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The Randić Index of Trees with given Total Domination Number

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ABSTRACT

In chemical graph theory, Randić index is among the most popular topological indices. We discovered an upper bound for the Randić index of trees in regards to the order and total domination number in this work. The extremal trees have also been identified and characterized.

1. INTRODUCTION

Most graphs presented in the current research are deemed connected and simple. Consider $G = (V, E)$ as a graph having $V = V(G)$ and $E = E(G)$ as its vertex and edge sets, respectively. Here, uv represents an edge in the graph G that connects two vertices given by u and v. Moreover, the amount of edges incident having u in graph G is indicated by $deg(u)$, which is also known as the vertex degree, u. Given that $deg(u) = 1$, a vertex u in G is termed pendant or leaf. In a G graph, the greatest vertex degree is expressed with the notation

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of $\Delta(G)$ (or simply Δ). The *open neighbourhood* of each vertex $v \in V$ denotes the $N(v) = \{u \in V | uv \in E\}$ set. Meanwhile, the *closed neighbourhood* denotes the $N[v] = N(v) \cup \{v\}$ set. The cycle and the path on n vertices are expressed as C_n and P_n, accordingly. Assume T is a tree. Then, the longest path that exists between the two leaves defines a tree's diameter. Provided that $v_1, v_2, \ldots, v_d$ denotes a path in which the diameter is obtained, we may state that it resembles a diametrical path in T. To designate the forest generated by T via eliminating the vertices of $u_1, u_2, \ldots, u_k$ or the edges $e_1, e_2, \ldots, e_k$ in T, we employ $T - \{u_1, u_2, \ldots, u_k\}$ or $T - \{e_1, e_2, \ldots, e_k\}$. For other notation and terminologies which are not defined here, please refer the book by West [12].

Provided that every vertex $V(G)\backslash D$ possess a neighbour in D, then the subset known as $D \subseteq V(G)$ is termed a *dominating set* that belongs to G. On the other hand, the minimal cardinality referring to a G dominating set is termed as the *domination number*, represented by $\gamma(G)$. If every vertex G has a neighbour in D, a subset known as $D \subseteq V(G)$ is termed as the *total dominating set*, expressed as TDS. For example, Cockayne *et al.* [3] established the TDS of G, indicated by $\gamma_t(G)$, as the minimal cardinality of a G TDS. Please see [5] for a summary of selected latest findings on total domination number in graphs. Domination in graphs has been an active research area in graph theory [8, 9].

The *Randić* index of a graph G was established by Randić [7], defined as follows:

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{deg(u)deg(v)}},$$

in which $deg(v)$ and $deg(u)$ resemble the vertices degrees $v, u \in V(G)$ while uv refers to the edge that connects the two vertices.

For instance, see [1, 2, 4, 10, 11] and their corresponding references for relationships between a variety of topological indices and domination number of graphs which has been a subject of concern for many years. Borović anin and Furtula [1] investigated the extremal Zagreb indices of trees with given domination number. Moreover, Bermudo et al. [2] discovered upper and lower bounds of the Randić index for trees in regards to the order and the domination number. Mojdeh *et al.* [10] found some upper bounds with regards to the Zagreb indices of trees, bicyclic and unicyclic graphs with given total domination number.

We provide an upper bound for the Randić index of trees in regards to the order and the total domination number in this research. Consequently, extremal trees can be characterized. We present several preliminary findings in Section 2, while in Section 3, we present our main results.

2. PRELIMINARIES RESULTS

The extremal values survey of the Randić index for major classes of graphs was detailed by Li and Shi [6]. The star S_n, for example, possess the lowest Randić index between trees having n vertices, whereas the path P_n possess the highest Randić index. The authors in [2] proposed new bounds specifically for the Randić index of trees with the order and the domination number. They introduced the function as follows to make the computations easier:

$$f(n,\gamma) = \frac{2n}{5} + \frac{3\gamma_t}{10} + \sqrt{2} - \frac{3}{2} + (n-3\gamma)\left(\frac{\sqrt{3}+1}{\sqrt{2}} - \frac{19}{10}\right).$$

Lemma 2.1. [2] Consider T as a tree having order n and a domination number γ, as well as a vertex $v \in V(T)$ provided that $N(v) = \{u_1, u_2, \dots, u_i\}$, $deg(v) = i \geq 3$, $deg(u_i) = j \geq 2$ and $deg(u_l) = 1$ for each $l \in \{1,2, \dots, i-1\}$. Now, by considering $T_1 = T - u_1$, we then obtain as follows:

I) Provided that $i \geq 4$ as well as $R(T_1) \leq f(n-1,\gamma)$, we now have $R(T) < f(n,\gamma)$.

II) Provided that $i = 3, j \leq 67$ as well as $R(T_1) \leq f(n-1,\gamma)$, we now have $R(T) < f(n,\gamma)$.

Lemma 2.2. [2] For any given tree T having order n as well as a domination number γ, we then obtain

$$R(T) \leq \frac{2n}{5} + \frac{3\gamma_t}{10} + \sqrt{2} - \frac{3}{2} + (n-3\gamma)\left(\frac{\sqrt{3}+1}{\sqrt{2}} - \frac{19}{10}\right).$$

3. Upper Bound for the Randić Index of Trees with Given Total Domination Number

We describe our main findings in this section. By using the order and total domination number, we will find an upper bound for Randić index of trees. To make our computations easier, we use the following abbreviation

$$f(n,\gamma_t) = \frac{2n+(-1)^n}{8} + \frac{\gamma_t}{2} + \sqrt{2} - \frac{13}{8} + (n-2\gamma_t+1)\left(\frac{\sqrt{14}-3}{2}\right).$$

Lemma 3.1. Consider T as a tree having order n and a total domination number γ_t, as well as a vertex $v \in V(T)$ provided that $N(v) = \{u_1, u_2, \cdots, u_i\}$, $deg(v) = i \geq 3$, $deg(u_i) = j \geq 2$ and $deg(u_l) = 1$ for each $l \in \{1,2, \dots, i-1\}$. Now, by taking $T_1 = T - u_1$ yields as follows:

I) Provided that $i \geq 4$ and $R(T_1) \leq f(n-1,\gamma_t)$, we now have $R(T) < f(n,\gamma_t)$.

