Journal of Mathematical Chemistry, Vol. 42, No. 3, October 2007 (© 2006)
DOI: 10.1007/s10910-006-9089-6

On the Randić index of quasi-tree graphs

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Received 12 January 2006; revised 8 February 2006

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 vertex u and v in G. A graph G is called quasi-tree, if there exists $u \in V(G)$ such that $G - u$ is a tree. In the paper, we give sharp lower and upper bounds on the Randić index of quasi-tree graphs.

KEY WORDS: Randić index, quasi-tree graph, cycle

1. Introduction

In studying branching properties of alkanes, several numbering schemes for the edges of the associated hydrogen-suppressed graph were proposed based on the degrees of the end vertices of an edge [11]. To preserve rankings of certain molecules, some inequalities involving the weights of edges needed to be satisfied. Randić [11] 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 and denoted by $R(G)$, has been closely correlated with many chemical properties [8] 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 [9]). It is said in [7] that Randić index "*together with its generalizations it is certainly the molecular-graph-based structure-descriptor, that found the most numerous applications in organic chemistry,*

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†Partially supported by NSFC (No. 10571105).

medicinal chemistry, and pharmacology". More data and additional references on the index can be found in [5, 6].

Let $G=(V, E)$ be a graph of order n $(n \geqslant 3)$. If G is a cycle, then we will call G an n-cycle. The degree and the neighborhood of a vertex $u \in V$ will be denoted by $d(u)$ and $N(u)$, respectively. The graph that arises from G by deleting the vertex $u \in V$ or the edge $uv \in E$ will be denoted by $G - u$ or $G - uv$, respectively. Similarly, the graph $G+uv$ arises from G by adding an edge $uv \notin E$ between the endpoints $u, v \in E(G)$. A graph G is called *an quasi-tree graph*, if there exists a vertex $u_0 \in V$ such that $G - u_0$ is a tree.

There are many results concerning Randić index. In [1], 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 [12] gave the sharp upper bound of $R(T) \leqslant (n + 2\sqrt{2} - 3)/2$ when T is a tree of order n. In [2], chemical trees with minimum Randić index are characterized and in [7], chemical trees of a given order and a number of pending vertices with minimum and with maximum Randić index are characterized. In [4], the sharp lower and upper bounds on Randić index of unicyclic graph were given. In the paper, we will give sharp lower and upper bounds on the Randić index of quasi-tree graphs.

2. Some lemmas

In the section, we will give some lemmas, which will be used in section 3.

Lemma 1 [3]. Let $G = (V, E)$ be a graph of order n and let $v_0, v_1, v_2 \in V$ with $N(v_0) = \{v_1, v_2\}$, $v_1v_2 \in E(G)$ and $d_1 = d(v_1)$, $d_2 = d(v_2) \geqslant 3$. Then

$$R(G) \geqslant R(G - v_0) + f(d_1, d_2)$$

for

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

and we have

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

Lemma 2 [10]. Let G be a simple connected graph of order n. Then

$$R(G) \leqslant \frac{n}{2}$$

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

Lemma 3 [4]. Let x, y be positive integers with $x \geqslant 1$ and $y \geqslant 2$. 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 monotonously decreasing in x.

Lemma 4 [4]. Let y be a positive integer with $y \geqslant 2$. Denote

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

Then $h(y)$ is monotonously decreasing in y.

Lemma 5. Let y be a positive integer with $y \geqslant 2$. Denote

$$h(y) = \frac{1}{\sqrt{y}} + \left(1 - \sqrt{\frac{y}{y-1}}\right)\frac{y-1}{\sqrt{2y}} = \left(\frac{\sqrt{y}}{\sqrt{2}} - \frac{\sqrt{y-1}}{\sqrt{2}}\right) + \frac{\sqrt{2}-1}{\sqrt{2y}}.$$

Then $h(y)$ is monotonously decreasing in y.

The proof of lemma 5 is very simple. We omit it here.

Let G be an quasi-tree graph and $u_0 \in V(G)$ such that $G - u_0$ is a tree. If $d(u_0) = 1$, then G is a tree and then $\sqrt{n-1} \leqslant R(G) \leqslant (n+2\sqrt{2}-3)/2$ (see [1,12]). Hence, in the following, we just consider the case that $d(u_0) \geqslant 2$. Denote

$$g(n) = \frac{n-4}{\sqrt{n-1}} + \frac{2}{\sqrt{2(n-1)}} + \frac{1}{\sqrt{3(n-1)}} + \frac{2}{\sqrt{6}},$$

$$\mathcal{QT}(n) = \{G \mid G \text{ is an quasi-tree graph with } V(G) = n \text{ and } d(u_0) \geqslant 2\}$$

and $PV = \{u \in V(G) \mid d(u) = 1\}$. Then we have the following lemma.

