MATCH
Communications in Mathematical and in Computer Chemistry

no. 51, April 2004
MATCDY (51) 155-166 (2004)

ISSN 0340 - 6253

Sharp Bounds for the General Randić Index*

Xueliang Li and Yiting Yang

Center for Combinatorics, LPMC
Nankai University, Tianjin 300071, People's Republic of China
Email: x.li@eyou.com; yitingyang@eyou.com

(Received September 10, 2003)

Abstract

The general Randić index of a (molecular) graph G is defined as the sum of the weights $(d(u)d(v))^{\alpha}$ of all edges uv of G, where $d(u)$ denotes the degree of a vertex u in G and α is an arbitrary real number. In this paper we obtain the lower and upper bounds for the general Randić index among graphs with n vertices and characterize the graphs whose general Randić indices reach the maximum and minimum. We give a clear picture depending on the real number α in different intervals.

1 Introduction

In 1975 Randić [6] proposed several numbering schemes for the edges of the associated hydrogen-suppressed graph based on the degrees of the end vertices of an edge in studying the properties of alkane. To preserve rankings of certain molecules, several inequalities involving the weights of edges needed to be satisfied. Randić stated that weighting all edges uv of the associated graph G by $(d_G(u)d_G(v))^{-1}$ or by $(d_G(u)d_G(v))^{-\frac{1}{2}}$ preserved these inequalities, where $d_G(u)$ denotes the degree of a vertex u in G. The sum of these latter weights over the edges of G is called the *Randić index* of G, denoted by $R(G)$. Some researchers often call it *connectivity index* [2]. Randić index is an important molecular descriptor and has been closely correlated with many chemical

*This work was done under the auspices of "973" Project on Mathematical Mechanization of the Ministry of Science and Technology, and the National Science Foundation of China.

properties [5]. So, finding the graphs having maximum and minimum Randić indices and related problem of finding lower and upper bounds for the Randić index, attracted recently the attention of many researchers, and many results have been achieved, see [1,2,3,4,8]. Clark and Moon [3] were interested in the former index and they gave a bound for trees. Bollobás and Erdös [1] generalized these indices by replacing $-\frac{1}{2}$ with any real number α, which was called the *general Randić index* in [3]. Here we denote it by $R_\alpha(G)$. When $\alpha = 1$, it is another important chemical index, called the Zagreb group index M_2, see [7]. In the following, we obtain the lower and upper bounds for the general Randić index among graphs with n vertices, and the corresponding extremal graphs. A clear picture is given depending on the real number α in different intervals.

2 Some notations and known results

For a graph $G = (V, E)$, we denote the number of vertices (order) by n and the number of edges (size) by m, and for any vertex $v \in V$ we denote its degree by $d(v)$. We deal with graphs without isolated vertex only, since isolated vertex contributes nothing to the sum. For a real number a, we use $\lfloor a \rfloor$ to denote the maximum integer smaller than or equal to a, and $\lceil a \rceil$ to denote the minimum integer greater than or equal to a. We call a tree an *r-star* if it is a star with r ($r \geq 1$) leaves. A 1-star is simply called a *stub*.

It seems that to obtain the lower and upper bounds for the general Randić index is somewhat more difficult than for other kinds of indices, in a given class of graphs, such as graphs of order n, trees of order n, etc. The following theorems are the main known results so far on the lower and upper bounds for the Randić index and general Randić index.

Theorem 2.1 *[1] Let G be a graph of order n, containing no isolated vertex. Then*

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

with equality if and only if G is a star.

Theorem 2.2 *[2, Theorem 1] Among graphs with n vertices, the graphs without isolated vertices, in which all components are regular, have the maximum Randić index, equal to $n/2$.*

Theorem 2.3 *[1] Every graph G of size m satisfies that*

$$R_\alpha(G) \leq m\left(\frac{\sqrt{8m+1}-1}{2}\right)^{2\alpha}$$

for $0 < \alpha \leq 1$, *and*

$$R_\alpha(G) \geq m\left(\frac{\sqrt{8m+1}-1}{2}\right)^{2\alpha}$$

for $-1 \leq \alpha < 0$.

Theorem 2.4 *[3] For a tree T of order* $n \geq 2$,

$$1 \leq R_{-1}(T) \leq \frac{5n+8}{18}.$$

In the next two sections, we investigate the lower and upper bounds for the general Randić index and the corresponding extremal graphs, among graphs of order n. We distinguish a few cases by considering the values of α.

