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On the Randić index of cacti

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Abstract

The Randić index of an organic molecule whose molecular graph is G is the sum of the weights $(d(u)d(v))^{-\frac{1}{2}}$ of all edges uv of G, where $d(u)$ and $d(v)$ are the degrees of the vertices u and v in G. In the paper, we give a sharp lower bound on the Randić index of cacti.

1. Introduction

In studying branching properties of alkanes, several numbering schemes for the edges of the associated hydrogen-suppressed graph were proposed based on the degrees of the end vertices of an edge [9]. To preserve rankings of certain molecules, some inequalities involving the weights of edges needed to be satisfied. Randić [9] stated that weighting all edges uv of the associated graph G by $(d(u)d(v))^{-1/2}$ preserved these inequalities, where $d(u)$ and $d(v)$ are the degrees of u and v. The sum of weights over all edges of G, which is called the *Randić index* of G and denoted by $R(G)$, has been closely correlated with many chemical properties [7] and found to parallel the boiling point, Kovats constants, and a calculated surface. In addition, the Randić index appears to predict the boiling points of alkanes more closely, and only it takes into account the bonding or adjacency degree among carbons in alkanes (see [8]). It is said in [6] that Randić index "*together with its generalizations it is certainly the molecular-graph-based structure-descriptor, that*

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found the most numerous applications in organic chemistry, medicinal chemistry, and pharmacology". More data and additional references on the index can be found in [4, 5].

Let $G = (V, E)$ be a graph. We call G a cactus if all of blocks of G are either edges or cycles. Denote $G(n, r)$ the set of cacti of order n and with r cycles. Obviously, $G(n, 0)$ are trees and $G(n, 1)$ are unicyclic graphs. The degree and the neighborhood of a vertex $u \in V$ will be denoted by $d(u)$ and $N(u)$, respectively and $\delta(G) = \min\{d(u) : u \in V(G)\}$. The graph that arises from G by deleting the vertex $u \in V$ will be denoted by $G - u$. Similarly, the graph $G + uv$ arises from G by adding an edge uv between two non-adjacent vertices u and v of G.

There are many results concerning Randić index. In [1], Bollobás and Erdös gave the sharp lower bound of $R(G) \geq \sqrt{n-1}$ when G is a graph of order n without isolated vertices. In the paper, we will give sharp lower bounds on the Randić index of cacti.

2. Some Lemmas

In the section, we use $G(n, r)$ to denote the set of cacti of order n and with r cycles and $G^0(n, r)$ to denote the cactus obtained from r triangles and $n - 2r - 1$ edges by taking one vertex of each triangle and each edge, and combining them as one vertex. Fig.1 illustrates the graph $G^0(n, r)$ with $n = 13,\ r = 3$.

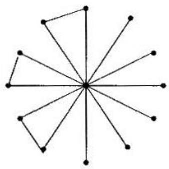

Fig. 1. $G^0(13, 3)$

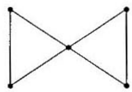

Fig. 2. $G^0(5, 2)$

Firstly, we will give some lemmas which will be used in Section 3.

Lemma 2.1 [3]. *Let $x,\ y$ be positive integers with $x \geq 1$ and $y \geq 2$. Denote*

$$h(x, y) = \frac{x+1}{\sqrt{y}} + \frac{y-1-x}{\sqrt{2y}} - \frac{x}{\sqrt{y-1}} - \frac{y-1-x}{\sqrt{2(y-1)}}.$$

Then $h(x, y)$ is monotonously decreasing in x.

Lemma 2.2 [3]. *Let y be a positive integer with $y \geq 2$. Denote*

$$h(y) = \frac{y-1}{\sqrt{y}} + \frac{1}{\sqrt{2y}} - \frac{y-2}{\sqrt{y-1}} - \frac{1}{\sqrt{2(y-1)}}.$$

Then $h(y)$ is monotonously decreasing in y.

Lemma 2.3. *Let y be a positive integer with $y \geq 2$. Denote*

$$h(y) = \left(\frac{\sqrt{y}}{\sqrt{2}} - \frac{\sqrt{y-k}}{\sqrt{2}}\right) + \frac{(\sqrt{2}-1)k}{\sqrt{2y}},$$

where $k \geq 1$. Then $h(y)$ is monotonously decreasing in y.

The proof of Lemma 2.3 is very simple. We omit it here.

