Maximum Randić Index on Unicyclic Graphs with k Pendant Vertices

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Abstract

Let G be a graph. The Randić index of 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. In this paper, we give a sharp upper bound for Randić index $R(G)$ among all unicyclic graphs G with n vertices, k pendant vertices with $n \geq 3k$ and $k \geq 3$.

Keywords: Randić index; Unicyclic graph; Pendant vertices

1. Introduction

Mathematical descriptors of molecular structure, such as various topological indices, have been widely used in structure-property-activity studies (see [11] and [12]). In order to measure the extent of branching of the carbon-atom skeleton of saturated hydrocarbons, Randić introduced the branching index which was called Randić index later. The Randić index of an organic molecule whose molecular graph is G is defined as (see [22]) $\sum(d(u)d(v))^{-1/2}$, where $d(u)$, $d(v)$ are the degrees of u and v and the sum

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is over all edges of G. This index is also called the *molecular connectivity index* or simply *connectivity index* of G and denoted by $R(G)$. The index has been closely correlated with many chemical properties [11] 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 [12]). In the past 30 years, the index has became one of the most popular molecular descriptors and has been extensively studied by both mathematicians and theoretical chemists [23]. More data and additional references on the index can be found in [7, 8].

There are many results concerning Randić index. In [2], 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. Yu [26] gave the sharp upper bound of $R(T) \leq (n + 2\sqrt{2} - 3)/2$ when T is a tree of order n. In [3], chemical trees with minimum Randić index are characterized and in [10], chemical trees of a given order and a number of pendant vertices with minimum and with maximum Randić index are characterized. Liu et al presented a upper bound on the Randić index for all chemical graphs with n vertices, $m \geq n$ edges and $k > 0$ pendant vertices in [20]. Zhang et al characterized trees of a given order and a number of pendant vertices with maximum Randić index in [27]. In [5], Gao and Lu gave the sharp lower bound of Randić index among unicyclic graphs and Lin et al gave the first three largest Randić indices among unicyclic graphs [17]. Lower bounds about unicyclic graphs with particular structure such as with given pendant vertices [21], or given girth [18], or given diameter [24] or with perfect matching [19] were considered. More research results about unicyclic graphs in other index can be found in [14] and [25].

For a comprehensive survey of the Randić index's mathematical properties and research results, see the book of Li and Gutman "Mathematical Aspects of Randić-Type Molecular Structure Descriptors" [13], the book of "Recent Results in the Theory of Randić Index" [9] and three survey papers [15, 16, 6].

Let $G = (V, E)$ be a graph of order n ($n \geq 3$). For $u \in V(G)$, we denote the degree of u by $d(u)$. A pendant vertex is a vertex of degree 1. Denote $V_i(G) = \{v \in V(G) | d(v) = i\}$ and $E_{ij}(G) = \{uv \in E(G) | d(u) = i, d(v) = j\}$. Then $V_1(G)$ is the set of pendant vertices.

Unicyclic graphs are connected graphs with n vertices and n edges. We denote by $\mathcal{U}(n, k)$ the set of all unicyclic graphs with n vertices and k pendant vertices.

In the paper, we will determine graphs with the largest Randić index among $\mathcal{U}(n, k)$ with $n \geq 3k$ and $k \geq 3$.

If v is a vertex of G or uv is an edge of G, then we denote by $G - v$ or $G - uv$ the graph obtained from G by deleting the vertex v and the edges incident with it or the edge $uv \in E(G)$. Let $P_s = v_0 v_1 \cdots v_s$ be a path of G with $d(v_1) = \cdots = d(v_{s-1}) = 2$ (unless $s = 1$). If $d(v_0) = 1$ and $d(v_s) \geq 3$, then we call P_s a pendant chain of G and we also call that s the length of the pendant chain P_s.

Let $G \in \mathcal{U}(n, k)$ and $uv \in E(G)$ with $d(u) = i$ and $d(v) = j$. Denote

$$x(uv) = x_{ij} = \left(\frac{1}{\sqrt{i}} - \frac{1}{\sqrt{j}}\right)^2.$$

If H is a subgraph of G, then we will denote $x(H) = \sum_{uv \in E(H)} x(uv)$. Thus another formula of $R(G)$ is (see [4])

$$R(G) = \frac{n}{2} - \frac{1}{2} \sum_{uv \in E(G)} x(uv) = \frac{n}{2} - \frac{1}{2} x(G).$$