3 The cases for α at $0, -\frac{1}{2}, -1$

The case for $\alpha = -\frac{1}{2}$ was completely solved by the above Theorems 2.1 and 2.2. So, there are two cases left.

For $\alpha = 0$, the general Randić index of a graph G is exactly equal to the number of edges in G. So we have the following simple result.

Theorem 3.1 *Let G be a graph of order n, containing no isolated vertex. Then*

$$\left\lceil\frac{n}{2}\right\rceil \leq R_0(G) \leq \frac{n(n-1)}{2}$$

with right equality if and only if G is a complete graph, and with left equality if and only if G is a forest composed of $\frac{n}{2}$ *stubs for n even, and a forest composed of* $\frac{n-3}{2}$ *stubs and a 2-star for n odd.*

From Theorem 2.2 one can see that the complete graph is a graph that has the maximum value of $R_{-\frac{1}{2}}$. However, for R_{-1} we show in the following that contrary to $R_{-\frac{1}{2}}$, the complete graph has the minimum value of R_{-1}.

Theorem 3.2 *Let G be a graph of order n, containing no isolated vertex. Then*

$$\frac{n}{2(n-1)} \leq R_{-1}(G) \leq \left\lfloor\frac{n}{2}\right\rfloor$$

with left equality if and only if G is a complete graph, and with right equality if and only if G is a forest composed of $\frac{n}{2}$ *stubs for n is even, and a forest composed of* $\frac{n-3}{2}$ *stubs and a 2-star for n is odd.*

Before proving it, let us show the following lemma first.

Lemma 3.3 *Let uv be an edge of minimum weight in a graph G such that uv is not a leaf. Then*

$$R_{-1}(G-uv) > R_{-1}(G)$$

Proof. Denote by S_u the sum of weights of the edges, other than uv, incident with the vertex u, and S_v the sum of weights of the edges, other than uv, incident with the vertex v. Then we have

$$S_u \geq \frac{d(u)-1}{d(v)d(u)} \text{ and } S_v \geq \frac{d(v)-1}{d(v)d(u)}.$$

So, we have

$$\begin{aligned}
&R_{-1}(G-uv) - R_{-1}(G) \\
&= S_u\left(\frac{d(u)}{d(u)-1}-1\right) + S_v\left(\frac{d(v)}{d(v)-1}-1\right) - \frac{1}{d(u)d(v)} \\
&\geq \frac{d(u)-1}{d(v)d(u)}\frac{1}{d(u)-1} + \frac{d(v)-1}{d(v)d(u)}\frac{1}{d(v)-1} - \frac{1}{d(u)d(v)} \\
&= \frac{1}{d(v)d(u)} > 0.
\end{aligned}$$

∎

Now we give the proof of our Theorem 3.2. We claim that a graph with the maximum value of R_{-1} must be composed of stars, for otherwise, from Lemma 3.3 we would get a graph with larger value of R_{-1} by deleting the edge with the minimum weight. Since any star has the same value 1 of R_{-1}, the graph with maximum value of R_{-1} must have most star components. The forest composed of $\frac{n}{2}$ stubs for n even, or the forest composed of $\frac{n-3}{2}$ stubs and a 2-star for n odd, has the maximum number of star components among graphs of order n. So we get that G has the maximum value of R_{-1} if and only if G is a forest composed of $\frac{n}{2}$ stubs for n even, and a forest composed of $\frac{n-3}{2}$ stubs and a 2-star for n odd.

In the following we show that the $R_{-1}(G)$ has the minimum value of R_{-1} if and only if G is a complete graph.

If we denote by S_u the sum of weights of the edges incident with the vertex u, Then

$$S_u \geq \frac{d(u)}{(n-1)d(u)} = \frac{1}{n-1}.$$

So we have

$$R_{-1}(G) = \sum_{uv \in E} \frac{1}{d(u)d(v)} = \frac{1}{2} \sum_{u \in V} S_u \geq \frac{n}{2} \cdot \frac{1}{n-1}$$

with equality only if each vertex in G has degree $n-1$, i.e., G is a complete graph. Now the proof of Theorem 3.2 is complete. ∎

4 The cases for α in different intervals

In this section we deal with our problem by considering the real number α in different intervals.

Case I. $\alpha > 0$.

