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On the Randić index

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The Randić index of an organic molecule whose molecular graph is G is defined as the sum of $(d(u)d(v))^{-1/2}$ over all pairs of adjacent vertices of G, where $d(u)$ is the degree of the vertex u in G. In Discrete Mathematics 257, 29–38 by Delorme et al. gave a best-possible lower bound on the Randić index of a triangle-free graph G with given minimum degree $\delta(G)$. In the paper, we first point out a mistake in the proof of their result (Theorem 2 of [2002]), and then we will show that the result holds when $\delta(G) \geqslant 2$.

KEY WORDS: connectivity index, Randić index, triangle-free graph, minimum degree

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1. Introduction

A single number which characterizes the graph of a molecular is called a graphtheoretical invariant or topological index. The structure property relationships quantity the connection between the structure and properties of molecules. The connectivity index is one of the most popular molecular-graph-based structure-descriptors (see [13]), and is defined in [11] as

$$C(\lambda) = C(\lambda; G) = \sum (\mathrm{d}(u)\mathrm{d}(v))^{\lambda},$$

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where d(u) denotes the degree of the vertex u of the molecular graph G, where the summation goes over all pairs of adjacent vertices of G and where λ is a pertinently chosen exponent. The respective structure-descriptor was introduced a quarter of century ago by Randić, who chose $\lambda = -(1/2)$, and now is referred to as the *Randić index* or *molecular connectivity index* or simply *connectivity index*. The *Randić index* has been closely correlated with many chemical properties [9]. It is viewed as a measure of branching of the carbon-atom skeleton, and hence the ordering of isomeric alkanes with respect to decreasing $C(-1/2)$-values basically represents their ordering according to the increasing extent of branching. This index was found to parallel closely the boiling point, Kovats constants, and a calculated surface. However, other choice of λ were also considered (see [2,7,8,11]) and the exponent λ was treated (see [5,4,12]) an adjustable parameter, chosen so as to optimize the correlation between $C(\lambda)$ and some selected class of organic compounds. Comparing with other topological indexes reported by Amidon and Anik (see [10]), 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. More data and additional references on $C(\lambda)$ can be found in [6,7].

In order to discuss the Randić index of the molecular graph, we first introduced some terminologies and notations of 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. The minimum degree of G is denoted by $\delta(G)$. We will use $G - x$ or $G - xy$ to denote the graph that arises from G by deleting the vertex $x \in V(G)$ or the edge $xy \in E(G)$. Similarly, $G + xy$ is a graph that arises from G by adding an edge $xy \notin E(G)$, where $x, y \in V(G)$.

Let G be a graph and $uv \in E(G)$. The *Randić weight* or simply *weight* of the edge uv is $R(uv) = 1/\sqrt{\mathrm{d}(u)\mathrm{d}(v)}$. Then, the *Randić index* of a graph G, $R(G) = C(-1/2; G)$, is the sum of the weights of its edges.

In [1], Bollobás and Erdös show that $R(G) \geqslant \sqrt{n-1}$ if G is a connected graph of order n.

In Delorme et al. [3], prove a lower bound on $R(G)$ for $\delta(G) \geqslant 2$.

Theorem 1 [3]. Let $G = (V, E)$ be a graph of order n with $\delta(G) \geqslant 2$. Then

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

with equality if and only if $G = K^*_{2,n-2}$. (Where $K^*_{2,n-2}$ is a graph that arises from a complete bipartite graph $K_{2,n-2}$ by joining the vertices in the part with 2 vertices by a new edge).

Note that $K^*_{2,n-2}$ contains triangles and $\sqrt{2(n-2)} > \sqrt{2(n-1)} + \frac{1}{n-1} - \frac{\sqrt{2}}{\sqrt{n-1}}$ for $n \geqslant 4$, and hence in [3], Delorme et al. gave a best-possible lower bound on $R(G)$ in terms of δ when G is triangle-free as follows.

(**Theorem 2** of [3]). Let $G = (V, E)$ be a triangle-free graph of order n with $\delta(G) \geqslant \delta \geqslant 1$. Then

$$R(G) \geqslant \sqrt{\delta(n-\delta)}$$

with equality if and only if $G = K_{\delta,n-\delta}$.

Although we find a mistake in the proof of Theorem 2 of [3], we still believe that Theorem 2 of [3] is correct. In section 3, we will show (Theorem 2 of [3]) which supports Theorem 2.