Lemma 6. Let $G \in \mathcal{QT}(n)$ with $n \geqslant 4$. If $PV = \emptyset$, then $R(G) > g(n)$.

Proof. By induction on n. If $n = 4$ or 5, then $g(4) = 1.9663$, $g(5) = 2.3123$, and the lemma holds clearly (see figures 1 and 2). Since G is a quasi-tree and $PV = \emptyset$, there exists $u \in V(G)$ such that $d(u) = 2$. Let $N(u) = \{v_1, v_2\}$, $d(v_1) = d_1$ and $d(v_2) = d_2$. We will complete the proof by considering the following two cases.

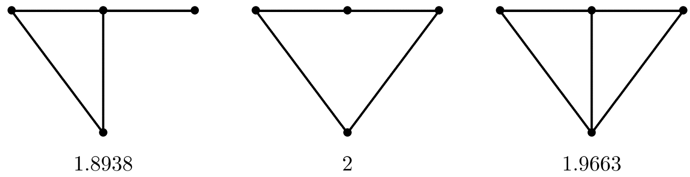

Figure 1. R(G) of QT(4).

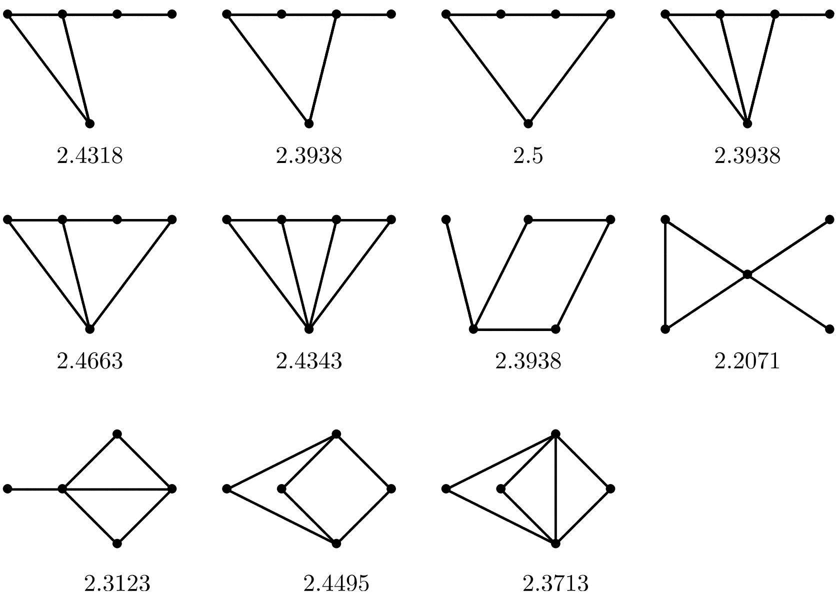

Figure 2. R(G) of QT(5).

Case 1. $v_1v_2 \notin E(G)$.

In this case, we have $d_1 \leqslant n-2$ and $d_2 \leqslant n-2$. Since $G' = G - u + v_1v_2 \in \mathcal{QT}(n-1)$, by induction, we have that

$$
\begin{aligned}
R(G) = & R(G') - \frac{1}{\sqrt{d_1 d_2}} + \frac{1}{\sqrt{2d_1}} + \frac{1}{\sqrt{2d_2}} \\
\geqslant & g(n) + \frac{n-5}{\sqrt{n-2}} + \frac{2}{\sqrt{2(n-2)}} + \frac{1}{\sqrt{3(n-2)}} - \frac{n-4}{\sqrt{n-1}} - \frac{2}{\sqrt{2(n-1)}} \\
& - \frac{1}{\sqrt{3(n-1)}} - \left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{d_1}}\right)\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{d_2}}\right) + \frac{1}{2} \\
\geqslant & g(n) + \frac{n-5}{\sqrt{n-2}} + \frac{2}{\sqrt{2(n-2)}} + \frac{1}{\sqrt{3(n-2)}} - \frac{n-4}{\sqrt{n-1}} - \frac{2}{\sqrt{2(n-1)}}
\end{aligned}
$$

$$
\begin{aligned}
&-\frac{1}{\sqrt{3(n-1)}}-\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{n-2}}\right)^2+\frac{1}{2}\\
&\geqslant g(n)+\left[\frac{n-4+\sqrt{2}+\sqrt{3}/3}{\sqrt{n-2}}-\frac{n-4+\sqrt{2}+\sqrt{3}/3}{\sqrt{n-1}}\right]\\
&\quad+\left[\frac{(\sqrt{2}-1)\sqrt{n-2}}{n-2}-\frac{1}{n-2}\right]\\
&> g(n).
\end{aligned}
$$

The last inequality holds obviously when $n \geqslant 8$ and it is not difficult to check that the inequality holds when $n = 6$ and 7.