II) Provided that $i = 3, j = 2$ and $R(T_1) \leq f(n-1,\gamma_t)$, we now have $R(T) < f(n,\gamma_t)$.

Proof. Since $T_1 = T - u_1$, we obtain

$$R(T) = R(T-u_1) - \frac{i-2}{\sqrt{i-1}} - \frac{1}{\sqrt{j(i-1)}} + \frac{i-1}{\sqrt{i}} + \frac{1}{\sqrt{ji}}$$

$$= R(T_1) + \left(\frac{1}{\sqrt{i}} - \frac{1}{\sqrt{i-1}}\right)\left(i-2+\frac{1}{\sqrt{j}}\right) + \frac{1}{\sqrt{i}}$$

$$\leq \frac{2(n-1)+(-1)^{n-1}}{8} + \frac{\gamma_t}{2} + \sqrt{2} - \frac{13}{8} + ((n-1) - 2\gamma_t + 1)\left(\frac{\sqrt{14}-3}{2}\right)$$
$$+\left(\frac{1}{\sqrt{i}} - \frac{1}{\sqrt{i-1}}\right)\left(i - 2 + \frac{1}{\sqrt{j}}\right) + \frac{1}{\sqrt{i}}$$
$$\leq f(n,\gamma_t) + \frac{5}{4} - \frac{(-1)^n}{4} - \frac{\sqrt{14}}{2} + \left(\frac{1}{\sqrt{i}} - \frac{1}{\sqrt{i-1}}\right)\left(i - 2 + \frac{1}{\sqrt{j}}\right) + \frac{1}{\sqrt{i}}.$$

Due to the function $\frac{5}{4} - \frac{(-1)^n}{4} - \frac{\sqrt{14}}{2} + \left(\frac{1}{\sqrt{i}} - \frac{1}{\sqrt{i-1}}\right)\left(i - 2 + \frac{1}{\sqrt{j}}\right) + \frac{1}{\sqrt{i}}$ yields a negative value for any $i \geq 4$, we then obtain (a).

Given that $j = 2$, we obtain

$$R(T) \leq f(n,\gamma_t) + \frac{5}{4} - \frac{(-1)^n}{4} - \frac{\sqrt{14}}{2} + \left(\frac{1}{\sqrt{i}} - \frac{1}{\sqrt{i-1}}\right)\left(i - 2 + \frac{1}{\sqrt{2}}\right) + \frac{1}{\sqrt{i}} < f(n,\gamma_t),$$

for $i = 3$, so we have (b). This then completes the proof. ■

Theorem 3.2. Consider any tree T having order n and a total domination number γ_t, we then obtain the following

$$R(T) \leq \frac{2n+(-1)^n}{8} + \frac{\gamma_t}{2} + \sqrt{2} - \frac{13}{8} + (n - 2\gamma_t + 1)\left(\frac{\sqrt{14}-3}{2}\right).$$

Proof. We express $f(n,\gamma_t) = \frac{2n+(-1)^n}{8} + \frac{\gamma_t}{2} + \sqrt{2} - \frac{13}{8} + (n - 2\gamma_t + 1)\left(\frac{\sqrt{14}-3}{2}\right)$. If $n = 4$, we have

$$R(P_4) = \sqrt{2} + \frac{1}{2} \leq f(4,2) \text{ and } R(S_4) = \sqrt{3} \leq f(4,2).$$

We make assumption that the findings holds for every tree with $n-1$ vertices, we then have to prove it for trees having n vertices. In T, by taking diameter $v_1, v_2, \ldots, v_d$, we make assumption that $deg(v_2) \leq 3$ according to Lemma 3.1. Therefore, we investigate two cases given below.

Case 1: Assume we have $deg(v_2) = 3$. Now, provided that $deg(v_3) = j \geq 3$, we express $N(v_2) = \{v_1, v_3, u_1\}$,

$N(v_3) = \{v_2, v_4, w_1, w_2, \ldots, w_{j-2}\}$, $deg(v_4) = k$ as well as $deg(w_l) = s_l$. Moreover, we set $T_2 = T - \{v_1, v_2, u_1\}$. Here, in this case, there exist a TDS $D \in T$ provided that $v_2 \in D$ as well as $v_3 \in N[D\backslash\{v_2\}]$. As a result, $\gamma_t(T) = \gamma_t(T_2) + 1$. Moreover, since $s_l \leq 3$, we obtain

$$R(T) = R(T_2) - \frac{1}{\sqrt{k(j-1)}} - \frac{1}{\sqrt{(j-1)s_1}} - \cdots - \frac{1}{\sqrt{(j-1)s_{j-2}}} + \frac{1}{\sqrt{kj}} + \frac{1}{\sqrt{js_1}}$$
$$+ \cdots + \frac{1}{\sqrt{js_{j-2}}} + \frac{1}{\sqrt{3j}} + \frac{2}{\sqrt{3}}$$
$$\leq \frac{2(n-3)+(-1)^{n-3}}{8} + \frac{\gamma_t - 1}{2} + \sqrt{2} - \frac{13}{8} + ((n-3) - 2(\gamma_t - 1) + 1)\left(\frac{\sqrt{14}-3}{2}\right)$$
$$-\left(\frac{1}{\sqrt{j-1}} - \frac{1}{\sqrt{j}}\right)\left(\frac{1}{\sqrt{k}} + \sum_{l=1}^{j-2} \frac{1}{\sqrt{s_l}}\right) + \left(\frac{1}{\sqrt{j}} + 2\right)\left(\frac{1}{\sqrt{3}}\right)$$

$$\leq f(n,\gamma_t)+\frac{1}{4}-\frac{(-1)^n}{4}-\frac{\sqrt{14}}{2}-\left(\frac{1}{\sqrt{j-1}}-\frac{1}{\sqrt{j}}\right)\left(\frac{1}{\sqrt{k}}+\sum_{l=1}^{j-2}\frac{1}{\sqrt{s_l}}\right)$$
$$+\left(\frac{1}{\sqrt{j}}+2\right)\left(\frac{1}{\sqrt{3}}\right).$$

Since $\frac{1}{4}-\frac{(-1)^n}{4}-\frac{\sqrt{14}}{2}-\left(\frac{1}{\sqrt{j-1}}-\frac{1}{\sqrt{j}}\right)\left(\frac{1}{\sqrt{k}}+\sum_{l=1}^{j-2}\frac{1}{\sqrt{s_l}}\right)+\left(\frac{1}{\sqrt{j}}+2\right)\left(\frac{1}{\sqrt{3}}\right)$ yields a negative value for every $j\geq 3$, we obtain $R(T)<f(n,\gamma_t)$.