Theorem 2. Let $G = (V, E)$ be a triangle-free graph of order n with $\delta(G) \geqslant 2$. Then

$$R(G) \geqslant \sqrt{2(n-2)}.$$

2. Examples

Let G be a triangle-free graph of order n with $\delta(G) \geqslant \delta \geqslant 1$ and v_0 a vertex of minimum degree of G. In the proof of Theorem 2, the authors claimed that

$$R(G - v_o) \geqslant \sqrt{\delta(n-\delta-1)}. \qquad (*)$$

We note that $(*)$ is not always true for all triangle-free graphs. The following graphs are the counterexamples. In order to depict construction of the counterexamples, we first define one kind of graph operation as follows.

For a given graph H with $V(H) = \{v_1, \dots, v_s\}$, we define the graph $G(H, m)(m \geqslant 2)$ as follows. Take m disjoint copies $H_1, \dots, H_m$ of H, with the vertex v_j^i in H_i corresponding to the vertex v_j in $H(1 \leqslant j \leqslant s, 1 \leqslant i \leqslant m)$. Let $G(H, m)$ be the graph obtained from $H_I \cup \cdots \cup H_m$ by joining v_j^k and $v_{j+1}^{k'}(k \neq k', 1 \leqslant j \leqslant s(v_{s+1}^{k'} = v_1^{k'})$ for $k, k' = 1, 2, \dots, m$.

Example 1. Regular graph. Let $H = (V, E)$ be a graph with $V = \{v_1, v_2, v_3, v_4\}$ and $E(H) = \{v_1v_2,\ v_3v_4\}$. Denote $G = G(H, m)$. Obviously, G is triangle-free. In the graph G, we have that $n = 4m$, $\delta(G) = 2m - 1$. Let v_0 be any vertex of G. It is easy to see that

$$R(G - v_0) = \frac{2m-1}{\sqrt{(2m-1)(2m-1)}} + \frac{(2m-1)(2m-2)}{\sqrt{(2m-1)(2m-2)}} = 1 + \sqrt{(2m-1)(2m-2)}$$

and

$$\sqrt{\delta(n-\delta-1)} = \sqrt{2m(2m-1)}.$$

Since

$$\begin{aligned}&\sqrt{(2m)(2m-1)}-\sqrt{(2m-1)(2m-2)}-1\\&=\frac{\left(\sqrt{2m-1}-\sqrt{2m-2}\right)-\left(\sqrt{2m}-\sqrt{2m-1}\right)}{\sqrt{2m}+\sqrt{2m-2}}>0,\end{aligned}$$

we have $R(G-v_0)<\sqrt{\delta(n-\delta-1)}$.

Example 2. Non-regular graph. Let $P_4 = v_1v_2v_3v_4$, a path of order 4, and let $G = G(P_4, m)$. Obviously, G is triangle-free. In the graph G, we have that $n = 4m, \delta(G) = 2m-1$. Let v_0 be any vertex of G with $d(v_0) = \delta(G) = 2m-1$. Then

$$\begin{aligned}R(G-v_0)=&\frac{m(m+1)}{\sqrt{2m(2m-1)}}+\frac{(m+1)(m-1)}{\sqrt{(2m-1)(2m-1)}}\\&+\frac{m(m-1)}{\sqrt{2m(2m-2)}}+\frac{(m-1)(m-2)}{\sqrt{(2m-1)(2m-2)}}\end{aligned}$$

and

$$\sqrt{\delta(n-\delta-1)}=\sqrt{2m(2m-1)}.$$

It is checked (in Appendix A) that $R(G-v_0)<\sqrt{\delta(n-\delta-1)}$.

Remark. Note that there is NO vertex with minimum degree such that $(*)$ holds in these graphs.

3. Proof of Theorem 2

In order to prove Theorem 2, we first need some lemmas.