This is a very simple case, since it is easy to see that adding edges to a graph will increase the sum, while deleting edges will decrease the sum. So, we get a result just like the case for $\alpha = 0$.

Theorem 4.1 *Let G be a graph of order n, containing no isolated vertex. When $\alpha > 0$, we have*

$$\frac{n}{2} \leq R_\alpha(G) \leq \frac{n(n-1)^{2\alpha} + 1}{2}$$

for n even, and

$$\frac{n-3}{2} + 2^{1+\alpha} \leq R_\alpha(G) \leq \frac{n(n-1)^{2\alpha} + 1}{2}$$

for n odd, with right equality if and only if G is a complete graph, and with left equality if and only if G is a forest composed of $\frac{n}{2}$ stubs for n even, and a forest composed of $\frac{n-3}{2}$ stubs and a 2-star for n odd.

Case II. $-\frac{1}{2} < \alpha < 0$.

Theorem 4.2 *Let G be a graph of order n, containing no isolated vertex. When $-\frac{1}{2} < \alpha < 0$, we have*

$$R_\alpha(G) \geq min\{\frac{n}{2}, (n-1)^{1+\alpha}\}$$

for n even, and

$$R_\alpha(G) \geq min\{\frac{n-3}{2} + 2^{1+2\alpha}, (n-1)^{1+\alpha}\}$$

for n odd.

The following two lemmas will be used in the proof.

Lemma 4.3 *Let uv be a leaf of a graph G. When $-\frac{1}{2} < \alpha < 0$, we have*

$$R_\alpha(G) - R_\alpha(G - uv) \geq (n-1)^{1+\alpha} - (n-2)^{1+\alpha}.$$

Proof. Let $d(u) = 1$. If $d(v) = 1$, then $R_\alpha(G) - R_\alpha(G - uv) = 1 > (n-1)^{1+\alpha} - (n-2)^{1+\alpha}$. Therefore, we may assume that $d(v) \geq 2$. Denote by S_v the sum of the weights of the edges, other than uv, incident with the vertex v. Then

$$R_\alpha(G) - R_\alpha(G - uv) = d(v)^\alpha + S_v \left(1 - \frac{(d(v)-1)^\alpha}{d(v)^\alpha}\right).$$

Since $S_v \leq (d(v)-1)d(v)^\alpha$, we have

$$\begin{aligned} R_\alpha(G) - R_\alpha(G - uv) &\geq d(v)^\alpha + (d(v)-1)d(v)^\alpha \left(1 - \frac{(d(v)-1)^\alpha}{d(v)^\alpha}\right) \\ &= d(v)^{1+\alpha} - (d(v)-1)^{1+\alpha} \\ &\geq (n-1)^{1+\alpha} - (n-2)^{1+\alpha}. \end{aligned}$$

∎

Lemma 4.4 *Let uv be an edge of maximum weight in a graph G. When $-\frac{1}{2} < \alpha < 0$, we have*

$$R_\alpha(G - uv) < R_\alpha(G).$$

Proof. Here we assume $min\{d(u), d(v)\} \geq 2$, otherwise, from Lemma 4.3 we can get the proof directly. Denote by S_u and S_v respectively the sum of weights of the edges incident with the vertex u and v. Then, we have

$$S_u \leq (d(u)-1)(d(u)d(v))^\alpha \; and \; S_v \leq (d(v)-1)(d(u)d(v))^\alpha.$$

So,

$$\begin{aligned} &R_\alpha(G) - R_\alpha(G - uv) \\ &= (d(u)d(v))^\alpha + S_u \left(1 - \frac{(d(u)-1)^\alpha}{d(u)^\alpha}\right) + S_v \left(1 - \frac{(d(v)-1)^\alpha}{d(v)^\alpha}\right) \\ &\geq (d(u)d(v))^\alpha \left\{1 + (d(u)-1)\left(1 - \frac{(d(u)-1)^\alpha}{d(u)^\alpha}\right) + (d(v)-1)\left(1 - \frac{(d(v)-1)^\alpha}{d(v)^\alpha}\right)\right\} \\ &> (d(u)d(v))^\alpha \left\{1 + (d(u)-1)\left(1 - \frac{(d(u)-1)^{-\frac{1}{2}}}{d(u)^{-\frac{1}{2}}}\right) + (d(v)-1)\left(1 - \frac{(d(v)-1)^{-\frac{1}{2}}}{d(v)^{-\frac{1}{2}}}\right)\right\} \end{aligned}$$

$$= (d(u)d(v))^{\alpha}\left(d(u) - \frac{1}{2} - \sqrt{d(u)(d(u)-1)} + d(v) - \frac{1}{2} - \sqrt{d(v)(d(v)-1)}\right)$$

$$> 0.$$

∎

Now we turn to the proof of our theorem by applying induction on $n + m$. From Lemma 4.4 we can delete the edges with maximum weights in a graph until all of them are leaves. So we can assume that the maximum weight edges in G are leaves. Let uv be one of such leaves.