Case 2: Suppose that $deg(v_2)=2$.

Case 2.1: Provided that $deg(v_3)=j\geq 3$, in this case, we express $N(v_3)=\{v_2,v_4,w_1,w_2,\dots,w_{j-2}\}$, $deg(v_4)=k$ as well as $deg(w_l)=s_l$. Moreover, we assume that $T_2=T-\{v_1,v_2\}$. Provided that we know the existance of a TDS $D\in T$ given by $v_2\in D$ as well as $v_3\in N[D\backslash\{v_2\}]$, then $\gamma_t(T)=\gamma_t(T_2)+1$ yielding

$$R(T)=R(T_2)-\frac{1}{\sqrt{k(j-1)}}-\frac{1}{\sqrt{(j-1)s_1}}-\cdots-\frac{1}{\sqrt{(j-1)s_{j-2}}}+\frac{1}{\sqrt{kj}}+\frac{1}{\sqrt{js_1}}\frac{1}{\sqrt{js_{j-2}}}$$
$$+\cdots++\frac{1}{\sqrt{2j}}+\frac{1}{\sqrt{2}}$$
$$\leq\frac{2(n-2)+(-1)^{n-2}}{8}+\frac{\gamma_t-1}{2}+\sqrt{2}-\frac{13}{8}+((n-2)-2(\gamma_t-1)+1)\left(\frac{\sqrt{14}-3}{2}\right)$$
$$-\left(\frac{1}{\sqrt{j-1}}-\frac{1}{\sqrt{j}}\right)\left(\frac{1}{\sqrt{k}}+\sum_{l=1}^{j-2}\frac{1}{\sqrt{s_l}}\right)+\left(\frac{1}{\sqrt{j}}+1\right)\left(\frac{1}{\sqrt{2}}\right)$$
$$\leq f(n,\gamma_t)-1-\left(\frac{1}{\sqrt{j-1}}-\frac{1}{\sqrt{j}}\right)\left(\frac{1}{\sqrt{k}}+\sum_{l=1}^{j-2}\frac{1}{\sqrt{s_l}}\right)+\left(\frac{1}{\sqrt{j}}+1\right)\left(\frac{1}{\sqrt{2}}\right).$$

Since $-1-\left(\frac{1}{\sqrt{j-1}}-\frac{1}{\sqrt{j}}\right)\left(\frac{1}{\sqrt{k}}+\sum_{l=1}^{j-2}\frac{1}{\sqrt{s_l}}\right)+\left(\frac{1}{\sqrt{j}}+1\right)\left(\frac{1}{\sqrt{2}}\right)$ yields a negative function for every $j\geq 3$, we then obtain $R(T)<f(n,\gamma_t)$.

Case 2.2: Provided that we have $deg(v_3)=2$, we then express $N(v_4)=\{v_3,v_5,z_1,z_2,\dots,z_{k-2}\}$ as well as $deg(z_l)=t_l$ for each $l\in\{1,2,\dots,k-2\}$. Also, provided that for every $l\in\{1,2,\dots,k-2\}$, let's say there exist $w_1,w_2\in V(T)$ given that $w_1\in N(z_l)$ as well as $w_2\in N(w_1)$, following from there $w_2,w_1,z_l,v_4,v_5,\dots v_d$ denotes a diameter (T). From here, following the cases mentioned above, we may make assumption that $t_l=deg(w_1)=2$. In addition, if z_l resembles a support vertex, thus, employing Lemma 3.1, we may make assumption that $t_l\leq 3$.

Case 2.2.1: Here, we assume that $k\geq 4$. Let say we set $T_3=T-\{v_1,v_2,v_3\}$, we then obtain

$$R(T)=R(T_3)-\frac{1}{\sqrt{(k-1)deg(v_5)}}-\frac{1}{\sqrt{(k-1)t_1}}-\cdots-\frac{1}{\sqrt{(k-1)t_{k-2}}}$$
$$+\frac{1}{\sqrt{kdeg(v_5)}}+\frac{1}{\sqrt{kt_1}}+\cdots+\frac{1}{\sqrt{kt_{k-2}}}+\frac{1}{\sqrt{2k}}+\frac{1}{2}+\frac{1}{\sqrt{2}}$$

$$\leq \frac{2(n-3)+(-1)^{n-3}}{8} + \frac{\gamma_t-2}{2} + \sqrt{2} - \frac{13}{8} + ((n-3) - 2(\gamma_t - 2) + 1)\left(\frac{\sqrt{14}-3}{2}\right)$$
$$- \left(\frac{1}{\sqrt{k-1}} - \frac{1}{\sqrt{k}}\right)\left(\frac{1}{\sqrt{deg(v_5)}} + \sum_{l=1}^{k-2} \frac{1}{\sqrt{t_l}}\right) + \frac{1}{\sqrt{2k}} + \frac{1}{2} + \frac{1}{\sqrt{2}}$$
$$\leq f(n,\gamma_t) - \frac{13}{4} - \frac{(-1)^n}{4} + \frac{\sqrt{14}}{2} - \left(\frac{1}{\sqrt{k-1}} - \frac{1}{\sqrt{k}}\right)\left(\frac{1}{\sqrt{\deg(v_5)}} + \sum_{l=1}^{k-2} \frac{1}{\sqrt{t_l}}\right)$$
$$+ \frac{1}{\sqrt{2k}} + \frac{1}{2} + \frac{1}{\sqrt{2}}.$$

Since the function $-\frac{13}{4} - \frac{(-1)^n}{4} + \frac{\sqrt{14}}{2} - \left(\frac{1}{\sqrt{k-1}} - \frac{1}{\sqrt{k}}\right)\left(\frac{1}{\sqrt{deg(v_5)}} + \sum_{l=1}^{k-2} \frac{1}{\sqrt{t_l}}\right) + \frac{1}{\sqrt{2k}} + \frac{1}{2} + \frac{1}{\sqrt{2}}$ yields a negative value for every $k \geq 4$, we then obtain $R(T) < f(n, \gamma_t)$.