Case 2. $v_1v_2 \in E(G)$.

Let $G' = G - u$. Then $G' \in \mathcal{QT}(n-1)$. By lemma 1, we have

$$
\begin{aligned}
R(G) &\geqslant R(G')+\frac{1}{\sqrt{2}}(\sqrt{d_1}-\sqrt{d_1-1})+\frac{1}{\sqrt{2}}(\sqrt{d_2}-\sqrt{d_2-1})\\
&\quad+\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{d_1}}\right)\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{d_2}}\right)-\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{d_1-1}}\right)\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{d_2-1}}\right)\\
&\geqslant g(n)+\frac{(n-2)-3}{\sqrt{n-2}}+\frac{2}{\sqrt{2(n-2)}}+\frac{1}{\sqrt{3(n-2)}}\\
&\quad-\frac{(n-1)-3}{\sqrt{n-1}}-\frac{2}{\sqrt{2(n-1)}}-\frac{1}{\sqrt{3(n-1)}}\\
&\quad+\sqrt{2}(\sqrt{n-1}-\sqrt{n-2})-\frac{\sqrt{2}}{\sqrt{n-1}}+\frac{1}{n-1}+\frac{\sqrt{2}}{\sqrt{n-2}}-\frac{1}{n-2}\\
&= g(n)+\left[(\sqrt{2}-1)(\sqrt{n-1}-\sqrt{n-2})-\frac{1}{(n-1)(n-2)}\right]\\
&\quad+(2\sqrt{2}+\sqrt{3}/3-3)\left(\frac{1}{\sqrt{n-2}}-\frac{1}{\sqrt{n-1}}\right)\\
&= g(n)+\left(\frac{\sqrt{2}-1}{\sqrt{n-1}+\sqrt{n-2}}-\frac{1}{(n-1)(n-2)}\right)\\
&\quad+(2\sqrt{2}+\sqrt{3}/3-3)\left(\frac{1}{\sqrt{n-2}}-\frac{1}{\sqrt{n-1}}\right)\\
&> g(n).
\end{aligned}
$$

□

Lemma 7. Let $G \in \mathcal{QT}(n)$ with $n \geqslant 5$ and $PV \neq \emptyset$. Let $u \in PV$ and v be the neighbor of u. Denote $d(v) = d$ and $N(v) \setminus \{u\} = \{y_1, y_2, \ldots, y_{d-1}\}$. If $d(y_i) \geqslant 2$ for $i = 1, \ldots, d-1$, then $R(G) > g(n)$.

Proof. By induction on n. If $n = 5$, then the lemma holds clearly (see figure 2). Since $u \in PV$ and v is the neighbor of u, $d(v) \geqslant 2$. Set $G' = G - u$. Then $G' \in \mathcal{QT}(n-1)$. Let S be the sum of the weights of the edges incident with v except for the edge uv in G and S' the sum of the weights of the edges incident with v in G'. Then $S = \sum_{i=1}^{d-1} \frac{1}{\sqrt{dd(y_i)}}$ and $S' = S\sqrt{\frac{d}{d-1}}$. Since $d(y_i) \geqslant 2$ for $i = 1, \ldots, d-1$, we have $S \leqslant \frac{d-1}{\sqrt{2d}}$. By lemma 5 and $d \leqslant n-1$, we have

$$
\begin{aligned}
R(G) &= R(G') + \frac{1}{\sqrt{d}} + S\left(1 - \sqrt{\frac{d}{d-1}}\right) \\
&\geqslant g(n) + \frac{n-5}{\sqrt{n-2}} + \frac{2}{\sqrt{2(n-2)}} + \frac{1}{\sqrt{3(n-2)}} - \frac{n-4}{\sqrt{n-1}} - \frac{2}{\sqrt{2(n-1)}} \\
&\quad - \frac{1}{\sqrt{3(n-1)}} + \frac{1}{\sqrt{d}} + \left(1 - \sqrt{\frac{d}{d-1}}\right)\frac{d-1}{\sqrt{2d}} \\
&\geqslant g(n) + \frac{n-5}{\sqrt{n-2}} + \frac{2}{\sqrt{2(n-2)}} + \frac{1}{\sqrt{3(n-2)}} - \frac{n-4}{\sqrt{n-1}} - \frac{2}{\sqrt{2(n-1)}} \\
&\quad - \frac{1}{\sqrt{3(n-1)}} + \frac{1}{\sqrt{n-1}} + \frac{n-2}{\sqrt{2(n-1)}} - \frac{n-2}{\sqrt{2(n-2)}} \\
&= g(n) + (\sqrt{6}(n-5) - \sqrt{3}(n-4) + \sqrt{2})\left(\frac{1}{\sqrt{6(n-2)}} - \frac{1}{\sqrt{6(n-1)}}\right) \\
&> g(n).
\end{aligned}
$$

□

Lemma 8. Let $G \in \mathcal{QT}(n)$ with $n \geqslant 5$ and $PV \neq \emptyset$. Let $u \in PV$ and v be the neighbor of u. Denote $d(v) = d$ and $N(v)\setminus\{u\} = \{y_1, y_2, \ldots, y_{d-1}\}$. If $d \leqslant n-2$ and there exists some y_i, say y_1, such that $d(y_1) = 1$, then $R(G) > g(n)$.