Lemma 2.4 [1]. *Let $G \in G(n, 0)$. Then*

$$R(G) \geq \sqrt{n-1},$$

and the equality holds if and only if $G \cong G^0(n, 0)$.

Lemma 2.5 [3]. *Let $G \in G(n, 1)$. Then*

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

and the equality holds if and only if $G \cong G^0(n, 1)$.

3. Main Result

Let $G(n, r)$ be the set of cacti of order n and with r cycles. Denote

$$f(n, r) = \frac{2r}{\sqrt{2(n-1)}} + \frac{r}{2} + \frac{n-1-2r}{\sqrt{n-1}}.$$

We have the following result.

Theorem 3.1. *Let $G \in G(n, r)$. Then*

$$R(G) \geq f(n, r),$$

and equality holds if and only if $G \cong G^0(n, r)$.

Proof. By induction on n and r. If $r = 0$ and 1, then the theorem holds clearly by Lemmas 2.4 and 2.5. Hence we can assume that $r \geq 2$ and then $n \geq 5$. If $n = 5$, then the theorem holds clearly by the facts that there are only one graph in $G(5, 2)$ (see Fig.2).

Let $G \in G(n, r)$ with $n \geq 6$ and $r \geq 2$. We will consider the following two cases.

Case 1. $\delta(G) = 1$.

Let $u \in V(G)$ with $d(u) = 1$ and $uv \in E(G)$. Denote $d(v) = d$ and $N(v) \setminus \{u\} = \{y_1, y_2, \cdots, y_{d-1}\}$. Then $2 \leq d \leq n-1$.

Assume, without loss of generality, that $d(y_1) = d(y_2) = \cdots = d(y_{k-1}) = 1$ and $d(y_i) \geq 2$ for $k \leq i \leq d-1$, where $k \geq 1$ and $k = 1$ implies $d(y_i) \geq 2$ for $1 \leq i \leq d-1$. Obviously, we have $r \leq \lfloor \frac{n-1-k}{2} \rfloor$. Set $G' = G - u - y_1 - \cdots - y_{k-1}$ (if $i = 1$, then let

$G' = G - u$). Then $G' \in G(n-k, r)$. Let S be the sum of the weights of the edges incident with v except for the edges $vu, vy_1, \cdots, vy_{k-1}$ in G and S' the sum of the weights of the edges incident with v in G'. Then $S = \sum_{i=k}^{d-1} \frac{1}{\sqrt{dd(y_i)}} \leq \frac{d-k}{\sqrt{2d}}$ and $S' = S\sqrt{\frac{d}{d-k}}$. By induction assumption and Lemma 2.3, we have

$$\begin{aligned}
R(G) &= R(G') + \frac{k}{\sqrt{d}} + S - S' \\
&\geq f(n-k, r) + \frac{k}{\sqrt{d}} + \left(1 - \sqrt{\frac{d}{d-k}}\right) S \\
&\geq f(n, r) + \frac{2r}{\sqrt{2(n-k-1)}} - \frac{2r}{\sqrt{2(n-1)}} + \frac{n-k-1-2r}{\sqrt{n-k-1}} \\
&\quad - \frac{n-1-2r}{\sqrt{n-1}} + \left(\frac{\sqrt{d}}{\sqrt{2}} - \frac{\sqrt{d-k}}{\sqrt{2}}\right) + \frac{(\sqrt{2}-1)k}{\sqrt{2d}} \\
&\geq f(n, r) + \frac{2r}{\sqrt{2(n-k-1)}} - \frac{2r}{\sqrt{2(n-1)}} + \frac{n-k-1-2r}{\sqrt{n-k-1}} \\
&\quad - \frac{n-1-2r}{\sqrt{n-1}} + \left(\frac{\sqrt{n-1}}{\sqrt{2}} - \frac{\sqrt{n-1-k}}{\sqrt{2}}\right) + \frac{(\sqrt{2}-1)k}{\sqrt{2(n-1)}} \\
&= f(n, r) + (n-k-1-2r)\left[\frac{\sqrt{2}-1}{\sqrt{2(n-k-1)}} - \frac{\sqrt{2}-1}{\sqrt{2(n-1)}}\right] \geq f(n, r).
\end{aligned}$$

The equality $R(G) = f(n, r)$ holds if and only if equalities hold throughout the above inequalities, that is, if and only if $d = n-1$, $2r = n-k-1$ and $G' \cong G^0(n-k, r)$. Thus we have $R(G) = f(n, r)$ holds if and only if $G \cong G^0(n, r)$.