Case 2.2.2: Provided that $k \leq 3$. Assume there exist a minimum TDS D of T given that $v_4 \in D$. We then set $T_2 = T - \{v_1, v_2\}$. In this case, we obtain

$$R(T) = R(T_2) - \frac{1}{\sqrt{k}} + \frac{1}{\sqrt{2k}} + \frac{1}{2} + \frac{1}{\sqrt{2}}$$
$$\leq \frac{2(n-2)+(-1)^{n-2}}{8} + \frac{\gamma_t-2}{2} + \sqrt{2} - \frac{13}{8} + ((n-2) - 2(\gamma_t - 2) + 1)\left(\frac{\sqrt{14}-3}{2}\right)$$
$$- \frac{1}{\sqrt{k}} + \frac{1}{\sqrt{2k}} + \frac{1}{2} + \frac{1}{\sqrt{2}}$$
$$\leq f(n,\gamma_t) - \frac{9}{2} + \sqrt{14} - \frac{1}{\sqrt{k}} + \frac{1}{\sqrt{2k}} + \frac{1}{2} + \frac{1}{\sqrt{2}} < f(n,\gamma_t),$$

for every $k \leq 3$.

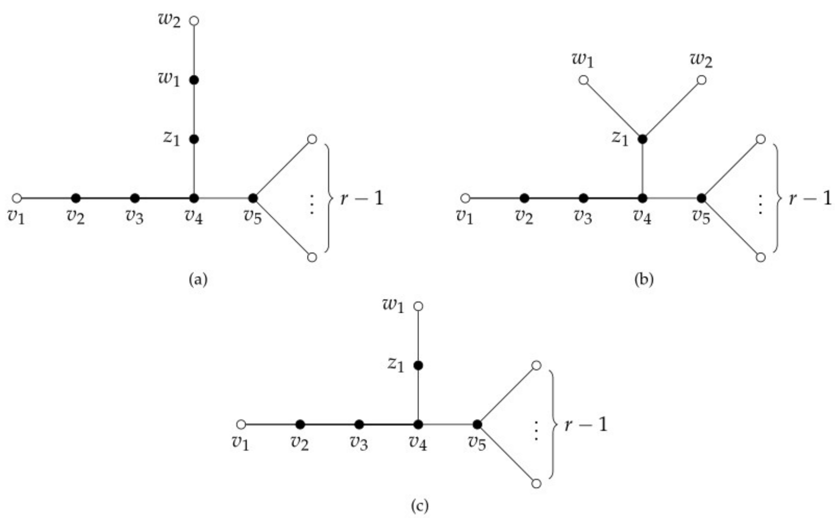

Figure 1: Three situation for the Case 2.2.2.1.

Case 2.2.2.1: Let $k = 3$. Here, in this case, we obtain the cases as portrayed in Figure 1, in which the black vertices denotes vertices having any minimum TDS D.

In Case (a), we express $N(v_5) = \{v_4, a_1, a_2, \dots, a_{r-1}\}$ as well as $deg(a_l) = q_l$ for each $l \in \{1,2, \dots, r-1\}$, in which we assume two cases.

Case (a.1): Let $r \geq 9$ and $T' = T - \{v_1, v_2, v_3, v_4, z_1, w_1, w_2\}$, here we obtain

$$\begin{aligned}
R(T) &= R(T') - \left(\tfrac{1}{\sqrt{r-1}} - \tfrac{1}{\sqrt{r}}\right)\left(\textstyle\sum_{l=1}^{r-1} \tfrac{1}{\sqrt{q_l}}\right) + \tfrac{1}{\sqrt{3r}} + \tfrac{2}{\sqrt{6}} + 1 + \sqrt{2} \\
&\leq \tfrac{2(n-7)+(-1)^{n-7}}{8} + \tfrac{\gamma_t-4}{2} + \sqrt{2} - \tfrac{13}{8} + ((n-7) - 2(\gamma_t - 4) + 1)\left(\tfrac{\sqrt{14}-3}{2}\right) \\
&- \left(\tfrac{1}{\sqrt{r-1}} - \tfrac{1}{\sqrt{r}}\right)\left(\textstyle\sum_{l=1}^{r-1} \tfrac{1}{\sqrt{q_l}}\right) + \tfrac{1}{\sqrt{3r}} + \tfrac{2}{\sqrt{6}} + 1 + \sqrt{2} \\
&\leq f(n, \gamma_t) - \tfrac{21}{4} - \tfrac{(-1)^n}{4} + \tfrac{\sqrt{14}}{2} - \left(\tfrac{1}{\sqrt{r-1}} - \tfrac{1}{\sqrt{r}}\right)\left(\textstyle\sum_{l=1}^{r-1} \tfrac{1}{\sqrt{q_l}}\right) \\
&+ \tfrac{1}{\sqrt{3r}} + \tfrac{2}{\sqrt{6}} + 1 + \sqrt{2} \\
&\leq f(n, \gamma_t) - \left(\tfrac{1}{\sqrt{r-1}} - \tfrac{1}{\sqrt{r}}\right)\left(\textstyle\sum_{l=1}^{r-1} \tfrac{1}{\sqrt{q_l}}\right) - \tfrac{17}{4} - \tfrac{(-1)^n}{4} + \tfrac{\sqrt{14}}{2} + \tfrac{1}{\sqrt{3r}} + \tfrac{2}{\sqrt{6}} + \sqrt{2},
\end{aligned}$$

and, since $-\frac{17}{4} - \frac{(-1)^n}{4} + \frac{\sqrt{14}}{2} + \frac{1}{\sqrt{3r}} + \frac{2}{\sqrt{6}} + \sqrt{2} < 0$ for $r \geq 9$, here we summarize that $R(T) < f(n, \gamma_t)$.