Proof. By induction on n. If $n = 5$, then the lemma holds clearly (see figure 2). Set $G' = G - u$. Then $G' \in \mathcal{QT}(n-1)$. Let S be the sum of the weights of the edges incident with v except for the edge uv in G and S' the sum of the weights of the edges incident with v in G'. Then $S = \sum_{i=1}^{d-1} \frac{1}{\sqrt{dd(y_i)}}$ and $S' = S\sqrt{\frac{d}{d-1}}$.

Assume, without loss of generality, that $d(y_1) = d(y_2) = \cdots = d(y_k) = 1$, where $k \geqslant 1$. Thus $S \leqslant k/\sqrt{d} + (d-1-k)/\sqrt{2d}$ and we have

$$\begin{aligned}
R(G) &= R(G') + \frac{1}{\sqrt{d}} + S\left(1 - \sqrt{\frac{d}{d-1}}\right) \\
&\geqslant g(n) + \frac{n-5}{\sqrt{n-2}} + \frac{2}{\sqrt{2(n-2)}} + \frac{1}{\sqrt{3(n-2)}} - \frac{n-4}{\sqrt{n-1}} - \frac{2}{\sqrt{2(n-1)}} \\
&\quad - \frac{1}{\sqrt{3(n-1)}} + \frac{k+1}{\sqrt{d}} + \frac{d-1-k}{\sqrt{2d}} - \frac{k}{\sqrt{d-1}} - \frac{d-1-k}{\sqrt{2(d-1)}}. \qquad (1)
\end{aligned}$$

If $d \leqslant n-3$, then $k \leqslant d-2$. By lemmas 3, 4 and (1), we have

$$\begin{aligned}
R(G) &\geqslant g(n) + \frac{n-5}{\sqrt{n-2}} + \frac{2}{\sqrt{2(n-2)}} + \frac{1}{\sqrt{3(n-2)}} - \frac{n-4}{\sqrt{n-1}} - \frac{2}{\sqrt{2(n-1)}} \\
&\quad - \frac{1}{\sqrt{3(n-1)}} + \frac{d-1}{\sqrt{d}} + \frac{1}{\sqrt{2d}} - \frac{d-2}{\sqrt{d-1}} - \frac{1}{\sqrt{2(d-1)}} \\
&\geqslant g(n) + \frac{n-5}{\sqrt{n-2}} + \frac{2}{\sqrt{2(n-2)}} + \frac{1}{\sqrt{3(n-2)}} - \frac{n-4}{\sqrt{n-1}} - \frac{2}{\sqrt{2(n-1)}} \\
&\quad - \frac{1}{\sqrt{3(n-1)}} + \frac{n-4}{\sqrt{n-3}} + \frac{1}{\sqrt{2(n-3)}} - \frac{n-5}{\sqrt{n-4}} - \frac{1}{\sqrt{2(n-4)}} \\
&= g(n) + \frac{n-5+\sqrt{2}+\sqrt{3}/3}{\sqrt{n-2}} + \frac{n-4+\sqrt{2}/2}{\sqrt{n-3}} - \frac{n-4+\sqrt{2}+\sqrt{3}/3}{\sqrt{n-1}} \\
&\quad - \frac{n-5+\sqrt{2}/2}{\sqrt{n-4}} \\
&= g(n) + (\sqrt{n-3} - \sqrt{n-4}) - (\sqrt{n-1} - \sqrt{n-2}) + \left(1 - \frac{\sqrt{2}}{2}\right) \\
&\quad \times \left(\frac{1}{\sqrt{n-4}} - \frac{1}{\sqrt{n-3}}\right) - \left(3 - \sqrt{2} - \frac{\sqrt{3}}{3}\right)\left(\frac{1}{\sqrt{n-2}} - \frac{1}{\sqrt{n-1}}\right) \\
&\geqslant g(n) + (\sqrt{n-3} - \sqrt{n-4}) - (\sqrt{n-1} - \sqrt{n-2}) + \left(1 - \frac{\sqrt{2}}{2}\right) \\
&\quad \times \left(\frac{1}{\sqrt{n-2}} - \frac{1}{\sqrt{n-1}}\right) - \left(3 - \sqrt{2} - \frac{\sqrt{3}}{3}\right)\left(\frac{1}{\sqrt{n-2}} - \frac{1}{\sqrt{n-1}}\right)
\end{aligned}$$

$$= g(n) + (\sqrt{n-3} - \sqrt{n-4}) - (\sqrt{n-1} - \sqrt{n-2}) \\ -0.72\left(\frac{1}{\sqrt{n-2}} - \frac{1}{\sqrt{n-1}}\right) \\ > g(n). \quad \text{(see Appendix)}$$