Lemma 1 [1]. Let x_1x_2 be an edge of maximal weight in a graph G. Then

$$R(G-x_1x_2)<R(G).$$

Lemma 2. Let d, d_1, d_2 be positive integers and

$$\begin{aligned}f(d_1,d_2)=&\frac{1}{\sqrt{2}}\left(\sqrt{d_1}-\sqrt{d_1-1}\right)+\frac{1}{\sqrt{2}}\left(\sqrt{d_2}-\sqrt{d_2-1}\right)\\&+\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{d_1}}\right)-\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{d_2}}\right)\\&-\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{d_1-1}}\right)\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{d_2-1}}\right).\end{aligned}$$

If $3\leqslant d_1, d_2, \leqslant d$, then

$$f(d_1,d_2)\geqslant\sqrt{2}(\sqrt{d}-\sqrt{d-1}).$$

Proof. From the proof of Lemma 1 in [3], we have

$$\begin{aligned} f(d_1, d_2) &\geqslant f(d, d) \\ &= \sqrt{2}\left(\sqrt{d} - \sqrt{d-1}\right) + \left(\frac{1}{\sqrt{d-1}} - \frac{1}{\sqrt{d}}\right)\left(\sqrt{2} - \frac{1}{\sqrt{d-1}} - \frac{1}{\sqrt{d}}\right). \end{aligned}$$

Obviously, $\frac{1}{\sqrt{d-1}} - \frac{1}{\sqrt{d}} > 0$. On the other hand, by $d \geqslant 3$, we have

$$\sqrt{2} - \frac{1}{\sqrt{d-1}} - \frac{1}{\sqrt{d}} \geqslant \sqrt{2} - \frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}} > 0,$$

hence $f(d_1, d_2) \geqslant \sqrt{2}(\sqrt{d} - \sqrt{d-1})$. □

The following result holds from the proof of Theorem 2 of [3].

Lemma 3. Let $G = (V, E)$ be a triangle-free graph of order n with $\delta(G) \geqslant \delta \geqslant 1$. Let $V_\delta = \{v : d(v) = \delta\}$. If there exists a vertex $v \in V_\delta$ such that $N(v) \cap V_\delta = \emptyset$, then

$$R(G) \geqslant \sqrt{\delta(n-\delta)}.$$

Now, we will prove our theorem.

Proof. We assume that G is a counterexample of minimal order for which $R(G)$ is minimal. Since G is a triangle-free graph and $\delta(G) \geqslant 2, n \geqslant 4$. If $\delta(G) > 2$, then, by Lemma 1, we have a triangle-free graph G' of minimum degree at least 2 and with $R(G') < R(G)$ by deleting the maximal weight edge, a contradiction with the choice of G. Hence $\delta(G) = 2$. Denote $T = \{v \in V(G) : d(v) = 2\}$. If there exists a vertex $v \in T$ such that $N(v) \cap T = \emptyset$, then $R(G) \geqslant \sqrt{2(n-2)}$ by Lemma 3, a contradiction with the choice of G. Thus we can assume that $N(v) \cap T \neq \emptyset$ for any $v \in T$. Choose a vertex $u \in T$ such that $|N(u) \cap T|$ is as small as possible. Let $N(u) = \{u_1, u_2\}$ with $u_l \in T$ and $d(u_2) = d_2 \geqslant 2$. □

Claim 1. $(N(u_1) \cap N(u_2))\ \{u\} \neq \emptyset$.

Proof. Suppose that $(N(u_1) \cap N(u_2)) \setminus \{u\} = \emptyset$. Then $n \geqslant 5$ and $G' = G - u + u_1u_2$ is no counterexample, i.e., $R(G') \geqslant \sqrt{2(n-3)}$. Thus

$$R(G) = R(G') + \frac{1}{\sqrt{2d_2}} + \frac{1}{2} - \frac{1}{\sqrt{2d_2}} \geqslant \sqrt{2(n-3)} + \frac{1}{2} > \sqrt{2(n-2)},$$

which is a contradiction. □

By Claim 1 and $u_1 \in T$, we can assume that $(N(u_1) \cap N(u_2)) = \{u, v\}$. Denote $d_1 = d(v)$. Since G is a triangle-free graph, $d_1 + d_2 \leqslant n$. Let S_1, S_2 be the sums of the weights of the edges incident with v and u_2 except for the edges u_1v, u_2v and uu_2, vu_2, respectively. Then $S_i \leqslant \frac{d_i-2}{\sqrt{2d_i}}$ for $i = 1, 2$.

Claim 2. $v \in T$.

