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On the Randić Index of acyclic conjugated molecules

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The Randić index of an organic molecule whose molecular graph is G is the sum of the weights $(d(u)d(v))^{-1/2}$ of all edges uv of G, where $d(u)$ and $d(v)$ are the degrees of the vertices u and v in G. We give a sharp lower bound on the Randić index of conjugated trees (trees with a perfect matching) in terms of the number of vertices. A sharp lower bound on the Randić index of trees with a given size of matching is also given.

KEY WORDS: Randić index, conjugated tree, given size of matching

1. Introduction

In studying branching properties of alkanes, several numbering schemes for the edges of the associated hydrogen-suppressed graph ware proposed based on the degrees of the end vertices of an edge [1]. To preserve certain rankings of certain molecules, some inequalities involving the weights of edges needed to be satisfied. Randić [7] 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* or *molecular connectivity index* or simply *connectivity index* of G

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and denoted by $R(G)$, has been closely correlated with many chemical properties [2] and found to parallel the boiling point, Kovats constants, and a calculated surface area. In addition, the Randić index appears to predict the boiling points of alkanes closely, while only taking into account the bonding or adjacency degree among carbons (see [3]). More data and additional references on the index can be found in [4,5].

A *tree* T is a graph in which any pair of vertices is linked by a unique path. Denote by S_n and P_n the star graph and the path graph with n vertices, respectively. In [6], Bollobás and Erdös gave the sharp lower bound of $R(G) \geqslant \sqrt{n-1}$ when G is a graph of order n without isolated vertices. Yu [7] gave the sharp upper bound of $R(T) \leqslant (n+2\sqrt{2}-3)/2$ when T is a tree of order n. In the present paper, we investigate the Randić index of a type graph, namely that of conjugated trees (trees with a perfect matching). Also a sharp lower bound on the Randić index of trees with a given size matching is given in Section 3.

For convenience, we first introduced some terminologies and notations for graphs. Let $G=(V,E)$ be a graph. For a vertex x of G, we denote the neighborhood and the degree of x by $N(x)$ and $d(x)$, respectively. We will use $G-x$ to denote the graph that arises from G by deleting the vertex $x \in V(G)$.

2. Some lemmas

Let G be a connected graph. Two edges of a graph G are said to be independent if they are not incident with a common vertex. An m-matching of G is a set of m mutually independent edges. In this paper, we say a tree T with an m-matching means that T has at least one m-matching, and T may or may not have a matching whose size is more than m. Let M be a matching of T. A vertex v of T is said to be M-saturated if v is incident with an edge in M; otherwise, v is M-unsaturated. A perfect matching M of T means that every vertex of T is M-saturated.

We begin with two important results from [8] about trees with an m-matching.

Lemma 2.1 [8]**.** Let T be a n-vertex tree ($n \geqslant 3$) with a perfect matching. Then T has at least two pendant vertices such that each are adjacent to vertices of degree 2.

Lemma 2.2 [8]**.** Let T be an n-vertex tree with an m-matching where $n > 2m$. Then there is an m-matching M and a pendant vertex v such that M does not saturate v.

The following two lemmas are used to prove our main results in Section 3.

Lemma 2.3. (1) For $x \geqslant 3$, the function

$$f(x) = \frac{1}{\sqrt{x}} + \frac{x-1}{\sqrt{2x}} - \frac{1}{\sqrt{x-1}} - \frac{x-2}{\sqrt{2(x-1)}}$$

is monotonicly decreasing in x.

(2) For $x \geqslant 2$, the function

$$g(x) = \frac{1}{\sqrt{x}} + \frac{x-1}{\sqrt{2x}} - \frac{x-1}{\sqrt{2(x-1)}}$$

is monotonicly decreasing in x.

Proof. (1) We consider the derivative of $f(x)$.

$$\begin{aligned}\frac{df(x)}{dx} &= -\frac{1}{2x\sqrt{x}} + \frac{x+1}{2x\sqrt{2x}} + \frac{1}{2(x-1)\sqrt{x-1}} - \frac{x}{2(x-1)\sqrt{2(x-1)}} \\ &= \frac{(\sqrt{2}-1)(x\sqrt{x}-(x-1)\sqrt{x-1})}{2x(x-1)\sqrt{2x(x-1)}} - \frac{1}{2(\sqrt{x-1}+\sqrt{x})\sqrt{2x(x-1)}} \\ &= \frac{(\sqrt{2}-1)\sqrt{x(x-1)} - x(x+1-2\sqrt{2}) - (\sqrt{2}-1)}{2x(x-1)(\sqrt{x}+\sqrt{x-1})\sqrt{2x(x-1)}}.\end{aligned}$$

Since $(\sqrt{2}-1)\sqrt{x(x-1)} - x(x+1-2\sqrt{2}) < 0$ for $x \geqslant 3$, we have $\frac{df(x)}{dx} < 0$. Thus (1) holds.