Case (a.2): Next, we assume that $r \leq 8$. Let's say now we consider $T' = T - \{v_1, v_2, v_3\}$, we then obtain

$$\begin{aligned}
R(T) &= R(T') - \tfrac{1}{2} - \tfrac{1}{\sqrt{2r}} + \tfrac{1}{\sqrt{3r}} + \tfrac{2}{\sqrt{6}} + \tfrac{1}{2} + \tfrac{1}{\sqrt{2}} \\
&\leq \tfrac{2(n-3)+(-1)^{n-3}}{8} + \tfrac{\gamma_t-2}{2} + \sqrt{2} - \tfrac{13}{8} + ((n-3) - 2(\gamma_t - 2) + 1)\left(\tfrac{\sqrt{14}-3}{2}\right) \\
&+ \tfrac{1}{\sqrt{2}} + \tfrac{2}{\sqrt{6}} + \left(\tfrac{1}{\sqrt{3}} - \tfrac{1}{\sqrt{2}}\right)\left(\tfrac{1}{\sqrt{r}}\right) \\
&\leq f(n, \gamma_t) - \tfrac{13}{4} - \tfrac{(-1)^n}{4} + \tfrac{\sqrt{14}}{2} + \tfrac{1}{\sqrt{2}} + \tfrac{2}{\sqrt{6}} + \left(\tfrac{1}{\sqrt{3}} - \tfrac{1}{\sqrt{2}}\right)\left(\tfrac{1}{\sqrt{r}}\right) < f(n, \gamma_t)
\end{aligned}$$

for any $r \leq 8$.

In Case (b), here we express $N(v_5) = \{v_4, a_1, a_2, \ldots, a_{r-1}\}$ as well as $deg(a_l) = q_l$ for each $l \in \{1, 2, \ldots, r-1\}$. From here, we take into account two more cases.

Case (b.1): Let's assume that $r \geq 4$. Let's say if we set $T' = T - \{v_1, v_2, v_3, v_4, z_1, w_1, w_2\}$, we then obtain

$$\begin{aligned}
R(T) &= R(T') - \left(\tfrac{1}{\sqrt{r-1}} - \tfrac{1}{\sqrt{r}}\right)\left(\textstyle\sum_{l=1}^{r-1} \tfrac{1}{\sqrt{q_l}}\right) + \tfrac{1}{\sqrt{3r}} + \tfrac{1}{3} + \tfrac{2}{\sqrt{3}} + \tfrac{1}{\sqrt{6}} + \tfrac{1}{2} + \tfrac{1}{\sqrt{2}} \\
&\leq \tfrac{2(n-7)+(-1)^{n-7}}{8} + \tfrac{\gamma_t-3}{2} + \sqrt{2} - \tfrac{13}{8} + ((n-7) - 2(\gamma_t - 3) + 1)\left(\tfrac{\sqrt{14}-3}{2}\right) \\
&- \left(\tfrac{1}{\sqrt{r-1}} - \tfrac{1}{\sqrt{r}}\right)\left(\textstyle\sum_{l=1}^{r-1} \tfrac{1}{\sqrt{q_l}}\right) + \tfrac{1}{\sqrt{3r}} + \tfrac{2}{\sqrt{3}} + \tfrac{1}{\sqrt{6}} + \tfrac{5}{6} + \tfrac{1}{\sqrt{2}} \\
&\leq f(n, \gamma_t) - \left(\tfrac{1}{\sqrt{r-1}} - \tfrac{1}{\sqrt{r}}\right)\left(\textstyle\sum_{l=1}^{r-1} \tfrac{1}{\sqrt{q_l}}\right)
\end{aligned}$$

$$-\frac{11}{12}-\frac{(-1)^n}{4}-\frac{\sqrt{14}}{2}+\frac{1}{\sqrt{3r}}+\frac{2}{\sqrt{3}}+\frac{1}{\sqrt{6}}+\frac{1}{\sqrt{2}}.$$

Since $-\frac{11}{12}-\frac{(-1)^n}{4}-\frac{\sqrt{14}}{2}+\frac{1}{\sqrt{3r}}+\frac{2}{\sqrt{3}}+\frac{1}{\sqrt{6}}+\frac{1}{\sqrt{2}}$ yields a negative value for every $r \geq 4$, we obtain $R(T) < f(n,\gamma_t)$.

Case (b.2): Next, assume that $r \leq 3$. Here, if we set $T' = T - \{v_1, v_2, v_3\}$, we obtain

$$\begin{aligned}R(T) &= R(T') - \frac{1}{\sqrt{6}} - \frac{1}{\sqrt{2r}} + \frac{1}{\sqrt{3r}} + \frac{1}{3} + \frac{1}{\sqrt{6}} + \frac{1}{2} + \frac{1}{\sqrt{2}}\\ &\leq \frac{2(n-3)+(-1)^{n-3}}{8} + \frac{\gamma_t-2}{2} + \sqrt{2} - \frac{13}{8} + ((n-3)-2(\gamma_t-2)+1)\left(\frac{\sqrt{14}-3}{2}\right)\\ &- \frac{1}{\sqrt{2r}} + \frac{1}{\sqrt{3r}} + \frac{5}{6} + \frac{1}{\sqrt{2}}\\ &\leq f(n,\gamma_t) - \frac{29}{12} - \frac{(-1)^n}{4} + \frac{\sqrt{14}}{2} + \frac{1}{\sqrt{2}} + \left(\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{2}}\right)\left(\frac{1}{\sqrt{r}}\right) < f(n,\gamma_t)\end{aligned}$$

for any $r \leq 3$.

In Case (c), let $N(v_5) = \{v_4, a_1, a_2, \dots, a_{r-1}\}$ as well as $deg(a_l) = q_l$ for each $l \in \{1,2, \dots, r-1\}$. From here, we take into account the following two cases.

Case (c.1): Here, we assume that $r \geq 5$. Now, by setting $T' = T - \{v_1, v_2, v_3, v_4, z_1, w_1\}$ yields

$$\begin{aligned}R(T) &= R(T') - \left(\frac{1}{\sqrt{r-1}} - \frac{1}{\sqrt{r}}\right)\left(\sum_{l=1}^{r-1}\frac{1}{\sqrt{q_l}}\right) + \frac{1}{\sqrt{3r}} + \frac{2}{\sqrt{6}} + \frac{1}{2} + \sqrt{2}\\ &\leq \frac{2(n-6)+(-1)^{n-6}}{8} + \frac{\gamma_t-3}{2} + \sqrt{2} - \frac{13}{8} + ((n-6)-2(\gamma_t-3)+1)\left(\frac{\sqrt{14}-3}{2}\right)\\ &- \left(\frac{1}{\sqrt{r-1}} - \frac{1}{\sqrt{r}}\right)\left(\sum_{l=1}^{r-1}\frac{1}{\sqrt{q_l}}\right) + \frac{1}{\sqrt{3r}} + \frac{2}{\sqrt{6}} + \frac{1}{2} + \sqrt{2}\\ &\leq f(n,\gamma_t) - \left(\frac{1}{\sqrt{r-1}} - \frac{1}{\sqrt{r}}\right)\left(\sum_{l=1}^{r-1}\frac{1}{\sqrt{q_l}}\right) - \frac{5}{2} + \frac{1}{\sqrt{3r}} + \frac{2}{\sqrt{6}} + \sqrt{2}.\end{aligned}$$

Since $-\frac{5}{2}+\frac{1}{\sqrt{3r}}+\frac{2}{\sqrt{6}}+\sqrt{2}$ yields a negative number for every $r \geq 5$, we now obtain $R(T) < f(n,\gamma_t)$.