Let $G_{n,k,s}$ ($n \geq 3k$, $3 \leq s \leq k$ and $2s \geq k$) be a graph of order n obtained from a cycle $C_s = v_1 v_2 \cdots v_s v_1$ by attaching $k-s$ edges to arbitrary $k-s$ vertices of C_s, and then attaching two pendant paths of length at least 2 to each vertex of degree 1, respectively and attaching $2s-k$ pendant paths of length at least 2 to each vertex of C_s with degree 2 (see Fig. 1). Then $G_{n,k,s} \in U(n,k)$ and

$$R(G_{n,k,s}) = \frac{n}{2} - \frac{1}{2}\left(k\sum_{i=1}^{2} x_{i(i+1)}\right) = \frac{n}{2} - \frac{k\left(7-3\sqrt{2}-\sqrt{6}\right)}{6}.$$

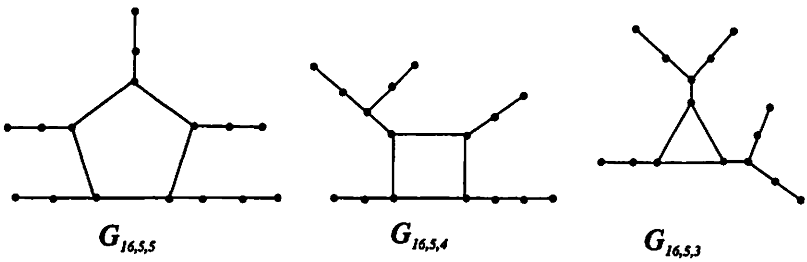

Figure 1:

The following three Lemmas had been shown in [1], we just cite them here.

Lemma 1.1 *Let* $0 < i < k < j$, *then* $x_{ij} > x_{ik} + x_{kj}$.

Lemma 1.2 *Let* G *be a graph. Let* $uv \in E(G)$ *with* $d(u) = i$ *and* $d(v) = j$. *If* $i < j$. *Then*

$$x(uv) = x_{ij} \geq \sum_{i \leq k \leq j-1} x_{k(k+1)}.$$

Moreover, the equality holds if and only if $j = i+1$.

Lemma 1.3 *Let* G *be a graph and* P *a path of* G *connecting* u *and* v. *Let* $d(u) = i$ *and* $d(v) = j$. *If* $i < j$, *then*

$$x(P) = \sum_{e \in E(P)} x(e) \geq \sum_{i \leq k \leq j-1} x_{k(k+1)}.$$

2. Main Result

Let $G^* \in U(n,k)$ such that $R(G^*) = \max\{R(G)|G \in U(n,k),\ n \geq 3k,\ k \geq 3\}$. Let $V_1 = \{v_1, \cdots, v_k\}$ be the set of pendant vertices. Since $G^* \in U(n,k)$ and $|V_1| = k$, there exist k pendant paths which denoted by $P_i = v_1^i v_2^i \cdots v_{s_i}^i$, where $v_1^i = v_i$ with $d(v_1^i) = 1$ and $d(v_{s_i}^i) \geq 3$ $(i = 1, 2, \cdots, k)$. Note that $v_{s_i}^i$ and $v_{s_j}^j$ may be the same vertex for some $i \neq j$. Firstly, we will give some lemmas which will be used later.

Lemma 2.1 *For every $v \in V(G^*)$, $d(v) \leq 3$.*

Proof. Suppose to the contrary that there is a vertex $v_0 \in V(G^*)$ such that $d(v_0) \geq 4$. If there exists some i $(1 \leq i \leq k)$ such that $v_0 = v_{s_i}^i$ or $d(v_{s_i}^i) \geq 4$, then by Lemmas 1.1 and 1.3, we have

$$\begin{aligned} R(G^*) &= \frac{n}{2} - \frac{1}{2}x(G) \\ &\leq \frac{n}{2} - \frac{1}{2}\sum_{i=1}^{k} x(P_i) \\ &\leq \frac{n}{2} - \frac{1}{2}\left(\sum_{i=1}^{k} \sum_{i=1}^{d(v_{s_i}^i)-1} x_{i(i+1)}\right) \\ &< \frac{n}{2} - \frac{1}{2}\left(k\sum_{i=1}^{2} x_{i(i+1)}\right) = R(G_{n,k,s}), \end{aligned}$$

a contradiction. Hence we can assume that $d(v_{s_i}^i) = 3$ for $i = 1, 2, \cdots, k$. Since $d(v_0) \geq 4$, $v_0 \neq v_{s_1}^1$. Then there is a path P in G^* joining $v_{s_1}^1$ and v_0 with $E(P) \cap E(P_i) = \emptyset$ for $i = 1, 2, \cdots, k$. Then