(2) Since

$$\begin{aligned}\frac{dg(x)}{dx} &= -\frac{1}{2x\sqrt{x}} + \frac{x+1}{2x\sqrt{2x}} - \frac{x-1}{2(x-1)\sqrt{2(x-1)}} \\ &= -\frac{\sqrt{2}-1}{2x\sqrt{2x}} + \left(\frac{1}{2\sqrt{2x}} - \frac{1}{2\sqrt{2(x-1)}}\right) < 0,\end{aligned}$$

(2) is obvious. □

Lemma 2.4. Let $x,\ y$ be positive integers with $1 \leqslant x \leqslant y-1$. 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 monotonicly decreasing in x and y, respectively.

Proof. We consider some partial derivatives. Since

$$\begin{aligned}\frac{\partial h(x,y)}{\partial x} &= \frac{1}{\sqrt{y}} - \frac{1}{\sqrt{2y}} - \frac{1}{\sqrt{y-1}} + \frac{1}{\sqrt{2(y-1)}} \\ &= \frac{\sqrt{2}-1}{\sqrt{2y}} - \frac{\sqrt{2}-1}{\sqrt{2(y-1)}} < 0,\end{aligned}$$

$h(x, y)$ is monotonicly decreasing in x. On the other hand,

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

Since $x \leqslant y-1$, we have

$$\frac{\partial h(x,y)}{\partial y} \leqslant \frac{(\sqrt{2}-1)(y\sqrt{y}-(y-1)\sqrt{y-1})}{2y\sqrt{2y(y-1)}} - \frac{(\sqrt{2}-1)\sqrt{y-1}}{2y\sqrt{2y(y-1)}} - \frac{\sqrt{y}-\sqrt{y-1}}{2\sqrt{2y(y-1)}}$$
$$= \frac{(\sqrt{y}-\sqrt{y-1})(\sqrt{2}-2)}{2\sqrt{2y(y-1)}} < 0.$$

Thus $h(x, y)$ is monotonicly decreasing in y. □

3. Main results

Let n and m be positive integers and $n \geqslant 2m$. We define a tree $T^0(n, m)$ with n vertices as follow: $T^0(n, m)$ is obtained from the star graph S_{n-m+1} by attaching a pendant edge to each of certain $m-1$ non-central vertices of S_{n-m+1}. Obviously, $T^0(n, m)$ is an n-vertex tree with an m-matching. Denote

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

We have the following initial result.

Theorem 3.1. Let T be an n-vertex ($n = 2m$) tree with a perfect matching. Then

$$R(T) \geqslant f(2m, m),$$

and equality holds if and only if $T \cong T^0(2m, m)$.

Proof. By induction on m. If $m = 1,\ 2,\ 3$, then the theorem holds clearly by the fact that there are at most two trees with $n = 2m$ vertices and a perfect matching for $m = 1,\ 2,\ 3$.

Let T be any $2m$-vertex tree with a perfect matching ($m \geqslant 4$). By Lemma 2.1, T has a pendant vertex x_1 which is adjacent to a vertex x_2 of degree 2. Then $x_1x_2 \in E(T)$ and there is a unique vertex $x_3 \neq x_1$ such that $x_2x_3 \in E(T)$. Let $T' = T - x_1 - x_2$. Then T' is a tree with $2(m-1)$ vertices and with an $(m-1)$-matching. Denote $d(x_3) = d$ and $N(x_3)\setminus\{x_2\} = \{y_1, y_2, \ldots, y_{d-1}\}$, then $d \geqslant 2$. Let S be the sum of the weights of the edges incident with x_3 except for the edge x_2x_3 in T, and let S' be the sum of the weights of the edges incident with x_3 in T'.