Case (c.2): Next, we assume that $r \leq 4$. Provided that we let $T' = T - \{v_1, v_2, v_3\}$, here we will obtain

$$\begin{aligned}R(T) &= R(T') - \frac{1}{\sqrt{2r}} - \frac{1}{2} + \frac{1}{\sqrt{3r}} + \frac{2}{\sqrt{6}} + \frac{1}{2} + \frac{1}{\sqrt{2}}\\ &\leq \frac{2(n-3)+(-1)^{n-3}}{8} + \frac{\gamma_t-2}{2} + \sqrt{2} - \frac{13}{8} + ((n-3)-2(\gamma_t-2)+1)\left(\frac{\sqrt{14}-3}{2}\right)\\ &+ \left(\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{2}}\right)\left(\frac{1}{\sqrt{r}}\right) + \frac{2}{\sqrt{6}} + \frac{1}{\sqrt{2}}\\ &\leq f(n,\gamma_t) - \frac{13}{4} - \frac{(-1)^n}{4} + \frac{\sqrt{14}}{2} + \frac{2}{\sqrt{6}} + \frac{1}{\sqrt{2}} + \left(\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{2}}\right)\left(\frac{1}{\sqrt{r}}\right),\end{aligned}$$

and since $-\frac{13}{4}-\frac{(-1)^n}{4}+\frac{\sqrt{14}}{2}+\frac{2}{\sqrt{6}}+\frac{1}{\sqrt{2}}+\left(\frac{1}{\sqrt{3}}-\frac{1}{\sqrt{2}}\right)\left(\frac{1}{\sqrt{r}}\right)<0$ for any $r \leq 4$, we obtain $R(T) < f(n, \gamma_t)$.

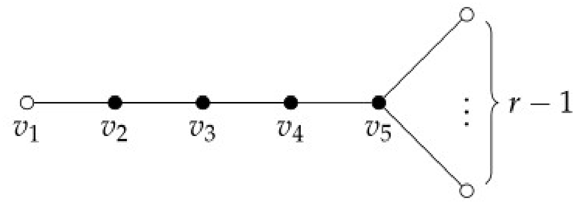

Figure 2: The situation yielded in Case 2.2.2.2.

Case 2.2.2.2: Let $k = 2$. Then, we obtain the condition portrayed in Figure 2.

We now express $N(v_5) = \{v_4, a_1, a_2, \dots, a_{r-1}\}$ as well as $deg(a_l) = q_l$ for each $l \in \{1,2, \dots, r-1\}$. We set $r = 2$ as well as $T' = T - \{v_1, v_2, v_3\}$, which yields

$$\begin{aligned}
R(T) &= R(T') - \tfrac{1}{\sqrt{2}} + \tfrac{3}{2} + \tfrac{1}{\sqrt{2}} \\
&\leq \tfrac{2(n-3)+(-1)^{n-3}}{8} + \tfrac{\gamma_t-2}{2} + \sqrt{2} - \tfrac{13}{8} \\
&+((n-3) - 2(\gamma_t - 2) + 1)\left(\tfrac{\sqrt{14}-3}{2}\right) + \tfrac{3}{2} \\
&\leq f(n, \gamma_t) - \tfrac{7}{4} - \tfrac{(-1)^n}{4} + \tfrac{\sqrt{14}}{2} < f(n, \gamma_t).
\end{aligned}$$

Following from here, we make assumption that $r \geq 3$ and take into account two more cases. Let $q_l \leq 2$ for each $l \in \{1,2, \dots, r-1\}$ and $T' = T - \{v_1, v_2, v_3, v_4\}$, we then obtain the following

$$\begin{aligned}
R(T) &= R(T') - \left(\tfrac{1}{\sqrt{r-1}} - \tfrac{1}{\sqrt{r}}\right)\left(\textstyle\sum_{l=1}^{r-1} \tfrac{1}{\sqrt{q_l}}\right) + \tfrac{1}{\sqrt{2r}} + 1 + \tfrac{1}{\sqrt{2}} \\
&\leq \tfrac{2(n-4)+(-1)^{n-4}}{8} + \tfrac{\gamma_t-2}{2} + \sqrt{2} - \tfrac{13}{8} + ((n-4) - 2(\gamma_t - 2) + 1)\left(\tfrac{\sqrt{14}-3}{2}\right) \\
&- \left(\tfrac{1}{\sqrt{r-1}} - \tfrac{1}{\sqrt{r}}\right)\left(\textstyle\sum_{l=1}^{r-1} \tfrac{1}{\sqrt{q_l}}\right) + \tfrac{1}{\sqrt{2r}} + 1 + \tfrac{1}{\sqrt{2}} \\
&\leq f(n, \gamma_t) - \left(\tfrac{1}{\sqrt{r-1}} - \tfrac{1}{\sqrt{r}}\right)\left(\textstyle\sum_{l=1}^{r-1} \tfrac{1}{\sqrt{q_l}}\right) - 1 + \tfrac{1}{\sqrt{2r}} + \tfrac{1}{\sqrt{2}} < f(n, \gamma_t)
\end{aligned}$$

for any $r \geq 3$.