Proof. Suppose $v \notin T$. Then by the choice of $u, u_2 \notin T$. Thus $d_1, d_2 \geqslant 3, n \geqslant 6$ and $G' = G - u - u_1$ is no counterexample, i.e., $R(G') \geqslant \sqrt{2(n-4)}$. In G', if we denote S_1', S_2' the sums of the weights of the edges incident with v and u_2 except for the edge u_2v, respectively. Then $S_i' = S_i\sqrt{d_i/(d_i-1)}$ for $i = 1, 2$. Since $d_1 + d_2 \leqslant n$ and $d_i \geqslant 3, d_i \leqslant n-3$ for $i = 1, 2$. Then

$$\begin{aligned}
R(G) &= R(G') + \frac{1}{2} + \frac{1}{\sqrt{2d_1}} + \frac{1}{\sqrt{2d_2}} + \frac{1}{\sqrt{d_1d_2}} + S_1 + S_2 \\
&\quad - \frac{1}{\sqrt{(d_1-1)(d_2-1)}} - S_1\sqrt{\frac{d_1}{d_1-1}} - S_2\sqrt{\frac{d_2}{d_2-1}} \\
&\geqslant \sqrt{2(n-4)} + \frac{1}{2} + \frac{1}{\sqrt{2d_1}} + \frac{1}{\sqrt{2d_2}} + \frac{1}{\sqrt{d_1d_2}} \\
&\quad - \frac{1}{\sqrt{(d_1-1)(d_2-1)}} - \frac{d_1-2}{\sqrt{2d_1}}\left(\sqrt{\frac{d_1}{d_1-1}} - 1\right) - \frac{d_2-2}{\sqrt{2d_2}}\left(\sqrt{\frac{d_2}{d_2-1}} - 1\right) \\
&= \sqrt{2(n-4)} + \frac{1}{2} + \frac{1}{\sqrt{2}}\left(\sqrt{d_1} - \sqrt{d_1-1}\right) + \frac{1}{\sqrt{2}}\left(\sqrt{d_2} - \sqrt{d_2-1}\right) \\
&\quad + \left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{d_1}}\right)\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{d_2}}\right) - \left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{d_1-1}}\right)\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{d_2-1}}\right).
\end{aligned}$$

Using the same notation as in Lemma 2, we have

$$R(G) \geqslant \sqrt{2(n-4)} + \frac{1}{2} + f(d_1, d_2).$$

Since $3 \leqslant d_1, d_2 \leqslant n-3$, we have $f(d_1, d_2) \geqslant \sqrt{2}(\sqrt{n-3} - \sqrt{n-4})$ by Lemma 2. Thus

$$\begin{aligned}
R(G) &\geqslant \sqrt{2(n-4)} + \frac{1}{2} + \sqrt{2}(\sqrt{n-3} - \sqrt{n-4}) \\
&= \sqrt{2(n-2)} + \frac{1}{2} + \sqrt{2}(\sqrt{n-3} - \sqrt{n-2})
\end{aligned}$$

Since

$$\frac{1}{2} + \sqrt{2}(\sqrt{n-3} - \sqrt{n-2}) \geqslant \frac{1}{2} + \sqrt{2}(\sqrt{6-3} - \sqrt{6-2}) > 0$$

we have $R(G) \geqslant \sqrt{2(n-2)}$, which is a contradiction. □

Claim 3. $u_2 \notin T$.

Proof. Suppose $u_2 \in T$. If $n = 4$, then $R(G) = 2 = \sqrt{2(4-2)}$, a contradiction with the choice of G. Therefore $n \neq 4$. By G being a triangle-free graph and $\delta(G) = 2$, we have $n \geqslant 8$. So $G' = G - u - u_1 - u_2 - v$ is no counterexample. Thus

$$R(G) = R(G') + 2 \geqslant \sqrt{2(n-6)} + 2 \geqslant \sqrt{2(n-2)},$$

which is a contradiction. □

By Claims 2 and 3, we have $v \in T$ and $d_2 \geqslant 3$, Thus $d_2 \leqslant n-2$ by G being triangle-free. Now, we will complete our proof by considering the following two cases.