Then $S = \sum_{i=1}^{d-1} \frac{1}{\sqrt{dd(y_i)}}$ and $S' = S\sqrt{\frac{d}{d-1}}$. By the induction assumption, we have

$$\begin{aligned} R(T) &= R(T') + \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2d}} + S - S' \\ &\geqslant f(2(m-1), m-1) + \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2d}} + S\left(1 - \sqrt{\frac{d}{d-1}}\right) \\ &= f(2m, m) + \frac{1}{\sqrt{m-1}} - \frac{1}{\sqrt{m}} + \frac{m-2}{\sqrt{2(m-1)}} \\ &\quad - \frac{m-1}{\sqrt{2m}} + \frac{1}{\sqrt{2d}} + \left(1 - \sqrt{\frac{d}{d-1}}\right) \sum_{i=1}^{d-1} \frac{1}{\sqrt{dd(y_i)}}. \end{aligned} \tag{1}$$

Now we complete the proof by considering two cases.

Case 1. $d = 2$.

Since $m \geqslant 4$, $d(y_1) \geqslant 2$. Thus by (1), we have

$$\begin{aligned} R(T) &\geqslant f(2m, m) + \frac{1}{\sqrt{m-1}} - \frac{1}{\sqrt{m}} + \frac{m-2}{\sqrt{2(m-1)}} - \frac{m-1}{\sqrt{2m}} + \frac{1}{2} + \frac{1}{2}(1 - \sqrt{2}) \\ &= f(2m, m) + \left(\frac{\sqrt{2}-1}{\sqrt{2(m-1)}} - \frac{\sqrt{2}-1}{\sqrt{2m}}\right) + \left(\frac{\sqrt{m-1}}{\sqrt{2}} - \frac{\sqrt{m}}{\sqrt{2}}\right) + \frac{2-\sqrt{2}}{2} \\ &> f(2m, m) + \left(\frac{\sqrt{4-1}}{\sqrt{2}} - \frac{\sqrt{4}}{\sqrt{2}}\right) + \frac{2-\sqrt{2}}{2} \\ &> f(2m, m). \end{aligned}$$

Case 2. $d \geqslant 3$.

Since T has a perfect matching, we have $d = d(x_3) \leqslant m$. If $d(y_i) \geqslant 2$ for $i = 1, 2, \ldots, d-1$, then by (1), we have

$$\begin{aligned} R(T) &\geqslant f(2m, m) + \frac{1}{\sqrt{m-1}} - \frac{1}{\sqrt{m}} + \frac{m-2}{\sqrt{2(m-1)}} \\ &\quad - \frac{m-1}{\sqrt{2m}} + \frac{1}{\sqrt{2d}} + \frac{d-1}{\sqrt{2d}}\left(1 - \sqrt{\frac{d}{d-1}}\right) \\ &= f(2m, m) + \frac{1}{\sqrt{m-1}} - \frac{1}{\sqrt{m}} + \frac{m-2}{\sqrt{2(m-1)}} - \frac{m-1}{\sqrt{2m}} + \frac{1}{\sqrt{2}}\left(\sqrt{d} - \sqrt{d-1}\right) \\ &\geqslant f(2m, m) + \frac{1}{\sqrt{m-1}} - \frac{1}{\sqrt{m}} + \frac{m-2}{\sqrt{2(m-1)}} - \frac{m-1}{\sqrt{2m}} + \frac{1}{\sqrt{2}}\left(\sqrt{m} - \sqrt{m-1}\right) \\ &= f(2m, m) + \frac{\sqrt{2}-1}{\sqrt{2(m-1)}} - \frac{\sqrt{2}-1}{\sqrt{2m}} > f(2m, m). \end{aligned}$$

Hence, we can assume that there exists some i ($1 \leqslant i \leqslant d-1$), say $i = 1$, such that $d(y_1) = 1$. Since T has a perfect matching, we have $d(y_i) \geqslant 2$ for $i = 2, \dots, d-1$. Thus

$$\begin{aligned} R(T) &\geqslant f(2m, m) + \frac{1}{\sqrt{m-1}} - \frac{1}{\sqrt{m}} + \frac{m-2}{\sqrt{2(m-1)}} \\ &\quad - \frac{m-1}{\sqrt{2m}} + \frac{1}{\sqrt{2d}} + \left(1 - \sqrt{\frac{d}{d-1}}\right)\left(\frac{1}{\sqrt{d}} + \frac{d-2}{\sqrt{2d}}\right) \\ &= f(2m, m) + \frac{1}{\sqrt{m-1}} - \frac{1}{\sqrt{m}} + \frac{m-2}{\sqrt{2(m-1)}} - \frac{m-1}{\sqrt{2m}} \\ &\quad + \frac{1}{\sqrt{d}} - \frac{1}{\sqrt{d-1}} + \frac{d-1}{\sqrt{2d}} - \frac{d-2}{\sqrt{2(d-1)}}. \end{aligned}$$