If $d = n-2$, then $k \leqslant n-5$ by $G \in \mathcal{QT}(n)$. Thus, by lemma 3 and (1), we have

$$R(G) \geqslant g(n) + \frac{n-5}{\sqrt{n-2}} + \frac{2}{\sqrt{2(n-2)}} + \frac{1}{\sqrt{3(n-2)}} - \frac{n-4}{\sqrt{n-1}} - \frac{2}{\sqrt{2(n-1)}} \\ - \frac{1}{\sqrt{3(n-1)}} + \frac{n-4}{\sqrt{n-2}} + \frac{2}{\sqrt{2(n-2)}} - \frac{n-5}{\sqrt{n-3}} - \frac{2}{\sqrt{2(n-3)}}$$

$$= g(n) + \frac{2n-9+2\sqrt{2}+\sqrt{3}/3}{\sqrt{n-2}} - \frac{n-4+\sqrt{2}+\sqrt{3}/3}{\sqrt{n-1}} - \frac{n-5+\sqrt{2}}{\sqrt{n-3}}$$

$$= g(n) + (\sqrt{n-2} - \sqrt{n-3}) - (\sqrt{n-1} - \sqrt{n-2}) + \left(2-\sqrt{2}\right) \\ \times \left(\frac{1}{\sqrt{n-3}} - \frac{1}{\sqrt{n-2}}\right) - \left(3 - \sqrt{2} - \frac{\sqrt{3}}{3}\right)\left(\frac{1}{\sqrt{n-2}} - \frac{1}{\sqrt{n-1}}\right) \\ \geqslant g(n) + (\sqrt{n-2} - \sqrt{n-3}) - (\sqrt{n-1} - \sqrt{n-2}) \\ -0.423\left(\frac{1}{\sqrt{n-2}} - \frac{1}{\sqrt{n-1}}\right) \\ > g(n). \quad \text{(see Appendix)}$$

□

3. Main result

Let n be a positive integer with $n \geqslant 3$. We define an quasi-tree graph $\mathcal{QT}^0(n)$ with n vertices as follow: $\mathcal{QT}^0(n)$ is obtained from the star graph $K_{1,n-1}$ by connecting two pendant vertices of $K_{1,n-1}$ (see figure 3). Also, we define another quasi-tree graph $\mathcal{QT}^1(n)$ with n vertices as follow: $\mathcal{QT}^1(n)$ is obtained from the graph $\mathcal{QT}^0(n)$ by connecting one pendant vertices and one vertex of degree two of $\mathcal{QT}^0(n)$ (see figure 3). Obviously, $\mathcal{QT}^0(n)$ and $\mathcal{QT}^1(n)$ are n-vertex quasi-tree graph. Let G be an quasi-tree graph and $u_0 \in V(G)$ such that $G - u_0$ is a tree. We just consider the case that $d(u_0) \geqslant 2$. Denote

$$\mathcal{QT}(n) = \{\ G \mid G \text{ is an quasi-tree graph with } |V(G)| = n \text{ and } d(u_0) \geqslant 2\}.$$

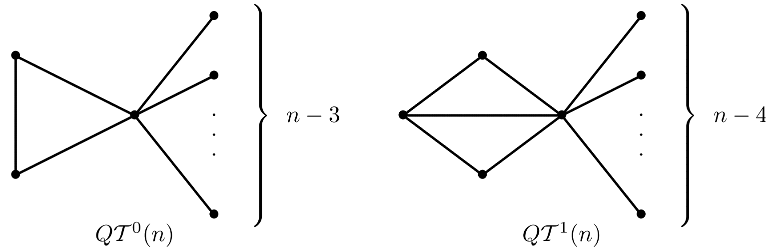

Figure 3.

Let

$$f(n) = R(\mathcal{QT}^0(n)) = \frac{n-3}{\sqrt{n-1}} + \frac{2}{\sqrt{2(n-1)}} + \frac{1}{2}.$$

We first have the following result.

Theorem 1. Let $G \in \mathcal{QT}(n)$ with $n \geqslant 3$. Then

$$f(n) \leqslant R(G) \leqslant \frac{n}{2}.$$

The left equality holds if and only if $G \cong \mathcal{QT}^0(n)$ and the right equality holds if and only if G is an n-cycle.