Consequently, we let $q_1 = max\{q_1, \dots, q_{r-1}\} \geq 3$. From Lemma 3.1 and the cases above, given that $N(a_1) = \{v_5, b_1, b_2, \dots, b_{q_1-1}\}$, we may make assumption that, for each $i \in \{1,2, \dots, q_1 - 1\}$, then every vertex in $N(b_i) \backslash \{a_1\}$ resembles a leaf while $1 \leq deg(b_i) \leq 3$. Here, we express p_i as the vertices quantity in $\{b_1, b_2, \dots, b_{q_1-1}\}$ having degree i. Moreover, assume that the two disjoint graphs of T' and T_{a_1} in $T - e$ and the edge $e = v_5 a_1$ contains the vertex v_5 and a_1, accordingly. Thus

$$
\begin{aligned}
R(T) &= R(T') + R(T_{a_1}) - \left(\tfrac{1}{\sqrt{r-1}} - \tfrac{1}{\sqrt{r}}\right)\left(\tfrac{1}{\sqrt{2}} + \textstyle\sum_{l=1}^{r-1} \tfrac{1}{\sqrt{q_l}}\right) - \tfrac{p_1}{\sqrt{q_1-1}} \\
&- \tfrac{p_2}{\sqrt{2q_1-1}} - \tfrac{p_3}{\sqrt{3q_1-1}} + \tfrac{p_1}{\sqrt{q_1}} + \tfrac{p_2}{\sqrt{2q_2}} + \tfrac{p_3}{3q_1} + \tfrac{1}{\sqrt{q_1 r}} \\
&\leq \tfrac{2n+(-1)^n}{8} + \tfrac{\gamma_t}{2} + \sqrt{2} - \tfrac{13}{8} + (n - 2\gamma_t + 1)\left(\tfrac{\sqrt{14}-3}{2}\right) + \sqrt{2} - \tfrac{3}{2} + \left(\tfrac{\sqrt{14}-3}{2}\right) \\
&- \left(\tfrac{1}{\sqrt{r-1}} - \tfrac{1}{\sqrt{r}}\right)\left(\tfrac{1}{\sqrt{2}} + \textstyle\sum_{l=1}^{r-1} \tfrac{1}{\sqrt{q_l}}\right) - \left(\tfrac{1}{\sqrt{q_1-1}} - \tfrac{1}{\sqrt{q_1}}\right)\left(\tfrac{p_1+p_2+p_3}{\sqrt{3}}\right) + \tfrac{1}{\sqrt{q_1 r}} \\
&\leq f(n,\gamma_t) + \sqrt{2} - \tfrac{3}{2} + \left(\tfrac{\sqrt{14}-3}{2}\right) - \left(\tfrac{1}{\sqrt{r-1}} - \tfrac{1}{\sqrt{r}}\right)\left(\tfrac{1}{\sqrt{2}} + \tfrac{1}{\sqrt{q_l}}\right) \\
&- \left(\tfrac{1}{\sqrt{q_1-1}} - \tfrac{1}{\sqrt{q_1}}\right)\left(\tfrac{q_1-1}{\sqrt{3}}\right) + \tfrac{1}{\sqrt{q_1 r}}.
\end{aligned}
$$

Now consider the function $h(r) = -\left(\frac{1}{\sqrt{r-1}} - \frac{1}{\sqrt{r}}\right)\left(\frac{1}{\sqrt{2}} + \frac{1}{\sqrt{q_l}}\right) + \frac{1}{\sqrt{q_1 r}}$. Since

$$
\begin{aligned}
h'(R) &= \left(\tfrac{1}{\sqrt{2}} - \tfrac{1}{\sqrt{q_1}}\right)\left(\frac{1}{\sqrt{2(r-1)^{\frac{3}{2}}}} - \frac{1}{\sqrt{2r^{\frac{3}{2}}}}\right) - \frac{1}{2\sqrt{q_1} r^{\frac{3}{2}}} \geq 0 \\
&\Leftrightarrow \left(\tfrac{1}{\sqrt{2}} - \tfrac{1}{\sqrt{q_1}}\right)\left(\left(\tfrac{r}{r-1}\right)^{\frac{3}{2}} - 1\right) \geq \tfrac{1}{\sqrt{q_1}} \\
&\Leftrightarrow \left(\tfrac{1}{\sqrt{2}} - \tfrac{1}{\sqrt{q_1}}\right)\left(\tfrac{r}{r-1}\right)^{\frac{3}{2}} \geq \tfrac{1}{\sqrt{2}} + \tfrac{2}{\sqrt{q_1}} \\
&\Leftrightarrow \tfrac{r}{r-1} \geq \left(\tfrac{\sqrt{q_1}+2\sqrt{2}}{\sqrt{q_1}+\sqrt{2}}\right)^{\frac{2}{3}} \\
&\Leftrightarrow r \leq \frac{1}{\left(\frac{\sqrt{q_1}+2\sqrt{2}}{\sqrt{q_1}+\sqrt{2}}\right)^{\frac{2}{3}} - 1} + 1 = \frac{\left(\frac{\sqrt{q_1}+2\sqrt{2}}{\sqrt{q_1}+\sqrt{2}}\right)^{\frac{2}{3}}}{\left(\frac{\sqrt{q_1}+2\sqrt{2}}{\sqrt{q_1}+\sqrt{2}}\right)^{\frac{2}{3}} - 1}.
\end{aligned}
$$

Therefore,

$$
\begin{aligned}
&\sqrt{2} - \tfrac{3}{2} + \left(\tfrac{\sqrt{14}-3}{2}\right) - \left(\tfrac{1}{\sqrt{r-1}} - \tfrac{1}{\sqrt{r}}\right)\left(\tfrac{1}{\sqrt{2}} + \tfrac{1}{\sqrt{q_l}}\right) - \left(\tfrac{1}{\sqrt{q_1-1}} - \tfrac{1}{\sqrt{q_1}}\right)\left(\tfrac{q_1-1}{\sqrt{3}}\right) + \tfrac{1}{\sqrt{q_1 r}} \\
&\leq \sqrt{2} - \tfrac{3}{2} + \left(\tfrac{\sqrt{14}-3}{2}\right) - \left(\sqrt{\left(\tfrac{\sqrt{q_1}+2\sqrt{2}}{\sqrt{q_1}+\sqrt{2}}\right)^{\frac{2}{3}} - 1} - \frac{\sqrt{\left(\frac{\sqrt{q_1}+2\sqrt{2}}{\sqrt{q_1}+\sqrt{2}}\right)^{\frac{2}{3}} - 1}}{\left(\frac{\sqrt{q_1}+2\sqrt{2}}{\sqrt{q_1}+\sqrt{2}}\right)^{\frac{1}{3}}}\right)\left(\tfrac{1}{\sqrt{2}} + \tfrac{1}{\sqrt{q_1}}\right) \\
&- \left(\tfrac{1}{\sqrt{q_1-1}} - \tfrac{1}{\sqrt{q_1}}\right)\left(\tfrac{q_1-1}{\sqrt{3}}\right) + \frac{\sqrt{\left(\frac{\sqrt{q_1}+2\sqrt{2}}{\sqrt{q_1}+\sqrt{2}}\right)^{\frac{2}{3}} - 1}}{\sqrt{q_1}\left(\frac{\sqrt{q_1}+2\sqrt{2}}{\sqrt{q_1}+\sqrt{2}}\right)^{\frac{1}{3}}}.
\end{aligned}
$$