Case 1. $d(u_2) = d_2 \geqslant 4$. In the case, $n \geqslant 6$ and $G' = G - u - u_1 - v$ is no counterexample, and then $R(G') \geqslant \sqrt{2(n-5)}$. Thus

$$\begin{aligned} R(G) &= R(G') + \frac{1}{\sqrt{2d_2}} + \frac{1}{\sqrt{2d_2}} + \frac{1}{2} + \frac{1}{2} + S_2\left(1 - \sqrt{\frac{d_2}{d_2-2}}\right) \\ &\geqslant \sqrt{2(n-5)} + 1 + \frac{\sqrt{d_2} - \sqrt{d_2-2}}{\sqrt{2}} \\ &\geqslant \sqrt{2(n-5)} + 1 + \frac{\sqrt{n-2} - \sqrt{n-4}}{\sqrt{2}} \\ &= \sqrt{2(n-5)} + \frac{\sqrt{2} + 2\sqrt{n-5} - \sqrt{n-2} - \sqrt{n-4}}{\sqrt{2}}. \end{aligned}$$

For $n \geqslant 6$, $\sqrt{2}+2\sqrt{n-5}-\sqrt{n-2}-\sqrt{n-4} \geqslant \sqrt{2}+2\sqrt{6-5}-\sqrt{6-2}-\sqrt{6-4} = 0$, and hence $R(G) \geqslant \sqrt{2(n-2)}$, which is a contradiction.

Case 2. $d(u_2) = d_2 = 3$.

Let $N(u_2) \setminus \{u, v\} = \{x\}$, $d(x) = d$ and $y \in N(x) \setminus \{u_2\}$. If $d = 2$, then $(N(y) \cap N(u_2)) \setminus \{x\} = \emptyset$ by $d(u) = d(v) = 2$ and $d_2 = 3$. Thus we can derive a contradiction by the same argument as the proof of Claim 1. Hence we can assume that $d \geqslant 3$ and then $n \geqslant 8$. Let S be the sum of the weights of the edges incident with x different from u_2x. Then $S \leqslant \frac{d-1}{\sqrt{2d}}$. Since $G' = G - u - u_1 - u_2 - v$ is no counterexample, i.e., $R(G') \geqslant \sqrt{2(n-6)}$, we have

$$
\begin{aligned}
R(G) &= R(G') + 1 + \frac{2}{\sqrt{6}} + \frac{1}{\sqrt{3d}} + S\left(1 - \sqrt{\frac{d}{d-1}}\right) \\
&\geqslant \sqrt{2(n-6)} + 1 + \frac{2}{\sqrt{6}} + \frac{\sqrt{d}}{\sqrt{2}} - \frac{\sqrt{d-1}}{\sqrt{2}} - \frac{1}{\sqrt{d}}\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}}\right) \\
&\geqslant \sqrt{2(n-6)} + 1 + \frac{2}{\sqrt{6}} - \frac{1}{\sqrt{d}}\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}}\right) \\
&\geqslant \sqrt{2(n-2)} + \sqrt{2(n-6)} + \sqrt{2(n-2)} + 1 + \frac{2}{\sqrt{6}} - \frac{1}{\sqrt{3}}\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}}\right).
\end{aligned}
$$

Since $\sqrt{2(n-6)} - \sqrt{2(n-2)} + 1 + \frac{2}{\sqrt{6}} - \frac{1}{\sqrt{3}}\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}}\right) \geqslant 3 - 2\sqrt{3} + \frac{1}{\sqrt{6}} + \frac{1}{3} > 0$, we have $R(G) > \sqrt{2(n-2)}$, which is a contradiction. Hence the proof of our Theorem is completed.

Appendix A

Let G be the graph of Example 2 and v_0 be any vertex of G with $d(v_0) = \delta(G)$. In the following, we will show that

$$\sqrt{\delta(n-\delta-1)} - R(G - v_0) > 0.$$

We have

$$
\begin{aligned}
&\sqrt{\delta(n-\delta-1)} - R(G - v_0) \\
&= \frac{3m(m-1)}{\sqrt{2m(2m-1)}} - \frac{(m+1)(m-1)}{2m-1} - \frac{m(m-1)}{\sqrt{2m(2m-2)}} - \frac{(m-1)(m-2)}{\sqrt{(2m-1)(2m-2)}} \\
&= (m-1)\left(\frac{3m}{\sqrt{2m(2m-1)}} - \frac{m+1}{2m-1} - \frac{m}{\sqrt{2m(2m-2)}} - \frac{m-2}{\sqrt{(2m-1)(2m-2)}}\right).
\end{aligned}
$$

Since $m - 1 > 0$, it just needs to check that

$$\frac{3m}{\sqrt{2m(2m-1)}} - \frac{m+1}{2m-1} - \frac{m}{\sqrt{2m(2m-2)}} - \frac{m-2}{\sqrt{(2m-1)(2m-2)}} > 0,$$

i.e.,

$$\frac{3m}{\sqrt{2m(2m-1)}} - \frac{m-2}{\sqrt{(2m-1)(2m-2)}} > \frac{m+1}{2m-1} + \frac{m}{\sqrt{2m(2m-2)}}.$$