Proof. By lemma 2, we have $R(G) \leqslant n/2$ and equality holds if and only if G is a regular graph. Since the n-cycle is the only regular graph in $\mathcal{QT}(n)$, we have that $R(G) = n/2$ if and only if G is an n-cycle. Hence, in the next proof, we just show that $f(n) \leqslant R(G)$ and equality holds if and only if $G \cong \mathcal{QT}^0(n)$.

By induction on n. If $n = 3$, the theorem holds obviously. If $n = 4, 5$, then the theorem holds clearly (see figures 1 and 2).

Assume that $G \in \mathcal{QT}(n)$ with $n \geqslant 6$. Denote $PV = \{u \in V(G) | d(u) = 1\}$. Note that when $n \geqslant 6$, we have

$$f(n) < \frac{n-4}{\sqrt{n-1}} + \frac{2}{\sqrt{2(n-1)}} + \frac{1}{\sqrt{3(n-1)}} + \frac{2}{\sqrt{6}} = g(n).$$

Thus we just need to consider the case that $PV \neq \emptyset$ by lemma 6. Let $u \in PV$ and v be the neighbor of u. Denote $d(v) = d$ and $N(v) \setminus \{u\} = \{y_1, y_2, \ldots, y_{d-1}\}$. Then $d \geqslant 2$. Set $G' = G - u$. Then $G' \in \mathcal{QT}(n-1)$. Let S be the sum of the weights of the edges incident with v except for the edge uv in G and S' the sum of the weights of the edges incident with v in G'. Then $S = \sum_{i=1}^{d-1} \frac{1}{\sqrt{dd(y_i)}}$ and $S' = S\sqrt{\frac{d}{d-1}}$. By lemmas 7 and 8, we can assume that there exists some i $(1 \leqslant i \leqslant d-1)$ such that $d(y_i) = 1$ and $d = n - 1$.

Assume, without loss of generality, that $d(y_1) = d(y_2) = \cdots = d(y_k) = 1$ and $d(y_i) \geqslant 2$ for $k+1 \leqslant i \leqslant d-1$, where $k \geqslant 1$. Thus $S \leqslant k/\sqrt{d} + (d-1-k)/\sqrt{2d}$ and we have

$$\begin{aligned}
R(G) &= R(G') + \frac{1}{\sqrt{d}} + S\left(1 - \sqrt{\frac{d}{d-1}}\right) \\
&\geqslant f(n) + \frac{n-4}{\sqrt{n-2}} - \frac{n-3}{\sqrt{n-1}} + \frac{2}{\sqrt{2(n-2)}} \\
&\quad - \frac{2}{\sqrt{2(n-1)}} + \frac{1}{\sqrt{d}} + \left(1 - \sqrt{\frac{d}{d-1}}\right)\left(\frac{k}{\sqrt{d}} + \frac{d-1-k}{\sqrt{2d}}\right) \\
&= f(n) + \frac{n-4}{\sqrt{n-2}} - \frac{n-3}{\sqrt{n-1}} + \frac{2}{\sqrt{2(n-2)}} \\
&\quad - \frac{2}{\sqrt{2(n-1)}} + \frac{k+1}{\sqrt{n-1}} + \frac{n-2-k}{\sqrt{2(n-1)}} - \frac{k}{\sqrt{n-2}} - \frac{n-2-k}{\sqrt{2(n-2)}} \\
&= f(n) + \frac{(\sqrt{2}-1)(n-k-4)(\sqrt{n-1} - \sqrt{n-2})}{\sqrt{2(n-2)(n-1)}} \\
&\geqslant f(n). \qquad (2)
\end{aligned}$$

In order for equality to hold, all inequalities in the above argument should be equalities. Thus we have

$$R(G') = f(n-1) \quad \text{and} \quad k = n-4.$$

By the induction hypothesis, $G' \in \mathcal{QT}^0(n-1)$. Note that G' has a unique vertex of degree greater than 3, and hence $G \in \mathcal{QT}^0(n)$. This completes the proof of theorem 1. □

Denote

$$g(n) = R(\mathcal{QT}^1(n)) = \frac{n-4}{\sqrt{n-1}} + \frac{2}{\sqrt{2(n-1)}} + \frac{1}{\sqrt{3(n-1)}} + \frac{2}{\sqrt{6}}$$

and $PV = \{u \in V(G) | d(u) = 1\}$.