By Lemma 2.3 (1) and $d \leqslant m$, we have

$$\begin{aligned} R(T) &\geqslant f(2m, m) + \frac{1}{\sqrt{m-1}} - \frac{1}{\sqrt{m}} + \frac{m-2}{\sqrt{2(m-1)}} \\ &\quad - \frac{m-1}{\sqrt{2m}} + \frac{1}{\sqrt{m}} - \frac{1}{\sqrt{m-1}} + \frac{m-1}{\sqrt{2m}} - \frac{m-2}{\sqrt{2(m-1)}} \\ &= f(2m, m). \end{aligned}$$

The equality $R(T) = f(2m, m)$ holds if and only if equality holds throughout the above inequalities, that is if and only if $T' \cong T^0(2(m-1), m-1)$, $d(y_1) = 1$, $d(y_i) = 2$ for $i = 2, 3, \dots, d-1$ and $d = m$. Thus $T \cong T^0(2m, m)$. □

Another result of the present paper is to give a sharp lower bound on the Randić index of the trees with an m-matching as follow.

Theorem 3.2. Let $T = (V, E)$ be an n-vertex tree with an m-matching, $n \geqslant 2m$. Then

$$R(T) \geqslant f(n, m),$$

with equality if and only if $T \cong T^0(n, m)$.

Proof. We prove the theorem by induction on n. Suppose $n = 2m$. Then the theorem holds by Theorem 2.1. Now we suppose $n > 2m$. Let T be any tree with n vertices and with an m-matching. By Lemma 2.2, T has an m-matching M and a pendant vertex v such that M does not saturate v. Let $uv \in E(T)$ with $d(u) = d$ and $N(u) \setminus \{v\} = \{v_1, v_2, \dots, v_{d-1}\}$. Obviously, $d \geqslant 2$. Denote $T' = T - v$. Then T' is a tree with $n-1$ vertices and with an m-matching. Let S be the sum of the weights of the edges incident with u except for the edge uv in T and S'

the sum of the weights of the edges incident with u in T'. Then $S = \sum_{i=1}^{d-1} \frac{1}{\sqrt{dd(v_i)}}$ and $S' = S\sqrt{\frac{d}{d-1}}$. By the induction assumption,

$$\begin{aligned} R(T) &= R(T') + \frac{1}{\sqrt{d}} + \left(1 - \sqrt{\frac{d}{d-1}}\right) S \\ &\geqslant f(n-1, m) + \frac{1}{\sqrt{d}} + \left(1 - \sqrt{\frac{d}{d-1}}\right) S \\ &= f(n, m) + \frac{m-1}{\sqrt{2(n-m-1)}} - \frac{m-1}{\sqrt{2(n-m)}} + \frac{n-2m}{\sqrt{n-m-1}} \\ &\quad - \frac{n-2m+1}{\sqrt{n-m}} + \frac{1}{\sqrt{d}} + \left(1 - \sqrt{\frac{d}{d-1}}\right) S. \end{aligned} \tag{2}$$

Case 1. $d(v_i) \geqslant 2$ for $i = 1, 2, \ldots, d-1$.

In the case, we have $S \leqslant (d-1)/\sqrt{2d}$. Then by (2), we have

$$\begin{aligned} R(T) &\geqslant f(n, m) + \frac{m-1}{\sqrt{2(n-m-1)}} - \frac{m-1}{\sqrt{2(n-m)}} + \frac{n-2m}{\sqrt{n-m-1}} \\ &\quad - \frac{n-2m+1}{\sqrt{n-m}} + \frac{1}{\sqrt{d}} + \left(1 - \sqrt{\frac{d}{d-1}}\right) \frac{d-1}{\sqrt{2d}} \\ &= f(n, m) + \frac{m-1}{\sqrt{2(n-m-1)}} - \frac{m-1}{\sqrt{2(n-m)}} + \frac{n-2m}{\sqrt{n-m-1}} \\ &\quad - \frac{n-2m+1}{\sqrt{n-m}} + \frac{1}{\sqrt{d}} + \frac{d-1}{\sqrt{2d}} - \frac{d-1}{\sqrt{2(d-1)}}. \end{aligned}$$

