $m \geqslant 5$, by the induction hypothesis and lemma 7, then

$$\begin{aligned} R(G) = (m-1) \cdot \left(\frac{1}{3} + \frac{1}{\sqrt{3}}\right) + \frac{1}{3} + \frac{1}{\sqrt{3}} > \psi(2m-2, m-1) + \frac{1}{3} \\ + \frac{1}{\sqrt{3}} > \psi(2m, m). \end{aligned}$$

Otherwise, there is at least a vertex of degree two on C. Since $G \ncong C_n$, there exists some $i \in \{1, 2, \ldots, n\}$ such that $d_G(u_i) = 3$ and $d_G(u_{i+1}) = 2$, where $u_{n+1} = u_1$. Without loss of generality, assume $d_G(u_2) = 3$ and $d_G(u_3) = 2$. Denote by v_2 the pendant vertex adjacent to u_2. Obviously, every pair of vertices of degree three can not be adjacent to a common vertex of degree two (since G has a perfect matching). Then each vertex of degree two on C must be adjacent to another vertex of degree two. Thus $d_G(u_4) = 2$.

Let $G' = (G \cdot u_2 v_2) \cdot u_2 u_3$ be a graph obtained from G by contracting $u_2 v_2$ and $u_2 u_3$ consecutively. Then $G' \in \mathscr{U}_{n-2,m-1} \backslash \{H_6, H_8\}$. By the induction hypothesis and lemma 7, if $d_G(u_1) = 3$, then

$$R(G) = R(G') + \frac{1}{\sqrt{3}} + \frac{1}{\sqrt{6}} + \frac{1}{3} - \frac{1}{\sqrt{6}} \geqslant \psi(2m-2, m-1) + \frac{1}{\sqrt{3}} + \frac{1}{3} > \psi(2m, m);$$

and if $d_G(u_1) = 2$, then

$$R(G) = R(G') + \frac{1}{\sqrt{3}} + \frac{2}{\sqrt{6}} - \frac{1}{2} \geqslant \psi(2m-2, m-1) + \frac{1}{\sqrt{3}} + \frac{2}{\sqrt{6}} - \frac{1}{2} > \psi(2m, m).$$

Hence the proof of theorem 8 is complete. □

Note 9. It is easy to calculate that $R(H_6) = 2.7321 < \psi(6,3) = 2.7678$ and $R(H_8) = 3.6260 < \psi(8,4) = 3.6263$, where H_6 and H_8 are shown in figure 1. Thus, by theorem 8, H_6 has the minimum Randić index in $\mathscr{U}_{6,3}$ and H_8 has the minimum Randić index in $\mathscr{U}_{8,4}$.

Theorem 10. Let $G \in \mathscr{U}_{n,m}$ $(n \geqslant 2m,\ m \geqslant 5)$, then

$$R(G) \geqslant \psi(n,m) \tag{4}$$

and equality in (4) holds if and only if $G \cong U_{n,m}$.

Proof. First we note that if $G \cong U_{n,m}$, then the equality in (4) holds clearly.

Now applying induction on n, we prove that if $G \in \mathscr{U}_{n,m}$, then (4) holds and the equality in (4) holds only if $G \cong U_{n,m}$.

If $n = 2m$, then the theorem holds by theorem 8.

Therefore we assume that $n > 2m$ and the result holds for smaller values of n.

If $G \cong C_n$, then $n = 2m + 1$, since G has an m-matching. If $m = 5$, then $R(G) = \frac{11}{2} > \psi(11,5) = 4.7136$. If $m \geqslant 6$, by the induction hypothesis and lemma 7, then

$$R(G) = R(C_{2(m-1)+1}) + 1 > \psi(2m-1, m-1) + 1 > \psi(2m+1, m).$$

So in the following proof, we can assume $G \ncong C_n$.

By lemma 2, G has an m-matching M and a pendant vertex v such that M does not saturate v. Let $uv \in E(G)$ with $d(u) = t$. Denote $N(u) \cap PV = \{v_1, \ldots, v_{r-1},\ v_r = v\}$ and $N(u) \backslash PV = \{x_1, \ldots, x_{t-r}\}$. Then all $d(x_j) = d_j \geqslant 2$.

Let $G' = G - v$. Then $G' \in \mathscr{U}_{n-1,m}$. By the induction hypothesis, we have

$$\begin{aligned} R(G) =\ & R(G') + \frac{r}{\sqrt{t}} - \frac{r-1}{\sqrt{t-1}} + \sum_{i=1}^{t-r}\left(\frac{1}{\sqrt{d_i t}} - \frac{1}{\sqrt{d_i(t-1)}}\right) \\ \geqslant\ & \psi(n-1,m) + \frac{r}{\sqrt{t}} - \frac{r-1}{\sqrt{t-1}} + (t-r)\cdot\left(\frac{1}{\sqrt{2t}} - \frac{1}{\sqrt{2(t-1)}}\right) \\ =\ & \psi(n,m) + \frac{m}{\sqrt{2(n-m)}} + \frac{n-2m}{\sqrt{n-m}} - \frac{m}{\sqrt{2(n-m+1)}} - \frac{n-2m+1}{\sqrt{n-m+1}} \\ & + \frac{t-r}{\sqrt{2t}} + \frac{r}{\sqrt{t}} - \frac{t-r}{\sqrt{2(t-1)}} - \frac{r-1}{\sqrt{t-1}} \\ =\ & \psi(n,m) + [h(n-m, n-2m) - h(n-m+1, n-2m+1)] \\ & -[h(t-1, r-1) - h(t,r)], \end{aligned} \tag{5}$$

where $h(x, y)$ is defined in (1). Since G has an m-matching, $n - m + 1 \geqslant t$ and $n - 2m \geqslant r - 1$. Thus, by (5) and lemma 4(i), we have

$$\begin{aligned} R(G) \geqslant\ & \psi(n, m) + h(n - m, n - 2m) - h(n - m + 1, n - 2m + 1) \\ & -[h(n - m, r - 1) - h(n - m + 1, r)] \\ \geqslant\ & \psi(n, m). \end{aligned}$$

In order for the equality to hold, all inequalities in the above argument should be equalities. Thus we have

$$R(G') = \psi(n - 1, m), \quad n - m + 1 = t, \quad r - 1 = n - 2m \text{ and } d_1 = \cdots = d_{t-r} = 2.$$

By the induction hypothesis, $G' \cong U_{n-1,m}$. Then it is not difficult to see $G \cong U_{n,m}$.

Hence the proof of theorem 10 is complete. □

3. Remarks

If $G \in \mathscr{U}_{2m,m}$, by Lemma 6, then $R(G) \leqslant m$ with equality if and only if $G \cong C_{2m}$, since C_{2m} is the only regular graph in $\mathscr{U}_{2m,m}$. Similarly, if $G \in \mathscr{U}_{2m+1,m}$, then $R(G) \leqslant (2m + 1)/2$ with equality if and only if $G \cong C_{2m+1}$.

As to $G \in \mathscr{U}_{n,m}$ $(n \geqslant 2m + 2)$, we do not know the sharp upper bounds on $R(G)$. The case maybe much more complicated.

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