If G contains no stubs, then $G - uv$ has only one isolated vertex. We assume that for smaller values of n+m the inequality $R_\alpha(G) \geq (n-1)^{1+\alpha}$ holds. Then

$$R_\alpha(G) \geq R_\alpha(G - uv) + (n-1)^{1+\alpha} - (n-2)^{1+\alpha} \geq (n-1)^{1+\alpha}.$$

We can see that only if G is a star the value of R_α for $-\frac{1}{2} < \alpha < 0$ is equal to $(n-1)^{1+\alpha}$, since the equality holds in the inequality of Lemma 4.3 only if $d(v) = 1$.

If G contains k stubs, from the above result we have that

$$R_\alpha(G) \geq k + (n - 2k - 1)^{1+\alpha},$$

with equality if and only if G is a graph composed of k stubs and a $(n - 2k - 1)$-star. We denote $k + (n - 2k - 1)^{1+\alpha}$ by $Q_n(k)$. So we only need to determine $min\{Q_n(k), k = 0, 1, 2, \ldots, \lfloor\frac{n-2}{2}\rfloor\}$.

When $1 + (n-3)^{1+\alpha} \leq (n-1)^{1+\alpha}$, since the function $f(x) = x^{1+\alpha} - (x-2)^{1+\alpha}$ for $-\frac{1}{2} < \alpha < 0$ is strictly decreasing in the interval $[2, +\infty)$, we have that

$$Q_n(0) \geq Q_n(1) > \ldots > Q_n(\lfloor\frac{n-2}{2}\rfloor)$$

So, we have that $min\{Q_n(k), k = 0, 1, 2, \ldots, \lfloor\frac{n-2}{2}\rfloor\} = Q_n(\lfloor\frac{n-2}{2}\rfloor)$.

When $1 + (n-3)^{1+\alpha} > (n-1)^{1+\alpha}$, we distinct the following two cases:

1. If there exists an integer i smaller than n such that $1 + (i-3)^{1+\alpha} < (i-1)^{1+\alpha}$, we have that

$$Q_n(0) \leq Q_n(1) \leq \ldots \geq Q_n(p) \geq Q_n(p+1) \ldots \geq Q_n(\lfloor\frac{n-2}{2}\rfloor)$$

for some $p \le i$. So, $min\{Q_n(k), k = 0, 1, 2, \ldots, \lfloor \frac{n-2}{2} \rfloor\} = min\{Q_n(0), Q_n(\lfloor \frac{n-2}{2} \rfloor)\}$.

2. If there exists no integer i smaller than n such that $1 + (i-3)^{1+\alpha} < (i-1)^{1+\alpha}$, we have that

$$Q_n(0) \le Q_n(1) \le \ldots \le Q_n(\lfloor \frac{n-2}{2} \rfloor).$$

So, $min\{Q_n(k), k = 0, 1, 2, \ldots, \lfloor \frac{n-2}{2} \rfloor\} = Q_n(0)$.

By now we have finished the proof of Theorem 4.2. We also note that $Q_n(\frac{n-2}{2})$ corresponds to the graph composed of $\frac{n}{2}$ stubs for n even, $Q_n(\frac{n-3}{2})$ corresponds to the graph composed of $\frac{n-3}{2}$ stubs and a 2-star for n odd, and $Q_n(0)$ corresponds to the $(n-1)$-star. ∎

Because the complete graph has the maximum value for both $R_{-\frac{1}{2}}$ and R_0, this naturally suggests us that for all α such that $-\frac{1}{2} < \alpha < 0$, the complete graph has the maximum value of R_α. So we get the following theorem.