Since T has an m-matching, $d \leqslant n-m$. Thus, by Lemma 2.3(2), we have

$$\begin{aligned} R(T) &\geqslant f(n, m) + \frac{m-1}{\sqrt{2(n-m-1)}} - \frac{m-1}{\sqrt{2(n-m)}} + \frac{n-2m}{\sqrt{n-m-1}} \\ &\quad - \frac{n-2m+1}{\sqrt{n-m}} + \frac{1}{\sqrt{n-m}} + \frac{n-m-1}{\sqrt{2(n-m)}} - \frac{n-m-1}{\sqrt{2(n-m-1)}} \\ &= f(n, m) + (n-2m)\left(\frac{\sqrt{2}-1}{\sqrt{2(n-m-1)}} - \frac{\sqrt{2}-1}{\sqrt{2(n-m)}}\right) \\ &> f(n, m). \end{aligned}$$

Case 2. There exists some i $(1 \leqslant i \leqslant d-1)$ such that $d(v_i) = 1$.

Suppose, without loss of generality, that $d(v_1) = d(v_2) = \cdots = d(v_k) = 1$ and $d(v_i) \geqslant 2$ for $k+1 \leqslant i \leqslant d-1$, where $k \geqslant 1$. Thus $S \leqslant k/\sqrt{d} + (d-1-k)/\sqrt{2d}$.

Then by (2), we have

$$\begin{aligned}
R(T) &\geqslant f(n,m) + \frac{m-1}{\sqrt{2(n-m-1)}} - \frac{m-1}{\sqrt{2(n-m)}} + \frac{n-2m}{\sqrt{n-m-1}} \\
&\quad - \frac{n-2m+1}{\sqrt{n-m}} + \frac{1}{\sqrt{d}} + \left(1 - \sqrt{\frac{d}{d-1}}\right)\left(\frac{k}{\sqrt{d}} + \frac{d-1-k}{\sqrt{2d}}\right) \\
&= f(n,m) + \frac{m-1}{\sqrt{2(n-m-1)}} - \frac{m-1}{\sqrt{2(n-m)}} + \frac{n-2m}{\sqrt{n-m-1}} \\
&\quad - \frac{n-2m+1}{\sqrt{n-m}} + \frac{k+1}{\sqrt{d}} + \frac{d-1-k}{\sqrt{2d}} - \frac{k}{\sqrt{d-1}} - \frac{d-1-k}{\sqrt{2(d-1)}}.
\end{aligned}$$

Since T has an m-matching, $k \leqslant n-2m$ and $d \leqslant n-m$. Thus by Lemma 2.4, we have

$$\begin{aligned}
R(T) &\geqslant f(n,m) + \frac{m-1}{\sqrt{2(n-m-1)}} - \frac{m-1}{\sqrt{2(n-m)}} + \frac{n-2m}{\sqrt{n-m-1}} \\
&\quad - \frac{n-2m+1}{\sqrt{n-m}} + \frac{n-2m+1}{\sqrt{n-m}} + \frac{m-1}{\sqrt{2(n-m)}} - \frac{n-2m}{\sqrt{n-m-1}} - \frac{m-1}{\sqrt{2(n-m-1)}} \\
&= f(n,m).
\end{aligned}$$

The equality $R(T) = f(2m,m)$ holds if and only if equality holds throughout the above inequalities, that is if and only if $T' \cong T^0(n-1,m)$, $d(v_i) = 1$ for $1 \leqslant i \leqslant n-2m$, $d(y_i) = 2$ for $n-2m+1 \leqslant i \leqslant d-1$ and $d = n-m$. Thus $T \cong T^0(n,m)$. □

References

[1] M. Randić, *J. Amer. Chem. Soc.* 97 (1975), 6609.
[2] L.B. Kier and L.H. Hall, *Molecular Connectivity in Chemistry and Drug Research* (Academic Press, San Francisco, 1976).
[3] L.B. Kier and L.H. Hall, *Molecular Connectivity in Structure-Activity Analysis* (Wiley, 1986).
[4] I. Gutman, D. Vidović and A. Nedić, J. Serb. Chem. Soc., in press.
[5] I. Gutman and M. Leporić, J. Serb. Chem. Soc. 66 (2001) 605.
[6] B. Bollobás and P. Erdös, Ars Combin. 50 (1998) 225.
[7] P. Yu, *J. Math. Study* (Chinese) 31 (1998) 225.
[8] Y. Hou and J. Li, Linear Algebra Appl. 342 (2002), 203.