Case 2. $\delta(G) \geq 2$.

By the definition of cactus and $\delta(G) \geq 2$, there exists an edge u_0u_1 in $E(G)$ such that $d(u_0) = d(u_1) = 2$. Let $\{u_2\} = N(u_0) \setminus \{u_1\}$. Denote $d(u_2) = d$. Then $d \geq 3$ by $n \geq 6$ and $r \geq 2$. We will finish the proof by considering two subcases.

Subcase 2.1. $u_1u_2 \notin E(G)$.

Let $G' = G - u_0 + u_1u_2$. Then $G' \in G(n-1, r)$. Thus we have

$$\begin{aligned}
R(G) &= R(G') + \frac{1}{\sqrt{2d}} + \frac{1}{2} - \frac{1}{\sqrt{2d}} \\
&\geq f(n-1, r) + \frac{1}{2} \\
&= f(n, r) + \frac{2r}{\sqrt{2(n-2)}} - \frac{2r}{\sqrt{2(n-1)}} + \frac{n-2-2r}{\sqrt{n-2}} - \frac{n-1-2r}{\sqrt{n-1}} + \frac{1}{2}
\end{aligned}$$

$$> \ f(n,r).$$

The last inequality holds obviously if $n \geq 7$. If $n = 6$, then $r \leq 2$ and it is not difficult to check that the inequality holds.

Subcase 2.2. $u_1u_2 \in E(G)$.

Let $G' = G - u_0 - u_1$. Then $G' \in G(n-2, r-1)$. Let S be the sum of the weights of the edges incident with u_2 except for the edges u_0u_2 and u_1u_2 in G and S' the sum of the weights of the edges incident with u_2 in G'. Denote $N(u_2) \setminus \{u_0, u_1\} = \{y_1, y_2, \cdots, y_{d-2}\}$. Then $S = \sum\limits_{i=1}^{d-2} \frac{1}{\sqrt{dd(y_i)}} \leq \frac{d-2}{\sqrt{2d}}$ by $\delta(G) \geq 2$ and $S' = S\sqrt{\frac{d}{d-2}}$. By induction assumption, we have

$$\begin{aligned}
R(G) &= R(G') + \frac{1}{2} + \frac{2}{\sqrt{2d}} + S - S' \\
&\geq f(n-2, r-1) + \frac{1}{2} + \frac{2}{\sqrt{2d}} + S\left(1 - \sqrt{\frac{d}{d-2}}\right) \\
&\geq f(n,r) + \frac{2(r-1)}{\sqrt{2(n-3)}} - \frac{2r}{\sqrt{2(n-1)}} + \frac{r-1}{2} - \frac{r}{2} \\
&\quad + \frac{n-3-2(r-1)}{\sqrt{n-3}} - \frac{n-1-2r}{\sqrt{n-1}} + \frac{1}{2} + \frac{2}{\sqrt{2d}} + \left(1 - \sqrt{\frac{d}{d-2}}\right)\frac{d-2}{\sqrt{2d}} \\
&= f(n,r) + \frac{2(r-1)}{\sqrt{2(n-3)}} - \frac{2r}{\sqrt{2(n-1)}} \\
&\quad + \frac{n-1-2r}{\sqrt{n-3}} - \frac{n-1-2r}{\sqrt{n-1}} + \frac{\sqrt{d}}{\sqrt{2}} - \frac{\sqrt{d-2}}{\sqrt{2}} \\
&\geq f(n,r) + \frac{2(r-1)}{\sqrt{2(n-3)}} - \frac{2r}{\sqrt{2(n-1)}} \\
&\quad + \frac{n-1-2r}{\sqrt{n-3}} - \frac{n-1-2r}{\sqrt{n-1}} + \frac{\sqrt{n-1}}{\sqrt{2}} - \frac{\sqrt{n-3}}{\sqrt{2}} \\
&= f(n,r) + (n-1-2r)\left(\frac{\sqrt{2}-1}{\sqrt{2(n-3)}} - \frac{\sqrt{2}-1}{\sqrt{2(n-1)}}\right) \\
&\geq f(n,r).
\end{aligned}$$

The equality $R(G) = f(n,r)$ holds if and only if equalities hold throughout the above inequalities, that is, if and only if $G' \cong G^0(n-2, r-1)$, $d = n-1$ and $2r = n-1$. Thus $R(G) = f(n,r)$ holds if and only if $G \cong G^0(n,r)$. ∎

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