Theorem 2. Let $G \in \mathcal{QT}(n)$ with $n \geqslant 4$ and $G \not\cong \mathcal{QT}^0(n)$. Then

$$R(G) \geqslant g(n) = \frac{n-4}{\sqrt{n-1}} + \frac{2}{\sqrt{2(n-1)}} + \frac{1}{\sqrt{3(n-1)}} + \frac{2}{\sqrt{6}}.$$

The equality holds if and only if $G \cong \mathcal{QT}^1(n)$.

Proof. By induction on n. If $n = 4, 5$, then the theorem holds clearly (see figures 1 and 2).

Assume that $G \in \mathcal{QT}(n)$ with $n \geqslant 6$. We just need to consider the case that $PV \neq \emptyset$ by lemma 7. Let $u \in PV$ and v be the neighbor of u. Denote $d(v) = d$ and $N(v) \setminus \{u\} = \{y_1, y_2, \dots, y_{d-1}\}$. Then $d \geqslant 2$. Set $G' = G - u$. Then $G' \in \mathcal{QT}(n-1)$. Let S be the sum of the weights of the edges incident with v except for the edge uv in G and S' the sum of the weights of the edges incident with v in G'. Then $S = \sum_{i=1}^{d-1} \frac{1}{\sqrt{dd(y_i)}}$ and $S' = S\sqrt{\frac{d}{d-1}}$. By lemmas 8 and 9, we can assume that there exists some i $(1 \leqslant i \leqslant d-1)$ such that $d(y_i) = 1$ and $d = n-1$.

Assume, without loss of generality, that $d(y_1) = d(y_2) = \cdots = d(y_k) = 1$ and $d(y_i) \geqslant 2$ for $k+1 \leqslant i \leqslant n-2$, where $k \geqslant 1$. Since $d(v) = n-1$ and $G \not\cong \mathcal{QT}^0(n)$, there exists y_i, say y_{n-2}, such that $d(y_{n-2}) \geqslant 3$. Thus $S \leqslant k/\sqrt{n-1} + (n-3-k)/\sqrt{2(n-1)} + 1/\sqrt{3(n-1)}$. Then we have

$$\begin{aligned}
R(G) &= R(G') + \frac{1}{\sqrt{d}} + S\left(1 - \sqrt{\frac{d}{d-1}}\right) \\
&\geqslant g(n) + \frac{n-5}{\sqrt{n-2}} + \frac{2}{\sqrt{2(n-2)}} + \frac{1}{\sqrt{3(n-2)}} \\
&\quad - \frac{n-4}{\sqrt{n-1}} - \frac{2}{\sqrt{2(n-1)}} - \frac{1}{\sqrt{3(n-1)}} \\
&\quad - \frac{2}{\sqrt{2(n-1)}} + \frac{1}{\sqrt{n-1}} + \left(1 - \sqrt{\frac{n-1}{n-2}}\right) \\
&\quad \times \left(\frac{k}{\sqrt{n-1}} + \frac{n-3-k}{\sqrt{2(n-1)}} + \frac{1}{\sqrt{3(n-1)}}\right) \\
&= g(n) + \left(\frac{(\sqrt{2}-1)(n-k-5)}{\sqrt{2(n-2)}} - \frac{(\sqrt{2}-1)(n-k-5)}{\sqrt{2(n-1)}}\right) \\
&\geqslant g(n).
\end{aligned}$$

In order for equality to hold, all inequalities in the above argument should be equalities. Thus we have

$$R(G') = g(n-1), \quad d(y_{n-2}) = 3 \quad \text{and} \quad k = n-5.$$

By the induction hypothesis, $G' \in \mathcal{QT}^1(n-1)$. Note that G' has a unique vertex of degree greater than 4, and hence $G \in \mathcal{QT}^1(n)$.

This completes the proof of our theorem. □

Appendix

Proposition 1. Let n be a positive integer with $n \geqslant 6$. Then

$$(\sqrt{n-3}-\sqrt{n-4})-(\sqrt{n-1}-\sqrt{n-2})-0.72\left(\frac{1}{\sqrt{n-2}}-\frac{1}{\sqrt{n-1}}\right)>0. \quad (1)$$

Proof. In order to show (1), we just need to show that

$$(\sqrt{n-3}-\sqrt{n-4})>(\sqrt{n-1}-\sqrt{n-2})+0.72\left(\frac{1}{\sqrt{n-2}}-\frac{1}{\sqrt{n-1}}\right),$$

i.e.,

$$\frac{1}{\sqrt{n-3}+\sqrt{n-4}}>\frac{\sqrt{n-1}\sqrt{n-2}+0.72}{\sqrt{n-1}\sqrt{n-2}(\sqrt{n-1}+\sqrt{n-2})},$$

i.e.,

$$\sqrt{n-1}\sqrt{n-2}(\sqrt{n-1}+\sqrt{n-2})>(\sqrt{n-3}+\sqrt{n-4})(\sqrt{n-1}\sqrt{n-2}+0.72),$$

i.e.,

$$\sqrt{n-1}\sqrt{n-2}[(\sqrt{n-1}-\sqrt{n-3})+(\sqrt{n-2}-\sqrt{n-4})]>0.72(\sqrt{n-3}+\sqrt{n-4}). \quad (2)$$