Note that this function has a negative value for every $q_1 \geq 3$. Thus, $R(T) < f(n,\gamma_t)$, completing the proof. ■

We analyse the given family of $\mathcal{F}$ graphs, which was created recursively to characterise all the trees that achieve the upper bound stated in Theorem 3.2. Here, the path $2k+1$ vertices is examined in $\mathcal{F}$ for every $k \geq 1$ and creating a new graph as follows:

(I). Provided that $T' \in \mathcal{F}$, then v denotes a leaf in T'. By taking any path P, in which subsequent vertices are denoted by $w_1, w_2, \ldots, w_{4k}$, the graph T provided that $V(T) = V(T') \cup V(P)$ as well as $E(T) = E(T') \cup E(P) \cup \{vw_1\}$ belongs to $\mathcal{F}$. Upon utilizing the function again yields

$$f(n, \gamma_t) = \frac{2n+(-1)^n}{8} + \frac{\gamma_t}{2} + \sqrt{2} - \frac{13}{8} + (n - 2\gamma_t + 1)\left(\frac{\sqrt{14}-3}{2}\right).$$

Lemma 3.3. If $T \in \mathcal{F}$, then $R(T) = f(n(T), \gamma_t(T))$.

Proof. Let T be a path having $2k+1$ vertices, here we may effortlessly determine that the finding holds. (i) Provided that $T \in \mathcal{F}$ agrees with $R(T') = f(n(T'), \gamma_t(T'))$, T' possess a leaf v, and P denotes a path having subsequent $w_1, w_2, \ldots, w_{4k}$ vertices. Moreover, we also take into account the graph T given that $V(T) = V(T') \cup V(P)$ as well as $E(T) = E(T') \cup E(P) \cup \{vw_1\}$. Furthermore, neighbor of v only possess degree 2, which yields

$$\begin{aligned}
R(T) &= R(T') + R(P) - \frac{2}{\sqrt{2}} + \frac{3}{2} \\
&= \frac{2n(T\prime)+(-1)^{n(T\prime)}}{8} + \frac{\gamma_t(T\prime)}{2} + \sqrt{2} - \frac{13}{8} + (n(T') - 2\gamma_t(T') + 1)\left(\frac{\sqrt{14}-3}{2}\right) \\
&+ \frac{2}{\sqrt{2}} + \frac{n(P)-3}{2} - \frac{2}{\sqrt{2}} + \frac{3}{2} \\
&= \frac{2n(T\prime)+(-1)^{n(T\prime)}}{8} + \frac{\gamma_t(T\prime)}{2} + \sqrt{2} - \frac{13}{8} + (n(T') - 2\gamma_t(T') + 1)\left(\frac{\sqrt{14}-3}{2}\right) \\
&+ \frac{2n(P)+(-1)^{n(P)}}{8} + \frac{\gamma_t(P)}{2} - \frac{1}{8} \\
&= \frac{2n(T)+(-1)^{n(T)}}{8} + \frac{\gamma_t}{2} + \sqrt{2} - \frac{13}{8} + (n(T) - 2\gamma_t + 1)\left(\frac{\sqrt{14}-3}{2}\right).
\end{aligned}$$

This completes the proof. ■

Theorem 3.4. $R(T) = f(n(T), \gamma_t(T))$ if and only if $T \in \mathcal{F}$.

Proof. Using Lemma 3.3, we are acquired to show that every tree T fullfiling $R(T) = f(n(T), \gamma_t(T))$ sits in the $\mathcal{F}$ family. Using contradiction, we assume the existence of a tree T given that $R(T) = f(n(T), \gamma_t(T))$ as well as $T \notin F$. Here, we now consider the tree T fullfiling the minimum number of vertices. Now, if we consider the Theorem 3.2 proof as well as the $v_1, v_2, \ldots, v_d$ as the diameter of T, we may make assumption that $i = j = k = 2$ as well as $r = 2$.

Provided that $r = 2$ and we assume $T' = T \backslash \{v_1, v_2\}$, we then obtain

$$R(T) = R(T') - \frac{1}{\sqrt{2}} + \frac{2}{\sqrt{4}} + \frac{1}{\sqrt{2}}$$
$$\leq \frac{2(n-2)+(-1)^{n-2}}{8} + \frac{\gamma_t - 1}{2} + \sqrt{2} - \frac{13}{8} + ((n-2) - 2(\gamma_t - 1) + 1)\left(\frac{\sqrt{14}-3}{2}\right) + 1$$
$$= \frac{2n+(-1)^n}{8} + \frac{\gamma_t}{2} + \sqrt{2} - \frac{13}{8} + (n - 2\gamma_t + 1)\left(\frac{\sqrt{14}-3}{2}\right).$$

Therefore,

$$R(T') = \frac{2n(T')+(-1)^{n(T')}}{8} + \frac{\gamma_t(T')}{2} + \sqrt{2} - \frac{13}{8} + (n(T') - 2\gamma_t(T') + 1)\left(\frac{\sqrt{14}-3}{2}\right).$$

Provided that $T' \in \mathcal{F}$, given v_3 denotes a leaf in T', we then have that T belongs to F. Thus, $T' \notin \mathcal{F}$, which contradicts with the minimality of T. This then completes the proof. ■

4. Concluding Remarks

The purpose of this research is to look at the link between the Randić index and the total domination number of trees. We provide an upper bound for the Randić index of trees in terms of total domination number, and characterizing all tree(s) that attain the equality case.

sTo sum up this paper, we want to suggest the following open problem.

Problem 3.5. Determine the lower bound for the Randić index of trees with respect to the order and the total domination number.

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