Theorem 4.5 *Let G be a graph of order n, containing no isolated vertex. When $-\frac{1}{2} < \alpha < 0$, we have*

$$R_\alpha \le \frac{n(n-1)^{1+2\alpha}}{2},$$

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

Proof. It follows directly from the inequalities that

$$\sum_{uv \in E} (d(u)d(v))^\alpha \le \sum_{uv \in E} \frac{d(u)^{2\alpha} + d(v)^{2\alpha}}{2} = \sum_{u \in V} \frac{d(u)^{1+2\alpha}}{2} \le \frac{n(n-1)^{1+2\alpha}}{2}.$$

From the above proof we can see that only if all the vertices in G have degree $n-1$, i.e., G is a complete graph, G has the maximum value of R_α for $-\frac{1}{2} < \alpha < 0$. ∎

Case III. $-1 < \alpha < -\frac{1}{2}$.

Theorem 4.6 *Let G be a graph of order n, containing no isolated vertex. When $-1 < \alpha < -\frac{1}{2}$, we have*

$$R_\alpha(G) \le \frac{n}{2}$$

for n even, with equality if and only if G is a forest composed of $\frac{n}{2}$ stubs.

Proof. It is clear that $R_a(G) \leq R_b(G)$ if $a \leq b$ and the maximum value of $R_{-\frac{1}{2}}$ is $\frac{n}{2}$. So we have $max\{R_\alpha(G)\} \leq \frac{n}{2}$. Since we know that the graph composed of $\frac{n}{2}$ stubs has the value of R_α equal to $\frac{n}{2}$, we have that $max\{R_\alpha(G)\} = \frac{n}{2}$ when n is even and $-1 < \alpha < -\frac{1}{2}$. So all the possible graphs with the maximum value of R_α must be among the graphs whose values of $R_{-\frac{1}{2}}$ are $\frac{n}{2}$. By checking, we can find that only the forest composed of $\frac{n}{2}$ stubs has the value of R_α equal to $\frac{n}{2}$ for $-1 < \alpha < -\frac{1}{2}$. ∎

Although we have examined the values of $R_\alpha(G)$ for $-1 < \alpha < -\frac{1}{2}$ for many graphs, we cannot find the common properties for graphs that have the maximum value of R_α when n is odd. We also find that it is very complicated to determine the minimum value.

Case IV. $\alpha < -1$.

Theorem 4.7 *Let G be a graph of order n, containing no isolated vertex. When $\alpha < -1$, we have*

$$\frac{n(n-1)^{1+2\alpha}}{2} \leq R_\alpha(G) \leq \frac{n}{2}$$

for n even, and

$$\frac{n(n-1)^{1+2\alpha}}{2} \leq R_\alpha(G) \leq \frac{n-3}{2} + 2^{1+\alpha}$$

for n odd, with left equality if and only if G is a complete graph, and with right equality if and only if G is a forest composed of $\frac{n}{2}$ stubs for n even, and a forest composed of $\frac{n-3}{2}$ stubs and a 2-star for n odd.

We can prove the latter part of the theorem in the same way as in the case for $\alpha = -1$.

Lemma 4.8 *Let uv be an edge of minimum weight in a graph G such that uv is not a leaf. When $\alpha < -1$, we have*

$$R_\alpha(G - uv) > R_\alpha(G).$$

Proof. Denote by S_u the sum of weights of the edges, other than uv, incident with the vertex u, and S_v the sum of weights of the edges, other than uv, incident with the vertex v. Then we have

$$S_v \geq \frac{d(v)-1}{(d(v)d(u))^{-\alpha}} \text{ and } S_u \geq \frac{d(u)-1}{(d(v)d(u))^{-\alpha}}.$$

So we have

$$
\begin{aligned}
&R_{-1}(G-uv)-R_{-1}(G)\\
&= S_u\left(\frac{d(u)^{-\alpha}}{(d(u)-1)^{-\alpha}}-1\right)+S_v\left(\frac{d(v)^{-\alpha}}{(d(v)-1)^{-\alpha}}-1\right)-(d(u)d(v))^{\alpha}\\
&\geq (d(u)d(v))^{\alpha}(d(u)-1)\left(\left(1+\frac{1}{(d(u)-1)}\right)^{-\alpha}-1\right)\\
&\quad + (d(u)d(v))^{\alpha}(d(v)-1)\left(\left(1+\frac{1}{(d(v)-1)}\right)^{-\alpha}-1\right)-(d(u)d(v))^{\alpha}\\
&> (d(u)d(v)^{\alpha})(d(u)-1)\left(1-\alpha\frac{1}{d(u)-1}-1\right)\\
&\quad + (d(u)d(v))^{\alpha}(d(u)-1)\left(1-\alpha\frac{1}{d(u)-1}-1\right)-(d(u)d(v))^{\alpha}\\
&= (d(u)d(v))^{\alpha}(-2\alpha-1)>0.
\end{aligned}
$$