Since $\sqrt{n-2}-\sqrt{n-4}>\sqrt{n-1}-\sqrt{n-3}$, to show (2), we just need to show that

$$2\sqrt{n-1}\sqrt{n-2}(\sqrt{n-1}-\sqrt{n-3})>0.72(\sqrt{n-3}+\sqrt{n-4}),$$

i.e.,

$$\frac{4\sqrt{n-1}\sqrt{n-2}}{\sqrt{n-1}+\sqrt{n-3}}>0.72(\sqrt{n-3}+\sqrt{n-4}),$$

i.e.,

$$\sqrt{n-1}\sqrt{n-2}>0.18(\sqrt{n-3}+\sqrt{n-4})(\sqrt{n-1}+\sqrt{n-3}). \quad (3)$$

Since $\sqrt{n-3}+\sqrt{n-4}<\sqrt{n-1}+\sqrt{n-3}$, to show (3), we just need to show that

$$\sqrt{n-1}\sqrt{n-2}>0.18(\sqrt{n-1}+\sqrt{n-3})^2. \quad (4)$$

Since $2\sqrt{n-2} > \sqrt{n-1} + \sqrt{n-3}$, to show (4), we just need to show that

$$\sqrt{n-1}\sqrt{n-2} > 0.18(2\sqrt{n-2})^2,$$

i.e.,

$$\sqrt{n-1} > 0.72\sqrt{n-2}.$$

The last inequality is obvious. Thus (3) holds, and then (2) and (1) holds immediately. □

Proposition 2. Let n be a positive integer with $n \geqslant 6$. Then

$$(\sqrt{n-2} - \sqrt{n-3}) - (\sqrt{n-1} - \sqrt{n-2}) - 0.423\left(\frac{1}{\sqrt{n-2}} - \frac{1}{\sqrt{n-1}}\right) > 0. \quad (5)$$

Proof. In order to show (5), we just need to show that

$$(\sqrt{n-2} - \sqrt{n-3}) > (\sqrt{n-1} - \sqrt{n-2}) + 0.423\left(\frac{1}{\sqrt{n-2}} - \frac{1}{\sqrt{n-1}}\right),$$

i.e.,

$$\frac{1}{\sqrt{n-2} + \sqrt{n-3}} > \frac{\sqrt{n-1}\sqrt{n-2} + 0.423}{\sqrt{n-1}\sqrt{n-2}(\sqrt{n-1} + \sqrt{n-2})},$$

i.e.,

$$\sqrt{n-1}\sqrt{n-2}(\sqrt{n-1} + \sqrt{n-2}) > (\sqrt{n-2} + \sqrt{n-3})(\sqrt{n-1}\sqrt{n-2} + 0.423),$$

i.e.,

$$\sqrt{n-1}\sqrt{n-2}(\sqrt{n-1} - \sqrt{n-3}) > 0.423(\sqrt{n-2} + \sqrt{n-3}).$$

By Cauchy–Schwarz inequality, we have

$$\sqrt{2(2n-5)} \geqslant \sqrt{n-2} + \sqrt{n-3}.$$

Thus, in order to show (5), we just need to show

$$\sqrt{n-1}\sqrt{n-2}(\sqrt{n-1} - \sqrt{n-3}) > 0.423\sqrt{2(2n-5)}.$$

Note that

$$\begin{aligned}&\left[\sqrt{n-1}\sqrt{n-2}(\sqrt{n-1} - \sqrt{n-3})\right]^2 - \left[0.423\sqrt{2(2n-5)}\right]^2\\ &\quad = 2(n^3 - 5n^2 + 7.64n - 3.1 - (n^2 - 3n + 2)\sqrt{(n-1)(n-3)}).\end{aligned}$$

On the other hand,

$$\begin{aligned}
&(n^3 - 5n^2 + 7.64n - 3.1)^2 - \left[(n^2 - 3n + 2)\sqrt{(n-1)(n-3)}\right]^2 \\
&\quad = (n^6 - 10n^5 + 40.28n^4 - 82.6n^3 + 89.37n^2 - 47.37n + 9.61) \\
&\qquad -(n^6 - 10n^5 + 40n^4 - 82n^3 + 91n^2 - 52n + 12) \\
&\quad = 0.28n^4 - 0.6n^3 - 1.63n^2 + 4.63n - 2.39 \\
&\qquad > 0. \qquad (n \geqslant 6)
\end{aligned}$$

Thus (5) holds. □

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