$$\begin{aligned} R(G^*) &= \frac{n}{2} - \frac{1}{2}x(G) \\ &\leq \frac{n}{2} - \frac{1}{2}\left(\sum_{i=1}^{k} x(P_i) + x(P)\right) \end{aligned}$$

$$
\begin{aligned}
&\leq \frac{n}{2}-\frac{1}{2}\left(\sum_{i=1}^{k}\sum_{i=1}^{d(v^i_{s_i})-1} x_{i(i+1)} + \sum_{i=3}^{d(v_0)-1} x_{i(i+1)}\right) \\
&< \frac{n}{2}-\frac{1}{2}\left(k\sum_{i=1}^{2} x_{i(i+1)}\right) = R(G_{n,k,s}),
\end{aligned}
$$

a contradiction. ∎

Lemma 2.2 $E_{13} = \emptyset$.

Proof. Suppose to the contrary that $E_{13} \neq \emptyset$. Without loss of generality, assume $v_1 \in V_1$ and $u_1 \in V_3$ with $u_1 v_1 \in E(G^*)$. Then $P_1 = v_1 u_1$. By Lemma 2.1, $d(v^i_{s_i}) = 3$ for $i = 2, \cdots, k$. By Lemma 1.3, we have

$$
\begin{aligned}
R(G^*) &= \frac{n}{2}-\frac{1}{2}x(G) \\
&\leq \frac{n}{2}-\frac{1}{2}\left(\sum_{i=2}^{k} x(P_i) + x_{13}\right) \\
&\leq \frac{n}{2}-\frac{1}{2}\left(\sum_{i=2}^{k}\sum_{i=1}^{d(v^i_{s_i})-1} x_{i(i+1)} + x_{13}\right) \\
&< \frac{n}{2}-\frac{1}{2}\left(k\sum_{i=1}^{2} x_{i(i+1)}\right) = R(G_{n,k,s}),
\end{aligned}
$$

a contradiction. ∎

By Lemma 2.2, the lengths of the pendant paths P_i $(1 \leq i \leq k)$ are at least 2. Combining Lemmas 2.1 and 2.2, we easily have the following result.

Lemma 2.3 $|E_{23}| \geq k$.

Now we give our main result as follows.

Theorem 2.4 *Let $G \in U(n,k)$ with $n \geq 3k$ and $k \geq 3$. Then*

$$
R(G) \leq \frac{n}{2}-\frac{1}{2}\left(k\sum_{i=1}^{2} x_{i(i+1)}\right) = \frac{n}{2} - \frac{k\left(7-3\sqrt{2}-\sqrt{6}\right)}{6}.
$$

Moreover, the equality holds if and only if $G \in \{G_{n,k,s} | n \geq 3k,\ 3 \leq s \leq k \text{ and } 2s \geq k\}$.

Proof. Let $G^* \in U(n,k)$ such that $R(G^*) = \max\{R(G) | G \in U(n,k),\ n \geq 3k,\ k \geq 3\}$. By Lemma 2.1, we have

$$\begin{cases} |V_1| & = & k \\ |V_1| + |V_2| + |V_3| & = & n \\ |V_1| + 2|V_2| + 3|V_3| & = & 2n, \end{cases}$$

which implies $|V_1| = |V_3| = k$ and $|V_2| = n - 2k$.

Obviously, $|E_{11}| = 0$. By Lemma 2.2, $|E_{13}| = 0$ and then $|E_{12}| = k$ by Lemma 2.1. Suppose $|E_{23}| = m > k$. Then

$$\begin{aligned} R(G^*) &\leq \frac{n}{2} - \frac{1}{2}(kx_{12} + mx_{23}) \\ &< \frac{n}{2} - \frac{1}{2}\left(k\sum_{i=1}^{2} x_{i(i+1)}\right) = R(G_{n,k,s}), \end{aligned}$$

a contradiction. Thus we have $|E_{23}| = k$ by Lemma 2.3.

Let C be the unique cycle of G^*. Now we will show that $d(v) = 3$ for all $v \in V(C)$. Suppose there exists a vertex $v \in V(C)$ such that $d(v) = 2$. Since $|V_1| = k$ and $|E_{13}| = 0$, we have $|E_{23}| \geq k + 2 > k$, a contradiction. Thus $d(v) = 3$ for all $v \in V(C)$ which implies $G^* \in \{G_{n,k,s} | 3 \leq s \leq k \text{ and } 2s \geq k\}$. ■

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