∎

Just like the case for $\alpha=-1$ we can obtain that the value of R_α for $\alpha<-1$ gets the maximum if and only if G is a forest composed of $\frac{n}{2}$ stubs for n even, or a forest composed of $\frac{n-3}{2}$ stubs and a 2-star for n odd. So, the right-hand part of Theorem 4.7 is proved.

Now we prove the left-hand part of Theorem 4.7. Since $\alpha<-1$, we have

$$\frac{1}{2(n-1)^{-\alpha}d(u)^{-\alpha}}+\frac{1}{2(n-1)^{-\alpha}d(v)^{-\alpha}}\leq\frac{1}{(d(u)d(v))^{-\alpha}}.$$

So,

$$
\begin{aligned}
R_\alpha(G)&=\sum_{uv\in E}\frac{1}{(d(u)d(v))^{-\alpha}}\geq\sum_{u\in V}\frac{d(u)}{2(n-1)^{-\alpha}d(u)^{-\alpha}}\\
&\geq\frac{n(n-1)}{2(n-1)^{-2\alpha}}.
\end{aligned}
$$

The last formula is the value of R_α for the complete graph, and from the above proof we know that only if G is a complete graph, $R_\alpha(G)$ for $\alpha<-1$ has the minimum value. ∎

5 Concluding remarks

In order to give a clear picture, we use the following table to summarize our main results.

α	min	max
$[0,\infty)$	$\frac{n}{2}$ (n even) and $\frac{n-3}{2}+2^{1+\alpha}$ (n odd)	$\frac{n(n-1)^{1+2\alpha}}{2}$
$(-\frac{1}{2},0)$	$\min\{(n-1)^{1+\alpha}$, $\frac{n}{2}$ (n even) and $\frac{n-3}{2}+2^{1+\alpha}$ (n odd)$\}$	$\frac{n(n-1)^{1+2\alpha}}{2}$
$-\frac{1}{2}$	$\sqrt{n-1}$	$\frac{n}{2}$
$(-1,-\frac{1}{2})$		$\frac{n}{2}$ (n even)
-1	$\frac{n}{2(n-1)}$	$\lfloor\frac{n}{2}\rfloor$
$(-\infty,-1)$	$\frac{n(n-1)^{1+2\alpha}}{2}$	$\frac{n}{2}$ (n even) and $\frac{n-3}{2}+2^{1+\alpha}$ (n odd)

There are two natural questions for further study along this line. As one can see that for the interval $(-1,-\frac{1}{2})$ there are one and a half blank places in the above table. So, the first question is to fill in the blank places of the table completely. Since in this paper we deal with general graphs, the second question is to consider some classes of interesting graphs, such as connected graphs, trees, chemical trees, etc.

Acknowledgment. The authors are grateful to the referees for their comments and suggestions, which are helpful to improving the presentation of the paper.

References

[1] B. Bollobás and P. Erdős, Graphs of extremal weights, Ars Combin. 50(1998) 225-233.

[2] G. Caporossi, I. Gutman, P. Hansen and L. Pavlović, Graphs with maximum connectivity index, Comput. Biol. and Chem. 27(2003) 85-90.

[3] L.H. Clark and J.W. Moon, On the general Randić index for certain families of trees, Ars Combin. 54(2000) 223-235.

[4] C. Delorme, O. Favaron and D. Rautenbach, On the Randić index, Discr. Math. 257(2002) 29-38.

[5] L.B. Kier and L.H. Hall, Molecular Connectivity in Chemistry and Drug Research, Academic Press, San Francisco, 1976.

[6] M. Randić, On characterization of molecular branching, J. Am. Chem. Soc. 97(1975) 6609-6615.

[7] N. Trinajstic, Chemical Graph Theory, CRC Press, Boca Raton, 1992.

[8] P. Yu, An upper bound for the Randić indices of trees, J. Math. Study (Chinese) 31(1998) 225-230.