Noting that

$$\frac{3m}{\sqrt{2m(2m-1)}} - \frac{m-2}{\sqrt{(2m-1)(2m-2)}} > \frac{3m}{2m} - \frac{m-2}{2m-2} = \frac{2m-1}{2m-2} > 0$$

and

$$\frac{m+1}{2m-1} + \frac{m}{\sqrt{2m(2m-2)}} > 0,$$

we will check that

$$\left(\frac{3m}{\sqrt{2m(2m-1)}} - \frac{m-2}{\sqrt{(2m-1)(2m-2)}}\right)^2 > \left(\frac{m+1}{2m-1} + \frac{m}{\sqrt{2m(2m-2)}}\right)^2,$$

i.e.,

$$\begin{aligned}&\frac{9m}{2(2m-1)} + \frac{(m-2)^2}{2(2m-1)(m-1)} - \frac{6m(m-2)}{2(2m-1)\sqrt{m(m-1)}}\\ &> \frac{(m+1)^2}{(2m-1)^2} + \frac{m}{4(m-1)} + \frac{2m(m+1)}{2(2m-1)\sqrt{m(m-1)}},\end{aligned}$$

i.e.,

$$\frac{5m-4}{2(m-1)} - \frac{(m+1)^2}{(2m-1)^2} - \frac{m}{4(m-1)} > \frac{m(4m-5)}{(2m-1)\sqrt{m(m-1)}},$$

i.e.,

$$32m^3 - 72m^2 + 45m - 4 > 4(2m-1)(4m-5)\sqrt{m(m-1)}.$$

Since $m \geqslant 2$, $32m^3 - 72m^2 + 45m - 4 = (m-1)(m(32m-40)+5)+1 > 0$ and $(2m-1)(4m-5)\sqrt{m(m-1)} > 0$. Hence we just need to check that

$$(32m^3 - 72m^2 + 45m - 4)^2 > \left(4(2m-1)(4m-5)\sqrt{m(m-1)}\right)^2,$$

i.e.,

$$\begin{aligned}&1024m^6 - 4608m^5 + 8064m^4 - 6736m^3 + 2601m^2 - 360m + 16\\ &> 16(m^2-m)(64m^4 - 224m^3 + 276m^2 - 140m + 25),\end{aligned}$$

i.e.,

$$64m^4 - 80m^3 - 39m^2 + 40m + 16 > 0.$$

Note that

$$64m^4 - 80m^3 - 39m^2 + 40m + 16 = m^2(8m-13)(8m+3) + 40m + 16 > 0$$

by $m \geqslant 2$, and hence $\sqrt{\delta(n-\delta-1)} - R(G - v_0) > 0$ holds.

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References

[1] B. Bollobás and P. Erdös, Graphs of extremal weights, Ars Combin. 50 (1998) 225.
[2] L.H. Clark and J.W. Moon, Ars Combinatorics 54 (1999) 223.
[3] C. Delorme, O. Favaron and D. Rautenbach, On the Randić index, Discrete Math. 257 (2002) 29.
[4] E. Estrada, Chem. Phys. Lett. 312 (1999) 556.
[5] E. Estrada, J. Chem. Inf. Comput. Sci. 35 (1995) 1022.
[6] I. Gutman, D. Vidović and A. Nedić, J. Serb. Chem. Soc. in press.
[7] I. Gutman and M. Leporić, J. Serb. Chem. Soc. 66 (2001) 605.
[8] I. Gutman and N. Trinajstić, Chem. Phys. Lett. 17 (1972) 535.
[9] L.B. Kier and L.H. Hall, *Molecular Connectivity in Chemistry and Drug Research* (Academic Press, San Francisco, 1976).
[10] L.B. Kier and L.H. Hall, *Molecular Connectivity in Structure-Activity Analysis* (Wiley, New york 1986).
[11] M. Randić, On characterization of molecular branching, J. Amer. Chem. Soc. 97 (1975) 6609.
[12] M. Randić, P.J. Hansen and P.C. Jurs, J. Chem. Inf. Comput. Sci. 28 (1988) 60.
[13] R. Todeschini and V. Consonni, *Handbook of Molecular Descriptors* (Wiley-VCH, Weinheim, 2000).